



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 22, 2024 – 08:17 AM EDT

PDB ID : 4KNG
Title : Crystal structure of human LGR5-RSPO1-RNF43
Authors : Chen, P.H.; He, X.
Deposited on : 2013-05-09
Resolution : 2.50 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 : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.20.1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

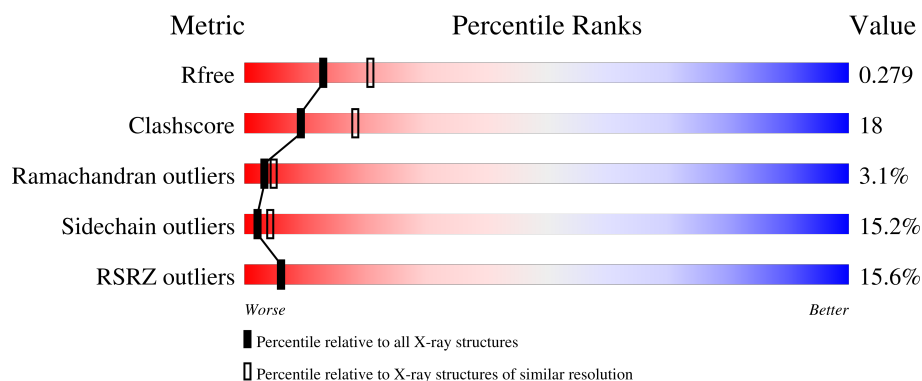
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	164625	5504 (2.50-2.50)
Clashscore	180529	6282 (2.50-2.50)
Ramachandran outliers	177936	6191 (2.50-2.50)
Sidechain outliers	177891	6193 (2.50-2.50)
RSRZ outliers	164620	5504 (2.50-2.50)

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	531	
1	B	531	
2	M	115	
2	P	115	
3	E	160	

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Mol	Chain	Length	Quality of chain
3	F	160	<div><div></div><div>40%</div><div>54%</div><div>29%</div><div>7%</div><div>•</div><div>8%</div></div>

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 11252 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 Leucine-rich repeat-containing G-protein coupled receptor 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	461	Total	C	N	O	S	0	1	0
			3622	2307	626	673	16			
1	B	463	Total	C	N	O	S	0	0	0
			3629	2312	627	674	16			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	GLY	-	expression tag	UNP O75473
A	31	PRO	-	expression tag	UNP O75473
A	558	ALA	-	expression tag	UNP O75473
A	559	ALA	-	expression tag	UNP O75473
A	560	ALA	-	expression tag	UNP O75473
B	30	GLY	-	expression tag	UNP O75473
B	31	PRO	-	expression tag	UNP O75473
B	558	ALA	-	expression tag	UNP O75473
B	559	ALA	-	expression tag	UNP O75473
B	560	ALA	-	expression tag	UNP O75473

- Molecule 2 is a protein called R-spondin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	98	Total	C	N	O	S	0	0	0
			750	465	131	136	18			
2	P	94	Total	C	N	O	S	0	0	0
			720	448	127	128	17			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	33	GLY	-	expression tag	UNP Q2MKA7
M	34	PRO	-	expression tag	UNP Q2MKA7

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Chain	Residue	Modelled	Actual	Comment	Reference
M	145	ALA	-	expression tag	UNP Q2MKA7
M	146	ALA	-	expression tag	UNP Q2MKA7
M	147	ALA	-	expression tag	UNP Q2MKA7
P	33	GLY	-	expression tag	UNP Q2MKA7
P	34	PRO	-	expression tag	UNP Q2MKA7
P	145	ALA	-	expression tag	UNP Q2MKA7
P	146	ALA	-	expression tag	UNP Q2MKA7
P	147	ALA	-	expression tag	UNP Q2MKA7

- Molecule 3 is a protein called E3 ubiquitin-protein ligase RNF43.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	149	Total	C	N	O	S	0	0	0
			1152	734	200	212	6			
3	F	148	Total	C	N	O	S	0	0	0
			1145	729	199	211	6			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	42	GLY	-	expression tag	UNP Q68DV7
E	43	PRO	-	expression tag	UNP Q68DV7
E	199	ALA	-	expression tag	UNP Q68DV7
E	200	ALA	-	expression tag	UNP Q68DV7
E	201	ALA	-	expression tag	UNP Q68DV7
F	42	GLY	-	expression tag	UNP Q68DV7
F	43	PRO	-	expression tag	UNP Q68DV7
F	199	ALA	-	expression tag	UNP Q68DV7
F	200	ALA	-	expression tag	UNP Q68DV7
F	201	ALA	-	expression tag	UNP Q68DV7

