



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:46 PM UTC

PDB ID : 2IU3 / pdb_00002iu3
Title : Crystal structures of transition state analogue inhibitors of inosine monophosphate cyclohydrolase
Authors : Xu, L.; Chong, Y.; Hwang, I.; D'Onofrio, A.; Amore, K.; Beardsley, G.P.; Li, C.; Olson, A.J.; Boger, D.L.; Wilson, I.A.
Deposited on : 2006-05-27
Resolution : 2.90 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

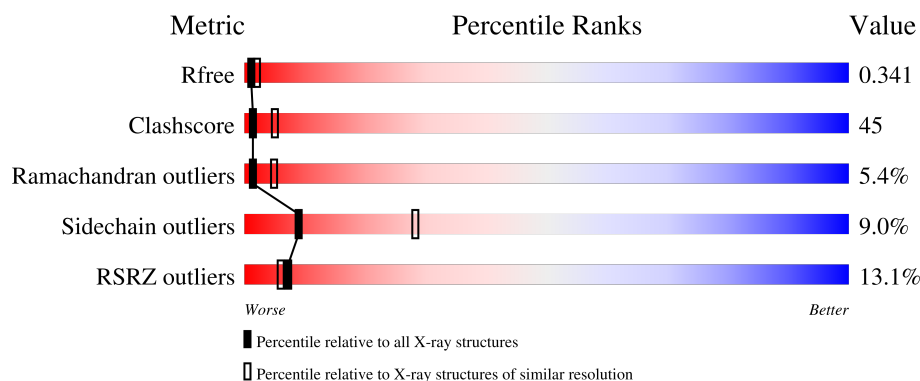
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	593	10% 34% 52% 12% ..
1	B	593	16% 36% 51% 12% ..

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9145 atoms, of which 0 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.

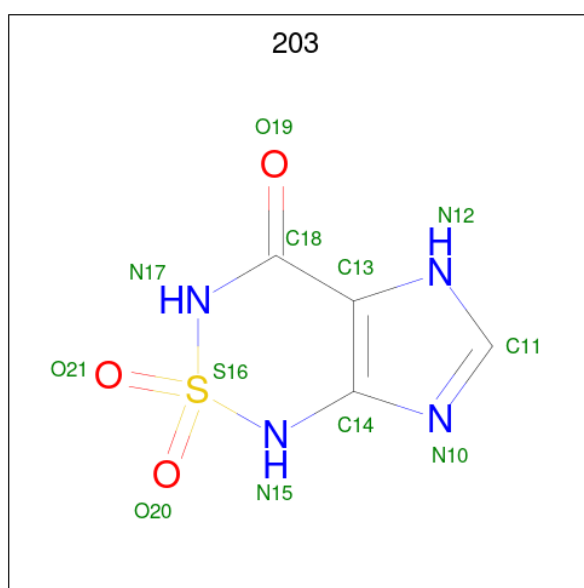
- Molecule 1 is a protein called BIFUNCTIONAL PURINE BIOSYNTHESIS PROTEIN PURH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	590	Total	C	N	O	S	0	1	0
			4523	2852	801	851	19			
1	B	590	Total	C	N	O	S	0	0	0
			4511	2843	800	849	19			

- Molecule 2 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	K	0	0
			1	1		
2	B	1	Total	K	0	0
			1	1		

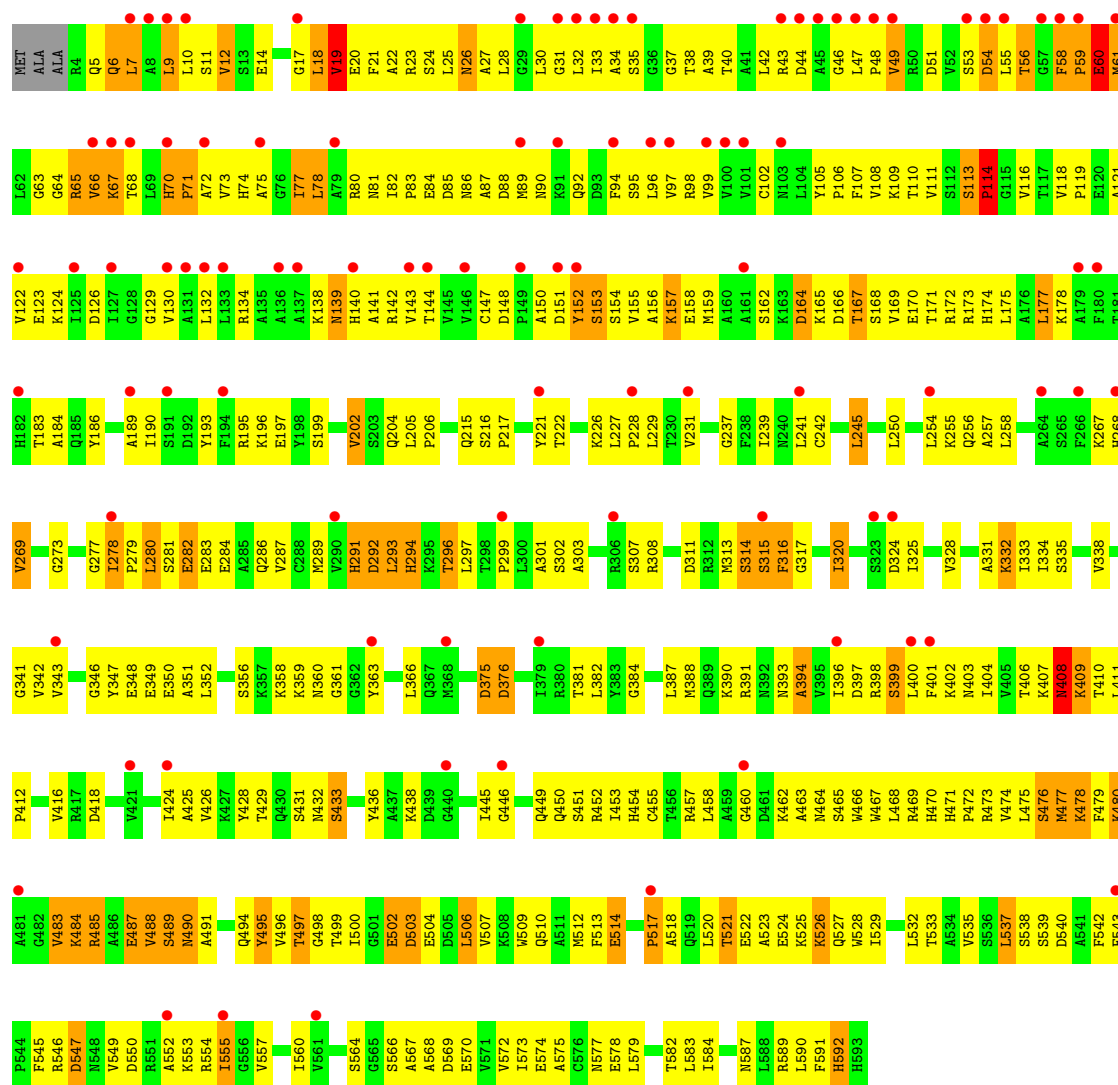
- Molecule 3 is 1,5-DIHYDROIMIDAZO[4,5-C][1,2,6]THIADIAZIN-4(3H)-ONE 2,2-DIOXIDE (CCD ID: 203) (formula: C₄H₄N₄O₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	S	0	0
			12	4	4	3	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	52	Total	O	0	0
			52	52		
4	B	45	Total	O	0	0
			45	45		



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	387.00Å 57.00Å 62.10Å 90.00° 98.90° 90.00°	Depositor
Resolution (Å)	35.20 – 2.90 35.20 – 2.90	Depositor EDS
% Data completeness (in resolution range)	91.5 (35.20-2.90) 91.6 (35.20-2.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 2.85Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.215 , 0.300 0.285 , 0.341	Depositor DCC
R_{free} test set	1210 reflections (3.99%)	wwPDB-VP
Wilson B-factor (Å ²)	50.6	Xtriage
Anisotropy	0.315	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 26.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.027 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	9145	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: K, 203

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	0.74	6/4608 (0.1%)	1.14	25/6249 (0.4%)
1	B	0.70	5/4595 (0.1%)	1.14	36/6230 (0.6%)
All	All	0.72	11/9203 (0.1%)	1.14	61/12479 (0.5%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	313	MET	SD-CE	6.70	1.96	1.79
1	A	527	GLN	CD-OE1	5.96	1.34	1.23
1	B	490	ASN	CG-OD1	5.79	1.34	1.23
1	B	139	ASN	CG-OD1	5.61	1.34	1.23
1	B	256	GLN	CD-OE1	5.44	1.33	1.23
1	B	289	MET	SD-CE	5.38	1.93	1.79
1	A	81	ASN	CG-OD1	5.35	1.33	1.23
1	B	291	HIS	ND1-CE1	5.33	1.37	1.32
1	A	103	ASN	CG-OD1	5.24	1.33	1.23
1	A	26	ASN	CG-OD1	5.23	1.33	1.23
1	A	432	ASN	CG-OD1	5.21	1.33	1.23

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	45	ALA	N-CA-C	-14.51	94.86	113.72
1	B	514	GLU	N-CA-C	-10.29	100.14	111.36
1	A	514	GLU	N-CA-C	-10.16	99.89	110.97
1	B	26	ASN	N-CA-C	-8.76	101.73	111.28
1	A	7	LEU	N-CA-C	8.72	122.62	109.63
1	B	495	TYR	N-CA-C	-8.60	101.85	111.14
1	B	65	ARG	N-CA-C	-8.32	102.23	112.38
1	A	39	ALA	N-CA-C	-7.81	102.71	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	587	ASN	N-CA-C	-7.48	104.18	113.38
1	A	65	ARG	N-CA-C	7.39	118.26	108.07
1	A	104	LEU	N-CA-C	7.36	120.26	109.07
1	A	433	SER	N-CA-C	7.25	120.23	107.61
1	B	480	LYS	N-CA-C	-7.20	99.50	110.30
1	B	587	ASN	N-CA-C	-7.16	105.07	114.31
1	A	590	LEU	N-CA-C	6.95	121.14	111.56
1	A	13	SER	N-CA-C	-6.66	104.90	113.16
1	A	34	ALA	N-CA-C	6.61	116.78	108.45
1	B	291	HIS	CB-CG-CD2	-6.58	122.64	131.20
1	B	320	ILE	N-CA-C	6.57	117.56	108.89
1	A	27	ALA	N-CA-C	-6.49	105.23	113.01
1	A	348	GLU	N-CA-C	-6.42	101.45	110.50
1	B	376	ASP	N-CA-C	6.20	120.57	112.89
1	B	12	VAL	N-CA-C	6.14	118.87	108.86
1	B	38	THR	N-CA-C	-6.13	104.22	111.03
1	A	28	LEU	N-CA-C	-6.09	104.49	112.41
1	B	49	VAL	N-CA-C	6.08	116.62	107.75
1	B	123	GLU	N-CA-C	-5.89	104.94	111.71
1	B	113	SER	CA-C-N	5.87	127.17	119.84
1	B	113	SER	C-N-CA	5.87	127.17	119.84
1	B	70	HIS	CA-C-N	5.85	127.16	119.84
1	B	70	HIS	C-N-CA	5.85	127.16	119.84
1	B	317	GLY	N-CA-C	-5.76	106.21	115.08
1	B	409	LYS	N-CA-C	5.75	119.88	112.41
1	A	572	VAL	N-CA-C	-5.74	104.73	110.30
1	B	6	GLN	N-CA-C	-5.74	101.20	110.32
1	B	408	ASN	N-CA-C	-5.73	101.42	109.96
1	B	291	HIS	CB-CG-ND1	5.63	131.14	122.70
1	B	487	GLU	N-CA-C	-5.58	105.09	111.07
1	A	9	LEU	N-CA-C	5.58	119.15	110.17
1	A	351	ALA	N-CA-C	-5.55	105.13	111.07
1	A	555	ILE	N-CA-C	5.49	119.84	112.98
1	B	77	ILE	N-CA-C	5.49	115.62	110.30
1	A	26	ASN	N-CA-C	-5.49	106.28	112.87
1	B	66	VAL	N-CA-C	-5.38	100.73	108.48
1	B	592	HIS	N-CA-C	5.36	117.16	108.26
1	B	521	THR	N-CA-C	-5.35	103.33	110.55
1	B	58	PHE	CA-C-N	5.33	126.50	119.84
1	B	58	PHE	C-N-CA	5.33	126.50	119.84
1	B	381	THR	N-CA-C	-5.32	101.86	110.32
1	B	301	ALA	N-CA-C	-5.22	104.84	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	414	SER	N-CA-C	-5.20	105.05	111.40
1	A	416	VAL	N-CA-C	-5.20	105.42	110.42
1	B	433	SER	N-CA-C	5.20	116.70	108.96
1	B	63	GLY	N-CA-C	-5.17	107.12	115.08
1	A	70	HIS	CA-C-N	5.14	126.27	119.84
1	A	70	HIS	C-N-CA	5.14	126.27	119.84
1	B	278	ILE	N-CA-C	-5.13	103.92	108.95
1	A	479	PHE	N-CA-C	5.08	121.61	110.80
1	A	377	ASN	N-CA-C	5.05	118.35	110.32
1	B	78	LEU	N-CA-C	5.05	119.15	112.89
1	B	245	LEU	N-CA-C	5.05	116.47	111.07

