



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 07:17 AM UTC

PDB ID : 3RRR / pdb_00003rrr
Title : Structure of the RSV F protein in the post-fusion conformation
Authors : McLellan, J.S.; Yongping, Y.; Graham, B.S.; Kwong, P.D.
Deposited on : 2011-04-30
Resolution : 2.82 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

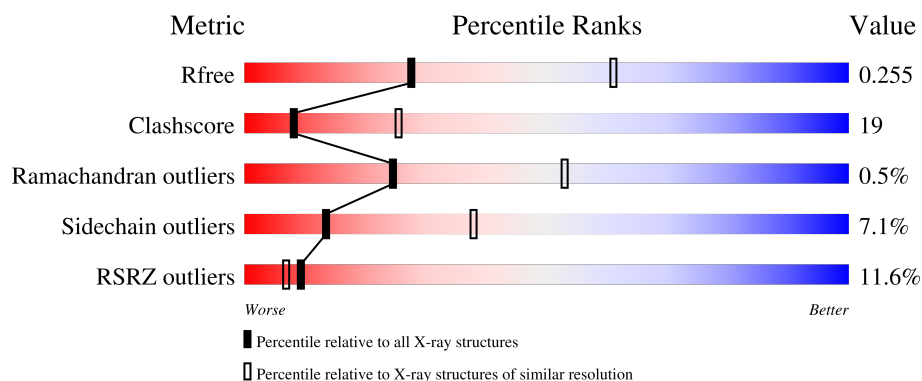
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.82 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	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (2.84-2.80)

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	84	11% 50% 35% • 13%
1	C	84	8% 60% 24% • 14%
1	E	84	13% 61% 24% • 13%
1	G	84	18% 50% 35% • 14%
1	I	84	10% 62% 20% • 15%

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Mol	Chain	Length	Quality of chain
1	M	84	
2	B	374	
2	D	374	
2	F	374	
2	H	374	
2	L	374	
2	N	374	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	F	800	X	-	-	-
3	NAG	H	800	X	-	-	-
3	NAG	I	770	X	-	-	-
3	NAG	N	800	X	-	-	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 40311 atoms, of which 20196 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 Fusion glycoprotein F0.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	73	Total	C	H	N	O	S	0	0	0
			1167	366	587	95	116	3			
1	C	72	Total	C	H	N	O	S	0	0	0
			1150	361	579	93	114	3			
1	E	73	Total	C	H	N	O	S	0	0	0
			1167	366	587	95	116	3			
1	G	72	Total	C	H	N	O	S	0	0	0
			1150	361	579	93	114	3			
1	I	71	Total	C	H	N	O	S	0	0	0
			1133	356	571	91	112	3			
1	M	72	Total	C	H	N	O	S	0	0	0
			1150	361	579	93	114	3			

- Molecule 2 is a protein called Fusion glycoprotein F0.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	358	Total	C	H	N	O	S	0	0	0
			5563	1744	2798	458	545	18			
2	D	355	Total	C	H	N	O	S	0	0	0
			5532	1735	2783	455	541	18			
2	F	351	Total	C	H	N	O	S	0	0	0
			5483	1720	2757	451	537	18			
2	H	359	Total	C	H	N	O	S	0	0	0
			5582	1750	2809	459	546	18			
2	L	354	Total	C	H	N	O	S	0	0	0
			5527	1733	2780	454	542	18			
2	N	355	Total	C	H	N	O	S	0	0	0
			5539	1737	2787	455	542	18			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	342	TYR	PHE	SEE REMARK 999	UNP Q84850

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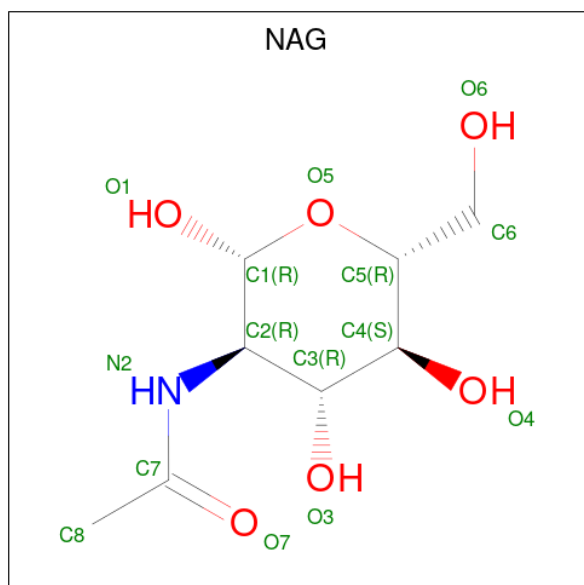
Chain	Residue	Modelled	Actual	Comment	Reference
B	514	GLY	-	expression tag	UNP Q84850
B	515	LEU	-	expression tag	UNP Q84850
B	516	GLU	-	expression tag	UNP Q84850
B	517	VAL	-	expression tag	UNP Q84850
B	518	LEU	-	expression tag	UNP Q84850
B	519	PHE	-	expression tag	UNP Q84850
B	520	GLN	-	expression tag	UNP Q84850
D	342	TYR	PHE	SEE REMARK 999	UNP Q84850
D	514	GLY	-	expression tag	UNP Q84850
D	515	LEU	-	expression tag	UNP Q84850
D	516	GLU	-	expression tag	UNP Q84850
D	517	VAL	-	expression tag	UNP Q84850
D	518	LEU	-	expression tag	UNP Q84850
D	519	PHE	-	expression tag	UNP Q84850
D	520	GLN	-	expression tag	UNP Q84850
F	342	TYR	PHE	SEE REMARK 999	UNP Q84850
F	514	GLY	-	expression tag	UNP Q84850
F	515	LEU	-	expression tag	UNP Q84850
F	516	GLU	-	expression tag	UNP Q84850
F	517	VAL	-	expression tag	UNP Q84850
F	518	LEU	-	expression tag	UNP Q84850
F	519	PHE	-	expression tag	UNP Q84850
F	520	GLN	-	expression tag	UNP Q84850
H	342	TYR	PHE	SEE REMARK 999	UNP Q84850
H	514	GLY	-	expression tag	UNP Q84850
H	515	LEU	-	expression tag	UNP Q84850
H	516	GLU	-	expression tag	UNP Q84850
H	517	VAL	-	expression tag	UNP Q84850
H	518	LEU	-	expression tag	UNP Q84850
H	519	PHE	-	expression tag	UNP Q84850
H	520	GLN	-	expression tag	UNP Q84850
L	342	TYR	PHE	SEE REMARK 999	UNP Q84850
L	514	GLY	-	expression tag	UNP Q84850
L	515	LEU	-	expression tag	UNP Q84850
L	516	GLU	-	expression tag	UNP Q84850
L	517	VAL	-	expression tag	UNP Q84850
L	518	LEU	-	expression tag	UNP Q84850
L	519	PHE	-	expression tag	UNP Q84850
L	520	GLN	-	expression tag	UNP Q84850
N	342	TYR	PHE	SEE REMARK 999	UNP Q84850
N	514	GLY	-	expression tag	UNP Q84850
N	515	LEU	-	expression tag	UNP Q84850

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Chain	Residue	Modelled	Actual	Comment	Reference
N	516	GLU	-	expression tag	UNP Q84850
N	517	VAL	-	expression tag	UNP Q84850
N	518	LEU	-	expression tag	UNP Q84850
N	519	PHE	-	expression tag	UNP Q84850
N	520	GLN	-	expression tag	UNP Q84850

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		
3	F	1	Total	C	N	O	0	0
			14	8	1	5		
3	G	1	Total	C	N	O	0	0
			14	8	1	5		
3	H	1	Total	C	N	O	0	0
			14	8	1	5		

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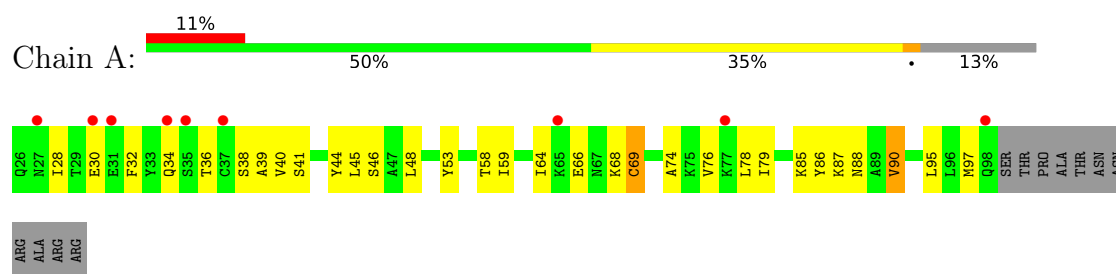
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	I	1	Total	C	N	O	0	0
			14	8	1	5		
3	L	1	Total	C	N	O	0	0
			14	8	1	5		
3	M	1	Total	C	N	O	0	0
			14	8	1	5		
3	N	1	Total	C	N	O	0	0
			14	8	1	5		

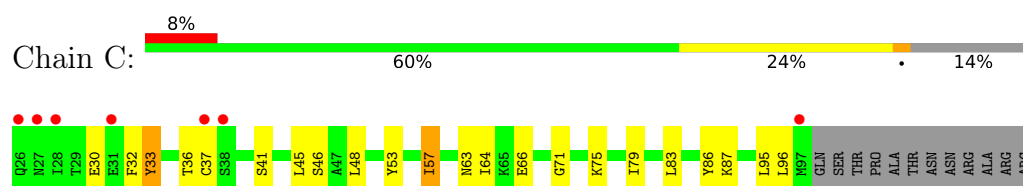
3 Residue-property plots

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.