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Ni	0	0
			1	1		

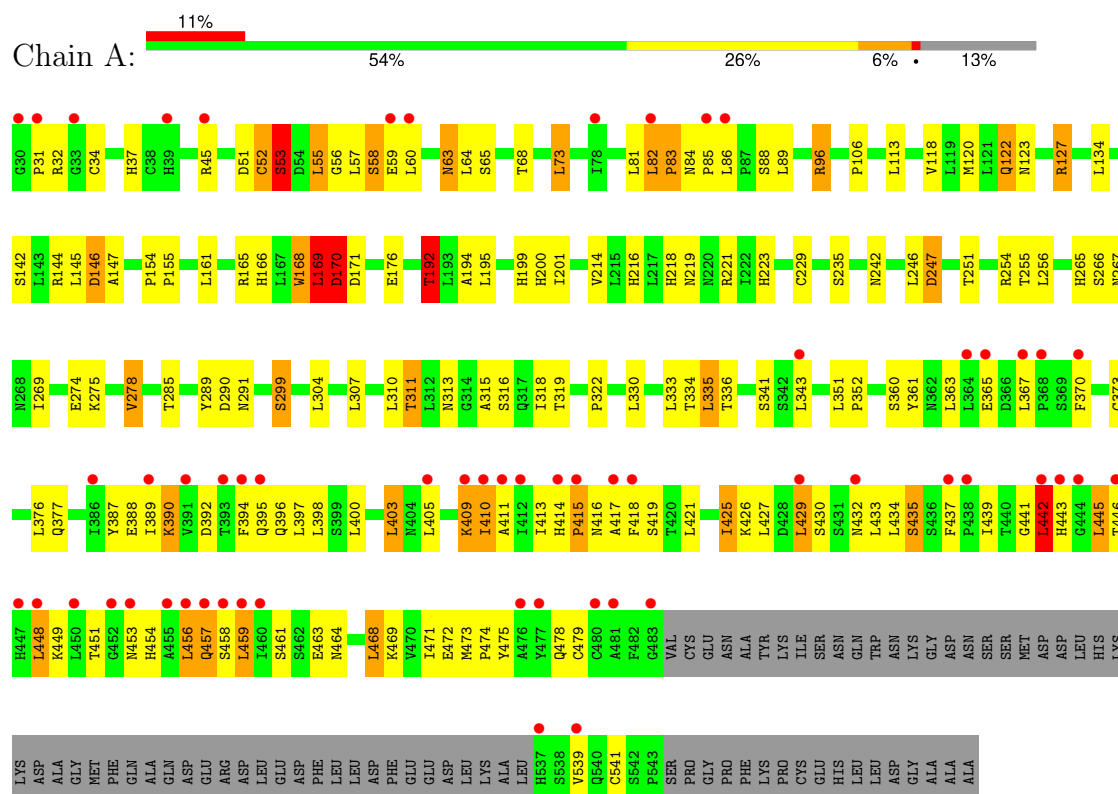
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	70	Total	O	0	0
			70	70		
6	B	85	Total	O	0	0
			85	85		
6	M	21	Total	O	0	0
			21	21		
6	P	7	Total	O	0	0
			7	7		
6	E	18	Total	O	0	0
			18	18		
6	F	4	Total	O	0	0
			4	4		

