



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 01:19 AM UTC

PDB ID : 7DQC / pdb_00007dqc
Title : Crystal structure of nucleotide-free mutant A(S23C)3B(N64C)3 complex from *Enterococcus hirae* V-ATPase
Authors : Maruyama, S.; Suzuki, K.; Mizutani, K.; Imai, F.L.; Ishizuka-Katsura, Y.; Shirouzu, M.; Murata, M.
Deposited on : 2020-12-23
Resolution : 2.71 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

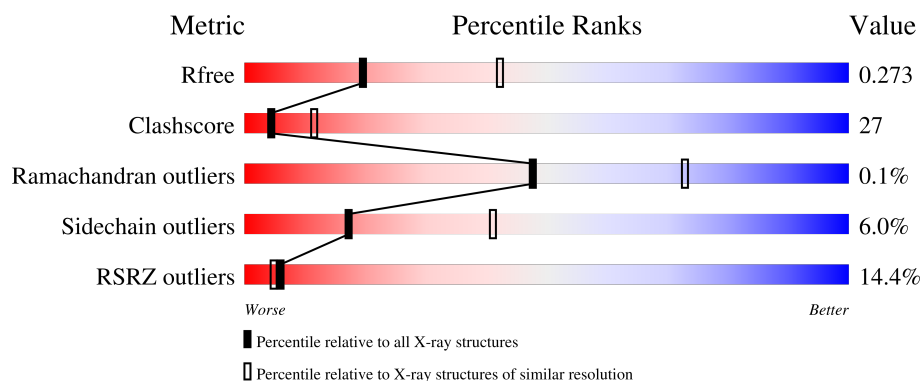
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.71 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	600	
1	B	600	
1	C	600	
2	D	465	
2	E	465	

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Mol	Chain	Length	Quality of chain
2	F	465	29% 47% 45% 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 23860 atoms, of which 48 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called V-type sodium ATPase catalytic subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	586	Total	C	N	O	S	0	0	0
			4529	2847	761	895	26			
1	B	586	Total	C	N	O	S	0	0	0
			4501	2827	758	889	27			
1	C	584	Total	C	N	O	S	0	0	0
			4456	2802	746	881	27			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLY	-	expression tag	UNP Q08636
A	-5	SER	-	expression tag	UNP Q08636
A	-4	SER	-	expression tag	UNP Q08636
A	-3	GLY	-	expression tag	UNP Q08636
A	-2	SER	-	expression tag	UNP Q08636
A	-1	SER	-	expression tag	UNP Q08636
A	0	GLY	-	expression tag	UNP Q08636
A	23	CYS	SER	engineered mutation	UNP Q08636
B	-6	GLY	-	expression tag	UNP Q08636
B	-5	SER	-	expression tag	UNP Q08636
B	-4	SER	-	expression tag	UNP Q08636
B	-3	GLY	-	expression tag	UNP Q08636
B	-2	SER	-	expression tag	UNP Q08636
B	-1	SER	-	expression tag	UNP Q08636
B	0	GLY	-	expression tag	UNP Q08636
B	23	CYS	SER	engineered mutation	UNP Q08636
C	-6	GLY	-	expression tag	UNP Q08636
C	-5	SER	-	expression tag	UNP Q08636
C	-4	SER	-	expression tag	UNP Q08636
C	-3	GLY	-	expression tag	UNP Q08636
C	-2	SER	-	expression tag	UNP Q08636
C	-1	SER	-	expression tag	UNP Q08636
C	0	GLY	-	expression tag	UNP Q08636

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Chain	Residue	Modelled	Actual	Comment	Reference
C	23	CYS	SER	engineered mutation	UNP Q08636

- Molecule 2 is a protein called V-type sodium ATPase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	448	Total	C	N	O	S	0	0	0
			3380	2137	590	638	15			
2	E	450	Total	C	N	O	S	0	0	0
			3347	2112	582	640	13			
2	F	450	Total	C	N	O	S	0	0	0
			3277	2068	568	627	14			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-6	GLY	-	expression tag	UNP Q08637
D	-5	SER	-	expression tag	UNP Q08637
D	-4	SER	-	expression tag	UNP Q08637
D	-3	GLY	-	expression tag	UNP Q08637
D	-2	SER	-	expression tag	UNP Q08637
D	-1	SER	-	expression tag	UNP Q08637
D	0	GLY	-	expression tag	UNP Q08637
D	64	CYS	ASN	engineered mutation	UNP Q08637
E	-6	GLY	-	expression tag	UNP Q08637
E	-5	SER	-	expression tag	UNP Q08637
E	-4	SER	-	expression tag	UNP Q08637
E	-3	GLY	-	expression tag	UNP Q08637
E	-2	SER	-	expression tag	UNP Q08637
E	-1	SER	-	expression tag	UNP Q08637
E	0	GLY	-	expression tag	UNP Q08637
E	64	CYS	ASN	engineered mutation	UNP Q08637
F	-6	GLY	-	expression tag	UNP Q08637
F	-5	SER	-	expression tag	UNP Q08637
F	-4	SER	-	expression tag	UNP Q08637
F	-3	GLY	-	expression tag	UNP Q08637
F	-2	SER	-	expression tag	UNP Q08637
F	-1	SER	-	expression tag	UNP Q08637
F	0	GLY	-	expression tag	UNP Q08637
F	64	CYS	ASN	engineered mutation	UNP Q08637

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			14	3	8	3		
3	A	1	Total	C	H	O	0	0
			14	3	8	3		
3	A	1	Total	C	H	O	0	0
			14	3	8	3		
3	A	1	Total	C	H	O	0	0
			14	3	8	3		
3	A	1	Total	C	H	O	0	0
			14	3	8	3		
3	A	1	Total	C	H	O	0	0
			14	3	8	3		

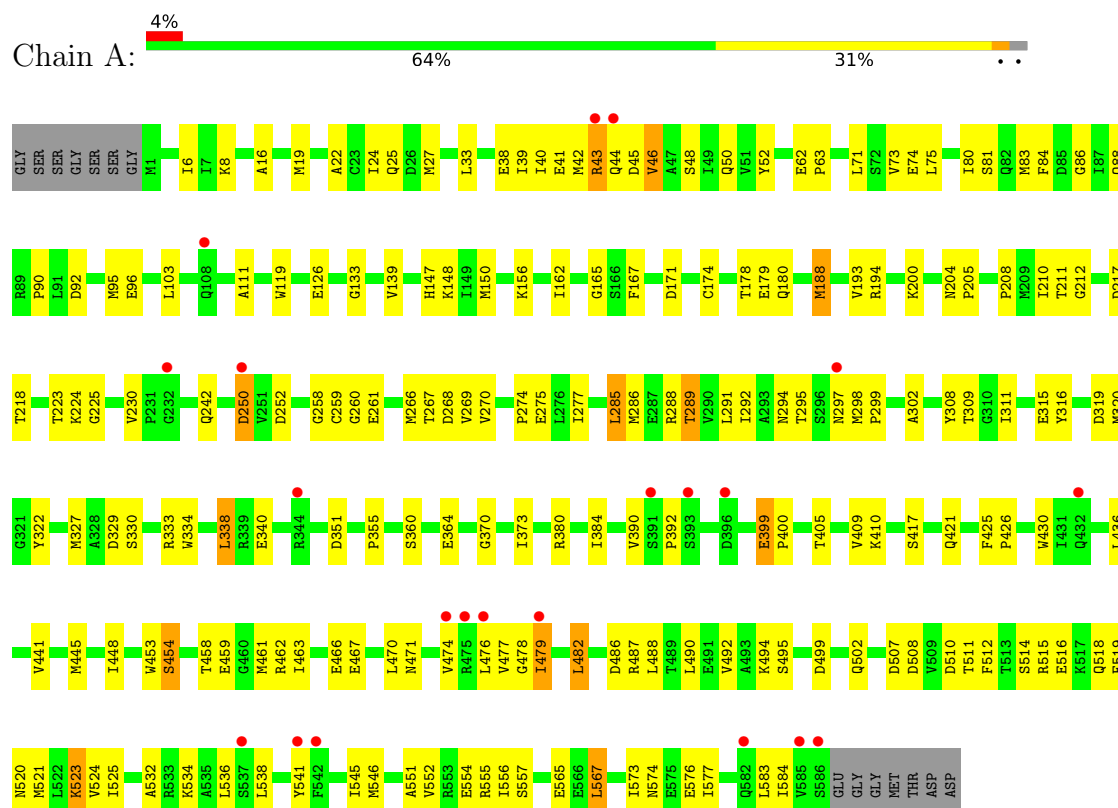
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	103	Total	O	0	0
			103	103		
4	B	45	Total	O	0	0
			45	45		
4	D	34	Total	O	0	0
			34	34		
4	E	42	Total	O	0	0
			42	42		
4	C	43	Total	O	0	0
			43	43		
4	F	19	Total	O	0	0
			19	19		

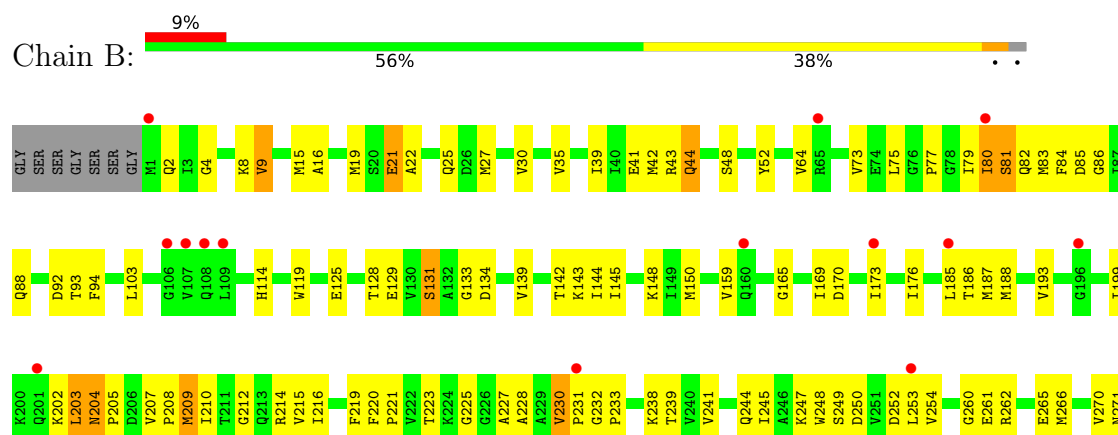
3 Residue-property plots [i](#)

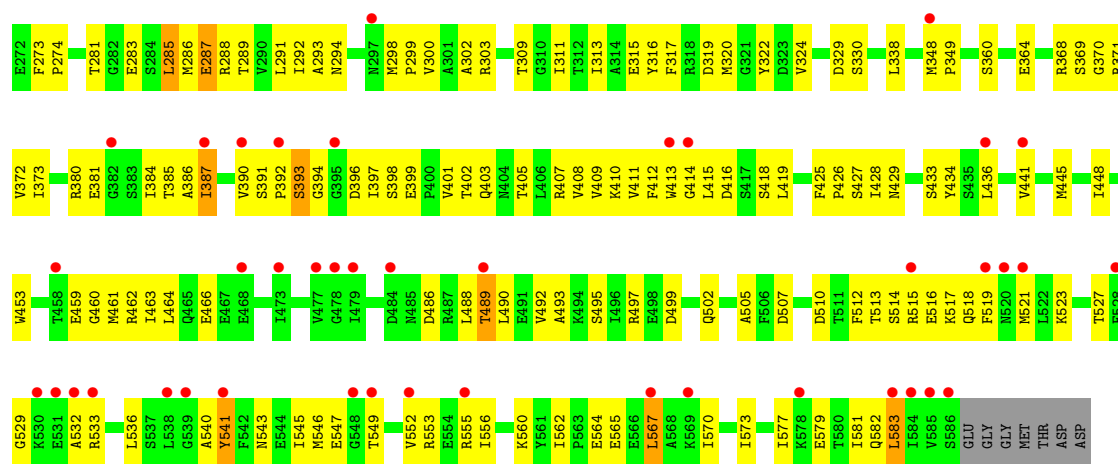
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: V-type sodium ATPase catalytic subunit A