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	4523	0	4570	457	0
1	B	4511	0	4561	393	4
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	B	12	0	4	1	0
4	A	52	0	0	2	0
4	B	45	0	0	3	0
All	All	9145	0	9135	816	4

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 45.

All (816) 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)
1:A:510:GLN:HE21	1:A:516:VAL:HG21	1.19	1.04
1:B:485:ARG:HG2	1:B:485:ARG:HH11	1.22	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:ILE:HG12	1:A:388:MET:HG3	1.34	1.04
1:A:510:GLN:NE2	1:A:516:VAL:HG21	1.76	1.00
1:B:479:PHE:HA	1:B:513:PHE:HA	1.46	0.97
1:A:502:GLU:HA	1:A:506:LEU:HB2	1.45	0.97
1:A:9:LEU:HD23	1:A:33:ILE:HB	1.45	0.95
1:B:407:LYS:O	1:B:409:LYS:HG3	1.67	0.93
1:A:520:LEU:H	1:A:520:LEU:HD12	1.33	0.92
1:B:80:ARG:HB2	1:B:82:ILE:HG12	1.51	0.92
1:B:408:ASN:HD21	1:B:577:ASN:HA	1.32	0.91
1:A:65:ARG:HD3	1:B:78:LEU:HD22	1.52	0.91
1:B:484:LYS:HB2	1:B:487:GLU:HG3	1.53	0.91
1:B:58:PHE:HD2	1:B:61:MET:HE1	1.35	0.91
1:A:545:PHE:HB2	1:A:547:ASP:OD1	1.70	0.90
1:A:212:ASN:OD1	1:B:589:ARG:HD2	1.72	0.90
1:A:106:PRO:HD2	1:A:109:LYS:HE2	1.54	0.89
1:B:468:LEU:HD23	1:B:528:TRP:CD1	2.09	0.88
1:B:356:SER:O	1:B:361:GLY:HA2	1.74	0.87
1:B:89:MET:HE2	1:B:96:LEU:HD23	1.56	0.87
1:B:406:THR:HG22	1:B:573:ILE:HG23	1.56	0.86
1:B:9:LEU:HD13	1:B:10:LEU:N	1.90	0.85
1:B:61:MET:HE2	1:B:61:MET:H	1.42	0.85
1:A:26:ASN:HB2	1:A:32:LEU:HD21	1.55	0.84
1:A:254:LEU:HD23	1:A:424:ILE:HD12	1.60	0.84
1:B:26:ASN:HB2	1:B:32:LEU:HD11	1.58	0.84
1:A:118:VAL:O	1:A:122:VAL:HG23	1.78	0.84
1:A:148:ASP:OD1	1:A:150:ALA:HB3	1.78	0.83
1:B:129:GLY:HA2	1:B:132:LEU:HD12	1.57	0.83
1:B:12:VAL:HG12	1:B:102:CYS:HA	1.60	0.82
1:B:22:ALA:HA	1:B:25:LEU:HD21	1.60	0.82
1:B:121:ALA:O	1:B:124:LYS:HB2	1.78	0.82
1:B:283:GLU:HG3	4:B:2018:HOH:O	1.80	0.81
1:B:485:ARG:HH11	1:B:485:ARG:CG	1.93	0.81
1:B:535:VAL:HB	1:B:557:VAL:HA	1.61	0.80
1:B:43:ARG:HG3	1:B:49:VAL:CG1	2.12	0.80
1:A:270:SER:OG	1:A:430:GLN:HG2	1.82	0.80
1:B:156:ALA:HB3	1:B:157:LYS:HE3	1.61	0.79
1:B:171:THR:O	1:B:175:LEU:HD23	1.83	0.79
1:A:522:GLU:C	1:A:524:GLU:H	1.88	0.78
1:A:200:LYS:HD3	1:A:200:LYS:C	2.07	0.78
1:A:544:PRO:O	1:A:568:ALA:HB3	1.83	0.78
1:B:74:HIS:HA	1:B:77:ILE:HD12	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:522:GLU:C	1:A:526:LYS:HE2	2.09	0.77
1:A:537:LEU:C	1:A:537:LEU:HD23	2.08	0.77
1:A:535:VAL:HB	1:A:557:VAL:HA	1.65	0.77
1:A:208:ARG:CZ	1:A:237:GLY:HA2	2.15	0.77
1:A:163:LYS:HG2	1:A:164:ASP:OD1	1.85	0.76
1:B:474:VAL:HA	1:B:477:MET:HG3	1.67	0.76
1:B:537:LEU:C	1:B:537:LEU:HD23	2.10	0.76
1:B:566:SER:HB3	1:B:569:ASP:OD1	1.84	0.76
1:A:56:THR:HG22	1:A:72:ALA:HB3	1.68	0.76
1:A:583:LEU:HD12	1:A:584:ILE:N	2.01	0.76
1:B:464:ASN:ND2	1:B:555:ILE:HD13	2.01	0.76
1:B:470:HIS:O	1:B:475:LEU:HD11	1.86	0.76
1:A:28:LEU:HG	1:A:165:LYS:HE2	1.68	0.75
1:A:174:HIS:HD2	1:A:175:LEU:HD22	1.51	0.75
1:A:410:THR:O	1:A:582:THR:HG21	1.86	0.74
1:B:83:PRO:HA	1:B:86:ASN:HD22	1.52	0.74
1:A:464:ASN:ND2	1:A:555:ILE:HD13	2.02	0.74
1:B:7:LEU:HA	1:B:31:GLY:H	1.53	0.74
1:B:89:MET:HE2	1:B:96:LEU:CD2	2.17	0.74
1:A:25:LEU:O	1:A:30:LEU:HD12	1.88	0.74
1:A:477:MET:HE2	1:A:492:ILE:HG12	1.69	0.74
1:A:50:ARG:HD2	1:A:54:ASP:OD2	1.87	0.74
1:B:167:THR:O	1:B:172:ARG:NH1	2.21	0.73
1:B:56:THR:OG1	1:B:58:PHE:HB2	1.87	0.73
1:B:118:VAL:O	1:B:122:VAL:HG23	1.88	0.73
1:A:289:MET:HG3	1:A:312:ARG:CZ	2.17	0.73
1:A:378:GLU:HG3	1:A:391:ARG:HB3	1.71	0.73
1:A:172:ARG:HG3	1:A:172:ARG:HH11	1.53	0.73
1:B:520:LEU:HB2	1:B:525:LYS:HE2	1.70	0.73
1:B:503:ASP:O	1:B:507:VAL:HG23	1.89	0.73
1:B:22:ALA:HA	1:B:25:LEU:CD2	2.19	0.72
1:A:471:HIS:ND1	1:A:472:PRO:HD2	2.05	0.72
1:A:520:LEU:HD13	1:A:525:LYS:HE2	1.70	0.72
1:A:241:LEU:O	1:A:245:LEU:HD23	1.88	0.71
1:B:408:ASN:ND2	1:B:577:ASN:HA	2.05	0.71
1:B:410:THR:O	1:B:582:THR:HG21	1.89	0.71
1:B:280:LEU:HD11	1:B:302:SER:HB2	1.71	0.71
1:B:410:THR:HG22	1:B:412:PRO:HD3	1.73	0.71
1:B:545:PHE:HB2	1:B:547:ASP:OD1	1.90	0.70
1:B:569:ASP:O	1:B:573:ILE:HG13	1.91	0.70
1:A:37:GLY:O	1:A:40:THR:HB	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:496:VAL:HG23	1:B:497:THR:H	1.56	0.70
1:B:80:ARG:HD2	1:B:82:ILE:CD1	2.22	0.70
1:A:458:LEU:HD21	1:A:462:LYS:HE3	1.73	0.70
1:A:547:ASP:OD1	1:A:547:ASP:N	2.24	0.70
1:A:38:THR:O	1:A:42:LEU:HG	1.92	0.70
1:A:70:HIS:CD2	1:A:72:ALA:H	2.10	0.70
1:A:61:MET:SD	1:B:92:GLN:HG3	2.31	0.70
1:B:521:THR:HG23	1:B:524:GLU:OE1	1.92	0.69
1:A:169:VAL:O	1:A:173:ARG:HG3	1.91	0.69
1:A:432:ASN:HD21	1:A:449:GLN:HB2	1.56	0.69
1:B:468:LEU:HD23	1:B:528:TRP:HD1	1.57	0.69
1:A:418:ASP:OD2	1:A:438:LYS:HA	1.92	0.69
1:B:485:ARG:HG2	1:B:485:ARG:NH1	2.03	0.69
1:B:583:LEU:HD12	1:B:584:ILE:N	2.08	0.69
1:B:43:ARG:HG3	1:B:49:VAL:HG11	1.75	0.69
1:A:104:LEU:O	1:A:106:PRO:HD3	1.93	0.68
1:A:106:PRO:HG2	1:A:109:LYS:HZ1	1.57	0.68
1:B:250:LEU:HD11	1:B:425:ALA:HA	1.76	0.68
1:A:9:LEU:CD2	1:A:33:ILE:HB	2.23	0.68
1:B:9:LEU:C	1:B:10:LEU:HD12	2.18	0.68
1:B:418:ASP:OD2	1:B:438:LYS:HA	1.94	0.68
1:B:472:PRO:HA	1:B:475:LEU:HD12	1.74	0.68
1:A:80:ARG:HG3	1:B:65:ARG:HH12	1.58	0.68
1:A:37:GLY:HA2	1:A:40:THR:HB	1.76	0.68
1:A:502:GLU:H	1:A:505:ASP:HB2	1.59	0.68
1:B:496:VAL:HG23	1:B:497:THR:N	2.09	0.68
1:A:289:MET:HG3	1:A:312:ARG:NH2	2.07	0.68
1:B:113:SER:OG	1:B:114:PRO:HD2	1.93	0.68
1:B:10:LEU:HB2	1:B:34:ALA:HB2	1.74	0.68
1:A:378:GLU:CG	1:A:391:ARG:HB3	2.23	0.67
1:A:153:SER:O	1:A:157:LYS:HG3	1.95	0.67
1:A:208:ARG:NH2	1:A:237:GLY:HA2	2.10	0.67
1:B:87:ALA:HA	1:B:90:ASN:OD1	1.95	0.67
1:B:151:ASP:O	1:B:152:TYR:C	2.35	0.67
1:B:280:LEU:N	1:B:280:LEU:HD12	2.09	0.67
1:A:200:LYS:HD3	1:A:201:GLY:N	2.09	0.67
1:A:53:SER:O	1:A:57:GLY:N	2.28	0.67
1:A:521:THR:OG1	1:A:524:GLU:HB2	1.95	0.67
1:A:522:GLU:OE2	1:A:522:GLU:HA	1.94	0.67
1:A:298:THR:HB	1:A:299:PRO:HD2	1.75	0.66
1:B:61:MET:HE2	1:B:61:MET:N	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:583:LEU:HD12	1:A:584:ILE:H	1.60	0.66
1:A:495:TYR:CE1	1:A:519:GLN:HA	2.31	0.66
1:A:106:PRO:HB2	1:A:109:LYS:HZ3	1.60	0.66
1:A:129:GLY:HA2	1:A:132:LEU:HD12	1.76	0.66
1:B:335:SER:HA	1:B:358:LYS:HD2	1.78	0.66
1:A:89:MET:HE2	1:A:96:LEU:HD23	1.76	0.66
1:A:282:GLU:HA	1:A:294:HIS:CE1	2.30	0.66
1:A:335:SER:HA	1:A:358:LYS:HD2	1.78	0.66
1:B:495:TYR:HD1	1:B:500:ILE:HD11	1.61	0.66
1:B:157:LYS:HE3	1:B:157:LYS:N	2.10	0.65
1:B:453:ILE:HD11	1:B:457:ARG:NH2	2.12	0.65
1:A:37:GLY:C	1:A:40:THR:HB	2.22	0.65
1:A:359:LYS:C	1:A:361:GLY:H	2.03	0.65
1:B:7:LEU:HA	1:B:31:GLY:N	2.11	0.65
1:A:74:HIS:HA	1:A:77:ILE:HD12	1.77	0.65
1:A:76:GLY:O	1:A:142:ARG:NH2	2.27	0.65
1:A:493:ASP:O	1:A:496:VAL:HG22	1.97	0.65
1:A:333:ILE:O	1:A:337:GLU:HG2	1.96	0.65
1:A:376:ASP:HB3	1:A:390:LYS:HD3	1.79	0.65
1:A:55:LEU:HD22	1:A:72:ALA:HB1	1.79	0.65
1:A:61:MET:HG3	1:A:62:LEU:H	1.62	0.65
1:A:426:VAL:CG1	1:A:540:ASP:HB3	2.27	0.65
1:A:148:ASP:HB3	1:A:178:LYS:HE3	1.79	0.65
1:A:277:GLY:N	1:A:303:ALA:HB2	2.11	0.65
1:B:51:ASP:O	1:B:54:ASP:HB2	1.96	0.65
1:A:198:TYR:CE1	1:B:173:ARG:HD3	2.32	0.65
1:A:280:LEU:HB3	1:A:284:GLU:HB3	1.78	0.64
1:B:299:PRO:O	1:B:303:ALA:N	2.29	0.64
1:A:28:LEU:HA	1:A:165:LYS:NZ	2.13	0.64
1:A:106:PRO:HG2	1:A:109:LYS:NZ	2.12	0.64