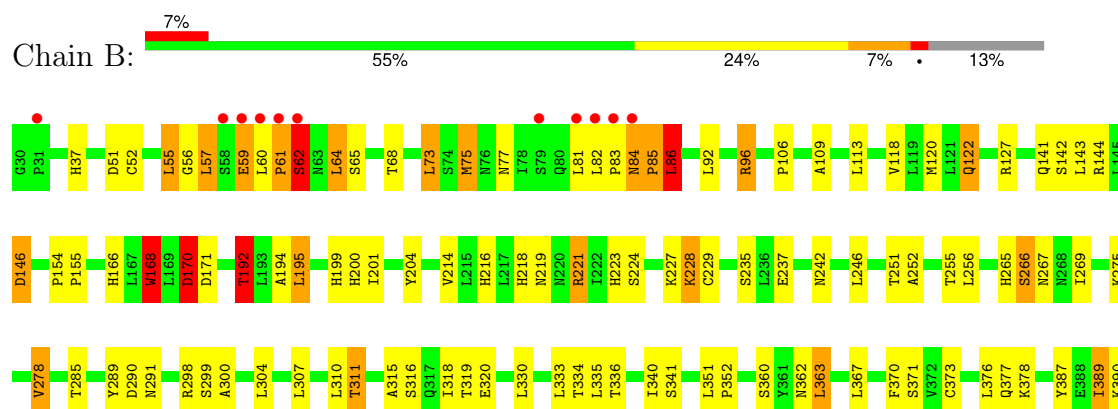
3 Residue-property plots

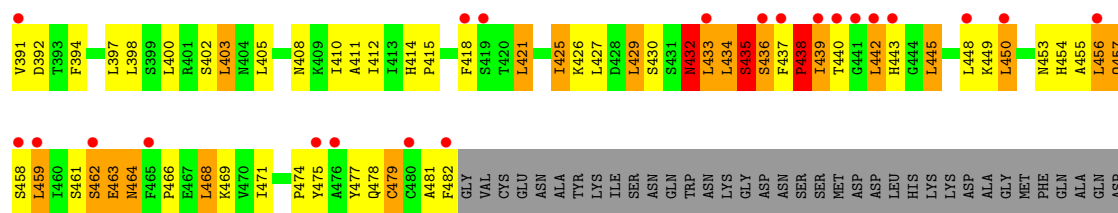
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Leucine-rich repeat-containing G-protein coupled receptor 5