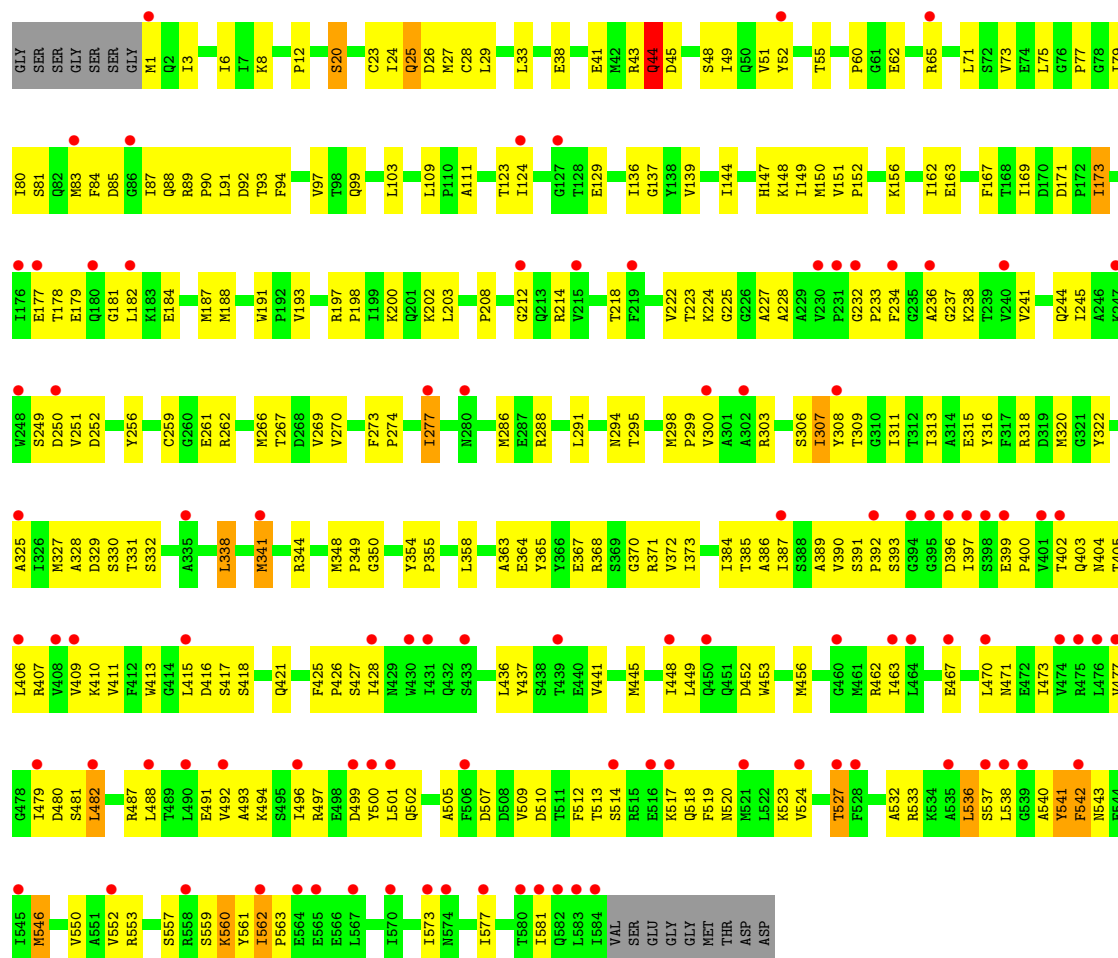


• Molecule 1: V-type sodium ATPase catalytic subunit A



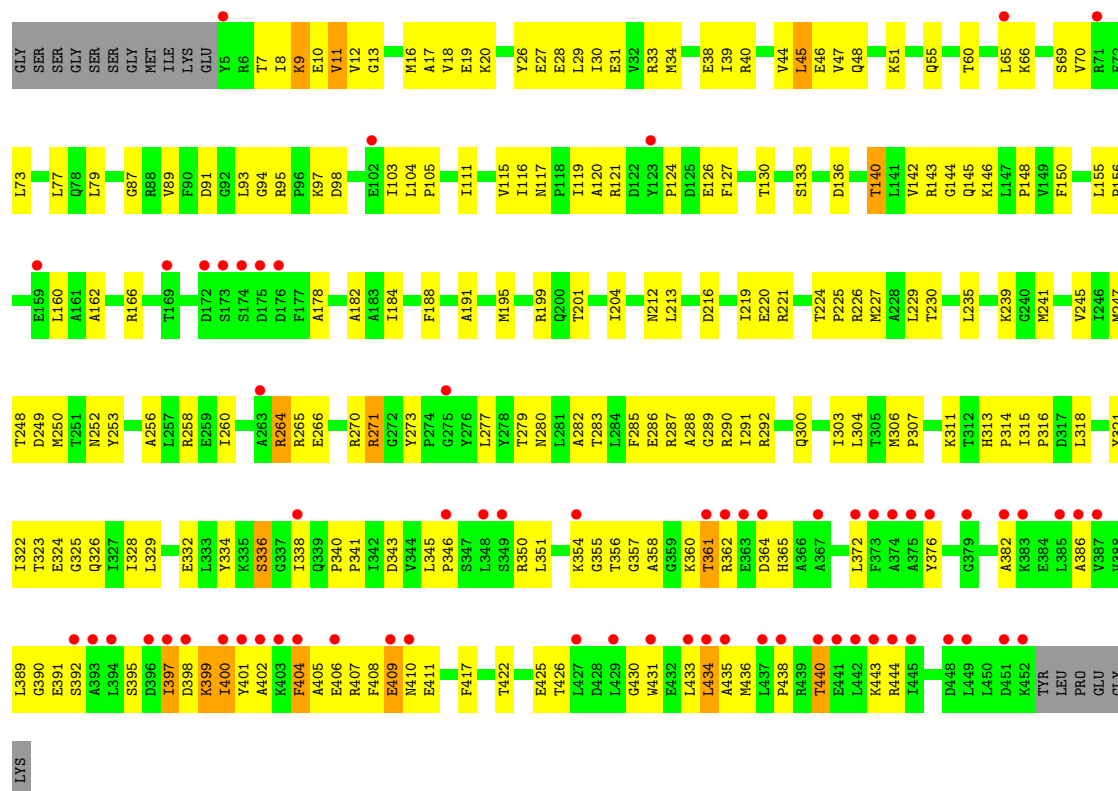


• Molecule 1: V-type sodium ATPase catalytic subunit A

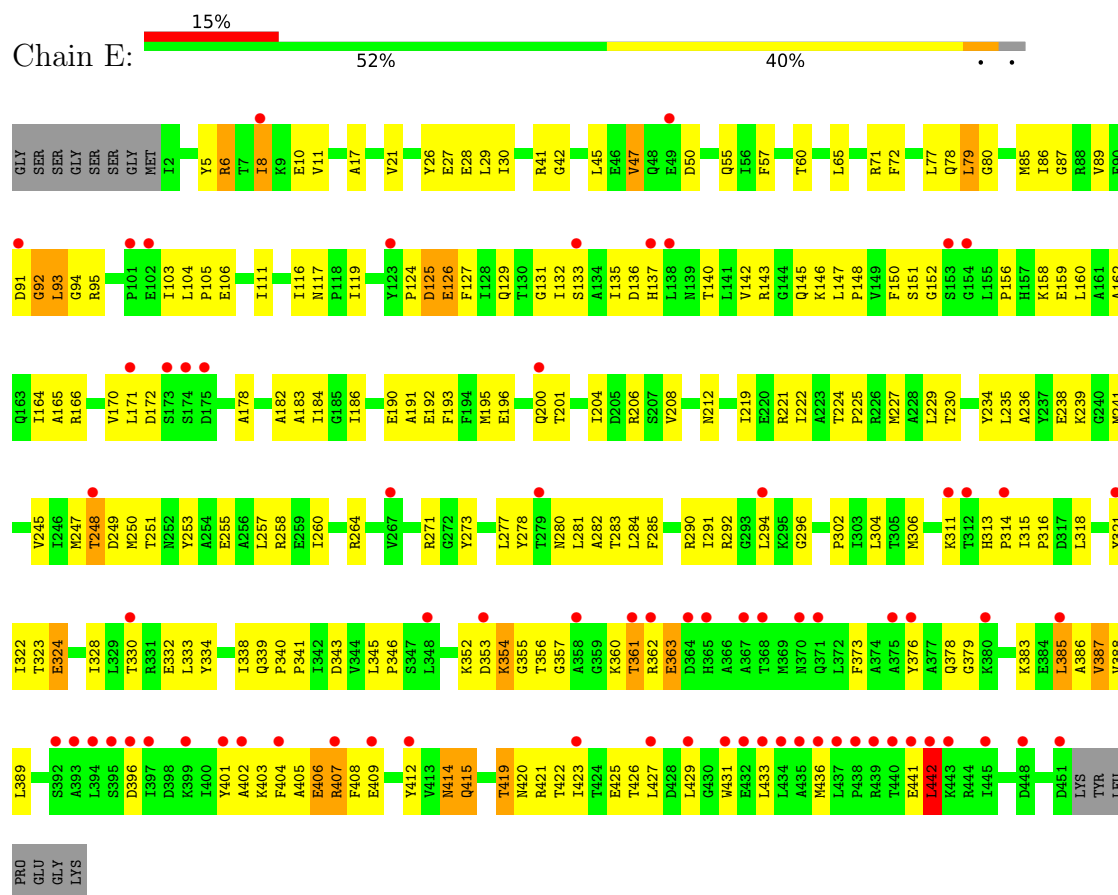


• Molecule 2: V-type sodium ATPase subunit B

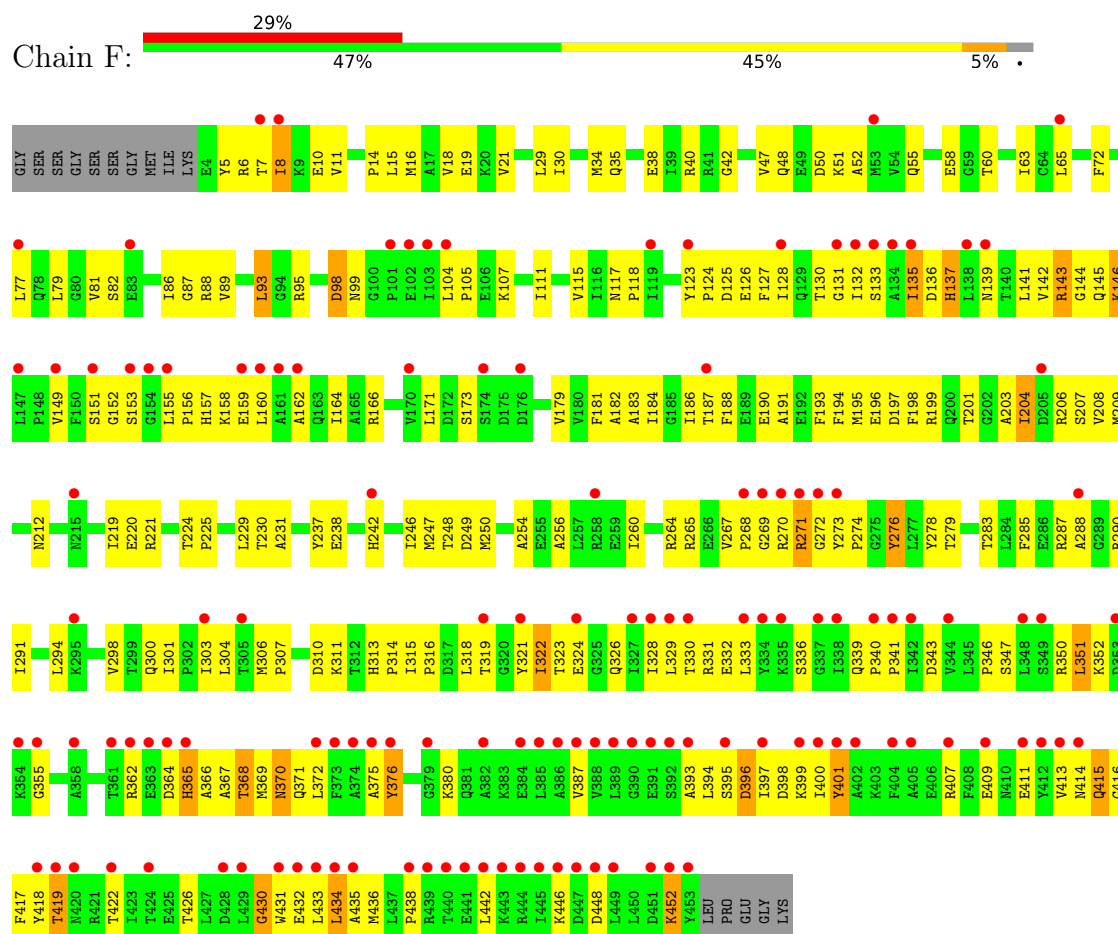




- Molecule 2: V-type sodium ATPase subunit B



● Molecule 2: V-type sodium ATPase subunit B



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	122.08Å 121.83Å 129.11Å 90.00° 90.22° 90.00°	Depositor
Resolution (Å)	44.30 – 2.71 44.30 – 2.71	Depositor EDS
% Data completeness (in resolution range)	99.8 (44.30-2.71) 99.8 (44.30-2.71)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.234 , 0.266 0.245 , 0.273	Depositor DCC
R_{free} test set	5266 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	61.6	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 72.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l 0.000 for -k,-h,-l 0.015 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	23860	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.25	0/4605	0.71	4/6234 (0.1%)
1	B	0.26	0/4577	0.74	4/6199 (0.1%)
1	C	0.25	0/4532	0.72	1/6148 (0.0%)
2	D	0.26	0/3441	0.71	0/4658
2	E	0.28	0/3406	0.76	3/4616 (0.1%)
2	F	0.30	0/3336	0.77	2/4536 (0.0%)
All	All	0.27	0/23897	0.73	14/32391 (0.0%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	399	GLU	CA-C-N	6.83	126.34	119.24
1	A	399	GLU	C-N-CA	6.83	126.34	119.24
1	B	230	VAL	CA-C-N	6.72	126.35	119.56
1	B	230	VAL	C-N-CA	6.72	126.35	119.56
2	E	92	GLY	N-CA-C	-5.95	107.53	115.32
2	E	396	ASP	CB-CA-C	-5.81	109.89	116.63
1	A	230	VAL	CA-C-N	5.75	125.29	119.19
1	A	230	VAL	C-N-CA	5.75	125.29	119.19
2	F	432	GLU	N-CA-C	-5.45	105.36	112.23
2	E	442	LEU	N-CA-C	5.22	116.78	108.79
1	B	393	SER	N-CA-C	5.13	117.77	111.82
2	F	430	GLY	N-CA-C	-5.13	106.43	112.64
1	C	44	GLN	CB-CA-C	-5.11	110.28	117.23
1	B	44	GLN	CB-CA-C	-5.11	110.29	117.23

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4529	0	4462	160	0
1	B	4501	0	4407	237	0
1	C	4456	0	4329	230	0
2	D	3380	0	3279	195	0
2	E	3347	0	3194	198	0
2	F	3277	0	3037	254	0
3	A	36	48	48	3	0
4	A	103	0	0	5	0
4	B	45	0	0	2	0
4	C	43	0	0	0	0
4	D	34	0	0	4	0
4	E	42	0	0	6	0
4	F	19	0	0	1	0
All	All	23812	48	22756	1230	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 27.