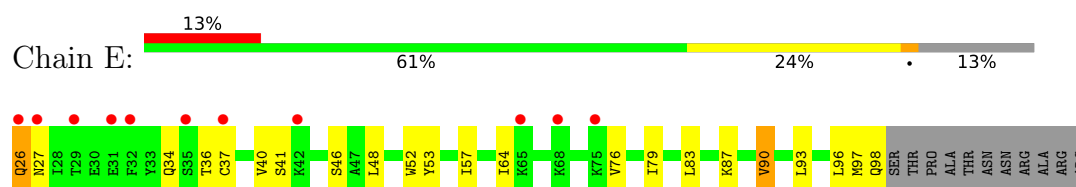
- Molecule 1: Fusion glycoprotein F0



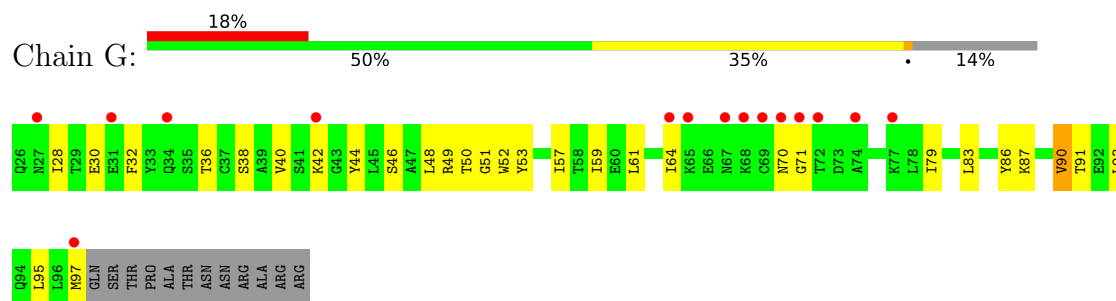
- Molecule 1: Fusion glycoprotein F0



- Molecule 1: Fusion glycoprotein F0

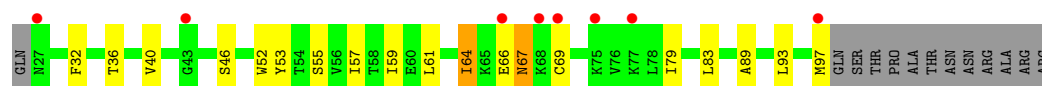


- Molecule 1: Fusion glycoprotein F0

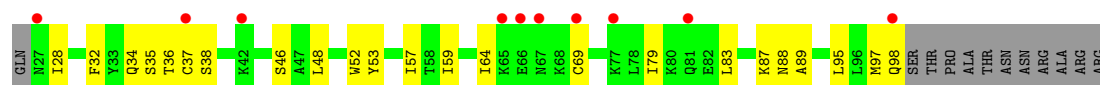


- Molecule 1: Fusion glycoprotein F0

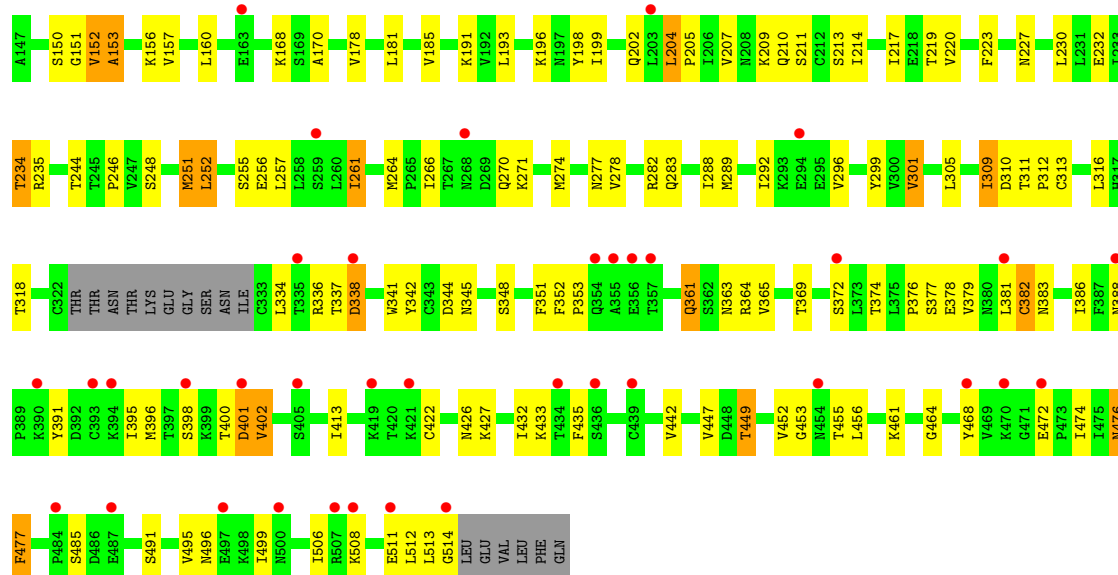




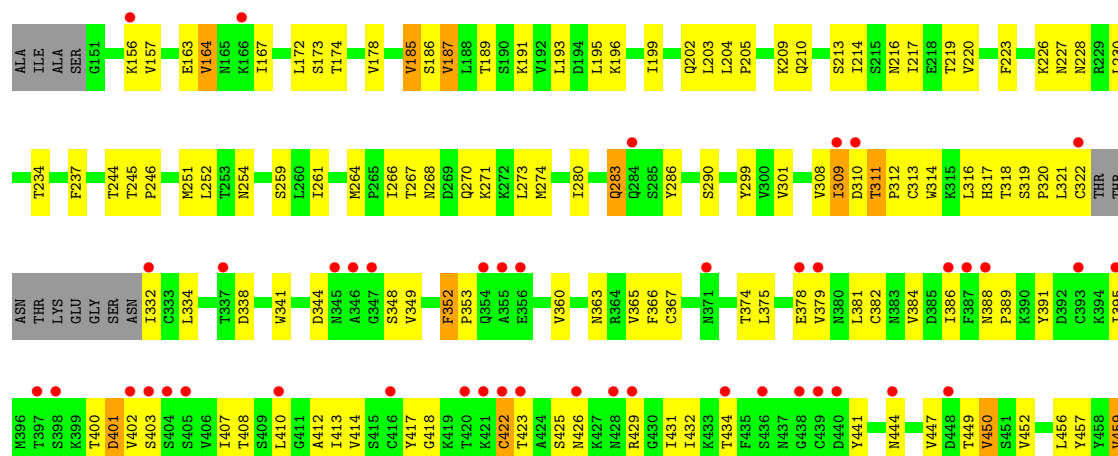
• Molecule 1: Fusion glycoprotein F0

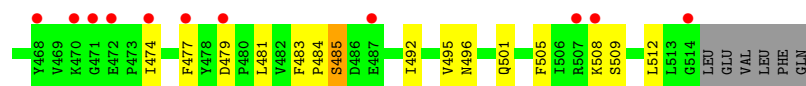


• Molecule 2: Fusion glycoprotein F0

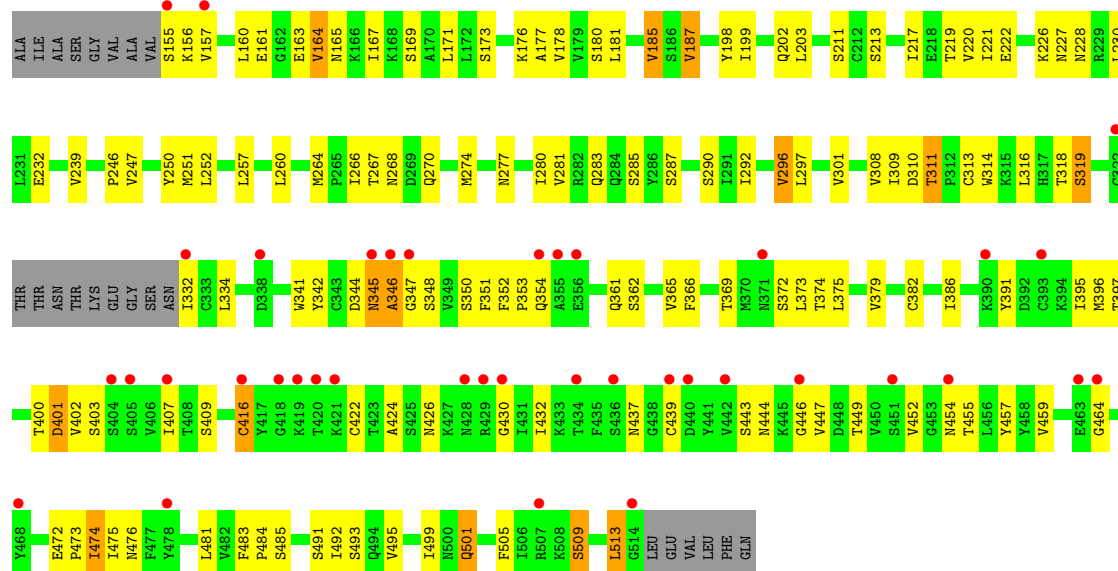


• Molecule 2: Fusion glycoprotein F0

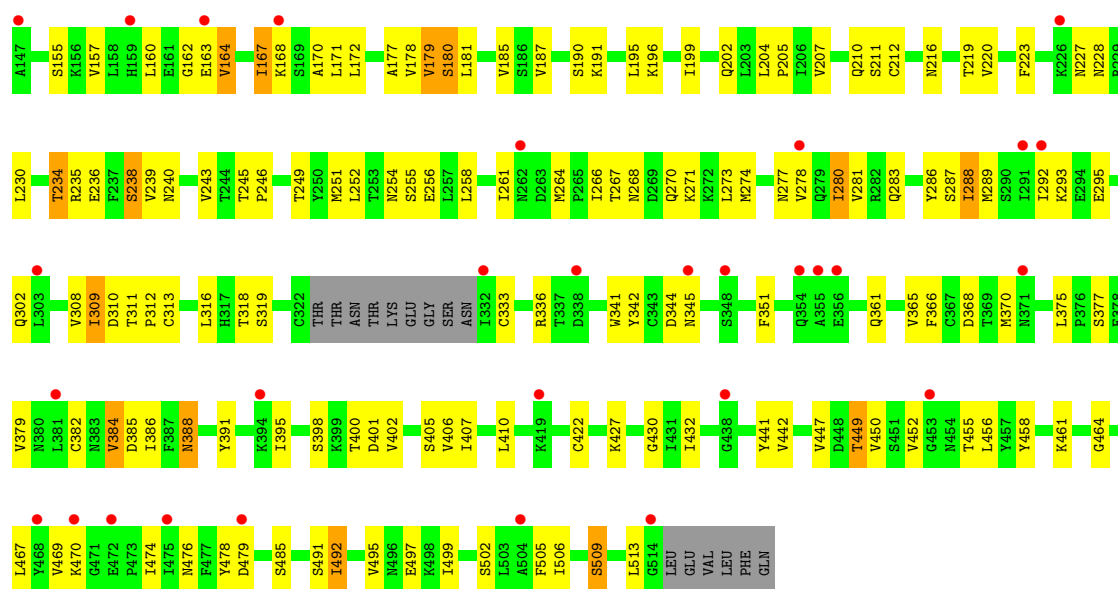




• Molecule 2: Fusion glycoprotein F0

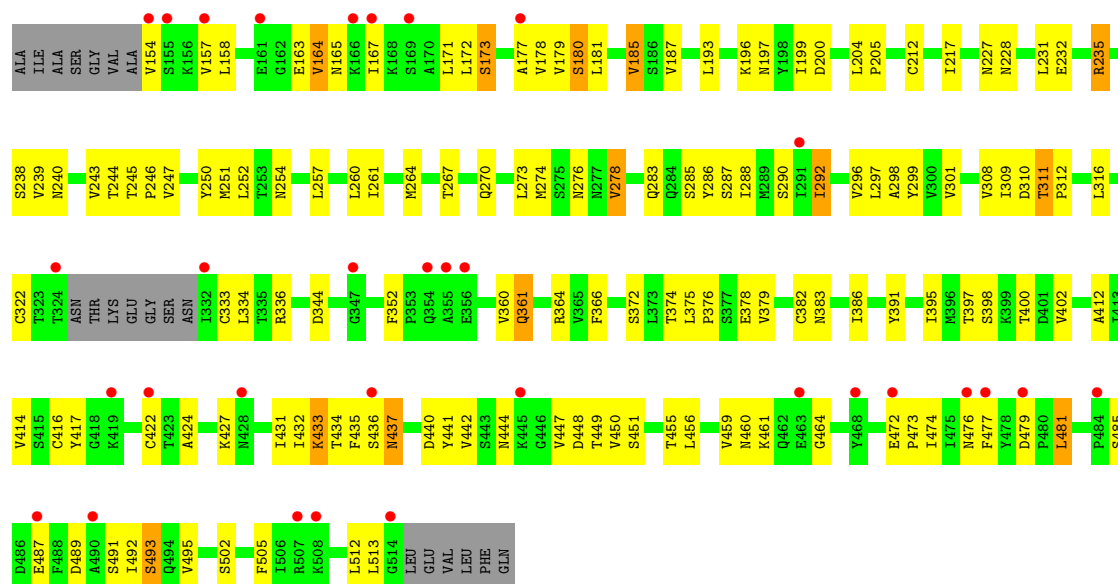


• Molecule 2: Fusion glycoprotein F0

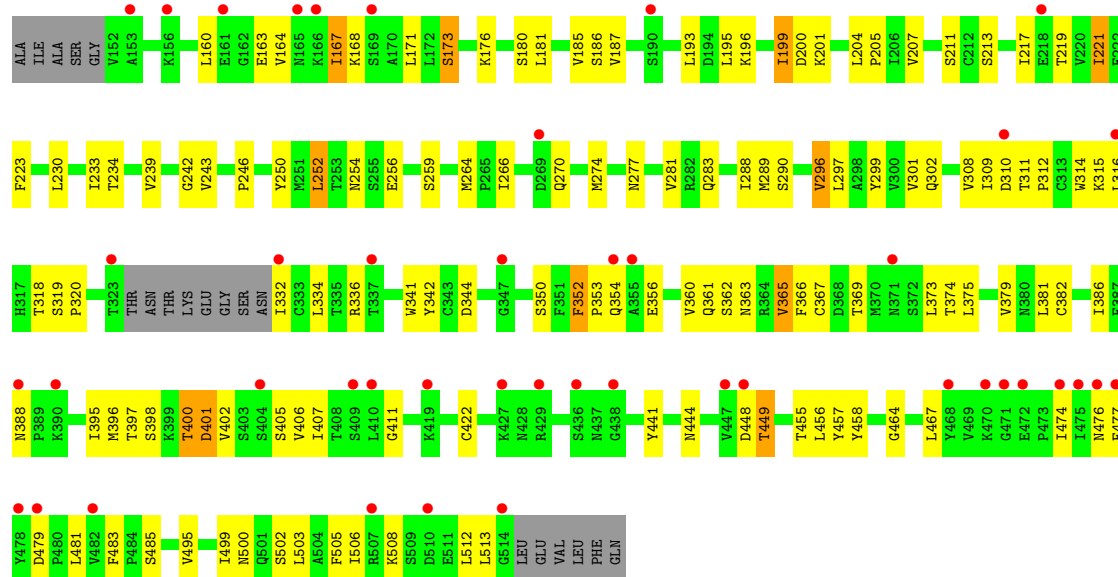


• Molecule 2: Fusion glycoprotein F0





• Molecule 2: Fusion glycoprotein F0



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	113.17Å 131.50Å 164.28Å 90.00° 103.17° 90.00°	Depositor
Resolution (Å)	44.21 – 2.82 44.21 – 2.82	Depositor EDS
% Data completeness (in resolution range)	63.7 (44.21-2.82) 63.7 (44.21-2.82)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	0.16	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.221 , 0.262 0.214 , 0.255	Depositor DCC
R_{free} test set	3590 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	30.4	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 36.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	40311	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% 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:
NAG

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	0.35	0/586	0.75	0/789
1	C	0.37	0/577	0.74	0/777
1	E	0.36	0/586	0.73	0/789
1	G	0.32	0/577	0.74	0/777
1	I	0.37	0/568	0.72	0/765
1	M	0.34	0/577	0.77	0/777
2	B	0.38	0/2805	0.75	0/3803
2	D	0.36	0/2789	0.74	2/3781 (0.1%)
2	F	0.39	0/2766	0.75	2/3749 (0.1%)
2	H	0.36	0/2813	0.75	0/3814
2	L	0.39	0/2787	0.75	0/3779
2	N	0.35	0/2792	0.74	2/3786 (0.1%)
All	All	0.37	0/20223	0.75	6/27386 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	472	GLU	CA-C-N	6.02	126.36	119.92
2	F	472	GLU	C-N-CA	6.02	126.36	119.92
2	D	352	PHE	CA-C-N	5.35	126.52	119.84
2	D	352	PHE	C-N-CA	5.35	126.52	119.84
2	N	352	PHE	CA-C-N	5.15	124.77	119.05
2	N	352	PHE	C-N-CA	5.15	124.77	119.05

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	580	587	588	37	0
1	C	571	579	579	38	0
1	E	580	587	588	25	0
1	G	571	579	580	36	0
1	I	562	571	572	29	0
1	M	571	579	580	33	0
2	B	2765	2798	2797	133	0
2	D	2749	2783	2782	149	0
2	F	2726	2757	2756	137	0
2	H	2773	2809	2808	155	0
2	L	2747	2780	2779	138	0
2	N	2752	2787	2786	142	0
3	A	14	0	13	0	0
3	B	14	0	13	4	0
3	C	14	0	13	1	0
3	D	14	0	13	0	0
3	E	14	0	13	0	0
3	F	14	0	13	1	0
3	G	14	0	13	1	0
3	H	14	0	13	1	0
3	I	14	0	13	1	0
3	L	14	0	13	0	0
3	M	14	0	13	4	0
3	N	14	0	13	2	0
All	All	20115	20196	20351	783	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 19.