1:A:40:THR:HG22	1:A:41:ALA:N	2.12	0.64
1:B:85:ASP:O	1:B:89:MET:HG2	1.97	0.64
1:A:452:ARG:NH2	1:A:541:ALA:HB3	2.13	0.64
1:A:154:SER:HA	1:A:157:LYS:HD2	1.78	0.64
1:A:401:PHE:HB3	1:A:584:ILE:HD13	1.80	0.64
1:A:325:ILE:HG23	1:A:346:GLY:C	2.22	0.64
1:A:171:THR:O	1:A:175:LEU:HD23	1.97	0.64
1:A:61:MET:HB2	1:B:88:ASP:HB3	1.80	0.63
1:B:25:LEU:HA	1:B:28:LEU:HD12	1.79	0.63
1:B:130:VAL:HG13	1:B:183:THR:HG22	1.78	0.63
1:A:451:SER:HB3	1:A:454:HIS:HB2	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:282:GLU:HA	1:B:294:HIS:HE1	1.62	0.63
1:A:458:LEU:C	1:A:458:LEU:HD23	2.23	0.63
1:A:522:GLU:C	1:A:524:GLU:N	2.49	0.63
1:A:151:ASP:O	1:A:152:TYR:C	2.40	0.63
1:B:205:LEU:HD12	1:B:206:PRO:HD2	1.80	0.63
1:B:542:PHE:HB3	1:B:564:SER:O	1.99	0.63
1:A:7:LEU:HD12	1:A:7:LEU:N	2.14	0.62
1:A:92:GLN:HG3	1:B:61:MET:SD	2.39	0.62
1:B:82:ILE:HG13	1:B:85:ASP:HB2	1.81	0.62
1:A:89:MET:HE3	1:A:94:PHE:O	1.99	0.62
1:A:163:LYS:HG2	1:A:164:ASP:N	2.14	0.62
1:A:480:LYS:O	1:A:483:VAL:HG23	2.00	0.62
1:A:143:VAL:O	1:A:172:ARG:HD2	1.99	0.62
1:A:163:LYS:HG2	1:A:164:ASP:H	1.63	0.62
1:A:163:LYS:H	1:A:163:LYS:HZ2	1.47	0.62
1:B:282:GLU:HA	1:B:294:HIS:CE1	2.35	0.62
1:A:85:ASP:O	1:A:89:MET:HG2	1.99	0.62
1:B:58:PHE:CD2	1:B:61:MET:HE1	2.26	0.62
1:B:229:LEU:C	1:B:229:LEU:HD23	2.25	0.62
1:B:320:ILE:O	1:B:342:VAL:HA	2.00	0.62
1:A:196:LYS:HG2	1:A:204:GLN:NE2	2.15	0.61
1:B:480:LYS:HA	1:B:514:GLU:CD	2.24	0.61
1:A:36:GLY:C	1:A:38:THR:N	2.57	0.61
1:A:220:LEU:HD13	1:B:387:LEU:HD12	1.82	0.61
1:B:254:LEU:HD23	1:B:424:ILE:HD12	1.81	0.61
1:B:471:HIS:ND1	1:B:472:PRO:HD2	2.15	0.61
1:A:37:GLY:CA	1:A:40:THR:HB	2.31	0.61
1:A:399:SER:O	1:A:402:LYS:HG3	2.00	0.61
1:A:15:LYS:O	1:A:18:LEU:HB3	1.99	0.61
1:A:208:ARG:HD3	1:A:208:ARG:H	1.66	0.61
1:B:9:LEU:HD13	1:B:10:LEU:H	1.60	0.61
1:B:480:LYS:O	1:B:483:VAL:HG12	2.00	0.61
1:A:36:GLY:C	1:A:38:THR:H	2.06	0.61
1:B:186:TYR:O	1:B:189:ALA:HB3	2.01	0.61
1:A:37:GLY:HA2	1:A:40:THR:CB	2.31	0.61
1:B:521:THR:O	1:B:525:LYS:HG3	2.01	0.61
1:A:378:GLU:CD	1:A:391:ARG:HB3	2.26	0.60
1:A:61:MET:HG3	1:A:62:LEU:N	2.16	0.60
1:A:208:ARG:NH1	1:A:237:GLY:HA2	2.15	0.60
1:A:19:VAL:HG12	1:A:20:GLU:N	2.17	0.60
1:B:514:GLU:OE2	1:B:514:GLU:HA	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:491:ALA:O	1:A:492:ILE:C	2.45	0.60
1:B:89:MET:HE3	1:B:94:PHE:O	2.01	0.60
1:B:547:ASP:OD1	1:B:547:ASP:N	2.35	0.60
1:B:61:MET:H	1:B:61:MET:CE	2.13	0.60
1:B:108:VAL:HG23	1:B:109:LYS:N	2.16	0.60
1:B:446:GLY:HA2	1:B:458:LEU:HD22	1.83	0.60
1:B:7:LEU:HD13	1:B:33:ILE:HD12	1.83	0.60
1:B:126:ASP:OD1	1:B:130:VAL:HG23	2.01	0.60
1:B:108:VAL:HG23	1:B:109:LYS:H	1.67	0.59
1:B:460:GLY:O	1:B:463:ALA:HB3	2.00	0.59
1:A:7:LEU:HD23	1:A:33:ILE:CG1	2.32	0.59
1:A:152:TYR:O	1:A:155:VAL:HB	2.02	0.59
1:A:432:ASN:C	1:A:432:ASN:HD22	2.11	0.59
1:B:490:ASN:O	1:B:494:GLN:HG2	2.01	0.59
1:B:105:TYR:CE1	1:B:109:LYS:HD3	2.37	0.59
1:B:7:LEU:CD1	1:B:33:ILE:HD12	2.33	0.59
1:B:384:GLY:N	4:B:2026:HOH:O	2.33	0.59
1:A:70:HIS:CD2	1:A:70:HIS:C	2.80	0.59
1:A:98:ARG:HG2	1:A:98:ARG:O	2.01	0.59
1:A:399:SER:HB3	4:A:2030:HOH:O	2.02	0.59
1:A:520:LEU:HD13	1:A:525:LYS:CE	2.32	0.59
1:A:159:MET:CE	1:A:166:ASP:HA	2.33	0.59
1:A:410:THR:O	1:A:411:LEU:HB2	2.02	0.59
1:B:108:VAL:O	1:B:111:VAL:HG22	2.03	0.59
1:A:394:ALA:CB	1:A:588:LEU:HD11	2.32	0.59
1:A:159:MET:HE2	1:A:166:ASP:HA	1.85	0.58
1:B:164:ASP:OD1	1:B:165:LYS:N	2.36	0.58
1:A:172:ARG:HG3	1:A:172:ARG:NH1	2.16	0.58
1:A:154:SER:HA	1:A:157:LYS:CD	2.33	0.58
1:A:398:ARG:NH1	1:A:398:ARG:HB2	2.18	0.58
1:B:37:GLY:HA2	1:B:40:THR:HB	1.85	0.58
1:B:64:GLY:C	1:B:66:VAL:N	2.57	0.58
1:A:492:ILE:O	1:A:493:ASP:C	2.47	0.58
1:B:26:ASN:HB2	1:B:32:LEU:HD21	1.85	0.58
1:A:506:LEU:O	1:A:510:GLN:HG3	2.04	0.58
1:B:159:MET:HA	1:B:162:SER:OG	2.04	0.58
1:B:376:ASP:HB3	1:B:390:LYS:NZ	2.19	0.58
1:A:382:LEU:HD21	1:B:242:CYS:HA	1.85	0.58
1:B:458:LEU:HD21	1:B:462:LYS:HE3	1.86	0.58
1:A:65:ARG:CD	1:B:78:LEU:HD22	2.29	0.58
1:A:156:ALA:O	1:A:157:LYS:C	2.47	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:ILE:HG23	1:A:400:LEU:HD23	1.85	0.58
1:B:156:ALA:HB3	1:B:157:LYS:CE	2.31	0.58
1:A:495:TYR:HD1	1:A:519:GLN:HE21	1.51	0.57
1:A:139:ASN:HB3	1:A:143:VAL:HG23	1.86	0.57
1:A:10:LEU:CD1	1:A:42:LEU:HD11	2.34	0.57
1:A:171:THR:O	1:A:174:HIS:HB3	2.05	0.57
1:B:64:GLY:HA2	1:B:66:VAL:O	2.05	0.57
1:A:75:ALA:O	1:A:79:ALA:HB2	2.05	0.57
1:A:198:TYR:CD1	1:B:173:ARG:HD3	2.40	0.57
1:A:7:LEU:HD23	1:A:33:ILE:HD11	1.85	0.57
1:B:7:LEU:HD23	1:B:7:LEU:N	2.19	0.57
1:B:164:ASP:O	1:B:165:LYS:HG2	2.05	0.57
1:A:87:ALA:HA	1:A:90:ASN:OD1	2.04	0.57
1:B:399:SER:HB2	1:B:402:LYS:NZ	2.19	0.57
1:A:18:LEU:O	1:A:19:VAL:C	2.47	0.57
1:A:398:ARG:HB2	1:A:398:ARG:HH11	1.69	0.57
1:B:25:LEU:HA	1:B:28:LEU:CD1	2.35	0.57
1:A:277:GLY:HA3	1:A:299:PRO:O	2.05	0.57
1:A:7:LEU:HD23	1:A:33:ILE:HG13	1.87	0.57
1:B:80:ARG:HD2	1:B:82:ILE:HD11	1.86	0.57
1:B:231:VAL:HG22	1:B:366:LEU:CD2	2.34	0.57
1:B:453:ILE:HD11	1:B:457:ARG:CZ	2.35	0.57
1:B:458:LEU:HD23	1:B:458:LEU:C	2.30	0.57
1:B:490:ASN:O	1:B:491:ALA:C	2.48	0.57
1:A:328:VAL:HG12	1:A:332:LYS:HE3	1.87	0.56
1:B:10:LEU:N	1:B:10:LEU:HD12	2.20	0.56
1:A:16:ALA:C	1:A:18:LEU:H	2.13	0.56
1:A:35:SER:O	1:A:39:ALA:HB3	2.05	0.56
1:A:386:GLN:HG3	1:B:221:TYR:CZ	2.40	0.56
1:A:495:TYR:HE1	1:A:519:GLN:HA	1.68	0.56
1:A:502:GLU:HA	1:A:506:LEU:CB	2.28	0.56
1:A:537:LEU:C	1:A:537:LEU:CD2	2.78	0.56
1:B:278:ILE:HG22	1:B:279:PRO:O	2.04	0.56
1:B:547:ASP:HA	1:B:550:ASP:OD2	2.04	0.56
1:B:483:VAL:O	1:B:484:LYS:O	2.23	0.56
1:B:506:LEU:O	1:B:510:GLN:HG3	2.05	0.56
1:A:58:PHE:CD2	1:A:59:PRO:HD2	2.41	0.56
1:A:70:HIS:HD2	1:A:72:ALA:N	2.04	0.56
1:A:163:LYS:H	1:A:163:LYS:NZ	2.04	0.56
1:B:500:ILE:HG23	1:B:509:TRP:CG	2.41	0.56
1:A:522:GLU:OE2	1:A:522:GLU:CA	2.53	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:PRO:O	1:B:75:ALA:N	2.35	0.55
1:A:35:SER:O	1:A:36:GLY:O	2.23	0.55
1:B:570:GLU:O	1:B:574:GLU:HG2	2.06	0.55
1:A:28:LEU:HA	1:A:165:LYS:HZ1	1.69	0.55
1:B:331:ALA:O	1:B:332:LYS:C	2.49	0.55
1:A:287:VAL:HG11	1:A:470:HIS:CE1	2.42	0.55
1:B:283:GLU:O	1:B:286:GLN:N	2.39	0.55
1:A:126:ASP:OD1	1:A:130:VAL:HG23	2.07	0.55
1:B:113:SER:O	1:B:116:VAL:HG12	2.06	0.55
1:A:106:PRO:CD	1:A:109:LYS:HE2	2.32	0.55
1:A:564:SER:HB3	1:A:585:HIS:ND1	2.22	0.55
1:B:31:GLY:O	1:B:33:ILE:HG13	2.07	0.55
1:B:216:SER:OG	1:B:217:PRO:HA	2.07	0.55
1:A:99:VAL:HG22	1:A:144:THR:HB	1.88	0.55
1:B:18:LEU:HD12	1:B:18:LEU:C	2.32	0.55
1:A:116:VAL:HG23	1:A:120:GLU:CD	2.32	0.55
1:A:151:ASP:O	1:A:155:VAL:HG23	2.07	0.55
1:B:432:ASN:HB2	1:B:452:ARG:NH2	2.22	0.55
1:A:12:VAL:HB	1:A:103:ASN:OD1	2.06	0.54
1:A:74:HIS:O	1:A:78:LEU:HB2	2.06	0.54
1:B:537:LEU:C	1:B:537:LEU:CD2	2.80	0.54
1:B:148:ASP:O	1:B:151:ASP:HB2	2.07	0.54
1:B:202:VAL:HG12	1:B:226:LYS:HG2	1.89	0.54
1:B:308:ARG:NH2	1:B:316:PHE:HA	2.22	0.54
1:B:426:VAL:CG1	1:B:540:ASP:HB3	2.37	0.54
1:A:70:HIS:CD2	1:A:72:ALA:N	2.74	0.54
1:A:130:VAL:HG13	1:A:183:THR:HG22	1.89	0.54
1:B:399:SER:O	1:B:402:LYS:HE2	2.07	0.54
1:A:464:ASN:HD22	1:A:555:ILE:HD13	1.72	0.54
1:A:89:MET:HE2	1:A:96:LEU:CD2	2.37	0.54
1:A:220:LEU:HD13	1:B:387:LEU:CD1	2.38	0.54
1:A:376:ASP:O	1:A:391:ARG:HG2	2.08	0.54