All (1230) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:267:VAL:HG22	2:F:268:PRO:HD2	1.31	1.10
2:F:155:LEU:HD22	2:F:156:PRO:HD2	1.25	1.09
1:A:27:MET:HE3	1:A:71:LEU:HB2	1.28	1.08
1:B:8:LYS:HD3	1:B:15:MET:HE2	1.40	1.00
1:B:260:GLY:HA3	1:B:261:GLU:HG2	1.39	1.00
2:D:89:VAL:HG21	2:D:195:MET:HE1	1.41	0.98
2:F:431:TRP:HE3	2:F:434:LEU:HD21	1.27	0.98
2:F:151:SER:HB2	2:F:329:LEU:HD12	1.44	0.97
1:B:540:ALA:HB1	1:B:545:ILE:HD11	1.47	0.96
1:C:150:MET:HE1	1:C:320:MET:HA	1.49	0.94
1:C:251:VAL:HG21	1:C:325:ALA:HB2	1.50	0.93
1:B:83:MET:HE1	1:B:270:VAL:HG13	1.48	0.93
2:E:278:TYR:HB2	2:E:318:LEU:HD13	1.47	0.93
2:D:390:GLY:N	2:D:391:GLU:HA	1.83	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:148:LYS:H	1:C:320:MET:HE3	1.32	0.92
2:D:306:MET:HE1	2:D:311:LYS:HG2	1.50	0.92
2:E:148:PRO:HB3	2:E:302:PRO:HG2	1.49	0.92
2:F:135:ILE:O	2:F:139:ASN:N	2.02	0.91
1:C:144:ILE:HG21	1:C:288:ARG:HD3	1.50	0.91
1:B:562:ILE:HB	1:B:570:ILE:HD11	1.52	0.91
2:F:436:MET:O	2:F:438:PRO:HD3	1.71	0.91
2:F:396:ASP:O	2:F:400:ILE:N	2.03	0.91
1:A:546:MET:HE2	1:A:546:MET:HA	1.50	0.90
1:A:150:MET:HE1	1:A:319:ASP:HB3	1.50	0.90
2:D:402:ALA:O	2:D:406:GLU:N	2.04	0.90
2:E:345:LEU:HG	2:E:376:TYR:HE2	1.37	0.90
2:D:328:ILE:HD12	2:D:346:PRO:HB2	1.55	0.87
1:C:562:ILE:HG22	1:C:563:PRO:HD2	1.55	0.86
2:F:431:TRP:CE3	2:F:434:LEU:HD21	2.10	0.86
2:F:267:VAL:CG2	2:F:268:PRO:HD2	2.05	0.86
1:B:461:MET:HA	1:B:461:MET:HE3	1.58	0.85
1:A:338:LEU:HD22	1:A:355:PRO:HG3	1.59	0.85
2:F:315:ILE:HB	2:F:316:PRO:HD3	1.60	0.84
2:D:11:VAL:HG11	1:C:24:ILE:HD11	1.60	0.83
2:E:357:GLY:O	2:E:361:THR:N	2.11	0.83
2:E:89:VAL:HG21	2:E:195:MET:HE1	1.60	0.83
2:D:407:ARG:O	2:D:411:GLU:N	2.11	0.83
2:D:401:TYR:O	2:D:405:ALA:N	2.11	0.83
1:B:393:SER:N	1:B:394:GLY:HA3	1.93	0.83
1:B:231:PRO:CG	1:B:414:GLY:HA2	2.09	0.82
1:B:445:MET:HE3	1:B:515:ARG:HG3	1.61	0.82
1:B:521:MET:HE1	1:B:560:LYS:HB3	1.60	0.82
1:C:410:LYS:HB3	1:C:436:LEU:HB2	1.60	0.82
1:C:266:MET:HE2	1:C:266:MET:HA	1.62	0.81
2:F:201:THR:HG23	2:F:203:ALA:H	1.45	0.81
2:D:399:LYS:HD2	2:D:400:ILE:H	1.46	0.81
1:A:148:LYS:HB2	1:A:320:MET:HE3	1.62	0.80
2:F:415:GLN:N	2:F:416:GLY:HA2	1.94	0.80
1:A:43:ARG:CB	1:A:46:VAL:HG13	2.12	0.80
2:D:340:PRO:HB3	2:D:417:PHE:HE1	1.45	0.80
1:B:489:THR:HG23	1:B:533:ARG:HH12	1.46	0.80
1:C:51:VAL:HG21	1:C:55:THR:CG2	2.12	0.80
1:B:231:PRO:HG2	1:B:414:GLY:HA2	1.62	0.79
1:C:41:GLU:HG2	1:C:48:SER:HB2	1.65	0.79
1:C:91:LEU:HD13	2:F:118:PRO:HG2	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:179:VAL:HB	2:F:207:SER:HB3	1.64	0.79
2:F:452:LYS:NZ	2:F:452:LYS:HA	1.98	0.79
2:D:116:ILE:HD13	2:D:291:ILE:HD11	1.64	0.79
2:F:135:ILE:HD12	2:F:136:ASP:H	1.47	0.79
2:F:219:ILE:HD12	2:F:219:ILE:H	1.48	0.79
2:E:219:ILE:HD13	2:E:260:ILE:HD13	1.65	0.79
1:B:77:PRO:HG2	1:B:187:MET:HE2	1.65	0.78
1:A:333:ARG:NH2	2:D:321:TYR:O	2.16	0.78
2:F:288:ALA:HB2	2:F:300:GLN:HG3	1.65	0.78
2:F:155:LEU:CD2	2:F:156:PRO:HD2	2.11	0.78
2:E:8:ILE:CD1	2:E:65:LEU:HG	2.14	0.77
2:D:124:PRO:HG2	2:D:351:LEU:HD13	1.66	0.77
1:B:8:LYS:HD3	1:B:15:MET:CE	2.14	0.76
2:D:166:ARG:HD2	2:D:201:THR:HG21	1.65	0.76
2:E:383:LYS:NZ	2:E:406:GLU:HG3	1.99	0.76
2:F:131:GLY:O	2:F:415:GLN:NE2	2.17	0.76
2:D:362:ARG:HH12	2:D:431:TRP:HE1	1.32	0.76
2:F:124:PRO:HB2	2:F:142:VAL:HG12	1.65	0.76
2:F:132:ILE:C	2:F:135:ILE:HD11	2.11	0.76
2:D:91:ASP:HB3	2:D:97:LYS:HE2	1.67	0.76
1:C:463:ILE:HD11	1:C:496:ILE:HD11	1.68	0.75
1:B:232:GLY:HA2	1:B:238:LYS:HD3	1.67	0.75
1:C:27:MET:HE3	1:C:71:LEU:HB2	1.67	0.75
1:A:44:GLN:CB	1:A:45:ASP:HA	2.17	0.75
1:C:27:MET:CE	1:C:71:LEU:HB2	2.16	0.75
1:A:266:MET:HE3	1:A:266:MET:HA	1.67	0.74
2:F:313:HIS:CE1	2:F:315:ILE:HG12	2.22	0.74
1:A:445:MET:HE1	1:A:515:ARG:HG3	1.69	0.74
1:B:398:SER:HA	1:B:403:GLN:HE21	1.52	0.74
1:C:232:GLY:HA3	1:C:238:LYS:HD3	1.69	0.74
1:C:129:GLU:N	1:C:129:GLU:OE1	2.20	0.73
2:D:398:ASP:CB	2:D:399:LYS:HB2	2.18	0.73
1:C:139:VAL:HG21	1:C:187:MET:HE3	1.69	0.73
2:D:224:THR:HB	2:D:225:PRO:HD3	1.70	0.73
1:A:103:LEU:HD21	2:D:117:ASN:HA	1.70	0.73
1:B:133:GLY:O	1:B:380:ARG:NH2	2.21	0.73
1:C:139:VAL:HG21	1:C:187:MET:CE	2.19	0.73
1:C:83:MET:HE2	1:C:270:VAL:HG13	1.70	0.72
1:B:9:VAL:HG13	2:E:47:VAL:HG23	1.70	0.72
2:D:399:LYS:HG3	2:D:401:TYR:H	1.51	0.72
1:A:43:ARG:HB2	1:A:46:VAL:HG13	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:410:LYS:HB3	1:B:436:LEU:HB2	1.71	0.72
2:D:258:ARG:HD2	2:D:273:TYR:CE1	2.24	0.72
2:F:368:THR:O	2:F:372:LEU:HG	1.89	0.71
1:B:150:MET:HE3	1:B:380:ARG:HH21	1.54	0.71
2:E:132:ILE:HA	2:E:415:GLN:HE22	1.54	0.71
2:F:224:THR:HB	2:F:225:PRO:HD3	1.73	0.71
1:C:562:ILE:CG2	1:C:563:PRO:HD2	2.20	0.71
2:F:393:ALA:N	2:F:394:LEU:HA	2.04	0.71
2:E:125:ASP:HB2	2:E:126:GLU:HA	1.72	0.70
2:E:222:ILE:HD12	2:E:260:ILE:HD12	1.72	0.70
1:C:256:TYR:HD1	1:C:327:MET:HE3	1.57	0.70
2:E:10:GLU:HG2	2:E:17:ALA:HB3	1.74	0.70
2:E:314:PRO:O	2:E:318:LEU:HG	1.91	0.70
1:B:260:GLY:HA3	1:B:261:GLU:CG	2.19	0.70
1:C:51:VAL:HG21	1:C:55:THR:HG23	1.73	0.70
2:F:365:HIS:HA	2:F:368:THR:CG2	2.22	0.70
1:B:416:ASP:OD1	1:B:418:SER:OG	2.10	0.69
2:F:395:SER:O	2:F:399:LYS:N	2.23	0.69
1:B:19:MET:HE1	1:B:64:VAL:CG1	2.22	0.69
1:B:81:SER:HB3	1:B:286:MET:O	1.92	0.69
1:A:24:ILE:HG22	1:A:25:GLN:HG2	1.74	0.69
1:B:133:GLY:HA2	1:B:150:MET:HE2	1.73	0.69
2:E:306:MET:HE3	2:E:311:LYS:HA	1.74	0.69
2:F:369:MET:HG3	2:F:370:ASN:N	2.06	0.69
2:E:45:LEU:HD13	2:E:264:ARG:HD3	1.73	0.69
1:A:95:MET:HE2	2:D:120:ALA:HB2	1.75	0.69
2:D:182:ALA:HB3	2:D:247:MET:HG2	1.75	0.69
1:B:579:GLU:O	1:B:583:LEU:HB2	1.91	0.69
2:F:339:GLN:O	2:F:414:ASN:HA	1.93	0.69
2:E:91:ASP:HB2	2:E:95:ARG:H	1.58	0.69
2:F:278:TYR:HB2	2:F:318:LEU:CD1	2.23	0.68
1:B:82:GLN:NE2	1:B:92:ASP:OD2	2.27	0.68
2:E:363:GLU:OE2	2:E:363:GLU:N	2.25	0.68
1:C:559:SER:HA	1:C:562:ILE:HD11	1.76	0.68
1:A:479:ILE:HD11	1:A:487:ARG:CZ	2.24	0.68
1:C:262:ARG:HH21	2:F:324:GLU:HG3	1.59	0.68
2:F:285:PHE:HB2	2:F:322:ILE:HD11	1.75	0.68
1:B:397:ILE:HG23	1:B:402:THR:HG21	1.74	0.68
1:C:546:MET:HE3	1:C:546:MET:HA	1.76	0.68
2:E:222:ILE:CD1	2:E:260:ILE:HD12	2.24	0.67
2:F:155:LEU:HD13	2:F:156:PRO:N	2.08	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:158:LYS:HG3	2:F:159:GLU:OE2	1.94	0.67
2:D:8:ILE:HD11	2:D:70:VAL:HG23	1.74	0.67
1:C:390:VAL:O	1:C:392:PRO:HD3	1.95	0.67
2:E:278:TYR:CB	2:E:318:LEU:HD13	2.22	0.67
2:F:229:LEU:HD13	2:F:287:ARG:HG3	1.76	0.67
2:F:395:SER:HB3	2:F:398:ASP:HB2	1.76	0.67
2:E:407:ARG:HG3	2:E:407:ARG:HH11	1.60	0.66
2:F:155:LEU:HD21	2:F:341:PRO:HG2	1.76	0.66
2:D:399:LYS:HD2	2:D:400:ILE:HG13	1.77	0.66
1:A:260:GLY:H	1:A:294:ASN:HB2	1.61	0.66
1:B:41:GLU:HB2	1:B:48:SER:HB2	1.77	0.66
2:E:345:LEU:HB2	2:E:346:PRO:HD3	1.78	0.66
2:F:137:HIS:CD2	2:F:369:MET:HB3	2.31	0.66
1:B:392:PRO:HG2	1:B:397:ILE:HD13	1.78	0.66
1:C:550:VAL:HG12	1:C:553:ARG:HH12	1.59	0.66
2:F:212:ASN:OD1	2:F:221:ARG:HG2	1.94	0.66
1:A:25:GLN:NE2	1:A:38:GLU:OE2	2.28	0.65
1:A:148:LYS:HE3	3:A:601:GOL:H31	1.76	0.65
1:B:397:ILE:O	1:B:403:GLN:NE2	2.29	0.65
2:D:260:ILE:O	2:D:264:ARG:HG3	1.96	0.65
2:E:136:ASP:O	2:E:137:HIS:ND1	2.29	0.65
1:C:29:LEU:HD12	1:C:65:ARG:HH12	1.60	0.65
2:E:363:GLU:CD	2:E:363:GLU:H	1.99	0.65
2:D:79:LEU:HD13	2:D:227:MET:CE	2.27	0.65
1:C:33:LEU:H	1:C:33:LEU:HD12	1.62	0.65
1:C:77:PRO:HG3	1:C:187:MET:HE2	1.78	0.65
1:B:232:GLY:CA	1:B:238:LYS:HD3	2.26	0.65
1:B:261:GLU:OE1	1:B:330:SER:N	2.28	0.65
1:B:4:GLY:HA3	1:B:19:MET:HE2	1.78	0.65
1:A:179:GLU:HB2	1:A:180:GLN:NE2	2.12	0.64
2:D:19:GLU:HB3	2:D:20:LYS:HD2	1.79	0.64
2:F:366:ALA:O	2:F:370:ASN:ND2	2.29	0.64
1:A:84:PHE:HB3	1:A:88:GLN:HA	1.79	0.64
1:C:320:MET:HE2	1:C:322:TYR:HE2	1.61	0.64
2:F:155:LEU:HD11	2:F:329:LEU:HD13	1.78	0.64
2:F:285:PHE:HD2	2:F:322:ILE:HG12	1.61	0.64
2:D:345:LEU:HB2	2:D:346:PRO:HD3	1.79	0.64
2:E:57:PHE:CE2	2:E:219:ILE:HG21	2.32	0.64
2:E:132:ILE:HA	2:E:415:GLN:NE2	2.12	0.64
1:B:392:PRO:HB2	1:B:394:GLY:O	1.97	0.64
1:C:218:THR:HG23	1:C:453:TRP:CZ2	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:376:TYR:OH	2:F:409:GLU:HG3	1.97	0.64
1:B:83:MET:CE	2:E:119:ILE:HG22	2.28	0.64
1:C:536:LEU:HA	1:C:540:ALA:HB3	1.80	0.64
1:A:476:LEU:N	1:A:477:VAL:HA	2.14	0.63
1:A:445:MET:HE1	1:A:515:ARG:CG	2.28	0.63
1:A:148:LYS:H	1:A:320:MET:CE	2.11	0.63
2:D:79:LEU:HD13	2:D:227:MET:HE1	1.79	0.63
2:E:129:GLN:OE1	2:E:423:ILE:N	2.29	0.63
2:F:128:ILE:HD11	2:F:143:ARG:HG2	1.79	0.63
2:F:397:ILE:HA	2:F:400:ILE:HG12	1.79	0.63
1:B:555:ARG:NH2	1:B:573:ILE:HA	2.13	0.63
1:C:320:MET:HE2	1:C:322:TYR:CE2	2.33	0.63
2:D:31:GLU:HG3	2:D:73:LEU:HD11	1.80	0.63
2:E:383:LYS:HG2	2:E:402:ALA:HB1	1.80	0.63
1:C:83:MET:CE	1:C:270:VAL:HG13	2.29	0.63
1:B:262:ARG:HB2	1:B:265:GLU:CD	2.24	0.63
2:E:156:PRO:HG3	2:E:334:TYR:CE1	2.34	0.63
2:E:280:ASN:O	2:E:283:THR:HG22	1.98	0.63
1:C:12:PRO:O	1:C:51:VAL:HG22	1.98	0.63
2:D:229:LEU:HG	2:D:247:MET:HE1	1.81	0.63
2:D:306:MET:CE	2:D:311:LYS:HA	2.29	0.63
1:A:148:LYS:H	1:A:320:MET:HE3	1.63	0.62
1:B:565:GLU:N	1:B:565:GLU:OE1	2.32	0.62
1:C:60:PRO:HD3	2:F:47:VAL:HG13	1.80	0.62
2:F:128:ILE:CD1	2:F:143:ARG:HG2	2.30	0.62
2:F:155:LEU:CD1	2:F:329:LEU:HD13	2.28	0.62
2:F:364:ASP:O	2:F:368:THR:HG22	1.98	0.62
2:E:249:ASP:OD1	2:E:304:LEU:HA	1.98	0.62
1:C:144:ILE:HG21	1:C:288:ARG:CD	2.28	0.62
2:E:258:ARG:NH2	2:E:271:ARG:O	2.31	0.62
2:F:135:ILE:HD13	2:F:136:ASP:OD1	1.99	0.62
2:F:313:HIS:CG	2:F:314:PRO:HD2	2.34	0.62
1:B:285:LEU:O	1:B:289:THR:HG23	2.00	0.62
1:C:315:GLU:HA	1:C:384:ILE:HD11	1.81	0.62
1:B:412:PHE:HB3	1:B:434:TYR:CE2	2.35	0.62
1:B:541:TYR:O	1:B:545:ILE:HG12	2.00	0.62
2:E:89:VAL:HG21	2:E:195:MET:CE	2.29	0.62
2:E:89:VAL:CG2	2:E:195:MET:HE1	2.29	0.62
2:E:407:ARG:HG3	2:E:407:ARG:NH1	2.14	0.62
1:C:269:VAL:O	1:C:273:PHE:HB2	2.00	0.62
1:A:148:LYS:HE3	3:A:601:GOL:C3	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:MET:CE	1:B:64:VAL:HB	2.30	0.62
2:E:345:LEU:CG	2:E:376:TYR:HE2	2.10	0.62
2:F:278:TYR:HB2	2:F:318:LEU:HD12	1.80	0.62
2:D:249:ASP:OD2	2:D:304:LEU:HA	2.00	0.62
2:F:184:ILE:N	2:F:248:THR:O	2.30	0.62
1:B:150:MET:HE1	1:B:319:ASP:HB3	1.82	0.62
2:E:245:VAL:HG11	2:E:247:MET:HE3	1.81	0.62
2:F:271:ARG:O	2:F:271:ARG:NE	2.31	0.62
2:D:252:ASN:OD1	1:C:407:ARG:NH2	2.32	0.61
1:C:214:ARG:HG2	1:C:518:GLN:HG2	1.82	0.61
1:A:19:MET:HG3	1:A:22:ALA:HB2	1.82	0.61
1:B:521:MET:CE	1:B:560:LYS:HB3	2.30	0.61
2:E:282:ALA:CA	2:E:322:ILE:HD13	2.29	0.61
1:C:497:ARG:HA	1:C:501:LEU:HB2	1.83	0.61
1:B:298:MET:HB3	1:B:299:PRO:HD2	1.82	0.61
2:D:66:LYS:HE3	1:C:20:SER:HB2	1.82	0.61
2:E:345:LEU:HG	2:E:376:TYR:CE2	2.28	0.61
1:C:331:THR:HG22	1:C:389:ALA:O	2.01	0.61
2:F:86:ILE:HA	2:F:208:VAL:HG22	1.81	0.61
2:F:184:ILE:HD11	2:F:225:PRO:HG3	1.82	0.61
1:C:123:THR:HG22	1:C:137:GLY:HA2	1.83	0.61
1:B:429:ASN:O	1:B:433:SER:OG	2.18	0.61
2:E:5:TYR:CE2	2:E:21:VAL:HG23	2.35	0.61
1:C:251:VAL:HG11	1:C:325:ALA:N	2.16	0.61
1:C:397:ILE:O	1:C:403:GLN:NE2	2.34	0.61
2:F:166:ARG:NH1	2:F:197:ASP:OD2	2.34	0.61
1:B:202:LYS:HG2	2:F:188:PHE:CE2	2.36	0.60
1:B:274:PRO:HA	1:B:286:MET:HG2	1.83	0.60
1:B:462:ARG:NH1	1:B:466:GLU:OE1	2.33	0.60
2:E:271:ARG:HG3	2:E:314:PRO:HG3	1.84	0.60
2:F:395:SER:CB	2:F:398:ASP:HB2	2.30	0.60
2:F:55:GLN:OE1	2:F:264:ARG:NH2	2.30	0.60
2:F:135:ILE:CD1	2:F:136:ASP:H	2.13	0.60
2:E:91:ASP:HB3	2:E:93:LEU:H	1.66	0.60
2:E:383:LYS:HZ1	2:E:406:GLU:HG3	1.65	0.60
2:F:187:THR:HG23	2:F:190:GLU:H	1.66	0.60
1:C:148:LYS:HG2	1:C:320:MET:HE3	1.83	0.60
1:C:167:PHE:HB3	1:C:171:ASP:HB2	1.83	0.60
1:C:560:LYS:HD2	1:C:561:TYR:CZ	2.36	0.60
2:F:130:THR:OG1	2:F:136:ASP:OD1	2.18	0.60
1:B:139:VAL:HG21	1:B:187:MET:CE	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:11:VAL:CG1	1:C:24:ILE:HD11	2.32	0.60
2:E:30:ILE:HD11	2:E:42:GLY:HA3	1.83	0.60
1:C:453:TRP:HZ3	1:C:519:PHE:HA	1.65	0.60
2:F:124:PRO:HB2	2:F:142:VAL:CG1	2.31	0.60
1:B:144:ILE:HD12	1:B:281:THR:HG21	1.84	0.60
1:B:445:MET:CE	1:B:515:ARG:HG3	2.29	0.60
2:D:178:ALA:HB2	2:D:241:MET:HE2	1.82	0.60
1:C:277:ILE:HD12	1:C:277:ILE:H	1.66	0.60
2:F:186:ILE:CD1	2:F:191:ALA:HB2	2.32	0.60
1:B:16:ALA:HB3	1:B:19:MET:HE3	1.83	0.60
1:B:300:VAL:HG22	1:B:303:ARG:NH2	2.17	0.60
2:F:166:ARG:NH2	2:F:417:PHE:O	2.35	0.60
2:F:452:LYS:HA	2:F:452:LYS:HZ3	1.65	0.60
2:E:282:ALA:HA	2:E:322:ILE:HD13	1.84	0.60
1:C:75:LEU:HD13	1:C:316:TYR:CD1	2.37	0.60
1:B:398:SER:HA	1:B:403:GLN:NE2	2.16	0.59
2:E:125:ASP:CB	2:E:126:GLU:HA	2.29	0.59
1:C:307:ILE:HD11	1:C:328:ALA:HB1	1.84	0.59
1:B:41:GLU:OE2	1:B:43:ARG:NH1	2.23	0.59
1:C:87:ILE:HD11	1:C:89:ARG:NE	2.17	0.59
2:F:407:ARG:O	2:F:411:GLU:N	2.35	0.59
2:D:280:ASN:O	2:D:283:THR:HG22	2.03	0.59
2:E:379:GLY:HA2	2:E:401:TYR:C	2.27	0.59
1:C:225:GLY:O	1:C:370:GLY:HA2	2.01	0.59
2:D:126:GLU:HG2	2:D:143:ARG:NH1	2.18	0.59
2:D:315:ILE:HB	2:D:316:PRO:HD3	1.85	0.59
2:F:267:VAL:HG22	2:F:268:PRO:CD	2.20	0.59
2:E:79:LEU:HD23	2:E:227:MET:HE1	1.85	0.59
1:A:148:LYS:CB	1:A:320:MET:HE3	2.31	0.59
2:D:26:TYR:CE2	2:D:27:GLU:HG3	2.37	0.59
2:D:288:ALA:HB2	2:D:300:GLN:HG3	1.84	0.59
2:D:357:GLY:N	2:D:361:THR:HG22	2.18	0.59
2:F:89:VAL:HB	2:F:98:ASP:HB2	1.83	0.59
1:B:139:VAL:HG21	1:B:187:MET:HE3	1.83	0.59
2:D:166:ARG:CD	2:D:201:THR:HG21	2.32	0.59
2:E:178:ALA:HB2	2:E:241:MET:CE	2.33	0.59
1:A:92:ASP:HA	2:D:119:ILE:HD11	1.85	0.59
1:B:19:MET:HE1	1:B:64:VAL:HB	1.85	0.59
2:F:371:GLN:OE1	2:F:442:LEU:HA	2.02	0.59
1:A:425:PHE:HA	1:A:426:PRO:C	2.28	0.59
1:B:285:LEU:HD21	1:B:288:ARG:NH2	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:315:ILE:HB	2:E:316:PRO:HD3	1.85	0.59
1:C:29:LEU:HD12	1:C:65:ARG:NH1	2.18	0.59
2:D:398:ASP:HB3	2:D:399:LYS:HB2	1.85	0.59
2:D:438:PRO:HB2	2:D:440:THR:HG23	1.84	0.59
2:E:79:LEU:HD11	2:E:85:MET:HE1	1.84	0.59