All (783) 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:B:496:ASN:HB3	3:B:800:NAG:H81	1.40	1.01
2:H:308:VAL:HB	2:N:455:THR:HG22	1.60	0.84
2:N:449:THR:HB	2:N:456:LEU:HD11	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:261:ILE:HA	2:L:264:MET:HE2	1.63	0.79
2:N:334:LEU:HB3	2:N:395:ILE:HD11	1.64	0.79
2:H:280:ILE:HD11	2:H:361:GLN:HB2	1.63	0.79
2:F:264:MET:HE1	2:F:274:MET:SD	2.23	0.79
2:L:264:MET:HE1	2:L:274:MET:SD	2.24	0.78
2:H:230:LEU:O	2:H:234:THR:HG23	1.84	0.77
2:F:270:GLN:HG2	2:F:309:ILE:HD12	1.67	0.76
2:L:270:GLN:HG2	2:L:309:ILE:HD12	1.67	0.76
2:N:375:LEU:HB3	2:N:379:VAL:HG11	1.68	0.75
2:L:164:VAL:HA	2:L:167:ILE:HG22	1.68	0.75
2:B:495:VAL:CG2	2:D:187:VAL:HG12	2.18	0.74
2:D:308:VAL:HB	2:F:455:THR:HG22	1.70	0.74
2:F:334:LEU:HB3	2:F:395:ILE:HD11	1.70	0.74
1:A:66:GLU:HA	1:A:79:ILE:HG21	1.70	0.73
1:G:28:ILE:HG22	2:H:410:LEU:HD11	1.71	0.73
1:A:46:SER:HB3	2:B:313:CYS:SG	2.29	0.72
1:C:46:SER:HB3	2:D:313:CYS:SG	2.29	0.72
2:N:264:MET:HE1	2:N:274:MET:SD	2.30	0.72
2:H:246:PRO:HB3	2:H:283:GLN:HA	1.70	0.72
1:I:57:ILE:HD11	2:L:252:LEU:HD13	1.73	0.71
2:N:311:THR:HG23	2:N:312:PRO:HD2	1.72	0.71
2:L:333:CYS:HB2	2:L:398:SER:HB3	1.73	0.71
2:F:246:PRO:HB3	2:F:283:GLN:HA	1.72	0.70
2:L:334:LEU:HB3	2:L:395:ILE:HD11	1.73	0.70
1:C:36:THR:HG21	2:D:382:CYS:O	1.92	0.70
2:L:386:ILE:HG21	2:L:395:ILE:HD12	1.73	0.69
2:D:477:PHE:CZ	2:D:479:ASP:HB2	2.28	0.69
1:G:38:SER:HB3	2:H:318:THR:HG22	1.75	0.69
2:H:191:LYS:HE3	2:L:491:SER:CB	2.23	0.69
2:N:246:PRO:HB3	2:N:283:GLN:HA	1.74	0.69
2:D:311:THR:HG23	2:D:344:ASP:HB2	1.75	0.68
2:B:230:LEU:O	2:B:234:THR:HG23	1.94	0.68
2:B:246:PRO:HB3	2:B:283:GLN:HA	1.74	0.68
2:D:449:THR:HB	2:D:456:LEU:HD11	1.76	0.68
2:L:311:THR:HG21	2:L:344:ASP:O	1.93	0.67
2:N:270:GLN:HG2	2:N:309:ILE:HD12	1.76	0.67
2:N:318:THR:O	2:N:406:VAL:HG21	1.93	0.67
1:A:45:LEU:O	2:B:364:ARG:HD3	1.94	0.67
2:B:181:LEU:HD23	2:F:181:LEU:HD23	1.75	0.67
1:C:57:ILE:HD11	2:D:252:LEU:HD13	1.77	0.66
1:E:46:SER:HB3	2:F:313:CYS:SG	2.35	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:345:ASN:OD1	2:N:455:THR:HG21	1.94	0.66
2:N:315:LYS:HD2	2:N:341:TRP:CE2	2.30	0.66
2:D:264:MET:HE1	2:D:274:MET:SD	2.35	0.66
2:L:232:GLU:HG3	2:L:250:TYR:CE1	2.30	0.66
2:B:453:GLY:HA3	2:F:346:ALA:HB1	1.78	0.66
2:D:401:ASP:OD1	2:D:417:TYR:C	2.38	0.66
1:E:36:THR:HG21	2:F:382:CYS:O	1.95	0.66
2:H:311:THR:HG23	2:H:312:PRO:HD2	1.76	0.66
2:L:177:ALA:HB2	2:N:505:PHE:HB2	1.76	0.66
2:N:252:LEU:CD2	2:N:256:GLU:HB2	2.25	0.65
2:B:270:GLN:HG2	2:B:309:ILE:HD12	1.76	0.65
2:B:334:LEU:HD22	2:B:395:ILE:HD13	1.77	0.65
2:D:246:PRO:HB3	2:D:283:GLN:HA	1.79	0.65
2:H:270:GLN:HG2	2:H:309:ILE:HD12	1.78	0.65
2:H:449:THR:CG2	2:H:456:LEU:HD11	2.25	0.65
2:H:163:GLU:O	2:H:167:ILE:HG22	1.97	0.65
2:H:185:VAL:HG12	2:N:499:ILE:HD11	1.78	0.65
2:L:164:VAL:HG12	2:L:164:VAL:O	1.97	0.65
1:C:57:ILE:CD1	2:D:252:LEU:HD13	2.27	0.65
2:L:288:ILE:N	2:L:288:ILE:HD12	2.11	0.65
2:L:455:THR:HG22	2:N:308:VAL:HB	1.79	0.65
1:I:36:THR:HG22	2:L:386:ILE:HG13	1.77	0.65
2:H:449:THR:HG23	2:H:456:LEU:HD11	1.80	0.64
1:I:36:THR:HG22	2:L:386:ILE:CG1	2.28	0.64
1:M:64:ILE:HG12	1:M:83:LEU:HD21	1.80	0.64
2:D:341:TRP:CH2	2:D:365:VAL:HG21	2.32	0.64
2:F:314:TRP:CE2	2:F:342:TYR:HB2	2.32	0.64
1:G:70:ASN:OD1	3:G:770:NAG:N2	2.31	0.64
1:M:59:ILE:HD12	2:N:233:ILE:HD12	1.80	0.64
2:D:334:LEU:HB3	2:D:395:ILE:HD11	1.80	0.64
2:F:311:THR:HG21	2:F:344:ASP:O	1.98	0.64
2:H:449:THR:CG2	2:H:450:VAL:N	2.59	0.64
2:B:386:ILE:HG21	2:B:395:ILE:HD12	1.77	0.64
1:G:36:THR:HG21	2:H:382:CYS:O	1.97	0.64
1:G:93:LEU:HB3	2:H:292:ILE:HD13	1.80	0.64
2:N:311:THR:HG21	2:N:344:ASP:O	1.98	0.64
2:B:449:THR:HG23	2:B:456:LEU:CD1	2.27	0.64
2:H:280:ILE:HD11	2:H:361:GLN:CB	2.27	0.64
1:I:46:SER:OG	2:L:311:THR:HB	1.98	0.63
2:D:505:PHE:HB3	2:F:173:SER:O	1.98	0.63
1:E:37:CYS:SG	2:F:319:SER:HB3	2.38	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:341:TRP:CZ3	2:F:365:VAL:HG21	2.34	0.63
2:H:308:VAL:CB	2:N:455:THR:HG22	2.29	0.63
2:H:469:VAL:HB	1:I:59:ILE:HG12	1.80	0.63
2:D:270:GLN:HG2	2:D:309:ILE:HD12	1.79	0.63
1:A:36:THR:HG21	2:B:382:CYS:O	1.99	0.63
1:I:57:ILE:CD1	2:L:252:LEU:HD13	2.28	0.63
1:M:69:CYS:HA	3:M:770:NAG:H62	1.81	0.63
2:H:499:ILE:HD11	2:L:185:VAL:HG12	1.81	0.62
2:D:375:LEU:HB3	2:D:379:VAL:HG11	1.81	0.62
1:M:83:LEU:HB3	1:M:87:LYS:HE2	1.80	0.62
3:M:770:NAG:O7	3:M:770:NAG:H3	2.00	0.62
2:H:199:ILE:HD11	2:L:199:ILE:HD11	1.82	0.62
1:C:64:ILE:HD12	1:C:79:ILE:HG23	1.81	0.61
2:H:235:ARG:O	2:H:239:VAL:HG23	2.00	0.61
1:M:37:CYS:SG	2:N:319:SER:HB3	2.40	0.61
2:H:333:CYS:HB2	2:H:398:SER:HB3	1.81	0.61
2:N:311:THR:HG23	2:N:344:ASP:HB2	1.82	0.61
2:L:474:ILE:HB	1:M:64:ILE:HG22	1.83	0.61
2:F:230:LEU:HD23	2:F:230:LEU:C	2.25	0.61
2:B:477:PHE:C	2:B:477:PHE:CD2	2.78	0.61
2:F:264:MET:HE3	2:F:266:ILE:HD13	1.82	0.61
2:L:364:ARG:HG3	2:L:366:PHE:CE2	2.35	0.61
1:E:36:THR:HG22	2:F:386:ILE:HG13	1.83	0.61
1:E:90:VAL:HG22	2:F:292:ILE:HD11	1.82	0.60
2:B:264:MET:HE1	2:B:274:MET:SD	2.42	0.60
2:L:477:PHE:CZ	2:L:479:ASP:HB2	2.37	0.60
2:L:442:VAL:CG1	2:L:447:VAL:HB	2.31	0.60
2:B:499:ILE:HD11	2:F:185:VAL:HG12	1.83	0.60
2:N:341:TRP:CH2	2:N:365:VAL:HG21	2.37	0.60
2:D:261:ILE:HA	2:D:264:MET:HE2	1.83	0.60
2:B:376:PRO:HB2	2:B:378:GLU:OE1	2.01	0.59
2:H:199:ILE:O	2:H:204:LEU:HB2	2.02	0.59
2:B:168:LYS:HA	2:F:167:ILE:HD11	1.82	0.59
2:D:156:LYS:HB3	2:F:157:VAL:HG11	1.85	0.59
2:F:407:ILE:HD11	2:F:457:TYR:HB3	1.84	0.59
1:G:64:ILE:HD12	1:G:79:ILE:HG23	1.84	0.59
2:D:407:ILE:HD11	2:D:457:TYR:HB3	1.85	0.59
2:H:168:LYS:HA	2:L:167:ILE:HD11	1.84	0.59
2:N:309:ILE:HG22	2:N:310:ASP:CG	2.27	0.59
1:C:64:ILE:HG22	2:F:474:ILE:CG1	2.31	0.59
2:B:506:ILE:HD11	2:F:178:VAL:HG11	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:97:MET:HE1	2:L:290:SER:O	2.02	0.59
2:D:223:PHE:O	2:D:227:ASN:HB2	2.03	0.59
1:M:64:ILE:CG1	1:M:83:LEU:HD21	2.33	0.59
2:N:242:GLY:HA2	2:N:289:MET:HE2	1.85	0.59
2:B:449:THR:HG23	2:B:456:LEU:HD11	1.84	0.59
1:E:79:ILE:HD13	2:F:220:VAL:HG23	1.85	0.59
2:H:181:LEU:HD21	2:N:181:LEU:HG	1.85	0.59
2:N:386:ILE:HG21	2:N:395:ILE:HD12	1.83	0.59
2:H:264:MET:HE1	2:H:274:MET:SD	2.43	0.58
2:F:232:GLU:HG3	2:F:250:TYR:CE1	2.38	0.58
2:N:332:ILE:O	2:N:332:ILE:HG13	2.03	0.58
2:B:152:VAL:O	2:B:153:ALA:C	2.46	0.58
2:B:449:THR:CG2	2:B:456:LEU:HD11	2.34	0.58
2:H:375:LEU:HD13	2:H:379:VAL:HG11	1.86	0.58
2:L:217:ILE:HG21	2:N:217:ILE:HG21	1.85	0.58
2:N:167:ILE:HG12	2:N:167:ILE:O	2.03	0.58
2:B:199:ILE:HD11	2:F:199:ILE:HD11	1.85	0.58
2:B:495:VAL:HG23	2:D:187:VAL:HG12	1.84	0.58
2:B:181:LEU:HD23	2:F:181:LEU:CD2	2.34	0.58
2:L:472:GLU:HB2	2:L:473:PRO:HD2	1.85	0.58
2:B:386:ILE:CG2	2:B:395:ILE:HD12	2.33	0.58
2:D:512:LEU:HD23	2:F:169:SER:HB3	1.85	0.58
2:L:386:ILE:CG2	2:L:395:ILE:HD12	2.34	0.57
1:A:64:ILE:HG22	2:D:474:ILE:HD11	1.86	0.57
1:M:48:LEU:CD2	2:N:367:CYS:HB2	2.34	0.57
2:B:251:MET:HG3	2:B:299:TYR:CE1	2.39	0.57
1:C:79:ILE:HD11	2:D:219:THR:HB	1.86	0.57
2:L:246:PRO:HB3	2:L:283:GLN:HA	1.87	0.57
2:L:442:VAL:HG11	2:L:447:VAL:HG11	1.86	0.57
2:H:280:ILE:HD12	2:H:366:PHE:CE2	2.39	0.57
2:B:341:TRP:CZ3	2:B:365:VAL:HG21	2.40	0.57
1:I:93:LEU:HD11	2:L:238:SER:OG	2.05	0.57
2:N:264:MET:CE	2:N:274:MET:SD	2.92	0.57
2:L:386:ILE:HG21	2:L:395:ILE:CD1	2.35	0.56
2:H:461:LYS:HG2	1:I:52:TRP:HB2	1.86	0.56
2:L:476:ASN:HB3	2:N:219:THR:OG1	2.05	0.56
2:F:277:ASN:O	2:F:281:VAL:HG23	2.05	0.56
2:H:273:LEU:HD23	2:H:309:ILE:HD13	1.88	0.56
2:H:311:THR:CG2	2:H:344:ASP:HB2	2.36	0.56
2:N:477:PHE:CZ	2:N:479:ASP:HB2	2.39	0.56
2:H:455:THR:HG22	2:L:308:VAL:CG2	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:251:MET:HG3	2:L:299:TYR:CE1	2.41	0.56
1:C:30:GLU:HG2	2:D:441:TYR:OH	2.06	0.56
2:D:264:MET:HE3	2:D:266:ILE:CD1	2.35	0.56
2:H:196:LYS:CE	2:N:485:SER:HB2	2.36	0.56
2:H:318:THR:HG21	2:H:336:ARG:HB2	1.88	0.56
2:L:247:VAL:HG23	2:L:285:SER:HB2	1.88	0.56
1:A:32:PHE:CE2	1:A:34:GLN:HG2	2.41	0.55
1:G:79:ILE:HD11	2:H:219:THR:HB	1.88	0.55
2:H:449:THR:HG22	2:H:450:VAL:N	2.21	0.55
1:E:36:THR:HG22	2:F:386:ILE:CG1	2.37	0.55
1:G:97:MET:HE2	2:H:289:MET:HE3	1.89	0.55
2:H:196:LYS:C	2:H:196:LYS:HD3	2.31	0.55
2:B:278:VAL:O	2:B:282:ARG:HG3	2.06	0.55
1:G:48:LEU:HD12	2:H:308:VAL:CG1	2.36	0.55
2:H:187:VAL:HB	2:L:495:VAL:HG22	1.88	0.55
2:H:384:VAL:CG2	2:H:385:ASP:N	2.70	0.55
2:L:489:ASP:O	2:L:493:SER:HB2	2.07	0.55
2:D:441:TYR:C	2:D:441:TYR:CD2	2.85	0.55
1:C:36:THR:HG22	2:D:386:ILE:HG12	1.88	0.55
1:E:97:MET:HE1	2:F:290:SER:O	2.06	0.55
1:M:97:MET:HE1	2:N:290:SER:O	2.06	0.55
1:A:78:LEU:HB3	2:B:220:VAL:HG21	1.89	0.55
2:B:181:LEU:O	2:B:185:VAL:HG23	2.07	0.55
2:D:322:CYS:SG	2:D:417:TYR:CD2	2.99	0.55
2:L:196:LYS:HD3	2:L:196:LYS:C	2.31	0.55
1:C:48:LEU:CD2	2:D:367:CYS:HB2	2.37	0.55
2:H:196:LYS:HG2	2:N:483:PHE:CE2	2.42	0.55
2:H:375:LEU:HD23	2:N:396:MET:CE	2.37	0.55
2:L:273:LEU:HD23	2:L:309:ILE:HD13	1.88	0.55
2:B:198:TYR:O	2:B:202:GLN:HB2	2.07	0.54
1:E:97:MET:C	1:E:98:GLN:HG3	2.31	0.54
1:A:28:ILE:HD11	2:B:363:ASN:HA	1.87	0.54
2:H:316:LEU:HD11	2:H:336:ARG:HH12	1.72	0.54
2:H:455:THR:HG22	2:L:308:VAL:HG21	1.88	0.54
2:D:196:LYS:HD3	2:D:196:LYS:C	2.32	0.54
2:H:311:THR:HG21	2:H:344:ASP:O	2.07	0.54
2:L:247:VAL:HG22	2:L:286:TYR:O	2.07	0.54
2:B:386:ILE:HG21	2:B:395:ILE:CD1	2.36	0.54
2:D:495:VAL:CG2	2:F:187:VAL:HG12	2.36	0.54
1:E:48:LEU:HD12	2:F:345:ASN:HD21	1.72	0.54
2:N:204:LEU:N	2:N:205:PRO:CD	2.70	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:352:PHE:CD1	2:B:372:SER:HB3	2.43	0.54
2:D:196:LYS:CE	2:F:485:SER:HB2	2.37	0.54
2:H:311:THR:HG23	2:H:344:ASP:HB2	1.89	0.54
1:A:38:SER:CB	2:B:318:THR:HG22	2.38	0.54
2:D:204:LEU:N	2:D:205:PRO:CD	2.71	0.54
1:G:57:ILE:HG12	2:N:467:LEU:HB2	1.90	0.54
2:L:171:LEU:HD13	2:N:171:LEU:HD13	1.89	0.54
1:A:85:LYS:HG3	2:D:228:ASN:ND2	2.23	0.54
2:B:491:SER:HB2	2:D:191:LYS:HE2	1.89	0.54
2:F:264:MET:HE1	2:F:274:MET:CE	2.37	0.54
2:H:204:LEU:N	2:H:205:PRO:CD	2.71	0.54
2:H:308:VAL:HG22	2:H:309:ILE:N	2.22	0.54
1:A:38:SER:HB3	2:B:318:THR:HG22	1.90	0.54
2:B:455:THR:HG22	2:F:308:VAL:CG2	2.37	0.54
1:G:90:VAL:HG22	2:H:292:ILE:HD11	1.89	0.54
2:F:309:ILE:CG2	2:F:310:ASP:N	2.72	0.53
2:F:316:LEU:HD22	2:F:318:THR:HG23	1.90	0.53
2:L:412:ALA:HB2	2:L:459:VAL:HG22	1.90	0.53
2:B:452:VAL:O	2:F:346:ALA:CB	2.57	0.53
2:B:513:LEU:HD11	2:F:171:LEU:HD23	1.89	0.53
2:B:513:LEU:N	2:B:514:GLY:HA2	2.24	0.53
2:D:374:THR:HG22	2:F:402:VAL:HG21	1.91	0.53
2:H:164:VAL:HA	2:H:167:ILE:HG23	1.90	0.53
2:H:202:GLN:C	2:H:205:PRO:HD2	2.33	0.53
2:N:405:SER:HB2	2:N:457:TYR:CE2	2.42	0.53
2:D:210:GLN:O	2:D:214:ILE:HG13	2.08	0.53
2:D:317:HIS:CG	2:D:408:THR:HG22	2.43	0.53
2:L:264:MET:HE1	2:L:274:MET:CE	2.38	0.53
2:F:164:VAL:HA	2:F:167:ILE:HG22	1.91	0.53
2:F:348:SER:HB3	2:F:375:LEU:O	2.09	0.53
2:F:509:SER:O	2:F:513:LEU:HG	2.09	0.53
2:H:497:GLU:HA	3:H:800:NAG:H83	1.90	0.53
1:G:64:ILE:CG2	2:N:474:ILE:HD11	2.38	0.53
2:L:311:THR:HG23	2:L:344:ASP:HB2	1.91	0.53
2:N:266:ILE:HD12	2:N:270:GLN:HB2	1.91	0.53
2:H:160:LEU:HD23	2:N:160:LEU:HD23	1.91	0.53
1:M:48:LEU:HD23	2:N:367:CYS:HB2	1.89	0.53
2:B:196:LYS:HD3	2:B:196:LYS:C	2.32	0.53
2:F:264:MET:HE1	2:F:274:MET:HE1	1.91	0.53
2:N:309:ILE:HG22	2:N:310:ASP:N	2.22	0.53
2:B:261:ILE:HA	2:B:264:MET:HE2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:164:VAL:HA	2:L:167:ILE:CG2	2.37	0.52
2:L:433:LYS:NZ	2:L:435:PHE:CE1	2.77	0.52
2:H:476:ASN:HD21	1:I:67:ASN:HB2	1.74	0.52
2:B:232:GLU:O	2:B:235:ARG:HB3	2.08	0.52
2:D:316:LEU:HD21	2:D:318:THR:CG2	2.39	0.52
3:I:770:NAG:O7	3:I:770:NAG:H3	2.08	0.52
2:L:416:CYS:O	2:L:417:TYR:CD1	2.62	0.52
1:C:32:PHE:CG	2:D:441:TYR:HB2	2.44	0.52
1:C:64:ILE:HG22	2:F:474:ILE:HD11	1.91	0.52