1:B:82:ILE:HD11	1:B:85:ASP:CG	2.32	0.54
1:A:174:HIS:CD2	1:A:175:LEU:HD22	2.37	0.54
1:A:386:GLN:HG3	1:B:221:TYR:CE1	2.42	0.54
1:A:186:TYR:O	1:A:189:ALA:HB3	2.08	0.54
1:A:383:TYR:HA	1:B:391:ARG:NH2	2.23	0.54
1:B:406:THR:HB	1:B:577:ASN:OD1	2.08	0.54
1:A:460:GLY:O	1:A:463:ALA:HB3	2.06	0.54
1:A:254:LEU:CD2	1:A:424:ILE:HD12	2.37	0.54
1:B:172:ARG:HG3	1:B:172:ARG:HH11	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:411:LEU:HD11	1:B:416:VAL:HG22	1.89	0.54
1:A:32:LEU:HD12	1:A:48:PRO:O	2.08	0.53
1:A:61:MET:SD	1:B:92:GLN:CG	2.95	0.53
1:A:566:SER:C	1:A:568:ALA:H	2.16	0.53
1:B:190:ILE:O	1:B:193:TYR:HB3	2.08	0.53
1:A:216:SER:OG	1:A:217:PRO:HA	2.09	0.53
1:B:359:LYS:HE2	1:B:363:TYR:HD1	1.73	0.53
1:A:40:THR:HA	1:A:43:ARG:CZ	2.37	0.53
1:A:113:SER:HB2	1:A:114:PRO:CD	2.39	0.53
1:A:220:LEU:CD1	1:B:387:LEU:HD12	2.37	0.53
1:A:330:THR:HG22	1:A:334:ILE:CD1	2.38	0.53
1:A:569:ASP:O	1:A:573:ILE:HG13	2.08	0.53
1:B:273:GLY:HA3	1:B:307:SER:O	2.08	0.53
1:B:83:PRO:HA	1:B:86:ASN:ND2	2.19	0.53
1:B:102:CYS:O	1:B:147:CYS:HA	2.09	0.53
1:B:484:LYS:CB	1:B:487:GLU:HG3	2.34	0.53
1:A:396:ILE:HG23	1:A:400:LEU:CD2	2.39	0.53
1:A:103:ASN:C	1:A:104:LEU:HG	2.33	0.53
1:A:25:LEU:C	1:A:27:ALA:N	2.66	0.53
1:A:326:CYS:O	1:A:348:GLU:HG3	2.09	0.53
1:B:53:SER:HG	1:B:60:GLU:CD	2.16	0.53
1:B:71:PRO:O	1:B:72:ALA:C	2.49	0.53
1:A:328:VAL:N	1:A:329:PRO:HD2	2.23	0.52
1:B:552:ALA:O	1:B:555:ILE:HG22	2.09	0.52
1:B:467:TRP:O	1:B:470:HIS:HB2	2.10	0.52
1:A:169:VAL:HG12	1:A:170:GLU:OE1	2.09	0.52
1:A:290:VAL:HA	1:A:336:ARG:HH22	1.73	0.52
1:A:328:VAL:CG1	1:A:332:LYS:HE3	2.40	0.52
1:A:490:ASN:O	1:A:493:ASP:HB3	2.09	0.52
1:A:396:ILE:HG21	1:A:423:SER:HB2	1.91	0.52
1:A:474:VAL:O	1:A:477:MET:HB2	2.10	0.52
1:B:465:SER:O	1:B:469:ARG:HG3	2.09	0.52
1:B:523:ALA:C	1:B:525:LYS:H	2.18	0.52
1:A:7:LEU:HD23	1:A:33:ILE:CD1	2.40	0.52
1:B:151:ASP:O	1:B:155:VAL:HG23	2.10	0.52
1:A:12:VAL:HG12	1:A:101:VAL:HG12	1.92	0.52
1:A:290:VAL:HA	1:A:336:ARG:NH2	2.25	0.52
1:A:348:GLU:O	1:A:351:ALA:HB3	2.09	0.52
1:A:65:ARG:HD3	1:B:78:LEU:HB3	1.90	0.52
1:B:483:VAL:O	1:B:484:LYS:C	2.53	0.52
1:B:537:LEU:HD23	1:B:538:SER:N	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:LEU:C	1:A:27:ALA:H	2.18	0.52
1:A:537:LEU:HD23	1:A:538:SER:N	2.25	0.52
1:A:63:GLY:O	1:B:80:ARG:NH2	2.43	0.51
1:A:103:ASN:HD22	1:A:104:LEU:N	2.08	0.51
1:A:289:MET:HA	1:A:289:MET:HE2	1.92	0.51
1:A:65:ARG:HD3	1:B:78:LEU:CD2	2.34	0.51
1:B:589:ARG:HG2	1:B:590:LEU:N	2.25	0.51
1:A:516:VAL:HG23	1:A:517:PRO:HD2	1.92	0.51
1:B:10:LEU:HD22	1:B:42:LEU:HD11	1.93	0.51
1:B:59:PRO:O	1:B:60:GLU:C	2.53	0.51
1:B:433:SER:HA	1:B:455:CYS:SG	2.50	0.51
1:B:523:ALA:C	1:B:525:LYS:N	2.65	0.51
1:B:589:ARG:HD3	1:B:591:PHE:CG	2.46	0.51
1:A:28:LEU:HA	1:A:165:LYS:CE	2.40	0.51
1:A:576:CYS:SG	1:A:583:LEU:HD22	2.51	0.51
1:B:64:GLY:C	1:B:66:VAL:H	2.18	0.51
1:A:309:GLY:O	1:A:469:ARG:NH2	2.42	0.51
1:B:58:PHE:O	1:B:60:GLU:N	2.41	0.51
1:A:325:ILE:HG23	1:A:346:GLY:O	2.11	0.51
1:A:445:ILE:HG23	1:A:445:ILE:O	2.11	0.51
1:B:408:ASN:HD21	1:B:577:ASN:CA	2.13	0.51
1:A:59:PRO:O	1:A:60:GLU:C	2.53	0.51
1:A:139:ASN:HB3	1:A:143:VAL:CG2	2.40	0.51
1:A:14:GLU:OE2	1:A:14:GLU:HA	2.11	0.51
1:A:414:SER:O	1:A:417:ARG:HB3	2.11	0.51
1:B:24:SER:O	1:B:28:LEU:HG	2.11	0.51
1:B:26:ASN:HB2	1:B:32:LEU:CD1	2.37	0.51
1:B:157:LYS:HE3	1:B:157:LYS:H	1.74	0.51
1:A:278:ILE:O	1:A:279:PRO:C	2.54	0.51
1:A:18:LEU:C	1:A:18:LEU:HD12	2.36	0.50
1:A:71:PRO:O	1:A:75:ALA:CB	2.59	0.50
1:A:102:CYS:O	1:A:147:CYS:HA	2.11	0.50
1:A:116:VAL:HG23	1:A:120:GLU:OE2	2.10	0.50
1:A:193:TYR:O	1:A:197:GLU:HG2	2.11	0.50
1:A:510:GLN:HA	1:A:513:PHE:HD1	1.76	0.50
1:A:50:ARG:HD2	1:A:54:ASP:CG	2.35	0.50
1:A:56:THR:O	1:A:57:GLY:C	2.54	0.50
1:A:84:GLU:OE1	1:A:84:GLU:N	2.38	0.50
1:A:28:LEU:HA	1:A:165:LYS:HE2	1.93	0.50
1:B:412:PRO:O	1:B:416:VAL:HG23	2.11	0.50
1:A:12:VAL:CG1	1:A:101:VAL:HG12	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:ALA:HB1	1:A:345:PRO:HD2	1.94	0.50
1:B:451:SER:HB3	1:B:454:HIS:HB2	1.92	0.50
1:A:286:GLN:C	1:A:288:CYS:N	2.68	0.50
1:B:522:GLU:O	1:B:526:LYS:HG3	2.12	0.50
1:A:376:ASP:HB3	1:A:390:LYS:CD	2.42	0.50
1:A:449:GLN:HB2	1:A:455:CYS:HB2	1.92	0.50
1:A:458:LEU:CD2	1:A:462:LYS:HE3	2.39	0.50
1:B:341:GLY:HA2	1:B:363:TYR:CZ	2.47	0.50
1:B:400:LEU:HG	1:B:400:LEU:O	2.11	0.50
1:B:432:ASN:HB2	1:B:452:ARG:HH22	1.76	0.50
1:B:506:LEU:O	1:B:506:LEU:HD12	2.11	0.50
1:A:19:VAL:O	1:A:22:ALA:HB3	2.12	0.50
1:A:476:SER:O	1:A:477:MET:C	2.53	0.50
1:A:520:LEU:HD12	1:A:520:LEU:N	2.12	0.50
1:A:458:LEU:HD23	1:A:458:LEU:O	2.11	0.50
1:A:525:LYS:O	1:A:529:ILE:HG13	2.12	0.50
1:A:562:ALA:O	1:A:585:HIS:HA	2.11	0.50
1:B:397:ASP:C	1:B:397:ASP:OD1	2.55	0.50
1:A:453:ILE:HG23	1:A:454:HIS:N	2.27	0.50
1:B:158:GLU:CD	1:B:168:SER:H	2.20	0.50
1:A:523:ALA:O	1:A:527:GLN:HB2	2.12	0.49
1:B:325:ILE:HA	1:B:346:GLY:O	2.11	0.49
1:A:168:SER:OG	1:A:171:THR:OG1	2.10	0.49
1:A:342:VAL:HG22	1:A:343:VAL:N	2.27	0.49
1:B:18:LEU:HG	1:B:19:VAL:N	2.26	0.49
1:B:148:ASP:OD1	1:B:150:ALA:HB3	2.11	0.49
1:B:426:VAL:HG13	1:B:540:ASP:HB3	1.93	0.49
1:A:229:LEU:C	1:A:229:LEU:HD23	2.37	0.49
1:A:255:LYS:HG3	1:A:323:SER:HB2	1.92	0.49
1:A:464:ASN:O	1:A:465:SER:C	2.54	0.49
1:B:44:ASP:C	1:B:46:GLY:H	2.20	0.49
1:B:172:ARG:NH1	1:B:172:ARG:HG3	2.27	0.49
1:A:426:VAL:HG13	1:A:540:ASP:HB3	1.94	0.49
1:B:7:LEU:HD13	1:B:33:ILE:CD1	2.42	0.49
1:B:496:VAL:C	1:B:498:GLY:H	2.20	0.49
1:A:64:GLY:C	1:A:65:ARG:HG3	2.37	0.49
1:A:522:GLU:O	1:A:526:LYS:HE2	2.11	0.49
1:B:376:ASP:HB3	1:B:390:LYS:HZ3	1.77	0.49
1:B:477:MET:C	1:B:478:LYS:HD2	2.37	0.49
1:B:572:VAL:O	1:B:575:ALA:N	2.43	0.49
1:A:520:LEU:HA	1:A:524:GLU:OE1	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:PHE:O	1:B:110:THR:HB	2.13	0.49
1:A:391:ARG:NH1	1:A:393:ASN:OD1	2.46	0.49
1:B:331:ALA:O	1:B:334:ILE:N	2.46	0.49
1:B:348:GLU:O	1:B:351:ALA:HB3	2.12	0.49
1:A:496:VAL:HG23	1:A:497:THR:HG23	1.94	0.49
1:A:537:LEU:HD22	1:A:560:ILE:HG23	1.93	0.49
1:A:145:VAL:O	1:A:175:LEU:HD12	2.13	0.48
1:B:250:LEU:HD12	1:B:428:TYR:HB2	1.95	0.48
1:B:431:SER:HB2	1:B:592:HIS:H	1.78	0.48
1:A:27:ALA:C	1:A:28:LEU:HD12	2.38	0.48
1:B:496:VAL:O	1:B:498:GLY:N	2.46	0.48
1:B:496:VAL:C	1:B:498:GLY:N	2.67	0.48
1:A:286:GLN:C	1:A:288:CYS:H	2.21	0.48
1:B:164:ASP:C	1:B:165:LYS:HG2	2.38	0.48
1:B:496:VAL:CG2	1:B:497:THR:H	2.25	0.48
1:A:161:ALA:HB3	4:A:2006:HOH:O	2.13	0.48
1:A:490:ASN:O	1:A:491:ALA:C	2.56	0.48
1:B:255:LYS:HE2	1:B:324:ASP:OD2	2.13	0.48
1:A:293:LEU:O	1:A:297:LEU:HG	2.14	0.48
1:B:375:ASP:N	1:B:375:ASP:OD2	2.44	0.48
1:A:106:PRO:CB	1:A:109:LYS:HZ3	2.26	0.48
1:A:226:LYS:HG2	1:A:227:LEU:N	2.29	0.48
1:A:275:ALA:HB2	1:A:441:GLN:HB2	1.96	0.48
1:A:350:GLU:O	1:A:354:ILE:HG13	2.13	0.48
1:A:471:HIS:CE1	1:A:472:PRO:HD2	2.47	0.48
1:A:485:ARG:HB2	1:A:485:ARG:CZ	2.43	0.48
1:A:71:PRO:O	1:A:75:ALA:HB2	2.13	0.48
1:A:269:VAL:HG12	1:A:269:VAL:O	2.14	0.48
1:A:544:PRO:HA	1:A:566:SER:OG	2.14	0.48
1:B:22:ALA:O	1:B:25:LEU:HD23	2.13	0.48
1:B:296:THR:O	1:B:297:LEU:HD23	2.14	0.48
1:B:464:ASN:ND2	1:B:555:ILE:CD1	2.76	0.48
1:B:473:ARG:HD3	1:B:518:ALA:O	2.14	0.48
1:A:21:PHE:CZ	1:A:155:VAL:HB	2.49	0.48
1:A:471:HIS:ND1	1:A:472:PRO:CD	2.75	0.48