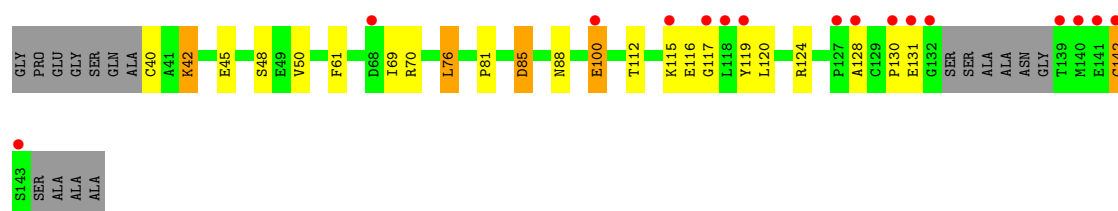


- Molecule 1: Leucine-rich repeat-containing G-protein coupled receptor 5

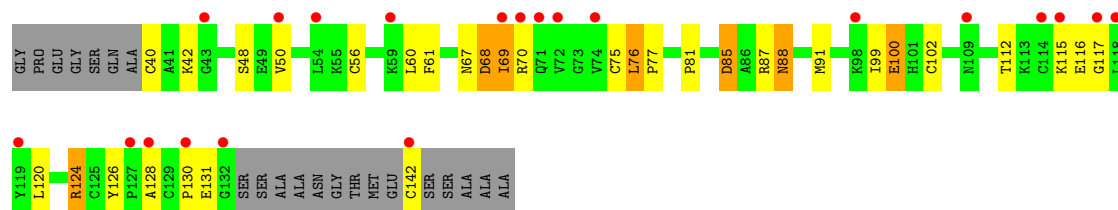




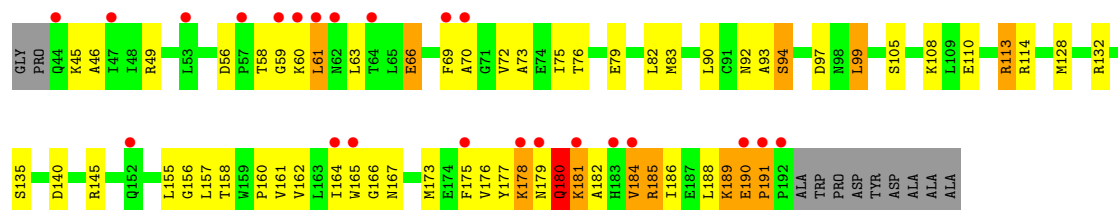
• Molecule 2: R-spondin-1



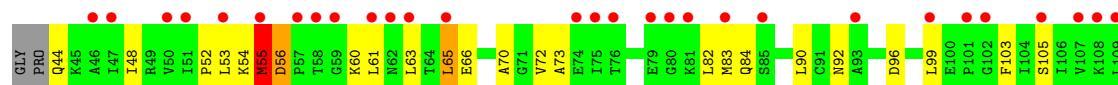
• Molecule 2: R-spondin-1

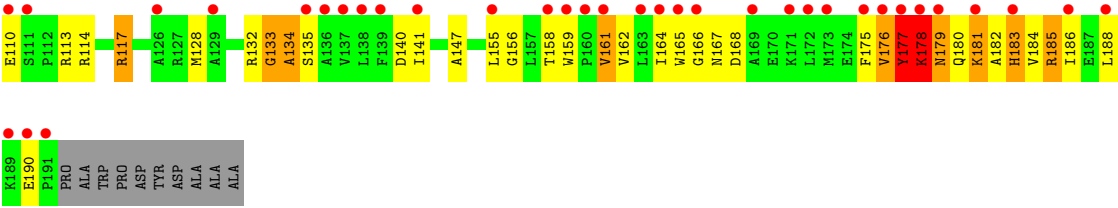


• Molecule 3: E3 ubiquitin-protein ligase RNF43



• Molecule 3: E3 ubiquitin-protein ligase RNF43





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.58Å 120.97Å 181.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.51 – 2.50 39.51 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.1 (39.51-2.50) 97.1 (39.51-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.232 , 0.276 0.232 , 0.279	Depositor DCC
R_{free} test set	3888 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	43.4	Xtriage
Anisotropy	0.321	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 51.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11252	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.19% 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: NI, 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	0.61	0/3704	0.87	9/5043 (0.2%)
1	B	0.72	1/3712 (0.0%)	0.93	8/5055 (0.2%)
2	M	0.73	0/765	0.90	0/1025
2	P	0.64	0/735	0.87	0/985
3	E	0.54	0/1175	0.80	0/1593
3	F	0.48	0/1167	0.88	2/1581 (0.1%)
All	All	0.64	1/11258 (0.0%)	0.89	19/15282 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	8
2	P	0	1
3	E	0	3
3	F	0	3
All	All	0	16

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	168	TRP	CG-CD1	5.66	1.44	1.36

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	86	LEU	CA-CB-CG	-7.22	98.69	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	442	LEU	CA-CB-CG	6.30	129.79	115.30
1	B	96	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	A	214	VAL	CB-CA-C	-6.15	99.71	111.40
1	A	170	ASP	N-CA-CB	-6.15	99.54	110.60
1	B	214	VAL	CB-CA-C	-6.08	99.85	111.40
1	A	96	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	B	170	ASP	N-CA-CB	-6.00	99.81	110.60
1	A	192	THR	CB-CA-C	-5.96	95.51	111.60
1	B	192	THR	CB-CA-C	-5.83	95.85	111.60
1	B	459	LEU	CA-CB-CG	5.69	128.38	115.30
1	A	169	LEU	CA-CB-CG	5.53	128.02	115.30
1	A	52	CYS	CA-CB-SG	-5.37	104.33	114.00
1	B	433	LEU	CB-CA-C	5.36	120.38	110.20
3	F	178	LYS	N-CA-C	5.36	125.46	111.00
1	A	168	TRP	CA-CB-CG	5.17	123.52	113.70
3	F	177	TYR	N-CA-C	-5.08	97.28	111.00
1	B	62	SER	N-CA-C	-5.03	97.41	111.00
1	A	335	LEU	CA-CB-CG	5.01	126.83	115.30

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	409	LYS	Peptide
1	B	432	ASN	Peptide
1	B	434	LEU	Peptide
1	B	435	SER	Peptide
1	B	438	PRO	Peptide
1	B	466	PRO	Peptide
1	B	57	LEU	Peptide
1	B	59	GLU	Peptide
1	B	61	PRO	Peptide
3	E	180	GLN	Peptide
3	E	61	LEU	Peptide
3	E	92	ASN	Peptide
3	F	134	ALA	Peptide
3	F	177	TYR	Peptide
3	F	179	ASN	Peptide
2	P	67	ASN	Peptide

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	3622	0	3626	129	0
1	B	3629	0	3634	146	0
2	M	750	0	719	17	0
2	P	720	0	692	26	0
3	E	1152	0	1182	43	0
3	F	1145	0	1175	47	0
4	A	14	0	13	0	0
4	B	14	0	13	0	0
5	B	1	0	0	0	0
6	A	70	0	0	8	0
6	B	85	0	0	7	0
6	E	18	0	0	4	0
6	F	4	0	0	1	0
6	M	21	0	0	2	0
6	P	7	0	0	8	0
All	All	11252	0	11054	394	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 18.