2:E:127:PHE:HB2	2:E:355:GLY:O	2.02	0.59
2:F:137:HIS:CE1	2:F:368:THR:HG23	2.38	0.59
2:F:151:SER:CB	2:F:329:LEU:HD12	2.27	0.59
1:B:260:GLY:CA	1:B:261:GLU:HG2	2.26	0.58
2:D:45:LEU:CD1	2:D:264:ARG:HD3	2.32	0.58
2:E:408:PHE:CE2	2:E:412:TYR:CD2	2.91	0.58
2:F:126:GLU:CB	2:F:143:ARG:HE	2.15	0.58
2:F:330:THR:OG1	2:F:333:LEU:HD13	2.04	0.58
1:A:224:LYS:HE2	1:A:250:ASP:HB3	1.85	0.58
2:D:191:ALA:O	2:D:195:MET:HG2	2.03	0.58
2:E:178:ALA:HB2	2:E:241:MET:HE2	1.84	0.58
1:B:371:ARG:HD2	1:B:381:GLU:OE2	2.03	0.58
2:D:264:ARG:NH1	2:D:266:GLU:OE2	2.35	0.58
2:F:370:ASN:ND2	2:F:370:ASN:H	2.01	0.58
2:D:389:LEU:CB	2:D:392:SER:H	2.16	0.58
2:F:125:ASP:OD2	2:F:290:ARG:NH1	2.36	0.58
2:F:153:SER:O	2:F:331:ARG:NH2	2.36	0.58
1:B:199:ILE:HD12	1:B:372:VAL:HB	1.84	0.58
1:C:148:LYS:H	1:C:320:MET:CE	2.10	0.58
1:B:73:VAL:CG1	1:B:309:THR:HG23	2.33	0.58
2:D:91:ASP:OD1	2:D:95:ARG:N	2.20	0.58
2:D:184:ILE:CD1	2:D:225:PRO:HG3	2.34	0.58
2:E:151:SER:OG	2:E:152:GLY:N	2.35	0.58
1:C:79:ILE:HD11	1:C:313:ILE:HD13	1.84	0.58
1:A:43:ARG:HD3	4:A:761:HOH:O	2.02	0.58
2:E:313:HIS:CG	2:E:314:PRO:HD2	2.39	0.58
2:E:357:GLY:O	2:E:360:LYS:N	2.33	0.58
2:F:332:GLU:N	2:F:332:GLU:OE2	2.36	0.58
2:D:9:LYS:HD3	2:D:19:GLU:CD	2.29	0.58
1:B:416:ASP:HB3	1:B:419:LEU:HG	1.86	0.58
1:A:225:GLY:O	1:A:370:GLY:HA2	2.03	0.57
1:C:73:VAL:HG11	1:C:309:THR:HG23	1.86	0.57
2:D:328:ILE:CD1	2:D:346:PRO:HB2	2.31	0.57
2:E:116:ILE:HD13	2:E:291:ILE:HD11	1.86	0.57
2:E:250:MET:HB2	2:E:304:LEU:HB3	1.85	0.57
2:F:166:ARG:HD2	2:F:201:THR:OG1	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:55:GLN:CD	2:D:219:ILE:HD11	2.28	0.57
1:C:386:ALA:C	1:C:387:ILE:HD12	2.29	0.57
2:F:184:ILE:CD1	2:F:225:PRO:HG3	2.33	0.57
2:E:386:ALA:HA	2:E:387:VAL:C	2.29	0.57
2:F:376:TYR:O	2:F:380:LYS:N	2.30	0.57
1:B:22:ALA:HB3	1:B:42:MET:HE1	1.85	0.57
2:D:11:VAL:HG12	2:D:65:LEU:HD21	1.87	0.57
2:D:213:LEU:N	2:D:216:ASP:OD2	2.30	0.57
1:C:41:GLU:CG	1:C:48:SER:HB2	2.33	0.57
1:C:124:ILE:HG22	1:C:162:ILE:HD13	1.86	0.57
1:C:523:LYS:O	1:C:527:THR:OG1	2.21	0.57
2:F:19:GLU:OE1	2:F:51:LYS:NZ	2.37	0.57
1:B:391:SER:O	1:B:391:SER:OG	2.22	0.57
2:F:77:LEU:HD12	2:F:77:LEU:O	2.04	0.57
1:A:156:LYS:O	1:A:178:THR:HG22	2.04	0.57
1:A:541:TYR:O	1:A:545:ILE:HG12	2.05	0.57
1:B:230:VAL:CG2	1:B:387:ILE:HD11	2.35	0.57
1:B:399:GLU:OE2	1:B:402:THR:OG1	2.22	0.57
1:C:298:MET:HB3	1:C:299:PRO:HD2	1.87	0.57
1:C:494:LYS:HA	1:C:497:ARG:NH1	2.20	0.57
2:E:79:LEU:HD22	2:E:80:GLY:N	2.20	0.56
1:C:406:LEU:HA	1:C:409:VAL:HG22	1.86	0.56
2:F:409:GLU:O	2:F:413:VAL:HB	2.05	0.56
1:B:30:VAL:HB	1:B:35:VAL:HG23	1.87	0.56
2:F:271:ARG:HD3	2:F:271:ARG:N	2.20	0.56
1:B:144:ILE:HG12	1:B:287:GLU:HB3	1.86	0.56
2:E:86:ILE:HD13	2:E:208:VAL:CG2	2.36	0.56
1:C:425:PHE:HA	1:C:426:PRO:C	2.28	0.56
2:F:313:HIS:ND1	2:F:315:ILE:HG12	2.19	0.56
2:F:315:ILE:O	2:F:319:THR:HG23	2.06	0.56
2:F:376:TYR:OH	2:F:409:GLU:N	2.38	0.56
2:F:415:GLN:O	2:F:419:THR:OG1	2.20	0.56
1:B:83:MET:HE1	1:B:270:VAL:CG1	2.29	0.56
1:B:176:ILE:HD12	1:B:185:LEU:HD11	1.86	0.56
2:F:314:PRO:O	2:F:318:LEU:HD23	2.05	0.56
1:A:298:MET:HB3	1:A:299:PRO:HD2	1.86	0.56
2:D:103:ILE:O	2:D:105:PRO:HD3	2.05	0.56
1:B:73:VAL:HG11	1:B:309:THR:HG23	1.88	0.56
2:D:155:LEU:HB3	2:D:156:PRO:HD2	1.87	0.56
1:C:546:MET:HA	1:C:546:MET:CE	2.36	0.56
2:D:386:ALA:HA	2:D:391:GLU:CB	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:379:GLY:O	2:E:383:LYS:HG3	2.06	0.56
1:C:90:PRO:HD3	1:C:111:ALA:HA	1.87	0.56
1:A:22:ALA:HB1	1:A:39:ILE:CD1	2.36	0.56
2:D:324:GLU:HB3	2:D:350:ARG:HB2	1.88	0.56
1:C:232:GLY:CA	1:C:238:LYS:HD3	2.36	0.56
2:D:146:LYS:HD3	2:D:285:PHE:O	2.06	0.56
2:D:354:LYS:HD2	2:D:354:LYS:N	2.21	0.56
2:E:148:PRO:HD3	2:E:323:THR:HB	1.87	0.56
1:C:513:THR:HG23	1:C:517:LYS:HE3	1.87	0.56
2:F:11:VAL:HG22	2:F:16:MET:HG3	1.88	0.56
1:B:212:GLY:HA3	1:B:512:PHE:CD1	2.42	0.55
1:B:489:THR:CG2	1:B:533:ARG:HH12	2.17	0.55
2:D:136:ASP:O	2:D:140:THR:HG23	2.05	0.55
2:E:405:ALA:O	2:E:408:PHE:HB3	2.07	0.55
1:B:397:ILE:O	1:B:397:ILE:HG22	2.07	0.55
2:D:332:GLU:O	2:D:336:SER:HB2	2.07	0.55
2:E:143:ARG:NH2	2:E:170:VAL:HB	2.21	0.55
2:E:345:LEU:HB2	2:E:346:PRO:CD	2.35	0.55
2:D:89:VAL:CG2	2:D:195:MET:HE1	2.25	0.55
2:E:352:LYS:O	2:E:356:THR:HG23	2.06	0.55
2:E:26:TYR:CE2	2:E:27:GLU:HG3	2.42	0.55
1:C:550:VAL:HA	1:C:553:ARG:NH1	2.21	0.55
2:D:399:LYS:HG3	2:D:401:TYR:N	2.22	0.55
2:E:106:GLU:OE1	2:E:234:TYR:OH	2.21	0.55
1:C:212:GLY:HA3	1:C:512:PHE:CD1	2.42	0.55
2:F:149:VAL:HB	2:F:303:ILE:HD13	1.88	0.55
1:A:523:LYS:HD2	1:A:574:ASN:HD21	1.72	0.55
2:E:150:PHE:HB2	2:E:328:ILE:HD13	1.89	0.55
1:C:191:TRP:CZ2	1:C:198:PRO:HD3	2.42	0.55
1:B:262:ARG:HB2	1:B:265:GLU:OE1	2.07	0.55
2:E:55:GLN:OE1	2:E:264:ARG:NH1	2.39	0.55
1:B:209:MET:SD	1:B:249:SER:HB3	2.46	0.55
2:D:292:ARG:HD2	4:D:502:HOH:O	2.06	0.55
2:F:123:TYR:O	2:F:290:ARG:NH1	2.40	0.55
2:D:282:ALA:HB2	2:D:322:ILE:HD13	1.89	0.55
2:F:340:PRO:HB3	2:F:417:PHE:HE1	1.71	0.55
2:F:343:ASP:OD2	2:F:346:PRO:HD3	2.06	0.55
2:D:34:MET:HE3	2:D:38:GLU:HB3	1.89	0.54
1:C:307:ILE:HG13	1:C:365:TYR:CE1	2.42	0.54
1:C:392:PRO:O	2:F:321:TYR:OH	2.25	0.54
2:D:94:GLY:HA3	2:D:227:MET:HE2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:150:MET:HE3	1:C:320:MET:HG2	1.88	0.54
1:A:27:MET:HE3	1:A:71:LEU:CB	2.20	0.54
1:B:210:ILE:HD11	1:B:515:ARG:HE	1.73	0.54
1:B:445:MET:HG2	1:B:453:TRP:CE3	2.42	0.54
2:D:357:GLY:H	2:D:361:THR:HG22	1.71	0.54
1:C:562:ILE:HD12	1:C:562:ILE:H	1.73	0.54
2:F:149:VAL:HB	2:F:303:ILE:CD1	2.37	0.54
1:A:95:MET:CE	2:D:120:ALA:HB2	2.37	0.54
1:A:462:ARG:O	1:A:466:GLU:HB2	2.07	0.54
2:D:389:LEU:C	2:D:391:GLU:HA	2.32	0.54
1:C:97:VAL:HG11	1:C:109:LEU:CD2	2.38	0.54
1:B:262:ARG:NH2	2:E:323:THR:O	2.40	0.54
2:D:184:ILE:N	2:D:248:THR:O	2.35	0.54
2:F:237:TYR:CZ	2:F:291:ILE:HD13	2.43	0.54
2:F:269:GLY:H	2:F:270:ARG:HA	1.72	0.54
1:A:83:MET:SD	1:A:270:VAL:HG13	2.48	0.54
1:A:285:LEU:O	1:A:289:THR:HG23	2.06	0.54
2:D:345:LEU:HG	2:D:376:TYR:HE2	1.71	0.54
2:D:356:THR:HG21	2:D:365:HIS:CE1	2.43	0.54
1:C:400:PRO:O	1:C:404:ASN:ND2	2.26	0.54
1:B:231:PRO:HG2	1:B:415:LEU:H	1.73	0.54
2:D:111:ILE:HA	2:D:230:THR:OG1	2.08	0.54
2:E:8:ILE:HD11	2:E:11:VAL:HG23	1.90	0.54
1:C:462:ARG:HH21	1:C:463:ILE:HG22	1.71	0.54
1:C:559:SER:CA	1:C:562:ILE:HD11	2.36	0.54
2:F:135:ILE:HD12	2:F:136:ASP:N	2.20	0.54
2:F:137:HIS:NE2	2:F:368:THR:HG23	2.23	0.54
2:F:340:PRO:HD3	2:F:416:GLY:O	2.08	0.54
1:A:126:GLU:HG2	1:A:162:ILE:HG22	1.89	0.54
2:D:10:GLU:HB2	2:D:17:ALA:HB3	1.90	0.54
2:D:398:ASP:CA	2:D:399:LYS:HB2	2.38	0.54
2:E:378:GLN:HA	2:E:378:GLN:OE1	2.07	0.54
1:C:156:LYS:O	1:C:178:THR:HG22	2.08	0.54
1:B:205:PRO:HB2	1:B:223:THR:OG1	2.08	0.54
2:E:184:ILE:N	2:E:248:THR:O	2.31	0.54
2:E:338:ILE:HA	2:E:414:ASN:OD1	2.08	0.54
2:F:306:MET:HG2	2:F:316:PRO:HG3	1.88	0.54
1:B:84:PHE:HB2	1:B:292:ILE:HD13	1.90	0.53
1:B:403:GLN:O	1:B:407:ARG:HG3	2.07	0.53
1:C:273:PHE:N	1:C:274:PRO:HD2	2.23	0.53
1:C:307:ILE:HD11	1:C:328:ALA:CB	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:529:GLY:O	1:B:533:ARG:HB2	2.08	0.53
2:D:431:TRP:O	2:D:435:ALA:N	2.41	0.53
1:A:43:ARG:CG	1:A:46:VAL:HG13	2.39	0.53
1:A:205:PRO:HB2	1:A:223:THR:OG1	2.09	0.53
2:D:33:ARG:O	2:D:33:ARG:HD3	2.08	0.53
2:E:306:MET:HE3	2:E:311:LYS:CA	2.37	0.53
1:C:222:VAL:HG22	1:C:411:VAL:HG11	1.90	0.53
2:D:345:LEU:HB2	2:D:346:PRO:CD	2.39	0.53
2:E:383:LYS:HZ2	2:E:406:GLU:HG3	1.74	0.53
1:C:497:ARG:O	1:C:502:GLN:HG3	2.08	0.53
1:A:546:MET:HA	1:A:546:MET:CE	2.32	0.53
1:B:266:MET:O	1:B:270:VAL:HG23	2.08	0.53
2:D:402:ALA:HA	2:D:405:ALA:HB3	1.91	0.53
2:E:87:GLY:HA2	2:E:204:ILE:O	2.08	0.53
1:C:533:ARG:HA	1:C:536:LEU:HB3	1.90	0.53
2:F:125:ASP:OD2	2:F:125:ASP:N	2.34	0.53
1:A:495:SER:O	1:A:499:ASP:HB2	2.09	0.53
1:B:549:THR:O	1:B:553:ARG:HG3	2.09	0.53
2:D:8:ILE:HD13	2:D:16:MET:CE	2.39	0.53
2:E:41:ARG:HB2	2:E:57:PHE:CD1	2.44	0.53
2:E:129:GLN:HE22	2:E:171:LEU:HD13	1.73	0.53
1:C:262:ARG:NH2	2:F:323:THR:O	2.42	0.53
2:F:126:GLU:O	2:F:142:VAL:HG13	2.09	0.53
2:F:151:SER:OG	2:F:157:HIS:HB3	2.08	0.53
2:F:306:MET:HE3	2:F:311:LYS:HA	1.90	0.53
1:B:208:PRO:HG3	1:B:441:VAL:HG22	1.91	0.53
1:C:467:GLU:OE2	1:C:497:ARG:NH1	2.42	0.53
1:B:273:PHE:HB3	1:B:274:PRO:HD3	1.91	0.53
1:B:405:THR:O	1:B:409:VAL:HG22	2.09	0.53
1:C:60:PRO:HD3	2:F:47:VAL:CG1	2.39	0.53
1:C:416:ASP:OD2	1:C:418:SER:HB2	2.08	0.53
1:C:480:ASP:OD1	1:C:481:SER:N	2.42	0.53
2:F:5:TYR:HB3	2:F:7:THR:HG22	1.91	0.53
2:F:269:GLY:N	2:F:270:ARG:HA	2.24	0.53
2:D:362:ARG:HH11	2:D:364:ASP:CB	2.22	0.53
2:E:111:ILE:HA	2:E:230:THR:OG1	2.09	0.53
1:C:25:GLN:HG3	1:C:38:GLU:OE1	2.09	0.53
2:F:95:ARG:HG3	4:F:518:HOH:O	2.09	0.53
2:F:339:GLN:HA	2:F:340:PRO:C	2.32	0.53
1:B:364:GLU:O	1:B:368:ARG:HG3	2.08	0.52
2:D:248:THR:HG22	2:D:249:ASP:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:LYS:O	1:B:320:MET:HE2	2.08	0.52
1:B:173:ILE:HD13	1:B:187:MET:HG2	1.92	0.52
2:E:71:ARG:HD2	4:E:527:HOH:O	2.08	0.52
2:E:376:TYR:CD1	2:E:408:PHE:HD1	2.27	0.52
1:C:173:ILE:HD13	1:C:173:ILE:H	1.73	0.52
1:C:552:VAL:HG11	1:C:577:ILE:HG12	1.91	0.52
2:F:204:ILE:HD13	2:F:204:ILE:O	2.10	0.52
2:F:307:PRO:HG2	2:F:313:HIS:CD2	2.44	0.52
1:A:40:ILE:HG13	1:A:50:GLN:HG2	1.90	0.52
1:B:507:ASP:HB3	1:B:510:ASP:HB3	1.91	0.52
4:B:601:HOH:O	2:E:322:ILE:HG23	2.08	0.52
2:E:125:ASP:HA	2:E:142:VAL:CG1	2.39	0.52
1:C:532:ALA:HA	1:C:581:ILE:HD11	1.90	0.52
1:A:315:GLU:HA	1:A:384:ILE:HD11	1.92	0.52
1:B:210:ILE:HD11	1:B:515:ARG:HH21	1.75	0.52
2:D:116:ILE:HD13	2:D:291:ILE:CD1	2.36	0.52
2:D:430:GLY:O	2:D:434:LEU:HB2	2.08	0.52
2:E:124:PRO:HA	2:E:290:ARG:HD3	1.92	0.52
2:F:135:ILE:CD1	2:F:136:ASP:N	2.72	0.52
2:F:270:ARG:CB	2:F:271:ARG:CA	2.88	0.52
2:F:306:MET:HE3	2:F:311:LYS:CA	2.40	0.52
2:F:319:THR:O	2:F:323:THR:HG23	2.10	0.52
1:A:162:ILE:HD13	1:A:174:CYS:HB2	1.91	0.52
1:A:459:GLU:O	1:A:463:ILE:HG13	2.10	0.52
1:B:380:ARG:HG2	4:B:614:HOH:O	2.09	0.52
1:C:84:PHE:HB3	1:C:88:GLN:HA	1.90	0.52
2:F:270:ARG:CB	2:F:271:ARG:HA	2.40	0.52
2:D:87:GLY:HA2	2:D:204:ILE:O	2.09	0.52
1:A:204:ASN:HD21	2:E:192:GLU:HG2	1.75	0.52
1:A:258:GLY:HA2	1:A:329:ASP:O	2.10	0.52
2:D:130:THR:OG1	2:D:136:ASP:OD1	2.21	0.52
1:C:27:MET:HE3	1:C:71:LEU:HD13	1.92	0.52
1:A:41:GLU:HB2	1:A:48:SER:HB2	1.92	0.52
2:D:306:MET:HE1	2:D:311:LYS:CG	2.32	0.52
2:F:34:MET:HE2	2:F:40:ARG:HG3	1.92	0.52
2:E:29:LEU:HD21	2:E:77:LEU:HG	1.91	0.52
2:F:431:TRP:HA	2:F:434:LEU:CD1	2.39	0.52
2:D:12:VAL:HG13	1:C:41:GLU:OE2	2.10	0.52
2:E:404:PHE:CZ	2:E:436:MET:CB	2.93	0.52
1:C:417:SER:O	1:C:421:GLN:HG3	2.10	0.52
1:A:43:ARG:HG2	1:A:46:VAL:HG13	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:GLY:HA3	1:A:512:PHE:CD1	2.45	0.51
1:A:320:MET:HE2	1:A:322:TYR:CE2	2.45	0.51
1:B:114:HIS:HB3	1:B:170:ASP:OD2	2.10	0.51
1:B:253:LEU:HD13	1:B:317:PHE:CG	2.45	0.51
1:B:397:ILE:CG2	1:B:402:THR:HG21	2.38	0.51
2:D:124:PRO:HG2	2:D:351:LEU:CD1	2.37	0.51
2:D:148:PRO:HD3	2:D:323:THR:HB	1.92	0.51
2:E:166:ARG:HD2	2:E:201:THR:HG21	1.92	0.51
2:E:182:ALA:HB3	2:E:247:MET:HG2	1.91	0.51
1:C:256:TYR:CD1	1:C:327:MET:HE3	2.41	0.51
1:A:399:GLU:HB2	1:A:400:PRO:HD2	1.91	0.51
2:E:408:PHE:HE2	2:E:412:TYR:CD2	2.27	0.51
2:F:58:GLU:OE1	2:F:58:GLU:N	2.42	0.51
2:F:237:TYR:CE2	2:F:291:ILE:HD13	2.45	0.51
1:B:564:GLU:O	1:B:567:LEU:HD11	2.10	0.51
1:C:234:PHE:CE2	2:F:350:ARG:HG2	2.45	0.51
1:C:245:ILE:O	1:C:249:SER:OG	2.23	0.51
2:F:132:ILE:CB	2:F:135:ILE:HD11	2.40	0.51
1:A:297:ASN:ND2	2:D:115:VAL:HG22	2.25	0.51
1:A:573:ILE:O	1:A:577:ILE:HG13	2.10	0.51
1:B:75:LEU:HD13	1:B:316:TYR:CD1	2.45	0.51
1:B:311:ILE:HD13	1:B:368:ARG:HB2	1.92	0.51
2:D:65:LEU:HD12	2:D:65:LEU:H	1.75	0.51
2:D:126:GLU:OE2	2:D:290:ARG:NH1	2.43	0.51
2:D:271:ARG:HB3	2:D:314:PRO:HG2	1.92	0.51
2:F:285:PHE:HB2	2:F:322:ILE:CD1	2.41	0.51
1:A:351:ASP:OD1	2:E:258:ARG:NH2	2.43	0.51
1:B:271:ASN:OD1	2:E:292:ARG:NH2	2.44	0.51
1:B:396:ASP:OD2	1:B:398:SER:N	2.39	0.51
1:B:497:ARG:O	1:B:502:GLN:HG3	2.11	0.51
2:D:45:LEU:CD1	2:D:264:ARG:CD	2.89	0.51
1:C:415:LEU:HD23	1:C:428:ILE:HG12	1.92	0.51
1:A:474:VAL:O	1:A:478:GLY:N	2.44	0.51
2:D:184:ILE:HD13	2:D:225:PRO:HG3	1.92	0.51
2:D:199:ARG:HD3	4:D:522:HOH:O	2.10	0.51
1:A:38:GLU:OE1	1:A:52:TYR:OH	2.29	0.51
1:A:224:LYS:CE	1:A:250:ASP:HB3	2.41	0.51
2:F:87:GLY:HA2	2:F:204:ILE:HD13	1.92	0.51
1:A:194:ARG:NH1	4:A:704:HOH:O	2.42	0.51
1:A:532:ALA:O	1:A:536:LEU:HG	2.11	0.51
1:A:545:ILE:HD13	1:A:584:ILE:HG21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:463:ILE:HD11	1:C:496:ILE:CD1	2.36	0.51
1:B:262:ARG:HB2	1:B:265:GLU:CG	2.40	0.51
1:C:51:VAL:HG21	1:C:55:THR:HG21	1.92	0.51
2:D:13:GLY:O	2:D:60:THR:HG21	2.11	0.51
2:E:376:TYR:CD1	2:E:408:PHE:CD1	2.99	0.51
1:C:492:VAL:O	1:C:496:ILE:HG13	2.11	0.51
1:A:551:ALA:O	1:A:554:GLU:HB3	2.11	0.50
1:B:254:VAL:HB	1:B:289:THR:HG22	1.93	0.50
2:F:328:ILE:N	2:F:347:SER:OG	2.30	0.50
2:F:369:MET:HG3	2:F:370:ASN:H	1.74	0.50
1:B:92:ASP:OD2	1:B:93:THR:N	2.42	0.50
1:B:562:ILE:HG13	1:B:570:ILE:HG12	1.92	0.50
2:F:203:ALA:O	2:F:206:ARG:HG2	2.11	0.50
2:F:396:ASP:O	2:F:400:ILE:HG23	2.11	0.50
1:A:43:ARG:HB2	1:A:46:VAL:O	2.11	0.50
1:A:71:LEU:HD23	1:A:193:VAL:HG21	1.93	0.50
1:B:461:MET:HE3	1:B:464:LEU:HB2	1.94	0.50
2:D:315:ILE:HB	2:D:316:PRO:CD	2.41	0.50
2:D:328:ILE:HD12	2:D:346:PRO:CB	2.33	0.50
1:B:266:MET:HE2	1:B:293:ALA:HB1	1.94	0.50
1:B:565:GLU:O	1:B:567:LEU:HD22	2.11	0.50
2:D:399:LYS:HD2	2:D:400:ILE:CG1	2.42	0.50
1:C:473:ILE:O	1:C:477:VAL:HG22	2.10	0.50
1:A:126:GLU:CG	1:A:162:ILE:HG22	2.40	0.50
1:A:218:THR:HG23	1:A:453:TRP:CZ2	2.46	0.50
1:B:225:GLY:O	1:B:370:GLY:HA2	2.10	0.50
2:E:315:ILE:HB	2:E:316:PRO:CD	2.41	0.50
2:F:144:GLY:HA2	2:F:298:VAL:O	2.12	0.50