2:D:217:ILE:HG23	2:F:221:ILE:HD11	1.92	0.52
2:N:213:SER:O	2:N:217:ILE:HG13	2.10	0.52
1:G:46:SER:OG	2:H:311:THR:HB	2.09	0.52
2:L:402:VAL:HG21	2:N:374:THR:HG22	1.92	0.52
2:B:442:VAL:CG1	2:B:447:VAL:HB	2.39	0.52
2:B:496:ASN:CB	3:B:800:NAG:H81	2.28	0.52
2:D:199:ILE:O	2:D:204:LEU:HB2	2.09	0.52
2:D:401:ASP:OD2	2:D:401:ASP:C	2.52	0.52
1:A:64:ILE:HD12	1:A:79:ILE:HG23	1.90	0.52
1:A:97:MET:SD	2:B:292:ILE:HG22	2.50	0.52
2:D:174:THR:O	2:D:178:VAL:HG23	2.09	0.52
2:H:168:LYS:CA	2:L:167:ILE:HD11	2.39	0.52
2:L:235:ARG:O	2:L:239:VAL:HG23	2.10	0.52
2:N:407:ILE:HD11	2:N:457:TYR:HB3	1.91	0.52
1:A:95:LEU:HB3	2:D:254:ASN:ND2	2.25	0.52
2:F:342:TYR:CE1	2:F:351:PHE:CD1	2.98	0.52
2:D:213:SER:O	2:D:217:ILE:HG13	2.11	0.51
2:D:311:THR:HG23	2:D:312:PRO:HD2	1.92	0.51
1:M:83:LEU:O	1:M:87:LYS:HG3	2.09	0.51
2:D:204:LEU:HD21	2:F:481:LEU:HB2	1.92	0.51
1:G:32:PHE:CG	2:H:441:TYR:HB2	2.44	0.51
2:L:361:GLN:O	2:L:361:GLN:HG3	2.10	0.51
1:E:83:LEU:HB3	1:E:87:LYS:HE2	1.92	0.51
2:F:361:GLN:NE2	2:F:362:SER:HB2	2.25	0.51
2:B:363:ASN:OD1	2:B:363:ASN:C	2.53	0.51
2:L:200:ASP:O	2:L:205:PRO:HD3	2.11	0.51
1:M:32:PHE:CD1	2:N:441:TYR:HB2	2.45	0.51
1:M:37:CYS:SG	1:M:37:CYS:O	2.67	0.51
2:N:411:GLY:HA2	2:N:444:ASN:N	2.26	0.51
2:H:400:THR:HG22	2:H:401:ASP:N	2.26	0.51
1:M:32:PHE:CG	2:N:441:TYR:HB2	2.46	0.51
2:B:400:THR:HG22	2:B:401:ASP:N	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:491:SER:CB	2:D:191:LYS:HE2	2.40	0.51
2:D:217:ILE:HG23	2:F:221:ILE:CD1	2.41	0.51
2:H:164:VAL:HA	2:H:167:ILE:CG2	2.39	0.51
1:I:64:ILE:CG1	1:I:83:LEU:HD21	2.41	0.51
2:L:322:CYS:SG	2:L:417:TYR:CD2	3.04	0.51
2:L:379:VAL:HG12	2:L:391:TYR:CZ	2.46	0.51
1:A:36:THR:HB	2:B:336:ARG:HD2	1.93	0.51
2:B:461:LYS:HG2	1:E:52:TRP:HB2	1.93	0.51
2:D:378:GLU:OE2	2:F:400:THR:HG21	2.11	0.51
2:H:375:LEU:HB3	2:H:379:VAL:HG11	1.93	0.50
2:N:500:ASN:HD22	3:N:800:NAG:C7	2.24	0.50
1:G:52:TRP:CE3	2:H:302:GLN:HG2	2.47	0.50
2:L:376:PRO:HB2	2:L:378:GLU:OE1	2.12	0.50
2:B:248:SER:CB	2:F:239:VAL:HA	2.41	0.50
2:D:216:ASN:O	2:D:220:VAL:HG23	2.12	0.50
2:N:164:VAL:HA	2:N:167:ILE:HG22	1.92	0.50
2:B:374:THR:HG22	2:D:402:VAL:CG2	2.40	0.50
2:L:180:SER:HB3	2:N:502:SER:HB2	1.94	0.50
2:N:252:LEU:HD23	2:N:256:GLU:HB2	1.93	0.50
2:N:400:THR:HG22	2:N:401:ASP:H	1.76	0.50
2:D:412:ALA:HB2	2:D:459:VAL:HG13	1.94	0.50
2:D:425:SER:O	2:D:447:VAL:HG13	2.12	0.50
2:L:451:SER:HB2	2:L:456:LEU:HD12	1.93	0.50
2:B:170:ALA:CB	2:F:513:LEU:HD21	2.41	0.50
2:F:247:VAL:HG23	2:F:285:SER:HB2	1.94	0.50
2:H:277:ASN:O	2:H:281:VAL:HG23	2.12	0.50
1:A:68:LYS:O	1:A:69:CYS:HB3	2.10	0.50
2:L:157:VAL:HG12	2:L:157:VAL:O	2.12	0.50
2:N:363:ASN:OD1	2:N:363:ASN:C	2.55	0.50
1:A:95:LEU:HD13	2:D:254:ASN:HD22	1.75	0.49
2:B:210:GLN:O	2:B:214:ILE:HG13	2.12	0.49
2:B:338:ASP:HB2	2:B:342:TYR:OH	2.12	0.49
3:F:800:NAG:O7	3:F:800:NAG:H3	2.11	0.49
2:H:506:ILE:HD11	2:L:178:VAL:HG11	1.94	0.49
2:L:228:ASN:O	2:L:232:GLU:HG2	2.12	0.49
2:D:163:GLU:OE2	2:D:163:GLU:HA	2.12	0.49
2:D:244:THR:OG1	2:D:251:MET:HE3	2.11	0.49
1:G:51:GLY:HA3	2:N:458:TYR:HB2	1.93	0.49
1:G:95:LEU:HD22	2:N:254:ASN:ND2	2.27	0.49
2:D:360:VAL:O	2:D:360:VAL:HG13	2.11	0.49
2:B:217:ILE:HG21	2:F:217:ILE:HD13	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:SER:OG	2:D:311:THR:HB	2.12	0.49
2:D:163:GLU:O	2:D:167:ILE:HG22	2.12	0.49
1:E:79:ILE:HD13	2:F:220:VAL:CG2	2.43	0.49
2:H:368:ASP:OD1	2:H:370:MET:HB2	2.13	0.49
2:H:455:THR:HG22	2:L:308:VAL:HB	1.94	0.49
2:N:199:ILE:HG22	2:N:200:ASP:N	2.27	0.49
2:N:309:ILE:CG2	2:N:310:ASP:N	2.75	0.49
2:H:264:MET:HE3	2:H:266:ILE:HD13	1.95	0.49
2:H:311:THR:CG2	2:H:312:PRO:HD2	2.42	0.49
2:L:477:PHE:CE2	2:L:479:ASP:HB2	2.47	0.49
2:B:309:ILE:CG2	2:B:310:ASP:N	2.76	0.49
2:B:374:THR:HG22	2:D:402:VAL:HG21	1.94	0.49
1:C:64:ILE:HD11	1:C:83:LEU:HG	1.95	0.49
1:M:79:ILE:O	1:M:83:LEU:HG	2.13	0.49
2:D:422:CYS:HB3	2:D:452:VAL:HG22	1.93	0.49
1:I:32:PHE:CG	2:L:441:TYR:HB2	2.47	0.49
2:B:449:THR:CG2	2:B:456:LEU:CD1	2.91	0.49
1:C:32:PHE:CD2	2:D:441:TYR:HB3	2.47	0.49
2:B:351:PHE:CE2	2:B:353:PRO:HB3	2.48	0.49
2:D:217:ILE:HG21	2:F:217:ILE:HG21	1.95	0.49
2:F:222:GLU:O	2:F:226:LYS:HG3	2.13	0.49
2:H:227:ASN:O	2:H:228:ASN:C	2.54	0.49
2:H:309:ILE:CG2	2:H:310:ASP:N	2.76	0.49
2:L:163:GLU:OE2	2:L:163:GLU:HA	2.13	0.49
2:L:267:THR:OG1	2:L:270:GLN:HG3	2.13	0.49
2:N:395:ILE:HG12	2:N:396:MET:N	2.28	0.49
2:B:452:VAL:O	2:F:346:ALA:HB3	2.13	0.48
2:F:296:VAL:HG13	2:F:296:VAL:O	2.12	0.48
2:F:447:VAL:HG12	2:F:459:VAL:HG21	1.95	0.48
2:H:171:LEU:HD13	2:N:171:LEU:HD13	1.95	0.48
2:H:180:SER:HB3	2:L:502:SER:HB2	1.95	0.48
2:H:495:VAL:CG2	2:N:187:VAL:HG12	2.43	0.48
1:A:95:LEU:HB3	2:D:254:ASN:HD22	1.77	0.48
2:B:264:MET:HE3	2:B:266:ILE:HD11	1.94	0.48
2:F:252:LEU:HD23	2:F:257:LEU:HD13	1.95	0.48
2:F:422:CYS:SG	2:F:452:VAL:HG22	2.53	0.48
2:N:366:PHE:N	2:N:366:PHE:CD2	2.82	0.48
2:D:311:THR:HG21	2:D:344:ASP:O	2.14	0.48
2:H:485:SER:HB2	2:L:196:LYS:CE	2.44	0.48
2:L:402:VAL:CG2	2:N:374:THR:HG22	2.43	0.48
1:A:48:LEU:HB3	2:B:369:THR:CG2	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:247:VAL:HG12	2:L:251:MET:HB3	1.95	0.48
2:D:280:ILE:HG21	2:D:366:PHE:CD2	2.48	0.48
1:G:61:LEU:HD22	1:G:86:TYR:CZ	2.49	0.48
2:D:273:LEU:HD23	2:D:309:ILE:CD1	2.44	0.48
2:F:345:ASN:O	2:F:346:ALA:C	2.56	0.48
2:L:375:LEU:HD13	2:L:379:VAL:HG11	1.96	0.48
2:B:496:ASN:C	3:B:800:NAG:H81	2.38	0.48
2:D:319:SER:OG	2:D:320:PRO:HD2	2.13	0.48
2:L:240:ASN:HB3	2:L:243:VAL:O	2.13	0.48
2:N:449:THR:CB	2:N:456:LEU:HD11	2.36	0.48
2:N:476:ASN:OD1	2:N:476:ASN:N	2.47	0.48
2:D:273:LEU:HD23	2:D:309:ILE:HD13	1.95	0.48
2:D:348:SER:HB3	2:D:375:LEU:O	2.14	0.48
2:F:228:ASN:O	2:F:232:GLU:HG2	2.14	0.48
2:F:334:LEU:HD22	2:F:395:ILE:CD1	2.44	0.48
2:L:481:LEU:O	2:N:204:LEU:HD21	2.13	0.48
2:L:492:ILE:HG13	2:N:193:LEU:HD13	1.96	0.48
1:A:36:THR:HG22	2:B:386:ILE:CG1	2.44	0.48
2:D:388:ASN:OD1	2:D:389:PRO:HD2	2.14	0.48
2:B:277:ASN:OD1	2:B:361:GLN:HG2	2.14	0.47
1:C:46:SER:HG	2:D:311:THR:HB	1.79	0.47
2:H:172:LEU:HD23	2:N:513:LEU:HD12	1.96	0.47
2:H:375:LEU:HD23	2:N:396:MET:HE1	1.95	0.47
2:L:173:SER:O	2:N:505:PHE:HB3	2.13	0.47
2:N:316:LEU:HD21	2:N:318:THR:CG2	2.44	0.47
2:D:332:ILE:O	2:D:332:ILE:HG13	2.14	0.47
2:D:492:ILE:O	2:D:496:ASN:ND2	2.46	0.47
2:B:311:THR:HG23	2:B:344:ASP:HB2	1.96	0.47
1:C:48:LEU:HD23	2:D:367:CYS:HB2	1.96	0.47
2:D:483:PHE:CD1	2:D:484:PRO:HD2	2.49	0.47
2:H:236:GLU:OE1	2:H:251:MET:HE2	2.13	0.47
2:H:432:ILE:HD11	2:H:447:VAL:HG22	1.95	0.47
1:C:45:LEU:HD22	2:D:310:ASP:HA	1.97	0.47
1:C:53:TYR:CE1	2:F:464:GLY:HA3	2.49	0.47
2:D:204:LEU:O	2:D:204:LEU:HD23	2.13	0.47
1:A:58:THR:HG22	1:A:59:ILE:N	2.29	0.47
1:A:79:ILE:HD11	2:B:219:THR:HB	1.95	0.47
2:L:336:ARG:HH12	2:L:383:ASN:ND2	2.12	0.47
2:B:264:MET:HE3	2:B:266:ILE:CD1	2.44	0.47
2:D:348:SER:OG	2:F:402:VAL:HG23	2.13	0.47
1:G:28:ILE:CD1	1:G:44:TYR:CE1	2.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:187:VAL:HB	2:N:495:VAL:HG22	1.97	0.47
2:L:424:ALA:O	2:L:432:ILE:HG12	2.14	0.47
1:C:32:PHE:CD2	2:D:441:TYR:CB	2.97	0.47
2:D:187:VAL:O	2:D:191:LYS:HG2	2.14	0.47
2:D:251:MET:HG3	2:D:299:TYR:CE1	2.50	0.47
2:D:316:LEU:CD2	2:D:318:THR:CG2	2.93	0.47
2:H:261:ILE:HA	2:H:264:MET:HE2	1.97	0.47
1:I:69:CYS:O	2:L:212:CYS:SG	2.72	0.47
2:L:254:ASN:HD22	1:M:95:LEU:HD13	1.79	0.47
2:L:297:LEU:HD12	2:L:298:ALA:N	2.30	0.47
1:M:46:SER:OG	2:N:311:THR:HB	2.14	0.47
2:B:156:LYS:O	2:B:160:LEU:HD13	2.15	0.47
2:H:240:ASN:HB3	2:H:243:VAL:O	2.15	0.47
1:C:63:ASN:O	2:F:473:PRO:HA	2.15	0.47
1:E:48:LEU:HB2	2:F:308:VAL:HG12	1.97	0.47
2:L:451:SER:HB2	2:L:456:LEU:CD1	2.45	0.47
1:G:57:ILE:HD11	2:H:252:LEU:HD13	1.97	0.47
2:H:407:ILE:HD13	2:H:458:TYR:O	2.14	0.47
1:A:53:TYR:CD2	2:B:264:MET:HG2	2.50	0.46
2:B:336:ARG:HH12	2:B:383:ASN:HD22	1.62	0.46
2:B:337:THR:CG2	2:B:396:MET:HB2	2.44	0.46
2:D:230:LEU:O	2:D:234:THR:HG23	2.15	0.46
1:G:44:TYR:HB2	2:H:313:CYS:HB2	1.97	0.46
2:D:202:GLN:C	2:D:205:PRO:HD2	2.40	0.46
2:D:363:ASN:OD1	2:D:363:ASN:C	2.59	0.46
2:D:410:LEU:HA	2:D:444:ASN:ND2	2.29	0.46
1:G:53:TYR:CZ	2:N:464:GLY:HA3	2.51	0.46
2:H:312:PRO:HG2	2:H:344:ASP:OD2	2.14	0.46
2:H:505:PHE:CD1	2:N:176:LYS:HB2	2.51	0.46
1:I:53:TYR:C	1:I:53:TYR:CD2	2.94	0.46
1:A:46:SER:CB	2:B:313:CYS:SG	3.02	0.46
2:B:476:ASN:HB3	2:F:219:THR:OG1	2.15	0.46
2:D:378:GLU:HG3	2:F:400:THR:OG1	2.15	0.46
2:H:177:ALA:HB2	2:L:505:PHE:HB2	1.96	0.46
2:H:336:ARG:HD2	2:H:386:ILE:HD11	1.96	0.46
2:H:386:ILE:HG21	2:H:395:ILE:HD12	1.96	0.46
2:L:185:VAL:O	2:L:185:VAL:CG1	2.64	0.46
2:L:252:LEU:HD22	2:L:301:VAL:HG11	1.97	0.46
2:D:164:VAL:HA	2:D:167:ILE:CG2	2.46	0.46
2:D:508:LYS:O	2:D:512:LEU:HD13	2.15	0.46
2:H:252:LEU:HD12	2:H:256:GLU:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:167:ILE:HG23	2:N:167:ILE:CD1	2.45	0.46
2:N:361:GLN:NE2	2:N:362:SER:HB2	2.30	0.46
2:B:168:LYS:CA	2:F:167:ILE:HD11	2.46	0.46
2:D:264:MET:HE3	2:D:266:ILE:HD11	1.97	0.46
1:I:36:THR:HG21	2:L:382:CYS:O	2.16	0.46
1:I:53:TYR:CD1	2:L:264:MET:HG2	2.50	0.46
1:I:93:LEU:HB2	2:L:292:ILE:HD13	1.97	0.46
2:B:193:LEU:HD13	2:D:492:ILE:HG13	1.97	0.46
2:B:311:THR:HG23	2:B:312:PRO:HD2	1.97	0.46
2:N:360:VAL:HG22	2:N:361:GLN:N	2.31	0.46
2:B:464:GLY:HA3	1:E:53:TYR:CZ	2.50	0.46
2:F:309:ILE:HG22	2:F:310:ASP:N	2.30	0.46
2:N:199:ILE:O	2:N:204:LEU:HB2	2.15	0.46
1:C:71:GLY:C	2:D:209:LYS:HB3	2.41	0.46
2:F:345:ASN:O	2:F:347:GLY:N	2.49	0.46
2:L:312:PRO:HG2	2:L:344:ASP:OD2	2.16	0.46
2:L:352:PHE:CD1	2:L:372:SER:HB3	2.51	0.46
2:B:381:LEU:HB2	2:B:388:ASN:ND2	2.31	0.46
2:B:508:LYS:O	2:B:512:LEU:HD13	2.16	0.46
1:C:33:TYR:N	1:C:33:TYR:CD2	2.84	0.46
2:D:316:LEU:HD23	2:D:318:THR:HG23	1.98	0.46
2:D:449:THR:C	2:D:450:VAL:HG23	2.41	0.46
2:H:342:TYR:CZ	2:H:351:PHE:CD1	3.04	0.46
2:L:287:SER:C	2:L:288:ILE:HD12	2.40	0.46
1:M:88:ASN:O	1:M:89:ALA:C	2.59	0.46
3:C:770:NAG:O7	3:C:770:NAG:H3	2.15	0.45
1:E:26:GLN:CG	1:E:27:ASN:H	2.29	0.45
2:H:181:LEU:HD23	2:L:181:LEU:HD23	1.98	0.45
2:B:426:ASN:OD1	2:B:427:LYS:N	2.49	0.45
2:H:379:VAL:HG12	2:H:391:TYR:CE2	2.52	0.45
2:H:455:THR:HG22	2:L:308:VAL:CB	2.46	0.45
2:B:248:SER:HB3	2:F:239:VAL:HA	1.97	0.45
2:F:352:PHE:CE1	2:F:372:SER:HB3	2.51	0.45
2:N:264:MET:HE3	2:N:266:ILE:HD13	1.97	0.45
1:G:48:LEU:O	1:G:50:THR:HG23	2.16	0.45
2:D:379:VAL:HG12	2:D:391:TYR:CZ	2.50	0.45
2:D:501:GLN:O	2:D:505:PHE:CD2	2.70	0.45
2:D:505:PHE:CD1	2:F:176:LYS:HB3	2.52	0.45
2:F:351:PHE:HD2	2:F:373:LEU:HD12	1.81	0.45
2:F:475:ILE:HG22	2:F:476:ASN:N	2.31	0.45
2:L:442:VAL:HG11	2:L:447:VAL:CG1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:167:ILE:HG12	2:D:167:ILE:O	2.16	0.45
2:D:423:THR:HG22	2:D:434:THR:HA	1.99	0.45
2:F:292:ILE:HB	2:F:297:LEU:HD13	1.99	0.45
2:L:199:ILE:CD1	2:N:199:ILE:HD11	2.47	0.45
2:L:414:VAL:CG2	2:L:450:VAL:HG11	2.46	0.45
2:N:277:ASN:O	2:N:281:VAL:HG23	2.17	0.45
2:D:334:LEU:HD13	2:D:395:ILE:CD1	2.46	0.45
2:H:223:PHE:CE1	2:H:227:ASN:ND2	2.85	0.45
1:M:28:ILE:HD11	2:N:363:ASN:HA	1.97	0.45
2:N:319:SER:OG	2:N:320:PRO:CD	2.65	0.45
2:B:433:LYS:HD3	2:B:435:PHE:CE1	2.52	0.45
1:C:64:ILE:HD11	1:C:83:LEU:CG	2.47	0.45
1:I:57:ILE:HD12	2:L:301:VAL:HG21	1.98	0.45
2:L:164:VAL:O	2:L:164:VAL:CG1	2.65	0.45
2:F:198:TYR:O	2:F:202:GLN:HB2	2.17	0.45
2:N:288:ILE:O	2:N:299:TYR:HB2	2.17	0.45
2:N:354:GLN:C	2:N:356:GLU:H	2.24	0.45
2:B:511:GLU:O	2:B:511:GLU:HG2	2.17	0.45
2:F:161:GLU:O	2:F:161:GLU:HG2	2.16	0.45
1:G:83:LEU:O	1:G:87:LYS:HG3	2.17	0.45
2:H:467:LEU:HB2	1:I:57:ILE:HG12	1.98	0.45
2:B:402:VAL:HG13	2:F:374:THR:HG22	1.98	0.44
2:D:203:LEU:HD21	2:F:203:LEU:CD2	2.47	0.44
2:F:227:ASN:O	2:F:228:ASN:C	2.60	0.44
2:F:386:ILE:HG21	2:F:395:ILE:HD12	1.99	0.44
2:H:163:GLU:C	2:H:167:ILE:HG22	2.42	0.44