1:A:118:VAL:C	1:A:122:VAL:HG23	2.39	0.47
1:A:311:ASP:OD2	1:A:314:SER:CB	2.62	0.47
1:A:392:ASN:OD1	1:A:427:LYS:HE3	2.14	0.47
1:B:566:SER:C	1:B:568:ALA:N	2.72	0.47
1:B:17:GLY:O	1:B:18:LEU:C	2.57	0.47
1:B:485:ARG:CG	1:B:485:ARG:NH1	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:ASN:HB2	1:A:32:LEU:HD11	1.96	0.47
1:A:73:VAL:HG12	1:A:74:HIS:N	2.29	0.47
1:A:81:ASN:O	1:A:81:ASN:CG	2.56	0.47
1:A:113:SER:CB	1:A:114:PRO:CD	2.92	0.47
1:B:44:ASP:C	1:B:46:GLY:N	2.70	0.47
1:B:18:LEU:O	1:B:19:VAL:C	2.56	0.47
1:B:67:LYS:NZ	3:B:1595:203:H12	2.13	0.47
1:B:121:ALA:C	1:B:124:LYS:HB2	2.39	0.47
1:B:431:SER:OG	1:B:432:ASN:HA	2.13	0.47
1:A:42:LEU:HD22	1:A:47:LEU:HD12	1.96	0.47
1:A:429:THR:HG22	1:A:433:SER:OG	2.15	0.47
1:A:36:GLY:O	1:A:39:ALA:N	2.47	0.47
1:B:347:TYR:OH	1:B:366:LEU:O	2.28	0.47
1:B:496:VAL:CG2	1:B:497:THR:N	2.78	0.47
1:A:58:PHE:CG	1:A:59:PRO:HD2	2.49	0.47
1:A:118:VAL:N	1:A:119:PRO:HD2	2.29	0.47
1:A:231:VAL:HG22	1:A:366:LEU:CD2	2.45	0.47
1:B:99:VAL:HG22	1:B:144:THR:HB	1.95	0.47
1:B:130:VAL:O	1:B:134:ARG:HG3	2.15	0.47
1:B:140:HIS:O	1:B:141:ALA:C	2.58	0.47
1:B:153:SER:HA	1:B:157:LYS:HZ1	1.79	0.47
1:B:495:TYR:HA	1:B:500:ILE:HD11	1.97	0.47
1:B:566:SER:HB3	1:B:569:ASP:CG	2.40	0.47
1:A:70:HIS:CD2	1:A:71:PRO:HG2	2.50	0.47
1:A:359:LYS:C	1:A:361:GLY:N	2.68	0.47
1:A:372:TYR:OH	1:B:384:GLY:HA3	2.15	0.47
1:A:467:TRP:O	1:A:470:HIS:HB2	2.15	0.47
1:A:553:LYS:O	1:A:554:ARG:C	2.57	0.47
1:B:193:TYR:O	1:B:197:GLU:HG2	2.15	0.47
1:A:148:ASP:O	1:A:151:ASP:HB2	2.14	0.47
1:A:522:GLU:O	1:A:524:GLU:N	2.48	0.47
1:A:566:SER:C	1:A:568:ALA:N	2.73	0.47
1:B:466:TRP:O	1:B:469:ARG:HB2	2.15	0.47
1:A:25:LEU:O	1:A:28:LEU:HB2	2.14	0.46
1:A:470:HIS:O	1:A:471:HIS:C	2.57	0.46
1:B:6:GLN:OE1	1:B:98:ARG:NH2	2.47	0.46
1:B:483:VAL:O	1:B:483:VAL:HG22	2.16	0.46
1:A:495:TYR:CD1	1:A:519:GLN:NE2	2.82	0.46
1:B:107:PHE:O	1:B:108:VAL:C	2.58	0.46
1:B:463:ALA:O	1:B:466:TRP:HB3	2.15	0.46
1:A:22:ALA:HB1	1:A:47:LEU:HD13	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:ASN:HD21	1:A:592:HIS:CE1	2.32	0.46
1:B:20:GLU:OE2	1:B:20:GLU:HA	2.16	0.46
1:B:280:LEU:HD12	1:B:280:LEU:H	1.79	0.46
1:A:73:VAL:O	1:A:77:ILE:HG13	2.15	0.46
1:A:138:LYS:C	1:A:140:HIS:H	2.23	0.46
1:A:330:THR:CG2	1:A:334:ILE:HD11	2.45	0.46
1:A:412:PRO:C	1:A:414:SER:N	2.72	0.46
1:B:81:ASN:CG	1:B:81:ASN:O	2.58	0.46
1:B:139:ASN:OD1	1:B:143:VAL:HG23	2.16	0.46
1:B:476:SER:O	1:B:478:LYS:HD2	2.15	0.46
1:B:572:VAL:O	1:B:575:ALA:HB3	2.15	0.46
1:A:330:THR:HG22	1:A:334:ILE:HD11	1.96	0.46
1:B:313:MET:C	1:B:315:SER:N	2.74	0.46
1:B:393:ASN:O	1:B:394:ALA:C	2.58	0.46
1:A:36:GLY:O	1:A:38:THR:N	2.49	0.46
1:A:70:HIS:O	1:A:73:VAL:HB	2.16	0.46
1:A:495:TYR:C	1:A:497:THR:H	2.23	0.46
1:B:342:VAL:HG22	1:B:343:VAL:N	2.31	0.46
1:B:553:LYS:C	1:B:555:ILE:H	2.22	0.46
1:A:493:ASP:O	1:A:494:GLN:C	2.59	0.46
1:A:200:LYS:C	1:A:200:LYS:CD	2.85	0.46
1:B:231:VAL:HG22	1:B:366:LEU:HD21	1.98	0.46
1:B:494:GLN:HA	1:B:497:THR:HB	1.97	0.46
1:A:149:PRO:C	1:A:151:ASP:N	2.73	0.46
1:B:22:ALA:O	1:B:23:ARG:C	2.59	0.46
1:B:352:LEU:HD12	1:B:352:LEU:O	2.16	0.46
1:A:177:LEU:C	1:A:177:LEU:CD2	2.89	0.46
1:A:429:THR:CG2	1:A:433:SER:OG	2.64	0.46
1:A:492:ILE:O	1:A:495:TYR:HB3	2.16	0.46
1:B:396:ILE:O	1:B:397:ASP:HB3	2.16	0.46
1:A:106:PRO:CG	1:A:109:LYS:NZ	2.79	0.45
1:A:298:THR:HG23	1:A:329:PRO:HG3	1.97	0.45
1:A:359:LYS:HB3	1:A:359:LYS:HE3	1.85	0.45
1:A:523:ALA:HA	1:A:526:LYS:CE	2.46	0.45
1:B:406:THR:CG2	1:B:583:LEU:HB3	2.47	0.45
1:B:438:LYS:HE2	1:B:533:THR:O	2.17	0.45
1:B:575:ALA:O	1:B:579:LEU:HG	2.16	0.45
1:B:589:ARG:HG2	1:B:590:LEU:H	1.82	0.45
1:A:25:LEU:O	1:A:28:LEU:N	2.44	0.45
1:A:38:THR:O	1:A:42:LEU:CG	2.64	0.45
1:A:390:LYS:O	1:B:215:GLN:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:492:ILE:O	1:A:495:TYR:N	2.49	0.45
1:A:102:CYS:O	1:A:147:CYS:CB	2.65	0.45
1:A:287:VAL:O	1:A:287:VAL:HG12	2.17	0.45
1:A:551:ARG:O	1:A:554:ARG:HB2	2.16	0.45
1:B:134:ARG:HB3	1:B:134:ARG:CZ	2.46	0.45
1:B:152:TYR:O	1:B:155:VAL:HB	2.16	0.45
1:A:39:ALA:O	1:A:40:THR:C	2.59	0.45
1:A:92:GLN:O	1:A:93:ASP:HB3	2.17	0.45
1:B:5:GLN:O	1:B:5:GLN:HG3	2.16	0.45
1:A:208:ARG:H	1:A:208:ARG:CD	2.29	0.45
1:A:502:GLU:N	1:A:505:ASP:HB2	2.29	0.45
1:B:26:ASN:C	1:B:28:LEU:H	2.24	0.45
1:A:208:ARG:NH2	1:A:237:GLY:CA	2.79	0.45
1:A:563:PRO:HG3	1:A:588:LEU:O	2.17	0.45
1:B:14:GLU:HA	1:B:14:GLU:OE1	2.16	0.45
1:B:398:ARG:O	1:B:401:PHE:HD2	1.99	0.45
1:B:464:ASN:O	1:B:465:SER:C	2.60	0.45
1:B:509:TRP:HH2	1:B:517:PRO:HG2	1.81	0.45
1:A:311:ASP:OD2	1:A:314:SER:HB2	2.17	0.45
1:A:494:GLN:O	1:A:498:GLY:N	2.50	0.45
1:B:39:ALA:O	1:B:40:THR:C	2.60	0.45
1:B:118:VAL:N	1:B:119:PRO:HD2	2.32	0.45
1:B:49:VAL:HG13	1:B:49:VAL:O	2.17	0.44
1:B:70:HIS:CD2	1:B:70:HIS:C	2.94	0.44
1:B:129:GLY:O	1:B:130:VAL:C	2.60	0.44
1:B:429:THR:O	1:B:592:HIS:HB3	2.16	0.44
1:B:497:THR:O	1:B:497:THR:HG22	2.17	0.44
1:A:26:ASN:HB2	1:A:32:LEU:CD2	2.37	0.44
1:A:37:GLY:HA2	1:A:40:THR:OG1	2.17	0.44
1:A:64:GLY:O	1:A:65:ARG:HG3	2.16	0.44
1:B:155:VAL:O	1:B:156:ALA:C	2.59	0.44
1:A:7:LEU:N	1:A:7:LEU:CD1	2.78	0.44
1:A:82:ILE:O	1:A:83:PRO:C	2.60	0.44
1:A:246:ASN:ND2	1:A:592:HIS:NE2	2.62	0.44
1:A:347:TYR:OH	1:A:366:LEU:O	2.35	0.44
1:A:429:THR:HG22	1:A:430:GLN:N	2.32	0.44
1:A:501:GLY:O	1:A:502:GLU:HB3	2.18	0.44
1:A:98:ARG:HD3	1:A:166:ASP:OD2	2.17	0.44
1:A:103:ASN:O	1:A:104:LEU:HD23	2.17	0.44
1:A:239:ILE:HG22	1:A:243:ASP:OD2	2.17	0.44
1:A:412:PRO:C	1:A:414:SER:H	2.24	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:ILE:HD11	1:B:85:ASP:OD1	2.17	0.44
1:B:495:TYR:CD1	1:B:500:ILE:HD11	2.47	0.44
1:B:546:ARG:O	1:B:549:VAL:N	2.50	0.44
1:A:80:ARG:HE	1:A:80:ARG:HB2	1.45	0.44
1:A:187:ASP:HB3	1:B:184:ALA:HB2	1.99	0.44
1:B:403:ASN:CG	1:B:403:ASN:O	2.59	0.44
1:A:103:ASN:O	1:A:104:LEU:HG	2.17	0.44
1:A:237:GLY:O	1:A:241:LEU:HG	2.18	0.44
1:B:22:ALA:CA	1:B:25:LEU:CD2	2.92	0.44
1:B:105:TYR:O	1:B:106:PRO:C	2.60	0.44
1:A:102:CYS:HB3	1:A:133:LEU:HD21	2.00	0.44
1:A:250:LEU:HD11	1:A:425:ALA:HA	1.98	0.44
1:A:407:LYS:O	1:A:409:LYS:HD3	2.17	0.44
1:A:436:TYR:CE2	1:A:555:ILE:HG21	2.53	0.44
1:B:156:ALA:CB	1:B:157:LYS:HE3	2.41	0.44
1:B:257:ALA:O	1:B:258:LEU:HD23	2.18	0.44
1:B:471:HIS:ND1	1:B:472:PRO:CD	2.81	0.44
1:B:169:VAL:O	1:B:173:ARG:HG3	2.17	0.44
1:A:10:LEU:HD13	1:A:42:LEU:HD11	2.00	0.44
1:B:7:LEU:HD21	1:B:95:SER:HB3	2.00	0.44
1:B:164:ASP:OD2	1:B:166:ASP:HB3	2.17	0.44
1:B:467:TRP:CE3	1:B:467:TRP:HA	2.53	0.44
1:B:71:PRO:O	1:B:75:ALA:CB	2.66	0.43
1:A:245:LEU:N	1:A:245:LEU:HD22	2.33	0.43
1:A:385:LEU:HD22	1:B:227:LEU:CD2	2.48	0.43
1:A:432:ASN:HD21	1:A:455:CYS:HB2	1.83	0.43
1:B:177:LEU:O	1:B:178:LYS:C	2.61	0.43
1:A:148:ASP:OD1	1:A:150:ALA:CB	2.59	0.43
1:A:163:LYS:NZ	1:A:163:LYS:N	2.66	0.43
1:A:281:SER:OG	1:A:284:GLU:HB2	2.19	0.43
1:B:473:ARG:HD2	1:B:520:LEU:HD21	2.01	0.43
1:B:474:VAL:O	1:B:475:LEU:C	2.60	0.43
1:A:192:ASP:HA	1:A:195:ARG:NH2	2.33	0.43
1:A:308:ARG:HG3	1:A:315:SER:HB3	2.01	0.43
1:B:311:ASP:OD1	1:B:314:SER:HB2	2.17	0.43
1:B:509:TRP:HE3	1:B:510:GLN:HG2	1.83	0.43
1:A:219:GLN:NE2	1:B:388:MET:CE	2.82	0.43
1:A:352:LEU:HD12	1:A:352:LEU:O	2.18	0.43
1:A:451:SER:HB3	1:A:454:HIS:CG	2.54	0.43