1:A:16:ALA:HB3	1:A:19:MET:CE	2.42	0.50
1:B:82:GLN:HE22	1:B:92:ASP:CG	2.20	0.50
1:B:311:ILE:CD1	1:B:368:ARG:HB2	2.41	0.50
2:F:8:ILE:O	2:F:8:ILE:HG13	2.11	0.50
2:F:155:LEU:HD21	2:F:341:PRO:CG	2.40	0.50
1:A:40:ILE:HG22	1:A:41:GLU:HG3	1.94	0.50
1:C:338:LEU:HD22	1:C:355:PRO:HG3	1.94	0.50
1:C:493:ALA:O	1:C:497:ARG:HG3	2.11	0.50
2:F:34:MET:HE3	2:F:38:GLU:HB3	1.94	0.50
1:B:230:VAL:HG21	1:B:387:ILE:HD11	1.94	0.50
1:B:425:PHE:HA	1:B:426:PRO:C	2.36	0.50
2:F:422:THR:O	2:F:426:THR:N	2.39	0.50
1:A:80:ILE:O	1:A:81:SER:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:ILE:HG22	1:B:81:SER:HB3	1.94	0.50
2:D:399:LYS:HD2	2:D:400:ILE:N	2.22	0.50
2:E:219:ILE:HD13	2:E:260:ILE:CD1	2.39	0.50
2:E:408:PHE:CE2	2:E:412:TYR:HD2	2.30	0.50
2:F:136:ASP:HA	2:F:139:ASN:O	2.11	0.50
1:B:567:LEU:HD13	1:B:567:LEU:N	2.27	0.49
1:B:573:ILE:O	1:B:577:ILE:HG13	2.11	0.49
1:C:139:VAL:CG2	1:C:187:MET:HE3	2.41	0.49
1:A:22:ALA:HB1	1:A:39:ILE:HD13	1.94	0.49
1:B:119:TRP:CZ3	1:B:165:GLY:HA2	2.47	0.49
1:C:33:LEU:HD12	1:C:33:LEU:N	2.28	0.49
1:C:300:VAL:HG22	1:C:303:ARG:NH2	2.27	0.49
2:F:107:LYS:NZ	2:F:238:GLU:OE2	2.34	0.49
1:B:399:GLU:OE2	1:B:401:VAL:HB	2.12	0.49
2:D:28:GLU:O	2:D:44:VAL:HG23	2.13	0.49
2:D:343:ASP:O	2:D:346:PRO:HD2	2.12	0.49
2:E:191:ALA:O	2:E:195:MET:HG2	2.12	0.49
1:C:499:ASP:O	1:C:560:LYS:NZ	2.41	0.49
1:A:405:THR:O	1:A:409:VAL:HG22	2.12	0.49
1:B:210:ILE:HD11	1:B:515:ARG:NH2	2.27	0.49
2:D:29:LEU:HD11	2:D:77:LEU:HD23	1.94	0.49
2:D:145:GLN:HG2	2:D:146:LYS:N	2.26	0.49
1:C:251:VAL:HG12	1:C:252:ASP:N	2.27	0.49
2:F:34:MET:CE	2:F:40:ARG:HG3	2.41	0.49
2:F:132:ILE:O	2:F:135:ILE:HD11	2.11	0.49
2:F:256:ALA:O	2:F:260:ILE:HG12	2.11	0.49
2:D:345:LEU:HG	2:D:376:TYR:CE2	2.47	0.49
2:E:30:ILE:C	2:E:30:ILE:HD12	2.37	0.49
1:C:92:ASP:OD1	1:C:93:THR:N	2.46	0.49
1:A:119:TRP:CZ3	1:A:165:GLY:HA2	2.47	0.49
1:A:208:PRO:HB3	1:A:441:VAL:HG13	1.93	0.49
2:D:89:VAL:HG21	2:D:195:MET:CE	2.27	0.49
1:C:12:PRO:HG2	1:C:344:ARG:HD2	1.94	0.49
1:C:177:GLU:HA	1:C:182:LEU:HD12	1.95	0.49
1:C:234:PHE:CD2	2:F:350:ARG:HG2	2.48	0.49
2:F:128:ILE:HB	2:F:141:LEU:HB3	1.94	0.49
1:A:297:ASN:HB2	2:D:286:GLU:CB	2.41	0.49
1:A:453:TRP:CZ3	1:A:519:PHE:HA	2.47	0.49
1:A:507:ASP:O	1:A:511:THR:HB	2.12	0.49
1:A:516:GLU:O	1:A:520:ASN:ND2	2.43	0.49
1:B:82:GLN:HG3	1:B:83:MET:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:THR:OG1	1:B:187:MET:N	2.46	0.49
2:E:236:ALA:O	2:E:296:GLY:HA3	2.13	0.49
1:C:87:ILE:HG13	1:C:89:ARG:HG3	1.93	0.49
2:F:254:ALA:CB	2:F:315:ILE:HD12	2.42	0.49
1:A:298:MET:HB3	1:A:299:PRO:CD	2.43	0.49
1:A:425:PHE:O	1:A:502:GLN:HA	2.12	0.49
2:D:45:LEU:HD11	2:D:264:ARG:HD3	1.95	0.49
2:D:245:VAL:HG11	2:D:247:MET:HE3	1.93	0.49
2:E:125:ASP:HB2	2:E:126:GLU:CA	2.42	0.49
2:F:191:ALA:O	2:F:195:MET:HG2	2.12	0.49
1:A:150:MET:HE1	1:A:319:ASP:CB	2.34	0.49
2:D:307:PRO:HG2	2:D:313:HIS:CE1	2.48	0.49
2:F:151:SER:OG	2:F:155:LEU:HB3	2.12	0.49
2:F:369:MET:CG	2:F:370:ASN:N	2.76	0.49
1:A:514:SER:O	1:A:518:GLN:HG3	2.13	0.49
1:B:19:MET:HE1	1:B:64:VAL:CB	2.41	0.49
1:B:453:TRP:HD1	1:B:519:PHE:HD1	1.60	0.49
2:D:235:LEU:O	2:D:239:LYS:HB2	2.13	0.49
2:D:408:PHE:HA	2:D:433:LEU:HD21	1.95	0.49
1:C:541:TYR:HB3	1:C:543:ASN:OD1	2.13	0.49
1:B:210:ILE:HD11	1:B:515:ARG:NE	2.27	0.48
1:B:562:ILE:HG21	1:B:570:ILE:HG13	1.95	0.48
2:D:249:ASP:HB3	2:D:252:ASN:ND2	2.28	0.48
2:E:135:ILE:O	2:E:140:THR:HA	2.12	0.48
2:E:313:HIS:CE1	2:E:315:ILE:HG13	2.47	0.48
2:E:343:ASP:O	2:E:346:PRO:HD2	2.13	0.48
2:F:14:PRO:HG2	2:F:15:LEU:CD1	2.43	0.48
2:F:365:HIS:HA	2:F:368:THR:HG22	1.94	0.48
1:A:467:GLU:HG2	1:A:471:ASN:ND2	2.29	0.48
2:D:271:ARG:CG	2:D:271:ARG:HH11	2.26	0.48
1:C:77:PRO:HG2	1:C:169:ILE:HG22	1.94	0.48
1:C:390:VAL:CG1	1:C:402:THR:HG22	2.42	0.48
2:F:397:ILE:CA	2:F:400:ILE:HG12	2.42	0.48
2:F:452:LYS:HA	2:F:452:LYS:CE	2.43	0.48
1:A:86:GLY:HA3	1:A:302:ALA:O	2.13	0.48
1:B:549:THR:HB	1:B:552:VAL:CG1	2.43	0.48
2:E:71:ARG:HD3	4:E:521:HOH:O	2.14	0.48
1:C:329:ASP:HA	1:C:330:SER:HA	1.48	0.48
1:A:454:SER:O	1:A:458:THR:HG23	2.13	0.48
1:A:499:ASP:OD2	1:A:557:SER:HA	2.13	0.48
1:B:252:ASP:HB2	1:B:322:TYR:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:92:GLY:O	2:E:227:MET:HG3	2.14	0.48
1:C:532:ALA:HA	1:C:581:ILE:CD1	2.43	0.48
1:A:103:LEU:HD23	2:D:115:VAL:HG12	1.96	0.48
1:C:514:SER:O	1:C:518:GLN:HG3	2.13	0.48
2:F:264:ARG:C	2:F:265:ARG:HE	2.20	0.48
2:F:395:SER:OG	2:F:398:ASP:HB2	2.13	0.48
1:A:267:THR:OG1	2:D:121:ARG:HD2	2.13	0.48
1:B:209:MET:HG2	1:B:250:ASP:OD2	2.13	0.48
2:D:8:ILE:HD13	2:D:16:MET:HE3	1.95	0.48
2:D:93:LEU:C	2:D:227:MET:HE2	2.39	0.48
2:D:126:GLU:N	2:D:126:GLU:OE1	2.46	0.48
2:E:245:VAL:CG1	2:E:247:MET:HE3	2.44	0.48
1:C:85:ASP:O	1:C:294:ASN:ND2	2.39	0.48
1:C:393:SER:HA	2:F:321:TYR:OH	2.13	0.48
2:F:270:ARG:CB	2:F:271:ARG:HB3	2.44	0.48
1:B:360:SER:O	1:B:364:GLU:HG3	2.14	0.48
1:B:393:SER:N	1:B:394:GLY:CA	2.73	0.48
1:C:23:CYS:O	1:C:26:ASP:HB2	2.14	0.48
1:C:467:GLU:O	1:C:471:ASN:HB2	2.13	0.48
1:A:392:PRO:HB3	1:A:399:GLU:HG2	1.95	0.48
2:D:18:VAL:O	2:D:51:LYS:HA	2.13	0.48
2:E:255:GLU:OE2	2:E:273:TYR:OH	2.31	0.48
2:F:315:ILE:HB	2:F:316:PRO:CD	2.39	0.48
1:A:482:LEU:HD22	1:A:486:ASP:HB3	1.96	0.48
1:B:9:VAL:CG1	2:E:47:VAL:HG23	2.41	0.48
2:E:278:TYR:CE1	2:E:321:TYR:HD2	2.32	0.48
1:B:577:ILE:O	1:B:581:ILE:HG12	2.14	0.48
2:D:382:ALA:O	2:D:386:ALA:N	2.44	0.48
2:E:282:ALA:HB2	2:E:322:ILE:HD13	1.96	0.48
1:C:224:LYS:HE2	1:C:250:ASP:HB3	1.96	0.48
1:C:295:THR:O	1:C:303:ARG:HD3	2.14	0.47
1:C:332:SER:HB2	1:C:391:SER:HB2	1.95	0.47
1:B:2:GLN:OE1	1:B:21:GLU:HB2	2.14	0.47
1:B:298:MET:HB3	1:B:299:PRO:CD	2.44	0.47
1:B:415:LEU:HA	1:B:427:SER:O	2.15	0.47
1:B:495:SER:O	1:B:499:ASP:N	2.40	0.47
2:D:260:ILE:CG2	2:D:264:ARG:HE	2.27	0.47
2:E:86:ILE:HD13	2:E:208:VAL:HG23	1.96	0.47
1:C:491:GLU:HG3	1:C:542:PHE:CZ	2.49	0.47
2:F:126:GLU:CB	2:F:143:ARG:HG3	2.43	0.47
2:F:285:PHE:CB	2:F:322:ILE:HD11	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:543:ASN:O	1:B:547:GLU:HG3	2.13	0.47
2:D:162:ALA:O	2:D:166:ARG:HG3	2.14	0.47
2:E:146:LYS:NZ	4:E:506:HOH:O	2.47	0.47
2:E:171:LEU:HA	2:E:172:ASP:HA	1.45	0.47
1:A:252:ASP:O	1:A:288:ARG:HG2	2.15	0.47
1:A:334:TRP:CH2	1:A:338:LEU:HD12	2.50	0.47
1:B:488:LEU:O	1:B:492:VAL:HG23	2.15	0.47
1:B:552:VAL:O	1:B:556:ILE:HG13	2.15	0.47
2:E:379:GLY:O	2:E:402:ALA:HA	2.14	0.47
1:C:415:LEU:HA	1:C:427:SER:O	2.15	0.47
1:A:583:LEU:C	1:A:583:LEU:HD23	2.40	0.47
1:B:231:PRO:HG2	1:B:415:LEU:N	2.30	0.47
2:E:28:GLU:OE1	2:E:72:PHE:HB3	2.14	0.47
2:E:103:ILE:O	2:E:105:PRO:HD3	2.13	0.47
2:E:412:TYR:O	2:E:421:ARG:NH1	2.47	0.47
1:C:94:PHE:CE2	1:C:103:LEU:HA	2.50	0.47
1:C:392:PRO:HB2	1:C:396:ASP:O	2.14	0.47
2:F:132:ILE:C	2:F:415:GLN:HE22	2.22	0.47
2:F:160:LEU:O	2:F:164:ILE:HG13	2.15	0.47
2:F:269:GLY:N	2:F:273:TYR:O	2.47	0.47
1:A:74:GLU:HA	1:A:188:MET:HE1	1.96	0.47
1:B:399:GLU:OE2	1:B:402:THR:N	2.41	0.47
2:D:156:PRO:HG3	2:D:334:TYR:CE1	2.50	0.47
2:D:166:ARG:NH2	2:D:417:PHE:O	2.47	0.47
2:D:282:ALA:CA	2:D:322:ILE:HD13	2.44	0.47
1:C:452:ASP:O	1:C:456:MET:HG3	2.14	0.47
1:B:565:GLU:C	1:B:567:LEU:HD13	2.39	0.47
2:E:131:GLY:HA3	2:E:420:ASN:OD1	2.15	0.47
2:E:415:GLN:O	2:E:419:THR:OG1	2.21	0.47
2:F:198:PHE:O	2:F:204:ILE:HB	2.15	0.47
2:F:246:ILE:CD1	2:F:301:ILE:HB	2.45	0.47
1:A:430:TRP:O	1:A:461:MET:HE1	2.15	0.47
1:B:145:ILE:HG13	1:B:253:LEU:HD21	1.96	0.47
1:B:523:LYS:O	1:B:527:THR:OG1	2.33	0.47
1:C:482:LEU:HD21	1:C:487:ARG:HD2	1.97	0.47
1:A:210:ILE:HG12	1:A:515:ARG:HH21	1.80	0.46
1:A:410:LYS:HB3	1:A:436:LEU:HB2	1.96	0.46
1:A:261:GLU:O	1:A:295:THR:HA	2.15	0.46
1:B:556:ILE:HG12	1:B:573:ILE:HG21	1.97	0.46
2:D:313:HIS:CG	2:D:314:PRO:HD2	2.50	0.46
2:D:324:GLU:HA	2:D:350:ARG:HD2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:285:PHE:CD2	2:F:322:ILE:HG12	2.47	0.46
1:A:133:GLY:O	1:A:380:ARG:NH2	2.27	0.46
1:A:266:MET:CE	1:A:269:VAL:HB	2.46	0.46
1:A:308:TYR:HA	1:A:311:ILE:HG22	1.97	0.46
1:B:209:MET:CE	1:B:385:THR:HG21	2.45	0.46
2:E:257:LEU:HD11	2:E:280:ASN:CG	2.40	0.46
1:C:44:GLN:HB3	1:C:45:ASP:H	1.51	0.46
2:F:186:ILE:HD12	2:F:186:ILE:O	2.14	0.46
1:B:220:PHE:CZ	1:B:433:SER:HB2	2.50	0.46
2:E:45:LEU:CD1	2:E:264:ARG:HD3	2.41	0.46
1:C:274:PRO:HA	1:C:286:MET:HG2	1.97	0.46
2:F:60:THR:HA	2:F:63:ILE:HD12	1.96	0.46
2:F:248:THR:OG1	2:F:303:ILE:HB	2.14	0.46
1:B:86:GLY:HA2	1:B:294:ASN:HD21	1.80	0.46
1:B:129:GLU:H	1:B:129:GLU:CD	2.22	0.46
1:B:329:ASP:HA	1:B:330:SER:HA	1.52	0.46
1:B:513:THR:HG23	1:B:517:LYS:HD3	1.97	0.46
2:F:279:THR:O	2:F:283:THR:HG23	2.16	0.46
1:B:80:ILE:HA	1:B:81:SER:HA	1.71	0.46
1:B:514:SER:O	1:B:518:GLN:HG3	2.15	0.46
1:A:329:ASP:HA	1:A:330:SER:HA	1.55	0.46
1:B:129:GLU:OE1	1:B:129:GLU:N	2.35	0.46
1:B:214:ARG:NH1	1:B:513:THR:OG1	2.48	0.46
2:D:142:VAL:HG21	2:D:351:LEU:O	2.16	0.46
2:E:94:GLY:HA3	2:E:227:MET:HE2	1.97	0.46
2:E:333:LEU:O	2:E:338:ILE:HG12	2.16	0.46
1:C:573:ILE:O	1:C:577:ILE:HG13	2.16	0.46
1:B:555:ARG:CZ	1:B:573:ILE:HG12	2.45	0.46
2:D:248:THR:HA	2:D:249:ASP:HA	1.68	0.46
2:E:415:GLN:H	2:E:415:GLN:HG2	1.56	0.46
1:C:123:THR:HG22	1:C:137:GLY:CA	2.46	0.46
1:B:315:GLU:HA	1:B:384:ILE:HD11	1.98	0.46
2:E:8:ILE:HD12	2:E:65:LEU:HG	1.93	0.46
1:C:410:LYS:HB2	1:C:437:TYR:CE2	2.51	0.46
1:A:417:SER:O	1:A:421:GLN:HG3	2.16	0.46
1:B:103:LEU:HD21	2:E:117:ASN:HA	1.98	0.46
1:B:300:VAL:HG22	1:B:303:ARG:HH22	1.78	0.46
2:F:186:ILE:HD11	2:F:191:ALA:HB2	1.96	0.46
2:F:446:LYS:C	2:F:448:ASP:H	2.23	0.46
1:C:75:LEU:HB3	1:C:316:TYR:CE1	2.51	0.45
1:C:341:MET:HA	1:C:341:MET:CE	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:30:ILE:C	2:F:30:ILE:HD12	2.41	0.45
2:F:30:ILE:HG13	2:F:42:GLY:C	2.41	0.45
2:F:179:VAL:HB	2:F:207:SER:CB	2.40	0.45
2:F:367:ALA:C	2:F:370:ASN:HD22	2.23	0.45
1:A:43:ARG:H	1:A:44:GLN:HA	1.80	0.45
1:B:176:ILE:CD1	1:B:185:LEU:HD11	2.46	0.45
2:E:224:THR:N	2:E:225:PRO:HD2	2.31	0.45
1:C:208:PRO:HA	1:C:223:THR:HA	1.97	0.45
1:C:259:CYS:HB3	1:C:306:SER:OG	2.16	0.45
1:B:128:THR:O	1:B:159:VAL:HG23	2.16	0.45
1:B:546:MET:CE	1:B:553:ARG:HD3	2.46	0.45
2:E:165:ALA:O	2:E:206:ARG:NH2	2.49	0.45
1:C:295:THR:OG1	1:C:298:MET:HG3	2.16	0.45
1:A:555:ARG:HD3	1:A:576:GLU:OE1	2.16	0.45
1:B:114:HIS:HA	1:B:169:ILE:HG12	1.99	0.45
2:D:250:MET:HB2	2:D:304:LEU:HB3	1.99	0.45
2:D:357:GLY:H	2:D:361:THR:CG2	2.30	0.45
2:E:29:LEU:HD11	2:E:77:LEU:HA	1.98	0.45
1:C:129:GLU:H	1:C:129:GLU:CD	2.22	0.45
1:C:363:ALA:O	1:C:367:GLU:HB2	2.16	0.45
2:F:8:ILE:HD11	2:F:65:LEU:HD22	1.99	0.45
2:F:393:ALA:HB3	2:F:394:LEU:HA	1.98	0.45
1:A:33:LEU:HD13	4:A:738:HOH:O	2.16	0.45
1:B:142:THR:HB	1:B:287:GLU:OE2	2.16	0.45
1:B:143:LYS:C	1:B:144:ILE:HD13	2.41	0.45
1:B:144:ILE:HD11	1:B:283:GLU:HB2	1.97	0.45
2:E:111:ILE:HG21	2:E:227:MET:SD	2.57	0.45
1:C:222:VAL:HG22	1:C:411:VAL:HG21	1.98	0.45
1:C:354:TYR:HB3	1:C:358:LEU:HD22	1.97	0.45
2:F:145:GLN:HG2	2:F:146:LYS:N	2.32	0.45
1:A:291:LEU:HD23	1:A:291:LEU:C	2.42	0.45
1:A:340:GLU:OE1	2:D:279:THR:OG1	2.35	0.45
1:B:173:ILE:HD13	1:B:187:MET:CG	2.46	0.45
1:B:227:ALA:HA	1:B:386:ALA:O	2.16	0.45
1:B:556:ILE:HD11	1:B:577:ILE:HD11	1.98	0.45
2:E:404:PHE:HZ	2:E:436:MET:CB	2.29	0.45
1:C:228:ALA:HA	1:C:411:VAL:O	2.16	0.45
1:C:479:ILE:O	1:C:482:LEU:HD22	2.16	0.45
1:C:562:ILE:HG22	1:C:563:PRO:CD	2.36	0.45
2:F:155:LEU:HD13	2:F:156:PRO:CD	2.47	0.45
1:A:448:ILE:HD13	1:A:515:ARG:HH11	1.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:278:TYR:CA	2:E:318:LEU:HD13	2.45	0.45
2:F:430:GLY:O	2:F:434:LEU:HD13	2.17	0.45
1:A:24:ILE:HD13	1:A:42:MET:HG2	1.98	0.45
1:A:84:PHE:HB2	1:A:292:ILE:CD1	2.47	0.45
1:A:274:PRO:HA	1:A:286:MET:HG2	1.97	0.45
2:E:271:ARG:CG	2:E:314:PRO:HG3	2.47	0.45
1:C:520:ASN:O	1:C:524:VAL:HG23	2.17	0.45
2:F:158:LYS:HA	2:F:194:PHE:HZ	1.81	0.45
1:A:476:LEU:N	1:A:477:VAL:CA	2.79	0.45
1:B:231:PRO:HG2	1:B:414:GLY:CA	2.40	0.45
1:B:416:ASP:OD1	1:B:418:SER:N	2.48	0.45
1:B:532:ALA:O	1:B:536:LEU:HG	2.16	0.45
2:D:148:PRO:HD2	2:D:325:GLY:O	2.17	0.45
2:E:125:ASP:HA	2:E:142:VAL:HG13	1.99	0.45
2:E:162:ALA:O	2:E:166:ARG:HG3	2.17	0.45
1:C:364:GLU:O	1:C:368:ARG:HG3	2.17	0.45
1:A:467:GLU:HG2	1:A:471:ASN:HD21	1.82	0.45
1:B:230:VAL:HA	1:B:231:PRO:HD3	1.70	0.45
1:B:311:ILE:O	1:B:315:GLU:HG3	2.16	0.45
1:C:348:MET:HA	1:C:349:PRO:HD3	1.83	0.45
1:B:150:MET:HE3	1:B:380:ARG:NH2	2.29	0.44
2:E:148:PRO:CB	2:E:302:PRO:HG2	2.35	0.44
1:C:227:ALA:HA	1:C:386:ALA:O	2.17	0.44
2:F:313:HIS:O	2:F:316:PRO:HD2	2.17	0.44
2:F:351:LEU:HD12	2:F:351:LEU:O	2.17	0.44
2:D:304:LEU:C	2:D:304:LEU:HD12	2.43	0.44
2:D:372:LEU:CD2	2:D:434:LEU:HD23	2.48	0.44
2:E:229:LEU:HG	2:E:247:MET:HE1	1.99	0.44
1:C:291:LEU:HD23	1:C:291:LEU:C	2.42	0.44
1:C:479:ILE:HD12	1:C:482:LEU:HD13	1.99	0.44
1:A:521:MET:O	1:A:524:VAL:HG22	2.18	0.44
1:B:84:PHE:HB3	1:B:88:GLN:HA	1.98	0.44
1:B:204:ASN:OD1	1:B:204:ASN:N	2.31	0.44
1:B:309:THR:O	1:B:313:ILE:HG13	2.17	0.44
2:D:127:PHE:HB2	2:D:355:GLY:O	2.17	0.44
2:E:29:LEU:HD11	2:E:77:LEU:HD23	1.99	0.44
2:E:183:ALA:HB1	2:E:186:ILE:CD1	2.47	0.44
2:F:274:PRO:HB2	2:F:276:TYR:CE2	2.51	0.44
1:A:24:ILE:CD1	1:A:42:MET:HG2	2.47	0.44
1:A:260:GLY:O	1:A:333:ARG:HD3	2.18	0.44
1:A:268:ASP:HB3	4:A:730:HOH:O	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:482:LEU:CD2	1:A:486:ASP:HB3	2.48	0.44
2:D:443:LYS:N	2:D:444:ARG:CA	2.79	0.44
2:E:304:LEU:HD12	2:E:304:LEU:O	2.17	0.44
2:E:330:THR:HB	2:E:332:GLU:OE1	2.17	0.44
2:E:429:LEU:O	2:E:429:LEU:HD12	2.17	0.44
1:C:318:ARG:HD2	1:C:372:VAL:CG2	2.48	0.44
1:C:559:SER:C	1:C:562:ILE:HD11	2.43	0.44
2:D:65:LEU:HD12	2:D:65:LEU:N	2.33	0.44
2:E:10:GLU:HG2	2:E:17:ALA:CB	2.46	0.44
2:E:221:ARG:NH1	4:E:502:HOH:O	2.30	0.44
1:C:327:MET:HA	1:C:387:ILE:O	2.18	0.44
1:C:538:LEU:HD12	1:C:538:LEU:O	2.18	0.44