All (394) 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)
3:F:177:TYR:O	3:F:179:ASN:HA	1.44	1.17
1:B:450:LEU:HD12	1:B:453:ASN:HD22	0.98	1.15
1:B:459:LEU:HD21	1:B:478:GLN:CB	1.76	1.14
1:B:459:LEU:CD2	1:B:478:GLN:HB2	1.78	1.14
1:B:459:LEU:HD21	1:B:478:GLN:HB2	1.22	1.08
1:B:450:LEU:HD12	1:B:453:ASN:ND2	1.72	1.04
3:F:54:LYS:HA	3:F:55:MET:HB2	1.48	0.95
1:B:84:ASN:HB3	1:B:85:PRO:HA	1.48	0.93
1:A:414:HIS:HB3	1:A:415:PRO:HD2	1.52	0.91
1:B:60:LEU:HB3	1:B:61:PRO:HD3	1.50	0.91
3:F:181:LYS:HA	3:F:182:ALA:HB3	1.54	0.90
1:B:410:ILE:HB	1:B:432:ASN:OD1	1.71	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:438:PRO:HB2	1:B:439:ILE:HG22	1.53	0.87
3:E:173:MET:HA	3:E:176:VAL:HG12	1.58	0.85
3:E:179:ASN:N	3:E:180:GLN:HA	1.95	0.81
2:P:75:CYS:HB3	6:P:203:HOH:O	1.80	0.80
1:B:363:LEU:HD13	3:E:113:ARG:HG2	1.64	0.80
1:B:84:ASN:HB3	1:B:85:PRO:CA	2.12	0.79
1:B:192:THR:HG23	1:B:216:HIS:HB2	1.65	0.79
1:B:450:LEU:CD1	1:B:453:ASN:HD22	1.89	0.78
1:B:389:ILE:HD11	1:B:418:PHE:HE1	1.48	0.78
1:A:468:LEU:HD11	1:A:471:ILE:HG12	1.64	0.78
3:E:113:ARG:HD2	6:E:312:HOH:O	1.84	0.78
1:B:55:LEU:O	1:B:57:LEU:HG	1.85	0.77
1:B:65:SER:O	1:B:68:THR:HG22	1.86	0.76
3:E:162:VAL:HG21	3:E:188:LEU:HD11	1.68	0.76
3:F:70:ALA:HB3	3:F:161:VAL:HG22	1.68	0.76
3:F:103:PHE:O	3:F:134:ALA:CB	2.33	0.76
1:A:55:LEU:O	1:A:57:LEU:HG	1.85	0.76
1:B:394:PHE:O	1:B:421:LEU:HD11	1.86	0.76
1:B:192:THR:HG22	1:B:194:ALA:H	1.51	0.75
1:A:192:THR:HG23	1:A:216:HIS:HB2	1.69	0.74
1:B:61:PRO:HG2	1:B:86:LEU:CD1	2.17	0.74
3:E:73:ALA:HB3	6:E:311:HOH:O	1.87	0.74
1:B:459:LEU:HD21	1:B:478:GLN:HB3	1.68	0.73
2:M:61:PHE:CZ	2:M:85:ASP:HB3	2.22	0.73
1:A:435:SER:CB	1:A:456:LEU:HD12	2.17	0.73
1:A:410:ILE:HG23	1:A:432:ASN:HB2	1.69	0.73
1:B:408:ASN:O	1:B:432:ASN:HB3	1.89	0.72
1:A:65:SER:O	1:A:68:THR:HG22	1.89	0.72
2:P:60:LEU:HD12	6:P:203:HOH:O	1.90	0.72
3:F:162:VAL:HG21	3:F:188:LEU:HD11	1.70	0.72
1:B:237:GLU:OE1	2:P:124:ARG:NH2	2.24	0.71
1:B:311:THR:CG2	6:B:739:HOH:O	2.38	0.71
2:P:61:PHE:CZ	2:P:85:ASP:HB3	2.25	0.71
1:B:52:CYS:SG	1:B:60:LEU:HD11	2.32	0.70
3:F:177:TYR:C	3:F:179:ASN:HA	2.10	0.70
1:B:459:LEU:O	1:B:459:LEU:HD23	1.92	0.70
1:B:61:PRO:HG2	1:B:86:LEU:HD13	1.73	0.69
3:E:128:MET:HE3	3:E:132:ARG:CZ	2.22	0.69
1:A:468:LEU:HD21	1:A:471:ILE:HD11	1.75	0.68