2:H:168:LYS:HB2	2:L:167:ILE:HD12	1.99	0.44
2:H:254:ASN:O	2:H:258:LEU:HD13	2.17	0.44
2:B:223:PHE:CD1	2:B:227:ASN:ND2	2.85	0.44
1:C:64:ILE:HG22	2:F:474:ILE:HG12	1.99	0.44
2:D:163:GLU:HB3	2:F:164:VAL:HG11	1.99	0.44
2:F:416:CYS:O	2:F:437:ASN:HA	2.18	0.44
2:N:500:ASN:ND2	3:N:800:NAG:C7	2.80	0.44
2:B:191:LYS:HE3	2:F:491:SER:HB2	2.00	0.44
2:B:491:SER:O	2:B:495:VAL:HG23	2.17	0.44
2:D:426:ASN:HB3	2:D:429:ARG:HB2	1.99	0.44
1:G:64:ILE:HD11	1:G:83:LEU:HG	2.00	0.44
2:H:402:VAL:HG13	2:L:374:THR:CG2	2.48	0.44
1:M:36:THR:HG22	2:N:386:ILE:HG13	1.99	0.44
1:M:38:SER:HB3	2:N:318:THR:HG22	1.99	0.44
1:A:44:TYR:HB2	2:B:313:CYS:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:341:TRP:CZ3	2:D:365:VAL:HG21	2.52	0.44
2:D:450:VAL:HG23	2:D:459:VAL:CG2	2.47	0.44
1:G:49:ARG:NH1	1:G:52:TRP:CE2	2.86	0.44
2:H:266:ILE:HD12	2:H:270:GLN:HB2	1.99	0.44
1:M:36:THR:HG21	2:N:382:CYS:O	2.17	0.44
1:C:41:SER:O	2:D:314:TRP:HA	2.18	0.44
1:C:64:ILE:HG22	2:F:474:ILE:CD1	2.48	0.44
2:D:374:THR:HG22	2:F:402:VAL:CG2	2.48	0.44
2:F:379:VAL:HG12	2:F:391:TYR:CE2	2.52	0.44
2:F:400:THR:HG22	2:F:401:ASP:N	2.32	0.44
2:L:171:LEU:CD1	2:N:171:LEU:HD13	2.47	0.44
2:F:501:GLN:O	2:F:505:PHE:HD2	1.99	0.44
2:H:379:VAL:HG12	2:H:391:TYR:CZ	2.53	0.44
2:H:384:VAL:HG23	2:H:385:ASP:N	2.32	0.44
1:M:32:PHE:CD2	2:N:441:TYR:HB3	2.52	0.44
2:B:266:ILE:HG13	2:B:271:LYS:HG3	2.00	0.44
2:B:432:ILE:HD11	2:B:447:VAL:HG22	2.00	0.44
2:D:378:GLU:HB2	2:D:391:TYR:HB2	1.99	0.44
1:G:97:MET:CE	2:H:289:MET:HE3	2.47	0.44
2:L:461:LYS:HG2	1:M:52:TRP:HB2	1.99	0.44
2:L:485:SER:HB2	2:N:196:LYS:NZ	2.32	0.44
3:M:770:NAG:O7	3:M:770:NAG:C3	2.65	0.44
2:N:296:VAL:HG13	2:N:296:VAL:O	2.18	0.44
2:B:205:PRO:O	2:B:209:LYS:HG3	2.17	0.44
2:B:318:THR:HG21	2:B:336:ARG:HB2	1.98	0.44
2:B:468:TYR:CZ	2:H:470:LYS:HE3	2.53	0.44
2:B:496:ASN:C	3:B:800:NAG:C8	2.90	0.44
2:D:226:LYS:HD2	2:F:474:ILE:HG21	1.99	0.44
2:D:400:THR:HG22	2:D:401:ASP:N	2.33	0.44
2:H:502:SER:HB2	2:N:180:SER:HB3	1.99	0.44
1:I:64:ILE:HG13	1:I:83:LEU:HD11	2.00	0.44
2:D:185:VAL:HG12	2:F:499:ILE:CD1	2.48	0.44
2:D:191:LYS:HA	2:D:191:LYS:HD2	1.85	0.44
2:D:413:ILE:HG22	2:D:414:VAL:N	2.33	0.44
2:F:342:TYR:CE1	2:F:351:PHE:HD1	2.35	0.44
2:B:196:LYS:HE2	2:D:485:SER:HB2	2.00	0.43
2:B:278:VAL:O	2:B:282:ARG:CG	2.66	0.43
2:B:348:SER:OG	2:D:402:VAL:HG23	2.17	0.43
2:D:193:LEU:HD22	2:F:492:ILE:HG21	2.00	0.43
2:F:266:ILE:HD12	2:F:270:GLN:HB3	1.99	0.43
1:G:93:LEU:O	1:G:97:MET:HE3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:267:THR:HB	2:H:270:GLN:HG3	2.00	0.43
2:H:308:VAL:CG2	2:H:309:ILE:N	2.81	0.43
2:H:492:ILE:HD13	2:H:492:ILE:HA	1.81	0.43
2:H:506:ILE:HG21	2:L:179:VAL:HG23	2.00	0.43
2:L:227:ASN:O	2:L:231:LEU:HG	2.18	0.43
1:M:52:TRP:CE3	2:N:302:GLN:HG2	2.53	0.43
2:B:379:VAL:HG12	2:B:391:TYR:CZ	2.54	0.43
2:B:452:VAL:O	2:B:452:VAL:HG12	2.18	0.43
1:C:75:LYS:NZ	2:H:427:LYS:HD2	2.33	0.43
2:D:309:ILE:CG2	2:D:310:ASP:N	2.80	0.43
2:H:179:VAL:HG23	2:N:506:ILE:HG21	1.99	0.43
1:I:93:LEU:HB2	2:L:292:ILE:CD1	2.48	0.43
2:L:487:GLU:N	2:L:487:GLU:CD	2.76	0.43
2:N:217:ILE:O	2:N:221:ILE:HG13	2.16	0.43
1:C:37:CYS:HB2	2:D:321:LEU:HD13	2.01	0.43
1:C:86:TYR:CD2	1:C:86:TYR:C	2.96	0.43
2:D:401:ASP:OD1	2:D:418:GLY:N	2.51	0.43
2:D:505:PHE:HB2	2:F:177:ALA:HB2	1.99	0.43
1:E:57:ILE:HD11	2:F:252:LEU:HD13	1.99	0.43
2:H:308:VAL:CG1	2:N:455:THR:HG22	2.49	0.43
2:N:361:GLN:O	2:N:361:GLN:HG3	2.16	0.43
1:A:39:ALA:HB2	2:B:413:ILE:HD11	1.99	0.43
2:L:163:GLU:C	2:L:165:ASN:H	2.25	0.43
2:N:239:VAL:O	2:N:239:VAL:CG1	2.65	0.43
2:N:334:LEU:CD2	2:N:397:THR:HG22	2.49	0.43
2:B:499:ILE:CD1	2:F:185:VAL:HG12	2.47	0.43
1:C:66:GLU:HG3	1:C:79:ILE:HG21	2.01	0.43
1:E:64:ILE:CG1	1:E:83:LEU:HD21	2.48	0.43
2:F:424:ALA:HB1	2:F:447:VAL:HG21	2.01	0.43
1:G:79:ILE:CD1	2:H:219:THR:CG2	2.97	0.43
2:H:207:VAL:O	2:H:207:VAL:HG12	2.19	0.43
2:H:292:ILE:O	2:H:292:ILE:HG23	2.19	0.43
2:L:276:ASN:HA	1:M:98:GLN:HE22	1.82	0.43
2:N:314:TRP:CE2	2:N:342:TYR:HB2	2.53	0.43
2:B:213:SER:HB3	2:D:214:ILE:HG21	2.01	0.43
1:E:48:LEU:HD13	2:F:369:THR:CG2	2.47	0.43
1:I:61:LEU:HD12	2:L:227:ASN:OD1	2.18	0.43
2:N:481:LEU:HD12	2:N:481:LEU:HA	1.89	0.43
1:A:58:THR:CG2	1:A:59:ILE:N	2.81	0.43
2:B:252:LEU:HD12	2:B:301:VAL:HG11	2.00	0.43
2:D:317:HIS:CD2	2:D:408:THR:HG22	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:452:VAL:O	2:D:452:VAL:HG12	2.17	0.43
1:G:28:ILE:HD11	1:G:44:TYR:CE1	2.54	0.43
2:H:210:GLN:NE2	2:N:211:SER:HB2	2.34	0.43
2:L:464:GLY:HA3	1:M:53:TYR:CZ	2.54	0.43
2:B:512:LEU:C	2:B:514:GLY:HA2	2.43	0.43
2:D:316:LEU:CD2	2:D:318:THR:HG23	2.49	0.43
2:N:196:LYS:HD3	2:N:196:LYS:C	2.43	0.43
2:N:318:THR:HG21	2:N:336:ARG:HB2	2.00	0.43
2:B:376:PRO:C	2:B:378:GLU:H	2.27	0.43
2:D:319:SER:OG	2:D:320:PRO:CD	2.67	0.43
2:H:266:ILE:HG13	2:H:271:LYS:HG3	2.00	0.43
1:I:40:VAL:HG22	2:L:316:LEU:HD13	2.00	0.43
1:A:48:LEU:HB3	2:B:369:THR:HG23	2.01	0.43
2:D:267:THR:O	2:D:271:LYS:HG3	2.19	0.43
2:F:400:THR:HG22	2:F:401:ASP:H	1.84	0.43
2:F:430:GLY:O	2:F:432:ILE:HG23	2.19	0.43
2:H:196:LYS:NZ	2:N:485:SER:HB2	2.33	0.43
2:H:492:ILE:HG21	2:L:193:LEU:HD22	2.01	0.43
2:L:432:ILE:HD11	2:L:447:VAL:CG2	2.49	0.43
2:L:442:VAL:HG11	2:L:447:VAL:CB	2.49	0.43
2:N:400:THR:HG22	2:N:401:ASP:N	2.34	0.43
2:B:252:LEU:HD23	2:B:256:GLU:HB2	2.01	0.42
2:H:216:ASN:O	2:H:220:VAL:HG23	2.19	0.42
2:H:318:THR:O	2:H:406:VAL:HG21	2.19	0.42
1:M:32:PHE:CG	2:N:441:TYR:CB	3.02	0.42
1:M:48:LEU:HB3	2:N:369:THR:HG23	2.01	0.42
2:H:251:MET:HG2	2:H:287:SER:CB	2.48	0.42
2:B:252:LEU:O	2:B:282:ARG:NH1	2.50	0.42
2:F:334:LEU:CD2	2:F:397:THR:HG22	2.49	0.42
2:H:388:ASN:O	2:H:388:ASN:ND2	2.52	0.42
2:H:513:LEU:CD1	2:L:172:LEU:HD21	2.49	0.42
2:L:379:VAL:HG12	2:L:391:TYR:CE2	2.55	0.42
1:M:59:ILE:HD12	2:N:233:ILE:CD1	2.48	0.42
2:N:201:LYS:O	2:N:205:PRO:HG2	2.18	0.42
1:A:74:ALA:C	1:A:76:VAL:H	2.27	0.42
2:B:150:SER:HB2	2:B:151:GLY:HA2	2.02	0.42
1:C:66:GLU:HA	2:F:476:ASN:ND2	2.34	0.42
2:D:167:ILE:HD11	2:F:167:ILE:HG23	2.00	0.42
2:D:267:THR:HG22	2:D:268:ASN:N	2.35	0.42
2:F:452:VAL:O	2:F:452:VAL:HG12	2.20	0.42
2:N:508:LYS:O	2:N:512:LEU:HD13	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:ILE:O	2:B:296:VAL:HG23	2.20	0.42
2:B:199:ILE:HD11	2:D:199:ILE:HD11	2.01	0.42
2:D:509:SER:HB2	2:F:173:SER:HB3	2.01	0.42
2:H:341:TRP:CH2	2:H:365:VAL:HG21	2.54	0.42
2:L:436:SER:O	2:L:437:ASN:C	2.62	0.42
1:A:36:THR:HG22	2:B:386:ILE:HG13	2.02	0.42
2:B:204:LEU:N	2:B:205:PRO:CD	2.82	0.42
1:C:95:LEU:O	1:C:96:LEU:HD23	2.19	0.42
2:F:483:PHE:CG	2:F:484:PRO:HD2	2.55	0.42
2:H:179:VAL:HG22	2:N:503:LEU:CD2	2.49	0.42
2:L:196:LYS:HD3	2:L:197:ASN:N	2.34	0.42
2:B:202:GLN:C	2:B:205:PRO:HD2	2.44	0.42
1:C:83:LEU:O	1:C:87:LYS:HG3	2.20	0.42
1:E:37:CYS:SG	1:E:37:CYS:O	2.77	0.42
2:L:157:VAL:O	2:L:157:VAL:CG1	2.67	0.42
2:L:442:VAL:CG1	2:L:447:VAL:CB	2.97	0.42
2:B:337:THR:HG21	2:B:396:MET:HB2	2.01	0.42
1:E:46:SER:OG	2:F:311:THR:HB	2.20	0.42
1:G:91:THR:O	1:G:95:LEU:HD12	2.20	0.42
1:G:93:LEU:CB	2:H:292:ILE:HD13	2.46	0.42
2:H:160:LEU:C	2:H:162:GLY:N	2.78	0.42
2:H:170:ALA:CB	2:L:513:LEU:HD21	2.50	0.42
1:I:64:ILE:HD12	1:I:79:ILE:HG23	2.02	0.42
1:A:53:TYR:HB2	2:B:305:LEU:HD11	2.02	0.42
2:B:213:SER:O	2:B:217:ILE:HG13	2.20	0.42
2:D:317:HIS:C	2:D:318:THR:HG23	2.44	0.42
1:E:26:GLN:CG	1:E:27:ASN:N	2.83	0.42
2:H:178:VAL:O	2:H:178:VAL:HG12	2.19	0.42
2:H:386:ILE:CG2	2:H:395:ILE:HD12	2.49	0.42
1:I:64:ILE:HG12	1:I:83:LEU:HD21	2.01	0.42
1:M:57:ILE:HD12	2:N:301:VAL:CG2	2.50	0.42
2:N:405:SER:HB2	2:N:457:TYR:CD2	2.55	0.42
1:C:53:TYR:CZ	2:F:464:GLY:HA3	2.55	0.41
1:E:64:ILE:HG12	1:E:83:LEU:HD21	2.02	0.41
1:G:30:GLU:HG3	1:G:40:VAL:O	2.19	0.41
1:G:57:ILE:HG12	2:N:467:LEU:HD12	2.01	0.41
1:G:71:GLY:HA2	2:H:212:CYS:HB3	2.01	0.41
2:H:430:GLY:O	2:H:432:ILE:HG23	2.19	0.41
1:I:89:ALA:O	1:I:93:LEU:HD13	2.20	0.41
2:N:316:LEU:CD2	2:N:318:THR:HG23	2.49	0.41
1:A:40:VAL:HG12	1:A:41:SER:N	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:444:ASN:OD1	2:F:444:ASN:C	2.63	0.41
2:H:191:LYS:HE3	2:L:491:SER:HB2	1.99	0.41
2:H:464:GLY:HA3	1:I:53:TYR:CZ	2.55	0.41
2:H:505:PHE:CE1	2:N:176:LYS:HB3	2.56	0.41
2:B:157:VAL:HG22	2:D:157:VAL:HG22	2.03	0.41
2:D:449:THR:CB	2:D:456:LEU:HD11	2.49	0.41
2:F:395:ILE:HG12	2:F:396:MET:N	2.36	0.41
2:L:309:ILE:CG2	2:L:310:ASP:N	2.83	0.41
1:C:79:ILE:CD1	2:D:219:THR:HB	2.48	0.41
2:L:154:VAL:HG23	2:L:154:VAL:O	2.19	0.41
2:L:171:LEU:O	2:L:171:LEU:HG	2.20	0.41
2:L:257:LEU:CD2	2:L:278:VAL:HG12	2.50	0.41
2:B:248:SER:HB2	2:F:239:VAL:HA	2.02	0.41
2:D:172:LEU:CD2	2:F:513:LEU:HD12	2.51	0.41
2:H:243:VAL:HG22	2:H:288:ILE:HG23	2.03	0.41
2:N:163:GLU:OE2	2:N:163:GLU:HA	2.19	0.41
2:N:252:LEU:HD21	2:N:256:GLU:HB2	2.02	0.41
2:N:256:GLU:O	2:N:259:SER:HB3	2.21	0.41
2:F:260:LEU:O	2:F:264:MET:HG3	2.21	0.41
2:F:280:ILE:HG21	2:F:366:PHE:CD2	2.55	0.41
2:H:167:ILE:O	2:H:167:ILE:CG1	2.69	0.41
2:H:223:PHE:CD1	2:H:227:ASN:ND2	2.88	0.41
2:H:267:THR:HG22	2:H:268:ASN:N	2.35	0.41
2:H:402:VAL:HG13	2:L:374:THR:HG22	2.03	0.41
2:H:476:ASN:ND2	1:I:67:ASN:HB2	2.35	0.41
2:D:505:PHE:HD1	2:F:176:LYS:HB2	1.86	0.41
1:E:79:ILE:CD1	2:F:220:VAL:HG23	2.50	0.41
1:E:93:LEU:HB2	2:F:292:ILE:HD13	2.03	0.41
2:F:163:GLU:O	2:F:165:ASN:N	2.53	0.41
2:F:426:ASN:ND2	2:F:446:GLY:O	2.54	0.41
2:H:479:ASP:O	2:H:479:ASP:CG	2.63	0.41
2:N:230:LEU:O	2:N:234:THR:HG23	2.21	0.41
2:B:257:LEU:HD23	2:B:278:VAL:CG1	2.51	0.41
2:H:273:LEU:CD2	2:H:309:ILE:HD13	2.50	0.41
1:I:55:SER:HB3	2:L:260:LEU:HD13	2.03	0.41
2:N:315:LYS:HD2	2:N:341:TRP:NE1	2.36	0.41
2:B:296:VAL:O	2:B:296:VAL:HG13	2.21	0.41
2:B:455:THR:HG22	2:F:308:VAL:HG21	2.02	0.41
1:C:64:ILE:CD1	1:C:79:ILE:HG23	2.51	0.41
2:D:172:LEU:HD23	2:F:513:LEU:HD12	2.03	0.41
2:D:245:THR:HB	2:D:286:TYR:CD1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:381:LEU:O	2:D:384:VAL:HG22	2.21	0.41
2:H:207:VAL:O	2:H:207:VAL:CG1	2.68	0.41
2:H:375:LEU:HD23	2:N:396:MET:HE3	2.02	0.41
2:H:509:SER:HB2	2:N:173:SER:HB2	2.03	0.41
1:M:69:CYS:CA	3:M:770:NAG:H62	2.49	0.41
2:N:164:VAL:O	2:N:168:LYS:HB2	2.21	0.41
2:N:252:LEU:HD12	2:N:301:VAL:HG11	2.03	0.41
2:N:352:PHE:HA	2:N:353:PRO:HD2	1.95	0.41
1:A:86:TYR:O	1:A:87:LYS:C	2.63	0.41
1:A:90:VAL:HG22	2:B:292:ILE:HD11	2.01	0.41
2:H:293:LYS:HE2	2:H:295:GLU:OE2	2.21	0.41
2:H:442:VAL:CG1	2:H:447:VAL:HG21	2.51	0.41
2:L:485:SER:HB2	2:N:196:LYS:CE	2.51	0.41
2:N:381:LEU:HB2	2:N:388:ASN:ND2	2.36	0.41
1:A:36:THR:HG22	2:B:386:ILE:HG12	2.02	0.40
1:A:38:SER:HB2	2:B:318:THR:HG22	2.03	0.40
2:F:267:THR:HG22	2:F:268:ASN:N	2.35	0.40
1:G:40:VAL:CG1	1:G:42:LYS:HG2	2.52	0.40
2:H:245:THR:HB	2:H:286:TYR:CD1	2.56	0.40
2:N:164:VAL:HA	2:N:167:ILE:CG2	2.51	0.40
2:B:178:VAL:O	2:B:178:VAL:HG12	2.21	0.40
2:D:352:PHE:HA	2:D:353:PRO:HD2	1.83	0.40
2:D:477:PHE:CE2	2:D:479:ASP:HB2	2.56	0.40
2:F:495:VAL:O	2:F:499:ILE:HG13	2.21	0.40
2:H:238:SER:HB3	2:N:250:TYR:CE2	2.56	0.40
2:B:204:LEU:CD2	2:D:481:LEU:HB3	2.51	0.40
2:L:177:ALA:HB3	2:N:506:ILE:HD11	2.03	0.40
2:L:427:LYS:HG2	2:L:448:ASP:OD2	2.22	0.40
2:B:257:LEU:HD23	2:B:278:VAL:HG12	2.04	0.40
2:F:332:ILE:O	2:F:332:ILE:HG13	2.21	0.40
2:N:195:LEU:HD23	2:N:195:LEU:HA	1.89	0.40
1:C:36:THR:CG2	2:D:382:CYS:O	2.66	0.40
2:D:185:VAL:HG12	2:F:499:ILE:HD11	2.03	0.40
2:F:251:MET:HG2	2:F:287:SER:OG	2.21	0.40
2:F:311:THR:HG23	2:F:344:ASP:HB2	2.02	0.40
2:H:405:SER:HB2	2:H:452:VAL:HG21	2.03	0.40
2:H:491:SER:O	2:H:495:VAL:HG23	2.21	0.40
2:L:375:LEU:HB3	2:L:376:PRO:HD2	2.04	0.40
2:L:444:ASN:HB2	2:L:460:ASN:OD1	2.21	0.40
1:M:64:ILE:HG21	2:N:223:PHE:HB2	2.04	0.40
2:N:233:ILE:CG2	2:N:297:LEU:HD21	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:319:SER:OG	2:N:320:PRO:HD2	2.20	0.40