2:F:201:THR:HG23	2:F:203:ALA:N	2.24	0.44
2:F:415:GLN:HG2	2:F:419:THR:O	2.16	0.44
1:A:8:LYS:HE3	2:D:46:GLU:OE1	2.18	0.44
2:D:256:ALA:O	2:D:260:ILE:HD13	2.17	0.44
2:E:6:ARG:H	2:E:6:ARG:HG2	1.66	0.44
2:E:277:LEU:O	2:E:281:LEU:HG	2.17	0.44
2:E:291:ILE:HB	2:E:294:LEU:HD12	2.00	0.44
1:C:151:VAL:HA	1:C:152:PRO:HD3	1.89	0.44
2:F:159:GLU:HG3	2:F:193:PHE:HZ	1.81	0.44
1:B:390:VAL:HG11	1:B:402:THR:OG1	2.18	0.44
2:D:94:GLY:HA3	2:D:227:MET:CE	2.47	0.44
2:D:150:PHE:HB3	2:D:306:MET:SD	2.57	0.44
2:D:156:PRO:HB2	2:D:417:PHE:CE2	2.52	0.44
2:D:358:ALA:HA	2:D:361:THR:O	2.17	0.44
2:D:395:SER:HA	2:D:398:ASP:O	2.18	0.44
2:E:145:GLN:HG3	2:E:324:GLU:HG3	2.00	0.44
2:E:166:ARG:CD	2:E:201:THR:HG21	2.47	0.44
2:E:212:ASN:OD1	2:E:221:ARG:HG3	2.16	0.44
2:E:313:HIS:CD2	2:E:314:PRO:HD2	2.53	0.44
2:E:334:TYR:HB2	2:E:341:PRO:HG3	1.99	0.44
1:C:507:ASP:HB3	1:C:510:ASP:HB3	1.99	0.44
1:C:560:LYS:HG2	1:C:561:TYR:CD2	2.52	0.44
1:B:73:VAL:HA	1:B:88:GLN:OE1	2.18	0.44
2:E:136:ASP:HB3	2:E:423:ILE:HD13	1.99	0.44
1:C:27:MET:HE3	1:C:71:LEU:CB	2.44	0.44
1:C:27:MET:HE1	1:C:52:TYR:OH	2.18	0.44
1:C:28:CYS:SG	1:C:49:ILE:HD13	2.57	0.44
1:C:85:ASP:HB3	1:C:91:LEU:HD21	1.98	0.44
1:C:200:LYS:HB3	1:C:373:ILE:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:29:LEU:HD12	2:F:42:GLY:O	2.18	0.44
1:A:92:ASP:O	1:A:96:GLU:HG3	2.18	0.44
1:B:43:ARG:HA	2:F:10:GLU:HB3	1.98	0.44
1:B:228:ALA:HA	1:B:411:VAL:O	2.18	0.44
1:B:408:VAL:HG23	1:B:409:VAL:N	2.33	0.44
2:D:111:ILE:O	2:D:226:ARG:HB3	2.18	0.44
2:E:282:ALA:CB	2:E:322:ILE:HD13	2.48	0.44
2:E:339:GLN:HA	2:E:340:PRO:HA	1.88	0.44
2:F:181:PHE:O	2:F:209:MET:HA	2.18	0.44
2:F:369:MET:HB2	2:F:369:MET:HE3	1.68	0.44
2:F:372:LEU:O	2:F:375:ALA:HB3	2.18	0.44
1:A:534:LYS:O	1:A:538:LEU:HG	2.18	0.43
2:D:184:ILE:HD11	2:D:225:PRO:HG3	1.99	0.43
2:F:143:ARG:HH12	2:F:242:HIS:CE1	2.36	0.43
2:F:152:GLY:HA2	2:F:153:SER:HA	1.68	0.43
1:A:567:LEU:HB2	4:A:753:HOH:O	2.17	0.43
1:B:231:PRO:HG3	1:B:412:PHE:CE1	2.53	0.43
2:D:29:LEU:HD11	2:D:77:LEU:HA	2.01	0.43
2:D:188:PHE:CE2	1:C:202:LYS:HG2	2.54	0.43
1:C:197:ARG:HG3	1:C:315:GLU:HB2	2.00	0.43
1:A:459:GLU:CD	1:A:462:ARG:HH21	2.22	0.43
2:D:422:THR:OG1	2:D:425:GLU:HG3	2.18	0.43
2:E:94:GLY:CA	2:E:227:MET:HE2	2.48	0.43
2:F:128:ILE:HD11	2:F:143:ARG:CG	2.47	0.43
2:F:271:ARG:HA	2:F:272:GLY:HA2	1.64	0.43
2:F:401:TYR:HD2	2:F:401:TYR:HA	1.67	0.43
1:A:43:ARG:HD2	1:A:43:ARG:HA	1.49	0.43
1:A:470:LEU:HB2	1:A:490:LEU:HD21	2.01	0.43
1:A:507:ASP:HB3	1:A:510:ASP:HB3	2.00	0.43
2:D:79:LEU:HD13	2:D:227:MET:HE3	1.98	0.43
2:F:19:GLU:HA	2:F:51:LYS:HA	2.00	0.43
2:F:201:THR:CG2	2:F:203:ALA:H	2.22	0.43
1:B:30:VAL:HB	1:B:35:VAL:CG2	2.47	0.43
1:B:461:MET:CE	1:B:464:LEU:HB2	2.48	0.43
2:D:408:PHE:HA	2:D:433:LEU:CD2	2.49	0.43
2:E:127:PHE:CE2	2:E:129:GLN:HB2	2.53	0.43
2:E:379:GLY:HA3	2:E:405:ALA:HB2	2.01	0.43
1:C:197:ARG:HG3	1:C:315:GLU:CB	2.49	0.43
2:F:127:PHE:HB2	2:F:355:GLY:O	2.18	0.43
2:F:246:ILE:HD13	2:F:301:ILE:HB	2.00	0.43
2:F:271:ARG:HD3	2:F:271:ARG:H	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:278:TYR:CB	2:F:318:LEU:HD12	2.48	0.43
1:A:75:LEU:HD13	1:A:316:TYR:CD1	2.53	0.43
2:D:38:GLU:C	2:D:39:ILE:HD12	2.42	0.43
2:D:288:ALA:HB3	4:D:501:HOH:O	2.17	0.43
2:E:251:THR:O	2:E:255:GLU:HG2	2.18	0.43
2:E:304:LEU:HD12	2:E:304:LEU:C	2.43	0.43
1:C:203:LEU:HD11	1:C:373:ILE:HG13	2.00	0.43
1:C:509:VAL:HG11	1:C:561:TYR:O	2.19	0.43
2:F:14:PRO:HG2	2:F:15:LEU:HD12	1.99	0.43
1:A:24:ILE:HG21	2:E:60:THR:HG23	2.00	0.43
1:B:291:LEU:C	1:B:291:LEU:HD23	2.44	0.43
2:E:318:LEU:O	2:E:322:ILE:HG13	2.18	0.43
1:A:441:VAL:O	1:A:445:MET:HG2	2.19	0.43
1:B:86:GLY:HA3	1:B:302:ALA:O	2.19	0.43
1:B:231:PRO:CD	1:B:414:GLY:HA2	2.49	0.43
2:D:126:GLU:HG2	2:D:143:ARG:CZ	2.49	0.43
2:D:229:LEU:HD13	2:D:287:ARG:HD3	2.01	0.43
1:C:222:VAL:HG23	1:C:413:TRP:CZ2	2.53	0.43
1:C:237:GLY:O	1:C:241:VAL:HG23	2.19	0.43
2:F:124:PRO:O	2:F:142:VAL:HG11	2.18	0.43
2:F:141:LEU:HD12	2:F:141:LEU:HA	1.86	0.43
2:F:269:GLY:HA3	2:F:273:TYR:O	2.18	0.43
2:D:362:ARG:NH1	2:D:431:TRP:HE1	2.08	0.43
2:D:404:PHE:HB2	2:D:436:MET:SD	2.59	0.43
2:E:30:ILE:CD1	2:E:42:GLY:HA3	2.47	0.43
2:F:21:VAL:HG22	2:F:50:ASP:O	2.19	0.43
2:F:183:ALA:O	2:F:212:ASN:HB3	2.18	0.43
1:B:27:MET:HE1	1:B:52:TYR:CZ	2.54	0.43
1:B:552:VAL:HG21	1:B:577:ILE:HG12	2.01	0.43
1:C:193:VAL:HG22	1:C:308:TYR:HB3	2.01	0.43
1:C:445:MET:O	1:C:449:LEU:HB2	2.18	0.43
1:B:231:PRO:HB2	1:B:233:PRO:HD3	2.01	0.42
2:D:397:ILE:H	2:D:397:ILE:HG13	1.50	0.42
2:E:352:LYS:HD3	4:E:501:HOH:O	2.18	0.42
1:C:97:VAL:HG11	1:C:109:LEU:HD23	2.01	0.42
1:C:214:ARG:HD2	1:C:500:TYR:CE1	2.53	0.42
2:F:290:ARG:C	2:F:291:ILE:HD12	2.44	0.42
2:D:30:ILE:HD12	2:D:30:ILE:C	2.44	0.42
2:D:66:LYS:CE	1:C:20:SER:HB2	2.47	0.42
2:E:385:LEU:O	2:E:388:VAL:N	2.52	0.42
1:C:273:PHE:H	1:C:274:PRO:HD2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:98:ASP:OD1	2:F:199:ARG:NH1	2.51	0.42
1:A:6:ILE:HD12	1:A:62:GLU:HB2	2.00	0.42
1:B:486:ASP:O	1:B:490:LEU:HG	2.19	0.42
1:B:546:MET:HE3	1:B:553:ARG:HD3	2.02	0.42
1:C:203:LEU:HB2	1:C:371:ARG:HG2	2.02	0.42
1:A:62:GLU:HB3	1:A:63:PRO:HD2	2.02	0.42
1:B:459:GLU:O	1:B:463:ILE:HG13	2.19	0.42
2:D:398:ASP:CG	2:D:399:LYS:HB2	2.44	0.42
1:C:6:ILE:HD12	1:C:62:GLU:HB2	2.01	0.42
1:C:93:THR:O	1:C:97:VAL:HG12	2.19	0.42
1:C:405:THR:O	1:C:409:VAL:HG22	2.19	0.42
2:F:30:ILE:HG22	2:F:72:PHE:CD2	2.54	0.42
2:F:182:ALA:HB3	2:F:247:MET:HG2	2.02	0.42
2:F:250:MET:HB2	2:F:304:LEU:HB3	2.01	0.42
2:F:304:LEU:C	2:F:304:LEU:HD12	2.44	0.42
2:F:369:MET:CG	2:F:370:ASN:H	2.32	0.42
1:A:73:VAL:CG1	1:A:309:THR:HG23	2.49	0.42
1:B:247:LYS:HE3	1:B:248:TRP:NE1	2.35	0.42
1:B:445:MET:O	1:B:448:ILE:HG22	2.19	0.42
2:D:45:LEU:N	2:D:45:LEU:HD23	2.34	0.42
1:C:147:HIS:HD2	1:C:149:ILE:HD12	1.85	0.42
2:F:153:SER:H	2:F:331:ARG:NH2	2.18	0.42
1:B:244:GLN:CD	1:B:505:ALA:HB1	2.45	0.42
1:B:463:ILE:HG22	1:B:493:ALA:HB2	2.01	0.42
2:E:133:SER:HB3	2:E:426:THR:HG23	2.02	0.42
2:E:190:GLU:O	2:E:193:PHE:HB3	2.20	0.42
1:C:144:ILE:CG2	1:C:288:ARG:HD3	2.37	0.42
1:C:318:ARG:HD3	1:C:384:ILE:HG13	2.01	0.42
1:C:482:LEU:HD23	1:C:482:LEU:O	2.19	0.42
2:F:162:ALA:O	2:F:166:ARG:HB2	2.20	0.42
1:A:567:LEU:HD12	1:A:567:LEU:HA	1.89	0.42
1:B:316:TYR:CE2	1:B:320:MET:HE3	2.55	0.42
2:E:143:ARG:HH21	2:E:170:VAL:HB	1.85	0.42
2:E:219:ILE:HG12	4:E:522:HOH:O	2.20	0.42
2:E:373:PHE:CD2	2:E:373:PHE:C	2.98	0.42
2:F:35:GLN:H	2:F:35:GLN:CD	2.27	0.42
2:F:77:LEU:HD13	2:F:111:ILE:CD1	2.49	0.42
2:F:135:ILE:HD13	2:F:136:ASP:CG	2.44	0.42
1:A:84:PHE:HB2	1:A:292:ILE:HD13	2.00	0.42
1:B:131:SER:N	1:B:134:ASP:OD2	2.37	0.42
2:D:133:SER:HB3	2:D:426:THR:HG23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:248:THR:OG1	2:D:303:ILE:HB	2.20	0.42
2:D:338:ILE:HD12	2:D:409:GLU:O	2.20	0.42
2:E:271:ARG:HG3	2:E:314:PRO:CG	2.49	0.42
1:C:318:ARG:HD2	1:C:372:VAL:HG22	2.01	0.42
2:F:159:GLU:HG3	2:F:193:PHE:CZ	2.55	0.42
2:E:235:LEU:O	2:E:239:LYS:HB2	2.18	0.42
2:E:441:GLU:O	2:E:442:LEU:HD12	2.19	0.42
1:C:233:PRO:HG2	1:C:236:ALA:HB2	2.01	0.42
1:C:266:MET:O	1:C:270:VAL:HG23	2.20	0.42
2:F:306:MET:HG2	2:F:316:PRO:CG	2.49	0.42
1:A:261:GLU:OE2	1:A:330:SER:N	2.47	0.42
1:B:207:VAL:HA	1:B:208:PRO:HD3	1.90	0.42
2:E:158:LYS:HG3	2:E:159:GLU:N	2.34	0.42
2:E:345:LEU:CG	2:E:376:TYR:CE2	2.98	0.42
2:E:362:ARG:CB	2:E:427:LEU:CD1	2.98	0.42
1:C:150:MET:CE	1:C:320:MET:HA	2.34	0.42
1:C:298:MET:HG2	2:F:115:VAL:HG11	2.01	0.42
1:C:308:TYR:O	1:C:311:ILE:HG22	2.20	0.42
1:C:533:ARG:O	1:C:537:SER:N	2.53	0.42
1:A:488:LEU:O	1:A:492:VAL:HG23	2.20	0.41
1:B:16:ALA:CB	1:B:19:MET:HE3	2.50	0.41
1:B:348:MET:HA	1:B:349:PRO:HD3	1.86	0.41
2:E:8:ILE:HD13	2:E:8:ILE:O	2.20	0.41
1:C:27:MET:HE2	1:C:71:LEU:HB2	1.98	0.41
1:C:41:GLU:CD	1:C:43:ARG:HH12	2.28	0.41
2:F:86:ILE:HA	2:F:208:VAL:CG2	2.49	0.41
2:F:93:LEU:HD13	2:F:220:GLU:HG2	2.01	0.41
2:F:431:TRP:HA	2:F:434:LEU:HD13	2.02	0.41
1:B:44:GLN:HA	1:B:44:GLN:OE1	2.20	0.41
1:B:139:VAL:CG2	1:B:187:MET:HE3	2.49	0.41
1:B:266:MET:CE	1:B:293:ALA:HB1	2.51	0.41
1:B:390:VAL:HG12	1:B:392:PRO:HD3	2.02	0.41
2:D:304:LEU:HD12	2:D:304:LEU:O	2.21	0.41
1:C:124:ILE:HB	1:C:136:ILE:HA	2.03	0.41
1:C:399:GLU:O	1:C:403:GLN:HG2	2.20	0.41
1:C:470:LEU:HD23	1:C:473:ILE:HD12	2.02	0.41
2:F:431:TRP:O	2:F:434:LEU:HD22	2.20	0.41
1:A:508:ASP:OD1	3:A:605:GOL:O2	2.37	0.41
1:B:81:SER:HB2	1:B:286:MET:HB3	2.02	0.41
1:B:245:ILE:O	1:B:249:SER:OG	2.33	0.41
1:B:516:GLU:OE1	1:B:516:GLU:N	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:144:GLY:CA	2:D:289:GLY:HA2	2.50	0.41
2:E:196:GLU:O	2:E:200:GLN:HB2	2.20	0.41
1:C:261:GLU:O	1:C:295:THR:HA	2.20	0.41
1:A:167:PHE:HB3	1:A:171:ASP:HB2	2.03	0.41
1:A:225:GLY:CA	1:A:370:GLY:HA2	2.49	0.41
2:D:406:GLU:O	2:D:410:ASN:N	2.47	0.41
2:E:253:TYR:CZ	2:E:284:LEU:HD11	2.56	0.41
1:C:224:LYS:CE	1:C:250:ASP:HB3	2.50	0.41
1:B:203:LEU:HD11	1:B:373:ILE:HG13	2.02	0.41
1:C:73:VAL:CG1	1:C:309:THR:HG23	2.49	0.41
1:C:385:THR:HG22	1:C:387:ILE:CD1	2.51	0.41
2:F:396:ASP:O	2:F:400:ILE:HG12	2.19	0.41
1:A:521:MET:O	1:A:525:ILE:HG13	2.21	0.41
2:D:282:ALA:CB	2:D:322:ILE:HD13	2.51	0.41
2:E:285:PHE:HB2	2:E:322:ILE:HG21	2.02	0.41
2:E:353:ASP:HB2	2:E:354:LYS:HE3	2.02	0.41
1:C:244:GLN:CD	1:C:505:ALA:HB1	2.46	0.41
1:C:488:LEU:HD21	1:C:532:ALA:HB3	2.02	0.41
1:C:536:LEU:C	1:C:536:LEU:HD23	2.45	0.41
2:F:304:LEU:CD2	2:F:319:THR:HG21	2.51	0.41
1:A:40:ILE:HG13	1:A:50:GLN:CG	2.49	0.41
1:A:200:LYS:HB3	1:A:373:ILE:O	2.21	0.41
1:A:242:GLN:O	1:A:327:MET:HE1	2.21	0.41
1:A:552:VAL:O	1:A:556:ILE:HG13	2.21	0.41
1:B:22:ALA:HB1	1:B:39:ILE:CD1	2.51	0.41
1:B:75:LEU:HB3	1:B:316:TYR:CE1	2.56	0.41
1:B:219:PHE:C	1:B:221:PRO:HD3	2.46	0.41
1:B:413:TRP:O	1:B:428:ILE:HG23	2.20	0.41
2:D:329:LEU:HG	2:D:341:PRO:O	2.21	0.41
2:F:18:VAL:O	2:F:52:ALA:N	2.43	0.41
2:F:111:ILE:HA	2:F:230:THR:OG1	2.21	0.41
2:F:117:ASN:HA	2:F:118:PRO:HD2	1.93	0.41
2:F:248:THR:HA	2:F:249:ASP:HA	1.69	0.41
2:F:333:LEU:O	2:F:336:SER:HB2	2.21	0.41
1:A:211:THR:OG1	1:A:217:ASP:OD2	2.37	0.41
1:B:85:ASP:HB2	1:B:298:MET:HE1	2.01	0.41
1:B:262:ARG:HH21	2:E:323:THR:C	2.27	0.41
1:B:562:ILE:CB	1:B:570:ILE:HD11	2.38	0.41
1:B:583:LEU:HD22	1:B:583:LEU:HA	1.82	0.41
1:C:8:LYS:HG3	2:F:48:GLN:HB2	2.01	0.41
1:C:80:ILE:O	1:C:81:SER:OG	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:274:PRO:HB3	1:C:286:MET:HG3	2.03	0.41
2:F:186:ILE:HD12	2:F:186:ILE:C	2.46	0.41
2:F:197:ASP:OD1	2:F:418:TYR:OH	2.16	0.41
1:A:275:GLU:O	1:A:277:ILE:HD12	2.20	0.41
1:B:73:VAL:HG13	1:B:193:VAL:CG1	2.51	0.41
1:B:460:GLY:O	1:B:464:LEU:HG	2.21	0.41
1:B:513:THR:HG22	1:B:518:GLN:HG3	2.03	0.41
2:D:33:ARG:HB3	2:D:69:SER:OG	2.21	0.41
2:D:34:MET:CE	2:D:40:ARG:HG3	2.51	0.41
2:D:98:ASP:N	2:D:98:ASP:OD1	2.53	0.41
2:D:160:LEU:HD12	2:D:160:LEU:O	2.21	0.41
2:D:212:ASN:OD1	2:D:221:ARG:HG3	2.21	0.41
2:E:26:TYR:CZ	2:E:27:GLU:HG3	2.55	0.41
2:E:93:LEU:HD12	2:E:93:LEU:HA	1.90	0.41
2:E:234:TYR:O	2:E:238:GLU:HB2	2.21	0.41
2:E:412:TYR:HA	2:E:429:LEU:HD21	2.02	0.41
1:C:109:LEU:HD12	1:C:109:LEU:O	2.21	0.41
1:C:178:THR:N	1:C:181:GLY:O	2.48	0.41
1:C:488:LEU:O	1:C:492:VAL:HG22	2.21	0.41
2:F:104:LEU:HA	2:F:105:PRO:HD3	1.87	0.41
2:F:137:HIS:HD2	2:F:369:MET:HB3	1.84	0.41
2:F:264:ARG:HG2	2:F:265:ARG:HH21	1.86	0.41
2:F:270:ARG:CB	2:F:271:ARG:CB	2.99	0.41
2:F:400:ILE:HG13	2:F:401:TYR:N	2.35	0.41
1:B:260:GLY:CA	1:B:261:GLU:CG	2.94	0.41
2:D:277:LEU:HD23	2:D:318:LEU:HD12	2.02	0.41
1:C:222:VAL:CG2	1:C:411:VAL:HG11	2.51	0.41
1:A:360:SER:O	1:A:364:GLU:HG3	2.20	0.40
1:A:520:ASN:O	1:A:524:VAL:HG13	2.21	0.40
1:B:73:VAL:HG13	1:B:193:VAL:HG12	2.03	0.40
1:B:215:VAL:HG13	1:B:216:ILE:N	2.37	0.40
2:D:225:PRO:HG2	2:D:253:TYR:CD1	2.56	0.40
2:E:93:LEU:C	2:E:227:MET:HE2	2.46	0.40
2:F:81:VAL:HG22	2:F:107:LYS:O	2.22	0.40
2:F:362:ARG:O	2:F:365:HIS:ND1	2.54	0.40
2:D:34:MET:HE2	2:D:40:ARG:HG3	2.03	0.40
2:D:93:LEU:HD21	2:D:220:GLU:HG2	2.04	0.40
2:D:136:ASP:HA	4:D:519:HOH:O	2.21	0.40
2:E:183:ALA:HB1	2:E:186:ILE:HD13	2.02	0.40
1:C:350:GLY:N	1:C:354:TYR:O	2.53	0.40
1:C:437:TYR:O	1:C:441:VAL:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:219:ILE:HD12	2:F:219:ILE:N	2.27	0.40
1:A:24:ILE:O	1:A:25:GLN:HB2	2.21	0.40
1:A:90:PRO:HD3	1:A:111:ALA:HA	2.02	0.40
1:A:139:VAL:O	1:A:147:HIS:N	2.52	0.40
1:A:148:LYS:N	1:A:320:MET:HE3	2.34	0.40
2:D:104:LEU:HD12	2:D:104:LEU:N	2.36	0.40
2:E:160:LEU:O	2:E:164:ILE:HG13	2.22	0.40
1:C:91:LEU:CD1	2:F:118:PRO:HG2	2.43	0.40
2:F:79:LEU:HD21	2:F:231:ALA:HB2	2.04	0.40
2:F:132:ILE:CB	2:F:135:ILE:CG1	2.99	0.40
1:B:241:VAL:O	1:B:245:ILE:HG12	2.22	0.40
1:B:369:SER:HB2	1:B:384:ILE:O	2.21	0.40
2:E:386:ALA:HB1	2:E:389:LEU:O	2.22	0.40
1:C:3:ILE:CD1	1:C:65:ARG:HG2	2.52	0.40
2:F:330:THR:HB	2:F:332:GLU:OE2	2.21	0.40
2:F:396:ASP:OD2	2:F:396:ASP:N	2.51	0.40
1:A:92:ASP:HA	2:D:119:ILE:CD1	2.51	0.40
1:A:103:LEU:CD2	2:D:117:ASN:HA	2.45	0.40
1:B:94:PHE:CE2	1:B:103:LEU:HA	2.56	0.40
1:B:103:LEU:N	1:B:103:LEU:HD22	2.36	0.40
1:B:324:VAL:O	1:B:384:ILE:HA	2.22	0.40
2:D:94:GLY:CA	2:D:227:MET:HE2	2.51	0.40
2:E:45:LEU:HD21	2:E:264:ARG:NH1	2.36	0.40
2:E:408:PHE:O	2:E:412:TYR:HB3	2.22	0.40
2:E:422:THR:OG1	2:E:425:GLU:HG3	2.22	0.40
1:C:203:LEU:HD11	1:C:373:ILE:CG1	2.51	0.40
2:F:433:LEU:O	2:F:435:ALA:N	2.50	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	584/600 (97%)	576 (99%)	8 (1%)	0	100	100
1	B	584/600 (97%)	573 (98%)	10 (2%)	1 (0%)	43	68
1	C	582/600 (97%)	569 (98%)	13 (2%)	0	100	100
2	D	446/465 (96%)	431 (97%)	15 (3%)	0	100	100
2	E	448/465 (96%)	427 (95%)	20 (4%)	1 (0%)	43	68
2	F	448/465 (96%)	431 (96%)	16 (4%)	1 (0%)	43	68
All	All	3092/3195 (97%)	3007 (97%)	82 (3%)	3 (0%)	48	73