1:A:218:HIS:HD2	1:A:219:ASN:HD22	1.41	0.68
1:A:192:THR:HG22	1:A:194:ALA:H	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:ASP:OD1	1:B:221:ARG:HD3	1.94	0.67
1:B:85:PRO:O	1:B:86:LEU:HG	1.93	0.67
1:B:200:HIS:N	6:B:767:HOH:O	2.26	0.67
1:A:146:ASP:HB3	1:A:170:ASP:HB3	1.76	0.67
2:M:45:GLU:OE2	6:M:205:HOH:O	2.13	0.67
3:F:141:ILE:CG2	3:F:165:TRP:HB3	2.25	0.67
1:B:218:HIS:HD2	1:B:219:ASN:HD22	1.43	0.66
1:A:435:SER:HB2	1:A:456:LEU:HD12	1.78	0.66
1:B:433:LEU:O	1:B:433:LEU:HD12	1.95	0.66
1:A:468:LEU:O	1:A:539:VAL:HG11	1.95	0.66
1:B:468:LEU:HD21	1:B:471:ILE:HB	1.78	0.65
1:B:432:ASN:O	1:B:434:LEU:N	2.21	0.65
3:F:176:VAL:O	3:F:178:LYS:HA	1.97	0.65
1:B:442:LEU:HG	1:B:443:HIS:H	1.60	0.65
1:B:146:ASP:HB3	1:B:170:ASP:HB3	1.79	0.65
1:A:64:LEU:HD12	1:A:86:LEU:HD23	1.79	0.64
1:A:85:PRO:O	1:A:86:LEU:HD22	1.97	0.64
3:F:103:PHE:O	3:F:134:ALA:HB1	1.96	0.64
1:B:168:TRP:CZ3	6:P:204:HOH:O	2.50	0.64
3:E:190:GLU:HB2	3:E:191:PRO:CD	2.27	0.64
1:B:52:CYS:SG	1:B:60:LEU:CD1	2.86	0.64
1:B:61:PRO:HG3	1:B:64:LEU:HD13	1.78	0.64
2:M:48:SER:OG	3:E:110:GLU:OE2	2.11	0.64
2:P:87:ARG:CZ	6:P:201:HOH:O	2.46	0.64
1:A:59:GLU:HG2	1:A:83:PRO:HD2	1.80	0.64
3:F:70:ALA:HB3	3:F:161:VAL:CG2	2.28	0.63
1:B:429:LEU:O	1:B:432:ASN:ND2	2.32	0.63
1:B:471:ILE:CG2	1:B:541:CYS:SG	2.87	0.63
3:F:141:ILE:HG22	3:F:165:TRP:HB3	1.81	0.63
3:E:83:MET:O	3:E:105:SER:HA	1.99	0.62
1:B:142:SER:OG	1:B:166:HIS:HD2	1.80	0.62
2:M:70:ARG:HG2	3:E:181:LYS:HB3	1.82	0.62
1:A:218:HIS:CD2	1:A:219:ASN:HD22	2.17	0.61
3:F:83:MET:O	3:F:105:SER:HA	1.99	0.61
3:F:103:PHE:CZ	3:F:133:GLY:HA3	2.35	0.61
1:B:168:TRP:HZ3	6:P:204:HOH:O	1.83	0.61
1:B:351:LEU:N	1:B:352:PRO:CD	2.63	0.61
1:A:416:ASN:C	1:A:418:PHE:H	2.04	0.61
2:P:88:ASN:HD22	2:P:91:MET:H	1.48	0.61
1:A:199:HIS:HB2	1:A:223:HIS:CE1	2.36	0.60
1:B:335:LEU:C	1:B:335:LEU:HD23	2.21	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:HIS:CD2	1:B:219:ASN:HD22	2.20	0.60
1:A:351:LEU:N	1:A:352:PRO:CD	2.65	0.60
1:A:274:GLU:O	1:A:299:SER:HB2	2.02	0.60
2:M:88:ASN:HB3	6:M:209:HOH:O	2.02	0.60
1:A:315:ALA:HB3	1:A:318:ILE:HD12	1.84	0.60
1:A:377:GLN:HA	1:A:400:LEU:HA	1.82	0.60
3:F:73:ALA:HB2	3:F:161:VAL:HG13	1.82	0.60
3:F:184:VAL:HG12	3:F:185:ARG:N	2.16	0.60
1:B:298:ARG:NH1	6:B:758:HOH:O	2.35	0.60