There are no symmetry-related clashes.

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	71/84 (84%)	65 (92%)	5 (7%)	1 (1%)	9	27
1	C	70/84 (83%)	68 (97%)	2 (3%)	0	100	100
1	E	71/84 (84%)	65 (92%)	5 (7%)	1 (1%)	9	27
1	G	70/84 (83%)	65 (93%)	5 (7%)	0	100	100
1	I	69/84 (82%)	65 (94%)	4 (6%)	0	100	100
1	M	70/84 (83%)	64 (91%)	6 (9%)	0	100	100
2	B	354/374 (95%)	336 (95%)	17 (5%)	1 (0%)	36	64
2	D	351/374 (94%)	326 (93%)	23 (7%)	2 (1%)	21	48
2	F	347/374 (93%)	320 (92%)	23 (7%)	4 (1%)	10	31
2	H	355/374 (95%)	327 (92%)	28 (8%)	0	100	100
2	L	350/374 (94%)	331 (95%)	17 (5%)	2 (1%)	21	48
2	N	351/374 (94%)	328 (93%)	22 (6%)	1 (0%)	36	64
All	All	2529/2748 (92%)	2360 (93%)	157 (6%)	12 (0%)	24	53

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	69	CYS
2	B	153	ALA
2	F	164	VAL