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	387	VAL
1	B	287	GLU
2	E	387	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	491/511 (96%)	475 (97%)	16 (3%)	33	63
1	B	484/511 (95%)	463 (96%)	21 (4%)	26	54
1	C	474/511 (93%)	449 (95%)	25 (5%)	20	46
2	D	335/387 (87%)	313 (93%)	22 (7%)	15	36
2	E	325/387 (84%)	298 (92%)	27 (8%)	10	26
2	F	304/387 (79%)	270 (89%)	34 (11%)	6	15
All	All	2413/2694 (90%)	2268 (94%)	145 (6%)	17	41

All (145) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	ARG
1	A	46	VAL

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Mol	Chain	Res	Type
1	A	188	MET
1	A	250	ASP
1	A	259	CYS
1	A	285	LEU
1	A	289	THR
1	A	338	LEU
1	A	390	VAL
1	A	454	SER
1	A	479	ILE
1	A	482	LEU
1	A	494	LYS
1	A	523	LYS
1	A	565	GLU
1	A	567	LEU
1	B	9	VAL
1	B	21	GLU
1	B	25	GLN
1	B	79	ILE
1	B	80	ILE
1	B	81	SER
1	B	125	GLU
1	B	131	SER
1	B	188	MET
1	B	203	LEU
1	B	204	ASN
1	B	209	MET
1	B	239	THR
1	B	285	LEU
1	B	338	LEU
1	B	387	ILE
1	B	489	THR
1	B	541	TYR
1	B	567	LEU
1	B	582	GLN
1	B	583	LEU
2	D	7	THR
2	D	9	LYS
2	D	11	VAL
2	D	45	LEU
2	D	47	VAL
2	D	48	GLN
2	D	140	THR

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Mol	Chain	Res	Type
2	D	264	ARG
2	D	265	ARG
2	D	270	ARG
2	D	271	ARG
2	D	326	GLN
2	D	336	SER
2	D	360	LYS
2	D	361	THR
2	D	397	ILE
2	D	399	LYS
2	D	400	ILE
2	D	404	PHE
2	D	409	GLU
2	D	434	LEU
2	D	440	THR
2	E	6	ARG
2	E	8	ILE
2	E	47	VAL
2	E	50	ASP
2	E	78	GLN
2	E	79	LEU
2	E	93	LEU
2	E	104	LEU
2	E	125	ASP
2	E	126	GLU
2	E	147	LEU
2	E	248	THR
2	E	324	GLU
2	E	354	LYS
2	E	361	THR
2	E	363	GLU
2	E	385	LEU
2	E	403	LYS
2	E	406	GLU
2	E	407	ARG
2	E	409	GLU
2	E	414	ASN
2	E	415	GLN
2	E	419	THR
2	E	431	TRP
2	E	433	LEU
2	E	442	LEU