1:B:21:PHE:O	1:B:25:LEU:HD23	2.17	0.43
1:B:328:VAL:HG21	1:B:350:GLU:OE1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:566:SER:C	1:B:568:ALA:H	2.26	0.43
1:A:268:HIS:NE2	1:B:432:ASN:HB3	2.33	0.43
1:A:382:LEU:CD2	1:B:242:CYS:HA	2.48	0.43
1:A:463:ALA:O	1:A:466:TRP:HB3	2.19	0.43
1:B:30:LEU:HD21	1:B:98:ARG:HD2	2.01	0.43
1:B:286:GLN:HG2	1:B:291:HIS:HB2	2.00	0.43
1:B:502:GLU:H	1:B:502:GLU:HG2	1.45	0.43
1:A:429:THR:CG2	1:A:447:ALA:HB2	2.49	0.43
1:A:484:LYS:HB2	1:A:487:GLU:HG3	2.01	0.43
1:B:174:HIS:O	1:B:178:LYS:HG3	2.18	0.43
1:A:205:LEU:HD23	1:A:205:LEU:C	2.44	0.43
1:A:330:THR:O	1:A:334:ILE:HG13	2.19	0.43
1:B:445:ILE:HG23	1:B:445:ILE:O	2.18	0.43
1:B:472:PRO:O	1:B:473:ARG:C	2.62	0.43
1:B:478:LYS:N	1:B:478:LYS:CD	2.82	0.43
1:B:520:LEU:O	1:B:525:LYS:HE3	2.19	0.43
1:A:130:VAL:O	1:A:134:ARG:HG3	2.19	0.43
1:A:163:LYS:C	1:A:165:LYS:H	2.27	0.43
1:A:385:LEU:HD21	1:B:228:PRO:HD2	2.01	0.43
1:B:283:GLU:O	1:B:284:GLU:C	2.62	0.43
1:B:432:ASN:OD1	1:B:432:ASN:C	2.62	0.43
1:B:474:VAL:CA	1:B:477:MET:HG3	2.45	0.43
1:A:139:ASN:C	1:A:141:ALA:N	2.76	0.42
1:A:162:SER:O	1:A:165:LYS:N	2.51	0.42
1:A:245:LEU:O	1:A:249:GLN:HG3	2.18	0.42
1:A:419:LEU:HD23	1:A:536:SER:HB3	2.01	0.42
1:B:118:VAL:HB	1:B:119:PRO:CD	2.49	0.42
1:B:195:ARG:HB3	1:B:204:GLN:HB2	2.01	0.42
1:B:510:GLN:C	1:B:512:MET:H	2.27	0.42
1:A:250:LEU:C	1:A:250:LEU:HD23	2.44	0.42
1:A:499:THR:O	1:A:500:ILE:C	2.62	0.42
1:B:84:GLU:H	1:B:84:GLU:CD	2.24	0.42
1:B:281:SER:HB2	4:B:2018:HOH:O	2.19	0.42
1:B:504:GLU:O	1:B:507:VAL:HB	2.19	0.42
1:A:40:THR:HA	1:A:43:ARG:NH2	2.34	0.42
1:A:89:MET:O	1:A:93:ASP:N	2.52	0.42
1:A:247:ALA:HB2	1:A:266:PHE:CD1	2.54	0.42
1:A:249:GLN:O	1:A:253:GLU:HG3	2.19	0.42
1:A:398:ARG:NH1	1:A:398:ARG:CB	2.83	0.42
1:B:237:GLY:O	1:B:241:LEU:HG	2.19	0.42
1:B:269:VAL:HG12	1:B:269:VAL:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:399:SER:O	1:B:402:LYS:HG2	2.18	0.42
1:A:15:LYS:O	1:A:18:LEU:CB	2.67	0.42
1:A:20:GLU:O	1:A:23:ARG:HB3	2.20	0.42
1:A:173:ARG:O	1:A:174:HIS:C	2.61	0.42
1:A:59:PRO:HG3	1:B:92:GLN:OE1	2.20	0.42
1:A:196:LYS:HD3	1:A:219:GLN:NE2	2.34	0.42
1:A:404:ILE:HG12	1:A:584:ILE:HG12	2.02	0.42
1:A:572:VAL:O	1:A:575:ALA:HB3	2.19	0.42
1:B:58:PHE:CD2	1:B:59:PRO:HD2	2.55	0.42
1:A:65:ARG:NH2	1:B:138:LYS:HE2	2.33	0.42
1:A:149:PRO:C	1:A:151:ASP:H	2.27	0.42
1:A:523:ALA:HA	1:A:526:LYS:HE3	2.00	0.42
1:A:555:ILE:HG13	1:A:555:ILE:O	2.19	0.42
1:B:33:ILE:HD13	1:B:55:LEU:HG	2.01	0.42
1:B:98:ARG:O	1:B:98:ARG:HG2	2.20	0.42
1:B:222:THR:O	1:B:222:THR:HG23	2.18	0.42
1:A:467:TRP:CD1	1:A:529:ILE:HA	2.54	0.42
1:B:286:GLN:HG2	1:B:291:HIS:CG	2.55	0.42
1:B:292:ASP:C	1:B:293:LEU:HD23	2.44	0.42
1:A:452:ARG:HG3	1:A:548:ASN:OD1	2.19	0.42
1:A:458:LEU:C	1:A:458:LEU:CD2	2.93	0.42
1:B:267:LYS:O	1:B:268:HIS:HB2	2.20	0.42
1:A:18:LEU:O	1:A:21:PHE:N	2.51	0.42
1:A:197:GLU:OE1	1:A:197:GLU:HA	2.19	0.42
1:A:280:LEU:HD12	1:A:280:LEU:N	2.35	0.42
1:A:282:GLU:HG3	1:A:291:HIS:CE1	2.54	0.42
1:A:379:ILE:CG1	1:A:388:MET:HG3	2.25	0.42
1:B:287:VAL:HG11	1:B:470:HIS:CE1	2.55	0.42
1:A:419:LEU:HD23	1:A:419:LEU:HA	1.87	0.42
1:B:25:LEU:HD23	1:B:25:LEU:H	1.85	0.42
1:B:118:VAL:O	1:B:119:PRO:C	2.63	0.42
1:A:155:VAL:O	1:A:156:ALA:C	2.63	0.41
1:A:330:THR:HG22	1:A:334:ILE:HD12	2.02	0.41
1:B:71:PRO:O	1:B:75:ALA:HB2	2.20	0.41
1:B:80:ARG:HD2	1:B:82:ILE:HD13	2.01	0.41
1:B:97:VAL:O	1:B:142:ARG:NH1	2.53	0.41
1:B:196:LYS:HG2	1:B:204:GLN:NE2	2.34	0.41
1:A:386:GLN:HG2	1:B:221:TYR:O	2.20	0.41
1:A:467:TRP:NE1	1:A:528:TRP:O	2.48	0.41
1:A:574:GLU:O	1:A:578:GLU:HG2	2.20	0.41
1:B:108:VAL:CG2	1:B:109:LYS:N	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:436:TYR:CE2	1:B:555:ILE:HG21	2.55	0.41
1:B:464:ASN:HD22	1:B:555:ILE:CD1	2.33	0.41
1:B:532:LEU:HD12	1:B:532:LEU:HA	1.74	0.41
1:B:542:PHE:C	1:B:542:PHE:CD1	2.98	0.41
1:B:553:LYS:O	1:B:555:ILE:N	2.52	0.41
1:A:177:LEU:C	1:A:177:LEU:HD23	2.45	0.41
1:A:356:SER:O	1:A:361:GLY:HA2	2.20	0.41
1:B:539:SER:HB2	1:B:543:PHE:CZ	2.55	0.41
1:A:520:LEU:H	1:A:520:LEU:CD1	2.13	0.41
1:B:537:LEU:HD22	1:B:560:ILE:HG23	2.02	0.41
1:A:87:ALA:O	1:A:90:ASN:HB2	2.20	0.41
1:A:267:LYS:HG2	1:B:450:GLN:HB3	2.02	0.41
1:B:521:THR:O	1:B:522:GLU:C	2.63	0.41
1:A:7:LEU:HB3	1:A:8:ALA:H	1.57	0.41
1:A:26:ASN:C	1:A:28:LEU:H	2.27	0.41
1:A:140:HIS:O	1:A:141:ALA:C	2.61	0.41
1:A:412:PRO:HD2	1:A:415:ALA:HB2	2.02	0.41
1:B:108:VAL:CG2	1:B:109:LYS:H	2.33	0.41
1:B:250:LEU:HG	1:B:424:ILE:HG22	2.03	0.41
1:B:453:ILE:O	1:B:453:ILE:HG13	2.20	0.41
1:B:479:PHE:O	1:B:480:LYS:C	2.61	0.41
1:B:480:LYS:N	1:B:512:MET:O	2.46	0.41
1:A:236:PRO:HB3	1:A:364:CYS:SG	2.61	0.41
1:A:378:GLU:HG3	1:A:391:ARG:CB	2.47	0.41
1:A:183:THR:O	1:A:184:ALA:C	2.63	0.41
1:A:212:ASN:OD1	1:B:591:PHE:HB2	2.21	0.41
1:A:418:ASP:N	1:A:418:ASP:OD1	2.54	0.41
1:B:6:GLN:O	1:B:30:LEU:HD23	2.21	0.41
1:B:53:SER:OG	1:B:60:GLU:CD	2.63	0.41
1:B:590:LEU:HD23	1:B:590:LEU:HA	1.91	0.41
1:A:13:SER:HB3	1:A:103:ASN:ND2	2.36	0.41
1:A:467:TRP:HA	1:A:467:TRP:CE3	2.55	0.41
1:B:26:ASN:CA	1:B:32:LEU:HD21	2.50	0.41
1:B:241:LEU:O	1:B:245:LEU:HG	2.20	0.41
1:B:280:LEU:N	1:B:280:LEU:CD1	2.80	0.41
1:B:331:ALA:O	1:B:333:ILE:N	2.53	0.41
1:B:527:GLN:C	1:B:529:ILE:N	2.76	0.41
1:B:575:ALA:O	1:B:578:GLU:HG2	2.21	0.41
1:A:121:ALA:O	1:A:124:LYS:HB2	2.21	0.41
1:A:347:TYR:CD1	1:A:347:TYR:N	2.88	0.41
1:B:406:THR:HG23	1:B:583:LEU:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:449:GLN:NE2	1:B:449:GLN:HA	2.35	0.41
1:A:10:LEU:HD12	1:A:42:LEU:HD11	2.02	0.40
1:A:16:ALA:O	1:A:18:LEU:N	2.54	0.40
1:A:271:PRO:HD2	1:A:429:THR:HA	2.03	0.40
1:A:288:CYS:O	1:A:289:MET:C	2.64	0.40
1:A:494:GLN:HA	1:A:499:THR:OG1	2.21	0.40
1:A:495:TYR:C	1:A:497:THR:N	2.79	0.40
1:B:31:GLY:O	1:B:32:LEU:C	2.64	0.40
1:B:360:ASN:HD22	1:B:360:ASN:HA	1.70	0.40
1:B:575:ALA:HA	1:B:578:GLU:HG2	2.03	0.40
1:A:65:ARG:HB3	1:A:66:VAL:H	1.68	0.40
1:A:254:LEU:HD23	1:A:254:LEU:HA	1.87	0.40
1:B:35:SER:N	1:B:39:ALA:HB2	2.37	0.40
1:B:164:ASP:O	1:B:165:LYS:CG	2.68	0.40
1:B:488:VAL:O	1:B:489:SER:C	2.64	0.40
1:A:7:LEU:CD2	1:A:33:ILE:HD11	2.49	0.40
1:A:523:ALA:N	1:A:526:LYS:HE2	2.34	0.40
1:A:26:ASN:C	1:A:28:LEU:N	2.79	0.40
1:A:474:VAL:C	1:A:476:SER:N	2.78	0.40
1:B:122:VAL:C	1:B:124:LYS:N	2.76	0.40
1:B:177:LEU:CD2	1:B:177:LEU:C	2.95	0.40
1:B:464:ASN:HD21	1:B:555:ILE:HD13	1.79	0.40
1:A:7:LEU:HA	1:A:31:GLY:H	1.85	0.40
1:A:55:LEU:CD2	1:A:72:ALA:HB1	2.49	0.40
1:A:71:PRO:O	1:A:75:ALA:N	2.46	0.40
1:A:103:ASN:O	1:A:104:LEU:CD2	2.70	0.40
1:A:144:THR:HG21	1:A:167:THR:HG21	2.04	0.40
1:A:219:GLN:HE21	1:B:388:MET:CE	2.34	0.40
1:A:229:LEU:HD23	1:A:229:LEU:O	2.21	0.40
1:A:464:ASN:HD22	1:A:555:ILE:CD1	2.32	0.40
1:A:520:LEU:CD1	1:A:525:LYS:HE2	2.47	0.40
1:B:446:GLY:CA	1:B:458:LEU:HD22	2.52	0.40
1:B:473:ARG:NH1	1:B:524:GLU:OE2	2.53	0.40
1:B:546:ARG:HA	1:B:549:VAL:HG23	2.03	0.40
1:B:583:LEU:HD12	1:B:584:ILE:H	1.81	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:LEU:O	1:B:47:LEU:O[2_656]	1.94	0.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:GLY:O	1:B:48:PRO:C[2_656]	2.02	0.18
1:B:46:GLY:CA	1:B:49:VAL:O[2_656]	2.07	0.13
1:B:46:GLY:O	1:B:48:PRO:CA[2_656]	2.11	0.09