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Mol	Chain	Res	Type
2	F	346	ALA
2	F	353	PRO
2	L	437	ASN
2	D	450	VAL
2	L	164	VAL
2	D	164	VAL
2	F	296	VAL
2	N	296	VAL
1	E	76	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	66/75 (88%)	63 (96%)	3 (4%)	24	57
1	C	65/75 (87%)	63 (97%)	2 (3%)	35	69
1	E	66/75 (88%)	60 (91%)	6 (9%)	9	27
1	G	65/75 (87%)	63 (97%)	2 (3%)	35	69
1	I	64/75 (85%)	61 (95%)	3 (5%)	23	55
1	M	65/75 (87%)	63 (97%)	2 (3%)	35	69
2	B	329/344 (96%)	299 (91%)	30 (9%)	9	27
2	D	328/344 (95%)	306 (93%)	22 (7%)	15	40
2	F	326/344 (95%)	299 (92%)	27 (8%)	10	31
2	H	330/344 (96%)	303 (92%)	27 (8%)	10	31
2	L	329/344 (96%)	304 (92%)	25 (8%)	12	35
2	N	329/344 (96%)	310 (94%)	19 (6%)	18	47
All	All	2362/2514 (94%)	2194 (93%)	168 (7%)	13	38

All (168) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	GLU

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Mol	Chain	Res	Type
1	A	88	ASN
1	A	90	VAL
2	B	152	VAL
2	B	204	LEU
2	B	207	VAL
2	B	211	SER
2	B	234	THR
2	B	244	THR
2	B	251	MET
2	B	252	LEU
2	B	255	SER
2	B	261	ILE
2	B	288	ILE
2	B	289	MET
2	B	301	VAL
2	B	309	ILE
2	B	316	LEU
2	B	338	ASP
2	B	345	ASN
2	B	361	GLN
2	B	377	SER
2	B	382	CYS
2	B	398	SER
2	B	401	ASP
2	B	402	VAL
2	B	422	CYS
2	B	449	THR
2	B	472	GLU
2	B	474	ILE
2	B	476	ASN
2	B	477	PHE
2	B	485	SER
1	C	33	TYR
1	C	57	ILE
2	D	173	SER
2	D	185	VAL
2	D	186	SER
2	D	187	VAL
2	D	189	THR
2	D	195	LEU
2	D	237	PHE
2	D	259	SER

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Mol	Chain	Res	Type
2	D	283	GLN
2	D	290	SER
2	D	301	VAL
2	D	309	ILE
2	D	311	THR
2	D	338	ASP
2	D	349	VAL
2	D	401	ASP
2	D	403	SER
2	D	422	CYS
2	D	431	ILE
2	D	432	ILE
2	D	459	VAL
2	D	485	SER
1	E	26	GLN
1	E	34	GLN
1	E	40	VAL
1	E	41	SER
1	E	90	VAL
1	E	96	LEU
2	F	155	SER
2	F	156	LYS
2	F	160	LEU
2	F	180	SER
2	F	185	VAL
2	F	187	VAL
2	F	211	SER
2	F	213	SER
2	F	301	VAL
2	F	311	THR
2	F	319	SER
2	F	345	ASN
2	F	350	SER
2	F	354	GLN
2	F	401	ASP
2	F	403	SER
2	F	409	SER
2	F	416	CYS
2	F	439	CYS
2	F	443	SER
2	F	449	THR
2	F	454	ASN

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Mol	Chain	Res	Type
2	F	474	ILE
2	F	493	SER
2	F	501	GLN
2	F	509	SER
2	F	513	LEU
1	G	59	ILE
1	G	90	VAL
2	H	155	SER
2	H	157	VAL
2	H	164	VAL
2	H	167	ILE
2	H	179	VAL
2	H	180	SER
2	H	190	SER
2	H	195	LEU
2	H	211	SER
2	H	234	THR
2	H	238	SER
2	H	249	THR
2	H	255	SER
2	H	278	VAL
2	H	280	ILE
2	H	288	ILE
2	H	309	ILE
2	H	319	SER
2	H	377	SER
2	H	384	VAL
2	H	388	ASN
2	H	422	CYS
2	H	449	THR
2	H	474	ILE
2	H	478	TYR
2	H	492	ILE
2	H	509	SER
1	I	64	ILE
1	I	66	GLU
1	I	67	ASN
2	L	158	LEU
2	L	173	SER
2	L	180	SER
2	L	185	VAL
2	L	204	LEU

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Mol	Chain	Res	Type
2	L	235	ARG
2	L	244	THR
2	L	245	THR
2	L	278	VAL
2	L	292	ILE
2	L	296	VAL
2	L	311	THR
2	L	360	VAL
2	L	361	GLN
2	L	397	THR
2	L	400	THR
2	L	422	CYS
2	L	431	ILE
2	L	433	LYS
2	L	434	THR
2	L	440	ASP
2	L	449	THR
2	L	481	LEU
2	L	493	SER
2	L	512	LEU
1	M	34	GLN
1	M	35	SER
2	N	167	ILE
2	N	173	SER
2	N	185	VAL
2	N	186	SER
2	N	199	ILE
2	N	207	VAL
2	N	221	ILE
2	N	243	VAL
2	N	252	LEU
2	N	350	SER
2	N	365	VAL
2	N	373	LEU
2	N	398	SER
2	N	400	THR
2	N	401	ASP
2	N	402	VAL
2	N	422	CYS
2	N	448	ASP
2	N	449	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	34	GLN
1	A	67	ASN
2	B	210	GLN
2	B	240	ASN
2	B	380	ASN
2	B	383	ASN
2	B	388	ASN
2	B	437	ASN
2	B	454	ASN
1	C	34	GLN
1	C	67	ASN
1	C	81	GLN
2	D	228	ASN
2	D	254	ASN
2	D	270	GLN
2	D	383	ASN
2	D	426	ASN
2	D	428	ASN
2	D	437	ASN
2	D	444	ASN
2	D	454	ASN
2	D	496	ASN
1	E	26	GLN
1	E	34	GLN
1	E	67	ASN
2	F	202	GLN
2	F	225	GLN
2	F	254	ASN
2	F	270	GLN
2	F	302	GLN
2	F	345	ASN
2	F	361	GLN
2	F	371	ASN
2	F	383	ASN
2	F	437	ASN
2	F	476	ASN
1	G	26	GLN
1	G	34	GLN
1	G	67	ASN
1	G	81	GLN
2	H	240	ASN

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Mol	Chain	Res	Type
2	H	254	ASN
2	H	262	ASN
2	H	276	ASN
2	H	277	ASN
2	H	383	ASN
2	H	388	ASN
2	H	454	ASN
2	H	476	ASN
1	I	34	GLN
2	L	210	GLN
2	L	254	ASN
2	L	276	ASN
2	L	284	GLN
2	L	380	ASN
2	L	383	ASN
2	L	437	ASN
2	L	454	ASN
1	M	34	GLN
1	M	88	ASN
1	M	94	GLN
1	M	98	GLN
2	N	254	ASN
2	N	270	GLN
2	N	317	HIS
2	N	361	GLN
2	N	371	ASN
2	N	383	ASN
2	N	428	ASN
2	N	437	ASN
2	N	454	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 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	NAG	N	800	2	14,14,15	0.49	0	17,19,21	0.78	0
3	NAG	G	770	1	14,14,15	0.63	0	17,19,21	1.34	1 (5%)
3	NAG	F	800	2	14,14,15	0.43	0	17,19,21	1.25	1 (5%)
3	NAG	A	770	1	14,14,15	0.46	0	17,19,21	0.75	1 (5%)
3	NAG	I	770	1	14,14,15	0.48	0	17,19,21	0.61	0
3	NAG	D	800	2	14,14,15	0.48	0	17,19,21	0.89	1 (5%)
3	NAG	H	800	2	14,14,15	0.47	0	17,19,21	1.23	1 (5%)
3	NAG	L	800	2	14,14,15	0.51	0	17,19,21	1.13	1 (5%)
3	NAG	B	800	2	14,14,15	0.41	0	17,19,21	1.43	1 (5%)
3	NAG	E	770	1	14,14,15	0.37	0	17,19,21	1.78	3 (17%)
3	NAG	M	770	1	14,14,15	0.45	0	17,19,21	1.68	2 (11%)
3	NAG	C	770	1	14,14,15	0.55	0	17,19,21	0.90	1 (5%)

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	NAG	N	800	2	1/1/5/7	3/6/23/26	0/1/1/1
3	NAG	G	770	1	-	4/6/23/26	0/1/1/1
3	NAG	F	800	2	1/1/5/7	3/6/23/26	0/1/1/1
3	NAG	A	770	1	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	I	770	1	1/1/5/7	3/6/23/26	0/1/1/1
3	NAG	D	800	2	-	3/6/23/26	0/1/1/1
3	NAG	H	800	2	1/1/5/7	3/6/23/26	0/1/1/1
3	NAG	L	800	2	-	3/6/23/26	0/1/1/1
3	NAG	B	800	2	-	3/6/23/26	0/1/1/1
3	NAG	E	770	1	-	3/6/23/26	0/1/1/1
3	NAG	M	770	1	-	3/6/23/26	0/1/1/1
3	NAG	C	770	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	770	NAG	C1-O5-C5	5.82	119.99	112.19
3	M	770	NAG	C1-O5-C5	5.75	119.89	112.19
3	B	800	NAG	C1-O5-C5	4.84	118.67	112.19
3	G	770	NAG	C1-O5-C5	4.69	118.47	112.19
3	F	800	NAG	C1-O5-C5	4.38	118.06	112.19
3	H	800	NAG	C1-O5-C5	4.29	117.93	112.19
3	L	800	NAG	C1-O5-C5	3.96	117.49	112.19
3	M	770	NAG	O5-C1-C2	3.00	115.94	111.29
3	E	770	NAG	O5-C1-C2	2.42	115.04	111.29
3	D	800	NAG	C1-O5-C5	2.36	115.35	112.19
3	E	770	NAG	C4-C3-C2	-2.26	107.71	111.02
3	C	770	NAG	C1-O5-C5	2.12	115.03	112.19
3	A	770	NAG	C1-O5-C5	2.08	114.97	112.19