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Mol	Chain	Res	Type
1	C	1	MET
1	C	20	SER
1	C	25	GLN
1	C	44	GLN
1	C	99	GLN
1	C	163	GLU
1	C	173	ILE
1	C	179	GLU
1	C	184	GLU
1	C	188	MET
1	C	267	THR
1	C	277	ILE
1	C	307	ILE
1	C	338	LEU
1	C	341	MET
1	C	448	ILE
1	C	482	LEU
1	C	527	THR
1	C	536	LEU
1	C	541	TYR
1	C	542	PHE
1	C	546	MET
1	C	557	SER
1	C	560	LYS
1	C	562	ILE
2	F	6	ARG
2	F	8	ILE
2	F	82	SER
2	F	88	ARG
2	F	93	LEU
2	F	98	ASP
2	F	99	ASN
2	F	133	SER
2	F	135	ILE
2	F	137	HIS
2	F	143	ARG
2	F	146	LYS
2	F	171	LEU
2	F	173	SER
2	F	196	GLU
2	F	204	ILE
2	F	271	ARG

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Mol	Chain	Res	Type
2	F	276	TYR
2	F	294	LEU
2	F	310	ASP
2	F	322	ILE
2	F	326	GLN
2	F	351	LEU
2	F	352	LYS
2	F	365	HIS
2	F	368	THR
2	F	370	ASN
2	F	376	TYR
2	F	396	ASP
2	F	401	TYR
2	F	415	GLN
2	F	419	THR
2	F	434	LEU
2	F	452	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	GLN
1	A	180	GLN
1	A	242	GLN
1	B	18	ASN
1	B	108	GLN
2	D	280	ASN
2	D	313	HIS
2	D	326	GLN
2	D	414	ASN
2	E	112	ASN
2	E	163	GLN
2	E	167	GLN
1	C	25	GLN
2	F	137	HIS
2	F	167	GLN
2	F	326	GLN
2	F	370	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	GOL	A	603	-	5,5,5	0.38	0	5,5,5	0.16	0
3	GOL	A	602	-	5,5,5	0.36	0	5,5,5	0.28	0
3	GOL	A	601	-	5,5,5	0.40	0	5,5,5	0.21	0
3	GOL	A	604	-	5,5,5	0.38	0	5,5,5	0.20	0
3	GOL	A	605	-	5,5,5	0.38	0	5,5,5	0.22	0
3	GOL	A	606	-	5,5,5	0.38	0	5,5,5	0.24	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	603	-	-	2/4/4/4	-
3	GOL	A	602	-	-	2/4/4/4	-
3	GOL	A	601	-	-	1/4/4/4	-
3	GOL	A	604	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	605	-	-	2/4/4/4	-
3	GOL	A	606	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	603	GOL	O1-C1-C2-C3
3	A	606	GOL	O1-C1-C2-C3
3	A	602	GOL	O1-C1-C2-C3
3	A	605	GOL	O1-C1-C2-C3
3	A	602	GOL	O1-C1-C2-O2
3	A	603	GOL	O1-C1-C2-O2
3	A	606	GOL	O1-C1-C2-O2
3	A	604	GOL	O1-C1-C2-O2
3	A	606	GOL	O2-C2-C3-O3
3	A	601	GOL	O1-C1-C2-O2
3	A	605	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	GOL	2	0
3	A	605	GOL	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	586/600 (97%)	0.28	21 (3%) 46 42	32, 52, 104, 139	0
1	B	586/600 (97%)	0.83	56 (9%) 13 11	42, 82, 137, 164	0
1	C	584/600 (97%)	1.18	99 (16%) 4 3	54, 87, 139, 158	0
2	D	448/465 (96%)	1.00	67 (14%) 5 4	48, 80, 152, 202	0
2	E	450/465 (96%)	0.91	72 (16%) 5 4	37, 72, 158, 209	0
2	F	450/465 (96%)	1.44	133 (29%) 1 1	51, 95, 172, 201	0
All	All	3104/3195 (97%)	0.92	448 (14%) 6 5	32, 77, 149, 209	0

All (448) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	396	ASP	5.8
1	C	545	ILE	5.2
1	C	479	ILE	4.9
2	E	137	HIS	4.8
2	E	393	ALA	4.7
2	E	451	ASP	4.7
2	E	434	LEU	4.7
2	F	412	TYR	4.7
2	F	353	ASP	4.6
2	F	342	ILE	4.5
2	D	397	ILE	4.4
1	C	463	ILE	4.4
2	D	373	PHE	4.4
1	C	397	ILE	4.4
2	F	338	ILE	4.4
2	E	375	ALA	4.3
2	E	448	ASP	4.3
2	E	392	SER	4.3
2	F	329	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
1	C	499	ASP	4.3
1	B	297	ASN	4.2
2	E	441	GLU	4.2
2	F	385	LEU	4.2
2	F	133	SER	4.1
2	E	399	LYS	4.1
1	A	44	GLN	4.1
2	D	123	TYR	4.1
2	F	154	GLY	4.1
2	F	449	LEU	4.1
2	F	364	ASP	4.0
1	C	448	ILE	4.0
2	E	435	ALA	4.0
2	F	344	VAL	4.0
1	C	396	ASP	3.9
2	F	440	THR	3.8
2	F	354	LYS	3.8
1	C	562	ILE	3.8
1	C	492	VAL	3.8
2	F	328	ILE	3.8
2	E	440	THR	3.7
1	C	490	LEU	3.7
1	B	548	GLY	3.7
2	D	442	LEU	3.7
1	A	393	SER	3.7
1	B	585	VAL	3.7
2	F	451	ASP	3.7
2	E	431	TRP	3.7
1	C	584	ILE	3.6
2	F	373	PHE	3.6
2	F	392	SER	3.6
1	C	232	GLY	3.6
2	F	401	TYR	3.6
2	D	400	ILE	3.6
2	D	392	SER	3.6
2	F	445	ILE	3.5
1	C	570	ILE	3.5
2	F	400	ILE	3.5
1	A	396	ASP	3.5
1	C	464	LEU	3.5
2	D	376	TYR	3.5
2	E	153	SER	3.5

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Mol	Chain	Res	Type	RSRZ
2	E	174	SER	3.5
2	F	355	GLY	3.5
1	C	65	ARG	3.5
1	A	586	SER	3.4
1	A	232	GLY	3.4
2	D	443	LYS	3.4
2	D	393	ALA	3.4
2	E	433	LEU	3.4
2	E	364	ASP	3.4
2	F	327	ILE	3.4
2	D	438	PRO	3.4
2	F	363	GLU	3.4
2	D	385	LEU	3.4
2	D	175	ASP	3.4
1	C	428	ILE	3.3
1	C	538	LEU	3.3
2	D	382	ALA	3.3
2	F	424	THR	3.3
1	A	297	ASN	3.3
2	E	396	ASP	3.3
2	D	440	THR	3.3
2	D	394	LEU	3.3
2	E	49	GLU	3.3
2	F	305	THR	3.3
1	B	414	GLY	3.3
2	E	402	ALA	3.3
2	F	358	ALA	3.3
2	F	428	ASP	3.3
1	C	182	LEU	3.2
1	B	477	VAL	3.2
2	D	433	LEU	3.2
2	F	433	LEU	3.2
2	F	174	SER	3.2
2	F	447	ASP	3.2
1	C	583	LEU	3.2
2	E	437	LEU	3.2
1	A	542	PHE	3.2
2	F	414	ASN	3.2
2	F	420	ASN	3.2
2	E	438	PRO	3.2
1	C	406	LEU	3.1
2	D	174	SER	3.1

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Mol	Chain	Res	Type	RSRZ
2	F	404	PHE	3.1
1	C	280	ASN	3.1
2	D	176	ASP	3.1
2	E	442	LEU	3.1
2	F	138	LEU	3.1
1	C	302	ALA	3.1
1	C	401	VAL	3.1
2	E	439	ARG	3.1
2	F	453	TYR	3.1
1	C	482	LEU	3.1
1	B	479	ILE	3.1
1	A	541	TYR	3.0
2	E	321	TYR	3.0
2	D	364	ASP	3.0
2	E	445	ILE	3.0
2	F	393	ALA	3.0
1	C	500	TYR	3.0
2	D	102	GLU	3.0
1	C	231	PRO	3.0
1	B	584	ILE	3.0
2	F	429	LEU	3.0
1	C	539	GLY	3.0
1	C	524	VAL	3.0
2	E	404	PHE	3.0
2	F	387	VAL	3.0
2	F	102	GLU	3.0
2	F	444	ARG	3.0
2	F	269	GLY	3.0
1	B	583	LEU	2.9
1	A	391	SER	2.9
1	C	392	PRO	2.9
2	F	341	PRO	2.9
2	F	390	GLY	2.9
1	C	230	VAL	2.9
2	D	437	LEU	2.9
2	E	385	LEU	2.9
1	B	108	GLN	2.9
1	C	127	GLY	2.9
2	F	131	GLY	2.9
2	E	330	THR	2.9
2	D	386	ALA	2.9
2	F	388	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	476	LEU	2.9
1	B	530	LYS	2.9
1	B	80	ILE	2.9
1	B	387	ILE	2.9
2	D	172	ASP	2.9
2	D	448	ASP	2.9
1	B	567	LEU	2.9
2	E	267	VAL	2.9
2	E	370	ASN	2.9
1	C	395	GLY	2.9
1	C	567	LEU	2.9
1	A	43	ARG	2.8
1	C	460	GLY	2.8
1	C	517	LYS	2.8
2	E	312	THR	2.8
2	E	358	ALA	2.8
2	F	330	THR	2.8
2	E	371	GLN	2.8
2	F	151	SER	2.8
2	E	380	LYS	2.8
1	B	484	ASP	2.8
2	F	386	ALA	2.8
1	C	234	PHE	2.8
2	F	441	GLU	2.8
2	F	397	ILE	2.8
2	D	379	GLY	2.8
2	F	337	GLY	2.8
2	F	348	LEU	2.8
2	F	389	LEU	2.8
1	C	219	PHE	2.8
2	F	379	GLY	2.8
1	B	107	VAL	2.8
1	C	580	THR	2.8
2	D	375	ALA	2.8
2	D	406	GLU	2.8
2	F	391	GLU	2.8
2	F	77	LEU	2.7
1	C	86	GLY	2.7
2	E	361	THR	2.7
2	F	448	ASP	2.7
1	C	582	GLN	2.7
2	E	200	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
2	E	443	LYS	2.7
1	A	476	LEU	2.7
2	E	429	LEU	2.7
2	F	442	LEU	2.7
1	B	489	THR	2.7
2	D	402	ALA	2.7
2	E	362	ARG	2.7
1	C	415	LEU	2.7
1	B	515	ARG	2.7
1	C	433	SER	2.7
1	C	177	GLU	2.7
1	A	474	VAL	2.7
1	A	250	ASP	2.7
1	B	539	GLY	2.7
2	D	71	ARG	2.7
2	E	102	GLU	2.7
2	D	387	VAL	2.7
1	B	458	THR	2.7
2	D	169	THR	2.7
2	E	279	THR	2.7
2	F	375	ALA	2.7
2	F	405	ALA	2.7
1	A	108	GLN	2.6
2	F	372	LEU	2.6
2	F	340	PRO	2.6
2	E	91	ASP	2.6
1	C	488	LEU	2.6
1	B	533	ARG	2.6
1	B	392	PRO	2.6
1	C	506	PHE	2.6
2	E	368	THR	2.6
2	F	438	PRO	2.6
1	C	496	ILE	2.6
1	C	558	ARG	2.6
1	C	212	GLY	2.6
2	E	173	SER	2.6
2	E	395	SER	2.6
1	B	173	ILE	2.6
2	F	128	ILE	2.6
1	B	436	LEU	2.6
2	D	434	LEU	2.6
2	E	171	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
2	F	155	LEU	2.6
1	B	541	TYR	2.6
1	C	475	ARG	2.6
2	D	452	LYS	2.6
2	D	409	GLU	2.6
1	C	477	VAL	2.6
2	E	367	ALA	2.6
2	F	431	TRP	2.5
2	E	436	MET	2.5
2	F	147	LEU	2.5
2	F	439	ARG	2.5
2	F	432	GLU	2.5
1	B	231	PRO	2.5
1	B	519	PHE	2.5
2	F	288	ALA	2.5
2	D	349	SER	2.5
2	F	103	ILE	2.5
2	F	399	LYS	2.5
1	B	441	VAL	2.5
1	C	300	VAL	2.5
2	D	410	ASN	2.5
2	D	362	ARG	2.5
2	D	427	LEU	2.5
2	F	365	HIS	2.5
2	E	376	TYR	2.5
2	F	268	PRO	2.5
2	F	413	VAL	2.5
2	F	435	ALA	2.5
1	C	574	ASN	2.5
2	F	422	THR	2.5
1	C	537	SER	2.5
2	D	348	LEU	2.5
2	F	8	ILE	2.5
2	F	153	SER	2.5
2	D	401	TYR	2.5
2	F	295	LYS	2.4
1	B	520	ASN	2.4
2	D	429	LEU	2.4
1	A	537	SER	2.4
1	C	248	TRP	2.4
1	A	582	GLN	2.4
1	B	201	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
2	F	452	LYS	2.4
2	F	361	THR	2.4
1	B	538	LEU	2.4
1	C	514	SER	2.4
1	C	1	MET	2.4
1	B	106	GLY	2.4
2	D	346	PRO	2.4
2	E	311	LYS	2.4
1	C	474	VAL	2.4
1	B	555	ARG	2.4
2	F	160	LEU	2.4
1	B	578	LYS	2.4
1	B	473	ILE	2.4
2	D	361	THR	2.4
1	B	531	GLU	2.4
2	F	349	SER	2.4
1	C	180	GLN	2.4
1	B	552	VAL	2.4
1	C	542	PHE	2.4
2	D	374	ALA	2.4
2	D	372	LEU	2.3
2	E	348	LEU	2.3
2	F	321	TYR	2.3
1	C	577	ILE	2.3
2	E	397	ILE	2.3
2	D	363	GLU	2.3
2	D	403	LYS	2.3
2	F	446	LYS	2.3
2	E	407	ARG	2.3
2	E	294	LEU	2.3
2	E	427	LEU	2.3
2	F	374	ALA	2.3
2	F	434	LEU	2.3
2	E	412	TYR	2.3
2	F	419	THR	2.3
2	F	139	ASN	2.3
1	C	341	MET	2.3
2	F	53	MET	2.3
1	B	569	LYS	2.3
2	D	451	ASP	2.3
1	C	450	GLN	2.3
1	C	408	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	532	ALA	2.3
1	C	470	LEU	2.3
2	D	65	LEU	2.3
2	F	65	LEU	2.3
1	C	581	ILE	2.3
1	B	1	MET	2.3
2	E	353	ASP	2.3
2	D	275	GLY	2.3
2	F	333	LEU	2.3
1	C	573	ILE	2.3
2	F	123	TYR	2.3
2	D	441	GLU	2.3
2	D	173	SER	2.3
1	B	382	GLY	2.3
2	E	154	GLY	2.3
2	E	394	LEU	2.3
1	C	528	PHE	2.3
1	C	387	ILE	2.2
1	C	431	ILE	2.2
2	F	161	ALA	2.2
2	F	162	ALA	2.2
2	F	303	ILE	2.2
1	C	402	THR	2.2
2	F	101	PRO	2.2
1	C	398	SER	2.2
2	D	398	ASP	2.2
2	E	175	ASP	2.2
2	F	149	VAL	2.2
2	F	170	VAL	2.2
1	B	528	PHE	2.2
1	C	277	ILE	2.2
2	D	383	LYS	2.2
2	D	435	ALA	2.2
2	F	242	HIS	2.2
1	C	527	THR	2.2
1	C	564	GLU	2.2
2	F	159	GLU	2.2
1	A	475	ARG	2.2
1	B	196	GLY	2.2
2	F	176	ASP	2.2
2	E	138	LEU	2.2
2	D	338	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
2	E	8	ILE	2.2
2	F	382	ALA	2.2
1	C	399	GLU	2.2
1	C	565	GLU	2.2
2	F	271	ARG	2.2
2	F	272	GLY	2.2
1	C	215	VAL	2.2
1	B	413	TRP	2.2
1	C	124	ILE	2.2
2	D	404	PHE	2.2
1	C	236	ALA	2.2
2	F	409	GLU	2.2
2	F	258	ARG	2.2
2	E	123	TYR	2.2
2	F	334	TYR	2.2
2	F	443	LYS	2.2
1	B	185	LEU	2.2
1	B	253	LEU	2.2
1	B	521	MET	2.2
1	C	552	VAL	2.2
2	D	263	ALA	2.1
2	D	367	ALA	2.1
2	D	431	TRP	2.1
2	F	324	GLU	2.1
2	F	411	GLU	2.1
1	C	439	THR	2.1
2	F	187	THR	2.1
1	C	52	TYR	2.1
2	F	418	TYR	2.1
2	D	445	ILE	2.1
1	C	535	ALA	2.1
1	B	468	GLU	2.1
2	E	432	GLU	2.1
2	F	384	GLU	2.1
1	B	549	THR	2.1
2	E	248	THR	2.1
2	F	7	THR	2.1
1	A	432	GLN	2.1
1	C	308	TYR	2.1
2	F	273	TYR	2.1
1	C	394	GLY	2.1
2	E	365	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	585	VAL	2.1
1	C	240	VAL	2.1
1	C	409	VAL	2.1
2	F	119	ILE	2.1
2	F	205	ASP	2.1
2	E	133	SER	2.1
2	F	395	SER	2.1
2	F	134	ALA	2.1
1	C	467	GLU	2.1
1	C	430	TRP	2.1
2	F	319	THR	2.1
2	F	335	LYS	2.1
2	E	314	PRO	2.1
1	B	348	MET	2.1
1	C	83	MET	2.1
1	B	478	GLY	2.1
2	E	401	TYR	2.1
1	C	250	ASP	2.1
1	C	335	ALA	2.1
2	D	159	GLU	2.1
2	F	407	ARG	2.1
1	C	247	LYS	2.1
2	F	215	ASN	2.1
1	B	395	GLY	2.1
2	E	423	ILE	2.1
2	F	132	ILE	2.1
2	F	376	TYR	2.1
1	C	516	GLU	2.0
2	F	83	GLU	2.0
2	E	101	PRO	2.0
1	C	501	LEU	2.0
2	F	104	LEU	2.0
1	C	176	ILE	2.0
2	F	135	ILE	2.0
1	B	390	VAL	2.0
2	D	5	TYR	2.0
1	A	344	ARG	2.0
1	B	65	ARG	2.0
2	F	270	ARG	2.0
2	F	362	ARG	2.0
2	E	409	GLU	2.0
1	C	325	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
2	D	354	LYS	2.0
2	F	402	ALA	2.0
1	B	586	SER	2.0
1	C	521	MET	2.0
1	B	109	LEU	2.0
1	B	160	GLN	2.0
2	D	449	LEU	2.0
1	A	479	ILE	2.0
2	D	444	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GOL	A	605	6/6	0.65	0.23	113,136,138,138	0
3	GOL	A	601	6/6	0.71	0.27	114,136,139,139	0
3	GOL	A	603	6/6	0.76	0.26	101,121,125,125	0
3	GOL	A	604	6/6	0.77	0.19	77,93,95,95	0
3	GOL	A	602	6/6	0.86	0.20	88,106,108,108	0
3	GOL	A	606	6/6	0.90	0.21	91,109,112,112	0

6.5 Other polymers [i](#)

There are no such residues in this entry.