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	589/593 (99%)	464 (79%)	90 (15%)	35 (6%)	1	4
1	B	588/593 (99%)	484 (82%)	75 (13%)	29 (5%)	1	6
All	All	1177/1186 (99%)	948 (80%)	165 (14%)	64 (5%)	1	5

All (64) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	SER
1	A	18	LEU
1	A	19	VAL
1	A	40	THR
1	A	66	VAL
1	A	83	PRO
1	A	114	PRO
1	A	152	TYR
1	A	403	ASN
1	B	18	LEU
1	B	114	PRO
1	B	152	TYR
1	B	164	ASP
1	B	477	MET
1	B	484	LYS
1	B	503	ASP
1	A	36	GLY

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Mol	Chain	Res	Type
1	A	67	LYS
1	A	269	VAL
1	A	402	LYS
1	A	477	MET
1	A	479	PHE
1	A	492	ILE
1	A	502	GLU
1	B	19	VAL
1	B	60	GLU
1	B	67	LYS
1	B	73	VAL
1	B	269	VAL
1	B	489	SER
1	B	554	ARG
1	A	41	ALA
1	A	162	SER
1	A	491	ALA
1	A	499	THR
1	B	27	ALA
1	B	316	PHE
1	A	5	GLN
1	A	17	GLY
1	A	160	ALA
1	A	311	ASP
1	A	316	PHE
1	A	493	ASP
1	B	59	PRO
1	B	394	ALA
1	B	476	SER
1	A	73	VAL
1	A	153	SER
1	A	411	LEU
1	B	153	SER
1	B	277	GLY
1	B	332	LYS
1	B	404	ILE
1	B	497	THR
1	A	113	SER
1	B	71	PRO
1	B	315	SER
1	B	526	LYS
1	B	567	ALA