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	F	800	NAG	C1
3	H	800	NAG	C1
3	I	770	NAG	C1
3	N	800	NAG	C1

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	770	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
3	B	800	NAG	C1-C2-N2-C7
3	D	800	NAG	C1-C2-N2-C7
3	D	800	NAG	C8-C7-N2-C2
3	D	800	NAG	O7-C7-N2-C2
3	E	770	NAG	C1-C2-N2-C7
3	G	770	NAG	C8-C7-N2-C2
3	G	770	NAG	O7-C7-N2-C2
3	H	800	NAG	C1-C2-N2-C7
3	H	800	NAG	C8-C7-N2-C2
3	H	800	NAG	O7-C7-N2-C2
3	L	800	NAG	C1-C2-N2-C7
3	N	800	NAG	C1-C2-N2-C7
3	N	800	NAG	C8-C7-N2-C2
3	N	800	NAG	O7-C7-N2-C2
3	B	800	NAG	C8-C7-N2-C2
3	B	800	NAG	O7-C7-N2-C2
3	L	800	NAG	C8-C7-N2-C2
3	L	800	NAG	O7-C7-N2-C2
3	M	770	NAG	C8-C7-N2-C2
3	A	770	NAG	C8-C7-N2-C2
3	E	770	NAG	C8-C7-N2-C2
3	I	770	NAG	C8-C7-N2-C2
3	A	770	NAG	O7-C7-N2-C2
3	E	770	NAG	O7-C7-N2-C2
3	F	800	NAG	C8-C7-N2-C2
3	I	770	NAG	O7-C7-N2-C2
3	M	770	NAG	O7-C7-N2-C2
3	F	800	NAG	O7-C7-N2-C2
3	C	770	NAG	C8-C7-N2-C2
3	F	800	NAG	C3-C2-N2-C7
3	M	770	NAG	C3-C2-N2-C7
3	C	770	NAG	O7-C7-N2-C2
3	C	770	NAG	C1-C2-N2-C7
3	I	770	NAG	C3-C2-N2-C7
3	G	770	NAG	C1-C2-N2-C7
3	C	770	NAG	C3-C2-N2-C7
3	G	770	NAG	C3-C2-N2-C7

There are no ring outliers.

8 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	N	800	NAG	2	0
3	G	770	NAG	1	0
3	F	800	NAG	1	0
3	I	770	NAG	1	0
3	H	800	NAG	1	0
3	B	800	NAG	4	0
3	M	770	NAG	4	0
3	C	770	NAG	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	73/84 (86%)	0.87	9 (12%) 8 6	29, 48, 94, 133	0
1	C	72/84 (85%)	0.59	7 (9%) 13 9	22, 39, 85, 158	0
1	E	73/84 (86%)	0.70	11 (15%) 5 4	21, 43, 94, 123	0
1	G	72/84 (85%)	1.07	15 (20%) 2 2	26, 51, 108, 171	0
1	I	71/84 (84%)	0.66	8 (11%) 10 7	17, 42, 97, 119	0
1	M	72/84 (85%)	0.81	10 (13%) 6 5	20, 45, 93, 146	0
2	B	358/374 (95%)	0.66	37 (10%) 12 9	20, 46, 88, 134	0
2	D	355/374 (94%)	0.92	55 (15%) 5 4	19, 52, 98, 181	0
2	F	351/374 (93%)	0.72	39 (11%) 10 7	18, 42, 90, 142	0
2	H	359/374 (95%)	0.68	30 (8%) 17 12	19, 47, 86, 130	0
2	L	354/374 (94%)	0.64	32 (9%) 15 11	17, 42, 88, 145	0
2	N	355/374 (94%)	0.86	44 (12%) 8 6	21, 52, 101, 201	0
All	All	2565/2748 (93%)	0.75	297 (11%) 9 7	17, 46, 94, 201	0

All (297) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	355	ALA	8.0
2	L	477	PHE	7.4
2	F	355	ALA	7.2
1	M	65	LYS	7.0
1	G	65	LYS	6.4
2	N	477	PHE	6.2
2	F	354	GLN	6.1
2	D	477	PHE	5.5
2	N	355	ALA	5.2
2	D	371	ASN	5.2
1	M	67	ASN	5.0

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Mol	Chain	Res	Type	RSRZ
1	M	27	ASN	5.0
2	N	472	GLU	4.9
2	B	436	SER	4.9
1	A	65	LYS	4.9
2	D	436	SER	4.9
2	H	371	ASN	4.9
2	H	472	GLU	4.8
1	C	26	GLN	4.8
2	F	356	GLU	4.8
2	B	381	LEU	4.7
1	E	35	SER	4.7
2	N	323	THR	4.6
2	N	371	ASN	4.6
2	H	332	ILE	4.5
2	D	332	ILE	4.5
1	A	35	SER	4.5
2	L	436	SER	4.5
2	D	356	GLU	4.5
2	N	436	SER	4.5
2	N	468	TYR	4.4
2	F	421	LYS	4.3
2	F	440	ASP	4.3
2	F	155	SER	4.3
2	F	404	SER	4.3
2	F	405	SER	4.3
2	N	479	ASP	4.3
2	H	470	LYS	4.2
2	B	355	ALA	4.2
2	D	514	GLY	4.2
2	N	354	GLN	4.2
1	I	69	CYS	4.2
2	L	463	GLU	4.1
2	D	310	ASP	4.1
2	B	388	ASN	4.1
2	L	154	VAL	4.1
2	L	355	ALA	4.1
2	F	332	ILE	4.1
2	B	439	CYS	4.1
2	L	169	SER	4.0
2	F	346	ALA	4.0
2	F	430	GLY	4.0
2	D	468	TYR	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	34	GLN	4.0
2	N	190	SER	4.0
2	D	322	CYS	3.9
2	D	471	GLY	3.9
2	H	356	GLU	3.8
2	N	332	ILE	3.8
2	D	438	GLY	3.8
2	F	393	CYS	3.7
2	D	346	ALA	3.7
2	N	156	LYS	3.7
2	N	419	LYS	3.7
2	L	155	SER	3.7
2	L	514	GLY	3.7
2	N	404	SER	3.6
2	D	429	ARG	3.6
2	B	268	ASN	3.6
2	D	354	GLN	3.6
1	G	77	LYS	3.6
2	N	475	ILE	3.6
2	F	478	TYR	3.6
1	A	77	LYS	3.5
2	D	388	ASN	3.5
2	D	398	SER	3.5
2	L	468	TYR	3.5
2	L	507	ARG	3.5
2	N	429	ARG	3.5
2	D	472	GLU	3.4
2	F	428	ASN	3.4
2	L	161	GLU	3.4
2	B	354	GLN	3.4
2	F	371	ASN	3.4
2	N	514	GLY	3.4
1	G	74	ALA	3.4
2	F	390	LYS	3.4
2	B	163	GLU	3.4
2	D	166	LYS	3.4
2	F	436	SER	3.4
2	F	347	GLY	3.3
1	G	69	CYS	3.3
2	B	357	THR	3.3
2	H	355	ALA	3.3
2	N	507	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
2	N	510	ASP	3.2
1	I	77	LYS	3.2
2	B	468	TYR	3.2
2	F	451	SER	3.2
2	F	463	GLU	3.2
2	H	345	ASN	3.2
2	N	388	ASN	3.2
2	F	507	ARG	3.2
1	M	77	LYS	3.2
2	L	419	LYS	3.2
1	G	31	GLU	3.2
2	L	508	LYS	3.2
2	L	332	ILE	3.2
2	B	393	CYS	3.1
1	E	32	PHE	3.1
1	I	27	ASN	3.1
2	H	514	GLY	3.1
1	M	66	GLU	3.1
2	L	324	THR	3.1
2	D	309	ILE	3.1
2	B	472	GLU	3.1
2	D	439	CYS	3.0
2	D	508	LYS	3.0
2	N	409	SER	3.0
2	H	168	LYS	3.0
2	H	468	TYR	3.0
2	D	347	GLY	3.0
1	G	72	THR	3.0
1	A	31	GLU	2.9
1	I	66	GLU	2.9
2	N	165	ASN	2.9
1	E	68	LYS	2.9
2	D	387	PHE	2.9
2	N	427	LYS	2.9
2	D	402	VAL	2.9
2	D	479	ASP	2.9
2	H	291	ILE	2.9
2	B	372	SER	2.8
1	A	37	CYS	2.8
1	G	71	GLY	2.8
2	N	347	GLY	2.8
1	I	75	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	M	37	CYS	2.8
2	B	394	LYS	2.8
2	N	166	LYS	2.8
1	A	27	ASN	2.8
2	B	508	LYS	2.8
1	C	37	CYS	2.7
2	D	421	LYS	2.7
2	D	345	ASN	2.7
1	M	69	CYS	2.7
1	C	31	GLU	2.7
1	E	37	CYS	2.7
2	H	226	LYS	2.7
2	D	434	THR	2.7
2	F	345	ASN	2.7
2	F	454	ASN	2.7
1	E	31	GLU	2.7
2	B	259	SER	2.7
2	B	470	LYS	2.7
2	N	390	LYS	2.7
2	D	337	THR	2.7
2	L	476	ASN	2.7
2	D	487	GLU	2.7
1	E	27	ASN	2.6
1	E	42	LYS	2.6
2	B	338	ASP	2.6
2	B	405	SER	2.6
2	B	514	GLY	2.6
2	N	471	GLY	2.6
2	B	203	LEU	2.6
2	F	420	THR	2.6
2	H	292	ILE	2.6
2	L	167	ILE	2.6
1	C	38	SER	2.6
2	H	419	LYS	2.6
2	N	478	TYR	2.6
2	F	439	CYS	2.6
2	N	337	THR	2.6
2	N	474	ILE	2.6
1	G	67	ASN	2.6
2	N	153	ALA	2.6
1	M	98	GLN	2.5
2	D	420	THR	2.5

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Mol	Chain	Res	Type	RSRZ
2	L	472	GLU	2.5
1	I	43	GLY	2.5
2	F	446	GLY	2.5
2	D	393	CYS	2.5
2	D	440	ASP	2.5
2	D	405	SER	2.5
2	H	303	LEU	2.5
2	L	484	PRO	2.5
2	F	322	CYS	2.5
1	G	97	MET	2.5
2	D	410	LEU	2.5
2	D	395	ILE	2.5
1	G	34	GLN	2.5
1	M	42	LYS	2.5
1	G	27	ASN	2.5
2	H	475	ILE	2.4
2	H	147	ALA	2.4
2	D	397	THR	2.4
2	D	426	ASN	2.4
2	F	416	CYS	2.4
2	D	448	ASP	2.4
1	G	68	LYS	2.4
2	L	445	LYS	2.4
2	H	479	ASP	2.4
2	N	448	ASP	2.4
2	B	507	ARG	2.4
2	D	470	LYS	2.4
1	A	30	GLU	2.4
2	H	159	HIS	2.4
2	D	428	ASN	2.4
2	D	156	LYS	2.4
2	N	310	ASP	2.4
2	B	497	GLU	2.4
2	H	381	LEU	2.4
2	L	291	ILE	2.4
1	C	27	ASN	2.3
1	G	70	ASN	2.3
2	N	482	VAL	2.3
2	L	356	GLU	2.3
2	D	284	GLN	2.3
2	L	354	GLN	2.3
2	B	398	SER	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	404	SER	2.3
1	I	68	LYS	2.3
2	D	444	ASN	2.3
2	L	347	GLY	2.3
1	C	97	MET	2.3
2	H	354	GLN	2.3
2	F	468	TYR	2.3
2	B	356	GLU	2.3
2	N	218	GLU	2.3
2	D	416	CYS	2.3
2	D	403	SER	2.3
1	E	65	LYS	2.3
2	L	422	CYS	2.3
2	H	348	SER	2.3
2	B	484	PRO	2.3
2	D	379	VAL	2.3
2	L	487	GLU	2.2
1	E	75	LYS	2.2
2	F	429	ARG	2.2
2	B	335	THR	2.2
2	F	157	VAL	2.2
2	N	169	SER	2.2
2	B	421	LYS	2.2
2	N	476	ASN	2.2
1	E	29	THR	2.2
2	D	422	CYS	2.2
2	D	423	THR	2.2
2	N	447	VAL	2.2
2	F	464	GLY	2.2
2	N	438	GLY	2.2
1	G	42	LYS	2.2
2	N	161	GLU	2.2
2	B	454	ASN	2.2
2	D	474	ILE	2.2
2	F	407	ILE	2.2
2	H	338	ASP	2.2
2	N	316	LEU	2.2
2	N	410	LEU	2.2
2	B	511	GLU	2.2
1	G	64	ILE	2.1
2	D	386	ILE	2.1
1	A	98	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	401	ASP	2.1
2	F	338	ASP	2.1
2	L	479	ASP	2.1
2	H	163	GLU	2.1
1	E	26	GLN	2.1
2	H	262	ASN	2.1
2	H	453	GLY	2.1
2	H	504	ALA	2.1
1	M	81	GLN	2.1
2	F	419	LYS	2.1
2	F	442	VAL	2.1
2	H	394	LYS	2.1
2	F	418	GLY	2.1
2	F	514	GLY	2.1
2	H	438	GLY	2.1
2	F	434	THR	2.1
2	B	487	GLU	2.1
2	B	390	LYS	2.1
2	H	278	VAL	2.1
2	L	157	VAL	2.1
2	B	434	THR	2.1
2	L	177	ALA	2.1
1	I	97	MET	2.0
2	B	419	LYS	2.0
2	N	470	LYS	2.0
2	B	500	ASN	2.0
2	D	507	ARG	2.0
1	C	28	ILE	2.0
2	B	294	GLU	2.0
2	L	428	ASN	2.0
2	L	490	ALA	2.0
2	D	378	GLU	2.0
2	N	269	ASP	2.0
2	L	166	LYS	2.0

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

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	NAG	I	770	14/15	0.46	0.32	128,147,151,151	0
3	NAG	H	800	14/15	0.53	0.24	88,106,112,113	0
3	NAG	D	800	14/15	0.60	0.23	58,76,82,82	0
3	NAG	N	800	14/15	0.62	0.22	62,80,85,86	0
3	NAG	A	770	14/15	0.65	0.24	62,81,84,86	0
3	NAG	G	770	14/15	0.68	0.22	95,113,119,120	0
3	NAG	B	800	14/15	0.70	0.21	57,74,81,82	0
3	NAG	F	800	14/15	0.70	0.23	71,89,94,95	0
3	NAG	M	770	14/15	0.71	0.28	91,110,114,115	0
3	NAG	E	770	14/15	0.71	0.24	99,117,122,124	0
3	NAG	L	800	14/15	0.76	0.18	64,82,87,87	0
3	NAG	C	770	14/15	0.80	0.23	82,100,106,107	0

6.5 Other polymers [i](#)

There are no such residues in this entry.