3:F:54:LYS:HA	3:F:55:MET:CB	2.28	0.60
3:F:182:ALA:O	3:F:183:HIS:HB2	2.02	0.60
1:B:333:LEU:C	1:B:333:LEU:HD23	2.22	0.59
1:B:315:ALA:HB3	1:B:318:ILE:HD12	1.84	0.59
3:E:46:ALA:HB2	3:E:69:PHE:CE1	2.37	0.59
1:B:267:ASN:HB2	1:B:291:ASN:HD21	1.68	0.59
1:A:63:ASN:H	1:A:63:ASN:HD22	1.50	0.58
1:B:377:GLN:HA	1:B:400:LEU:HA	1.84	0.58
1:B:141:GLN:HB2	6:B:713:HOH:O	2.02	0.58
2:P:85:ASP:N	2:P:85:ASP:OD1	2.37	0.58
1:B:144:ARG:HG2	1:B:168:TRP:CD1	2.38	0.58
1:A:86:LEU:HD12	1:A:88:SER:OG	2.03	0.58
1:A:267:ASN:HB2	1:A:291:ASN:HD21	1.68	0.58
1:A:142:SER:OG	1:A:166:HIS:HD2	1.86	0.58
1:B:435:SER:HB3	1:B:455:ALA:HB3	1.86	0.58
1:A:387:TYR:HA	1:A:410:ILE:N	2.18	0.57
1:B:389:ILE:CD1	1:B:418:PHE:HE1	2.17	0.57
1:B:410:ILE:CB	1:B:432:ASN:OD1	2.48	0.57
1:B:459:LEU:CD2	1:B:478:GLN:CB	2.54	0.57
1:B:192:THR:HG21	6:B:779:HOH:O	2.04	0.57
1:B:200:HIS:HD2	1:B:224:SER:HB2	1.70	0.57
1:A:416:ASN:HB3	1:A:419:SER:HB3	1.87	0.57
2:M:85:ASP:OD1	2:M:85:ASP:N	2.37	0.57
3:F:90:LEU:HA	3:F:128:MET:HE2	1.86	0.57
1:B:408:ASN:O	1:B:432:ASN:CB	2.53	0.57
2:P:87:ARG:NH1	6:P:201:HOH:O	2.36	0.57
1:A:415:PRO:O	1:A:439:ILE:HD13	2.05	0.56
3:F:54:LYS:CA	3:F:55:MET:HB2	2.30	0.56
3:F:175:PHE:HE2	3:F:184:VAL:HG21	1.71	0.56
1:A:82:LEU:HD23	1:A:106:PRO:HG2	1.86	0.56
1:A:85:PRO:C	1:A:86:LEU:HD22	2.26	0.56
1:A:165:ARG:HH22	2:M:120:LEU:HD23	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:ILE:HG22	1:A:439:ILE:HD12	1.88	0.56
1:A:442:LEU:C	1:A:442:LEU:HD22	2.26	0.56
1:A:333:LEU:HD23	1:A:333:LEU:C	2.26	0.56
1:A:373:CYS:HB3	1:A:376:LEU:HD22	1.86	0.56
1:A:82:LEU:HA	1:A:84:ASN:N	2.21	0.56
3:E:82:LEU:HB3	3:E:184:VAL:HG23	1.87	0.56
3:F:175:PHE:CE2	3:F:184:VAL:HG21	2.40	0.56
2:P:128:ALA:O	2:P:130:PRO:HD3	2.05	0.56
3:E:73:ALA:HB2	3:E:161:VAL:HG13	1.88	0.56
3:E:179:ASN:N	3:E:180:GLN:CA	2.69	0.56
1:B:60:LEU:HD23	1:B:60:LEU:C	2.27	0.56
1:B:373:CYS:HB3	1:B:376:LEU:HD22	1.86	0.55
2:M:76:LEU:HD23	2:M:76:LEU:N	2.21	0.55
1:B:389:ILE:HD11	1:B:418:PHE:CE1	2.35	0.55
1:B:387:TYR:O	1:B:410:ILE:HA	2.06	0.55
2:P:76:LEU:N	2:P:76:LEU:HD23	2.22	0.55
3:E:70:ALA:HB2	3:E:161:VAL:HG22	1.89	0.55
1:A:86:LEU:HB3	1:A:89:LEU:HG	1.88	0.55
1:B:199:HIS:HB2	1:B:223:HIS:CE1	2.42	0.55
1:B:61:PRO:CG	1:B:64:LEU:HD22	2.37	0.55
1:B:471:ILE:HG21	1:B:541:CYS:SG	2.46	0.55