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Mol	Chain	Res	Type
1	A	496	VAL
1	B	488	VAL
1	A	290	VAL
1	A	71	PRO
1	A	106	PRO

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	485/485 (100%)	439 (90%)	46 (10%)	8	26
1	B	484/485 (100%)	443 (92%)	41 (8%)	10	31
All	All	969/970 (100%)	882 (91%)	87 (9%)	9	28

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	11	SER
1	A	12	VAL
1	A	18	LEU
1	A	21	PHE
1	A	24	SER
1	A	30	LEU
1	A	32	LEU
1	A	43	ARG
1	A	54	ASP
1	A	55	LEU
1	A	60	GLU
1	A	68	THR
1	A	70	HIS
1	A	81	ASN
1	A	83	PRO
1	A	103	ASN
1	A	120	GLU

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Mol	Chain	Res	Type
1	A	154	SER
1	A	159	MET
1	A	163	LYS
1	A	164	ASP
1	A	170	GLU
1	A	177	LEU
1	A	187	ASP
1	A	202	VAL
1	A	208	ARG
1	A	255	LYS
1	A	289	MET
1	A	340	ASP
1	A	350	GLU
1	A	359	LYS
1	A	360	ASN
1	A	386	GLN
1	A	390	LYS
1	A	406	THR
1	A	432	ASN
1	A	477	MET
1	A	502	GLU
1	A	504	GLU
1	A	519	GLN
1	A	520	LEU
1	A	522	GLU
1	A	524	GLU
1	A	537	LEU
1	A	547	ASP
1	B	7	LEU
1	B	9	LEU
1	B	11	SER
1	B	19	VAL
1	B	54	ASP
1	B	56	THR
1	B	60	GLU
1	B	61	MET
1	B	68	THR
1	B	114	PRO
1	B	154	SER
1	B	157	LYS
1	B	167	THR
1	B	170	GLU

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Mol	Chain	Res	Type
1	B	177	LEU
1	B	199	SER
1	B	202	VAL
1	B	239	ILE
1	B	280	LEU
1	B	282	GLU
1	B	292	ASP
1	B	293	LEU
1	B	294	HIS
1	B	296	THR
1	B	314	SER
1	B	338	VAL
1	B	349	GLU
1	B	375	ASP
1	B	382	LEU
1	B	399	SER
1	B	408	ASN
1	B	478	LYS
1	B	483	VAL
1	B	485	ARG
1	B	499	THR
1	B	502	GLU
1	B	506	LEU
1	B	517	PRO
1	B	537	LEU
1	B	547	ASP
1	B	555	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	70	HIS
1	A	81	ASN
1	A	86	ASN
1	A	174	HIS
1	A	204	GLN
1	A	219	GLN
1	A	246	ASN
1	A	249	GLN
1	A	286	GLN
1	A	291	HIS

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Mol	Chain	Res	Type
1	A	294	HIS
1	A	371	ASN
1	A	386	GLN
1	A	403	ASN
1	A	430	GLN
1	A	432	ASN
1	A	464	ASN
1	A	510	GLN
1	B	5	GLN
1	B	70	HIS
1	B	86	ASN
1	B	185	GLN
1	B	360	ASN
1	B	377	ASN
1	B	386	GLN
1	B	393	ASN
1	B	449	GLN
1	B	454	HIS
1	B	464	ASN
1	B	494	GLN
1	B	510	GLN
1	B	527	GLN
1	B	558	GLN

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 ⓘ

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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	203	B	1595	-	10,13,13	6.63	5 (50%)	8,20,20	8.21	7 (87%)

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	203	B	1595	-	-	-	0/1/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1595	203	O20-S16	16.52	1.65	1.43
3	B	1595	203	O21-S16	10.57	1.57	1.43
3	B	1595	203	C13-C18	4.63	1.55	1.41
3	B	1595	203	C11-N12	4.58	1.42	1.35
3	B	1595	203	C13-N12	2.45	1.41	1.38

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1595	203	O21-S16-O20	-17.17	97.97	118.87
3	B	1595	203	C11-N12-C13	-11.31	93.89	106.59
3	B	1595	203	N12-C11-N10	7.54	121.73	112.98
3	B	1595	203	C18-C13-N12	-4.88	121.81	131.14
3	B	1595	203	O19-C18-C13	-3.85	117.98	127.26
3	B	1595	203	C14-C13-N12	2.99	114.57	106.71
3	B	1595	203	O19-C18-N17	2.86	124.53	120.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1595	203	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	590/593 (99%)	1.08	57 (9%) 13 11	22, 43, 66, 74	1 (0%)
1	B	590/593 (99%)	1.21	97 (16%) 4 3	27, 46, 63, 72	0
All	All	1180/1186 (99%)	1.15	154 (13%) 7 6	22, 45, 65, 74	1 (0%)

All (154) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	96	LEU	4.9
1	A	31	GLY	4.8
1	B	46	GLY	4.8
1	B	43	ARG	4.5
1	A	72	ALA	4.2
1	B	49	VAL	4.1
1	B	47	LEU	4.1
1	B	48	PRO	4.0
1	B	100	VAL	4.0
1	B	10	LEU	4.0
1	A	10	LEU	3.9
1	A	128	GLY	3.8
1	A	132	LEU	3.6
1	A	105[A]	TYR	3.5
1	B	53	SER	3.5
1	B	146	VAL	3.5
1	B	99	VAL	3.4
1	B	144	THR	3.4
1	B	55	LEU	3.3
1	B	79	ALA	3.3
1	B	8	ALA	3.2
1	B	57	GLY	3.2
1	B	379	ILE	3.2
1	B	33	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	97	VAL	3.1
1	A	315	SER	3.1
1	A	188	ALA	3.0
1	A	78	LEU	3.0
1	A	87	ALA	3.0
1	B	133	LEU	3.0
1	B	54	ASP	3.0
1	B	32	LEU	2.9
1	B	517	PRO	2.9
1	B	143	VAL	2.9
1	B	396	ILE	2.9
1	A	213	PRO	2.9
1	A	33	ILE	2.9
1	B	9	LEU	2.9
1	B	446	GLY	2.9
1	B	221	TYR	2.9
1	B	231	VAL	2.9
1	B	7	LEU	2.9
1	A	135	ALA	2.8
1	B	31	GLY	2.8
1	B	101	VAL	2.8
1	B	180	PHE	2.8
1	A	19	VAL	2.7
1	B	132	LEU	2.7
1	B	58	PHE	2.7
1	B	75	ALA	2.7
1	A	182	HIS	2.7
1	A	355	LEU	2.7
1	A	145	VAL	2.7
1	B	264	ALA	2.7
1	B	555	ILE	2.7
1	B	103	ASN	2.6
1	B	122	VAL	2.6
1	B	424	ILE	2.6
1	B	34	ALA	2.6
1	A	29	GLY	2.6
1	A	64	GLY	2.6
1	B	45	ALA	2.6
1	B	131	ALA	2.6
1	A	433	SER	2.6
1	A	66	VAL	2.6
1	B	44	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	189	ALA	2.6
1	A	238	PHE	2.6
1	A	15	LYS	2.5
1	A	62	LEU	2.5
1	A	223	THR	2.5
1	B	70	HIS	2.5
1	B	191	SER	2.5
1	A	362	GLY	2.5
1	B	127	ILE	2.5
1	A	58	PHE	2.5
1	A	65	ARG	2.5
1	B	89	MET	2.5
1	A	16	ALA	2.5
1	A	63	GLY	2.5
1	B	29	GLY	2.5
1	B	561	VAL	2.5
1	A	207	LEU	2.4
1	B	94	PHE	2.4
1	B	136	ALA	2.4
1	B	61	MET	2.4
1	A	52	VAL	2.4
1	B	149	PRO	2.4
1	A	576	CYS	2.4
1	A	543	PHE	2.4
1	B	72	ALA	2.4
1	B	59	PRO	2.4
1	A	191	SER	2.3
1	A	198	TYR	2.3
1	A	127	ILE	2.3
1	A	46	GLY	2.3
1	A	479	PHE	2.3
1	A	519	GLN	2.3
1	B	35	SER	2.3
1	A	71	PRO	2.3
1	B	130	VAL	2.3
1	B	460	GLY	2.3
1	A	314	SER	2.3
1	B	67	LYS	2.3
1	B	137	ALA	2.3
1	B	481	ALA	2.3
1	B	68	THR	2.3
1	A	237	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	266	PHE	2.2
1	B	299	PRO	2.2
1	A	277	GLY	2.2
1	A	547	ASP	2.2
1	B	66	VAL	2.2
1	B	440	GLY	2.2
1	A	107	PHE	2.2
1	A	7	LEU	2.2
1	A	125	ILE	2.2
1	B	125	ILE	2.2
1	A	74	HIS	2.2
1	B	151	ASP	2.2
1	B	324	ASP	2.2
1	A	221	TYR	2.2
1	B	268	HIS	2.2
1	B	91	LYS	2.2
1	B	323	SER	2.2
1	B	401	PHE	2.2
1	A	9	LEU	2.2
1	B	368	MET	2.1
1	B	152	TYR	2.1
1	A	288	CYS	2.1
1	B	552	ALA	2.1
1	B	140	HIS	2.1
1	B	17	GLY	2.1
1	B	194	PHE	2.1
1	B	241	LEU	2.1
1	B	278	ILE	2.1
1	B	182	HIS	2.1
1	B	543	PHE	2.1
1	B	306	ARG	2.1
1	A	136	ALA	2.1
1	A	265	SER	2.1
1	A	228	PRO	2.1
1	B	254	LEU	2.1
1	A	184	ALA	2.1
1	B	179	ALA	2.1
1	A	146	VAL	2.0
1	B	290	VAL	2.0
1	B	343	VAL	2.0
1	B	161	ALA	2.0
1	B	363	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	315	SER	2.0
1	B	421	VAL	2.0
1	B	228	PRO	2.0
1	B	400	LEU	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($\text{\AA}^2$)	Q<0.9
2	K	A	1594	1/1	0.65	0.17	56,56,56,56	0
3	203	B	1595	12/12	0.67	0.16	68,71,74,74	0
2	K	B	1594	1/1	0.93	0.07	48,48,48,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.