3:E:162:VAL:HA	6:E:309:HOH:O	2.05	0.55
1:B:61:PRO:HG2	1:B:86:LEU:HD11	1.88	0.55
1:B:438:PRO:C	1:B:439:ILE:HG22	2.27	0.54
3:F:82:LEU:HB2	3:F:186:ILE:HD13	1.89	0.54
3:F:141:ILE:HG13	3:F:147:ALA:HB3	1.89	0.54
1:A:254:ARG:HD3	6:A:754:HOH:O	2.06	0.54
2:M:128:ALA:O	2:M:130:PRO:HD3	2.06	0.54
1:A:442:LEU:HD21	1:A:445:LEU:HD13	1.88	0.54
1:A:446:THR:HA	1:A:468:LEU:HA	1.90	0.54
1:B:195:LEU:N	1:B:195:LEU:HD23	2.22	0.54
1:B:64:LEU:HD21	1:B:86:LEU:HD13	1.90	0.54
1:B:265:HIS:HD2	1:B:266:SER:OG	1.90	0.54
3:E:45:LYS:HB3	3:E:66:GLU:OE2	2.07	0.54
3:F:184:VAL:CG1	3:F:185:ARG:N	2.71	0.54
3:E:90:LEU:HA	3:E:128:MET:HE2	1.90	0.53
3:F:180:GLN:O	3:F:181:LYS:C	2.46	0.53
1:B:456:LEU:O	1:B:459:LEU:HB2	2.09	0.53
1:B:252:ALA:HB1	6:B:727:HOH:O	2.09	0.53
1:A:410:ILE:CG2	1:A:432:ASN:HB2	2.37	0.53
1:A:429:LEU:O	1:A:432:ASN:HB3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:79:GLU:HB3	3:E:185:ARG:NH2	2.23	0.52
1:B:411:ALA:HB2	1:B:433:LEU:HD11	1.91	0.52
1:B:432:ASN:O	1:B:453:ASN:OD1	2.28	0.52
1:A:435:SER:HB3	1:A:456:LEU:HD12	1.90	0.52
1:A:58:SER:O	1:A:60:LEU:O	2.28	0.52
1:A:265:HIS:HD2	1:A:266:SER:OG	1.92	0.52
1:B:461:SER:OG	1:B:461:SER:O	2.20	0.52
1:B:336:THR:HG22	1:B:360:SER:HB3	1.91	0.52
1:A:395:GLN:O	1:A:396:GLN:HB2	2.09	0.52
1:A:127:ARG:CD	6:A:744:HOH:O	2.58	0.51
1:A:411:ALA:O	1:A:434:LEU:HD23	2.09	0.51
1:A:468:LEU:CD2	1:A:471:ILE:HD11	2.38	0.51
3:E:82:LEU:HB2	3:E:186:ILE:HD13	1.91	0.51
1:A:118:VAL:HG22	1:A:142:SER:HB2	1.92	0.51
2:M:119:TYR:HB3	2:M:142:CYS:HB2	1.92	0.51
1:A:435:SER:HB3	1:A:456:LEU:HA	1.93	0.51
3:F:65:LEU:HB2	3:F:168:ASP:HB3	1.93	0.51
1:A:414:HIS:CB	1:A:415:PRO:HD2	2.34	0.51
3:F:96:ASP:OD2	3:F:132:ARG:HG3	2.11	0.51
1:A:459:LEU:HG	1:A:478:GLN:HB2	1.92	0.51
1:B:55:LEU:O	1:B:56:GLY:C	2.49	0.51
1:B:370:PHE:O	1:B:397:LEU:HD21	2.11	0.50
1:B:242:ASN:ND2	1:B:265:HIS:H	2.10	0.50
1:B:448:LEU:HB3	1:B:471:ILE:HD12	1.92	0.50
1:A:418:PHE:HA	1:A:421:LEU:HD23	1.92	0.50
1:A:59:GLU:HG2	1:A:83:PRO:CD	2.41	0.50
1:A:442:LEU:HD21	1:A:445:LEU:HD22	1.92	0.50
2:M:61:PHE:CE2	2:M:85:ASP:HB3	2.47	0.50
3:F:135:SER:HB3	3:F:159:TRP:HB3	1.93	0.50
1:B:201:ILE:HG22	1:B:229:CYS:HB2	1.93	0.50
3:E:58:THR:O	3:E:60:LYS:N	2.45	0.50
1:B:462:SER:O	1:B:464:ASN:N	2.41	0.50
1:A:311:THR:HB	1:A:334:THR:HB	1.93	0.50
1:A:370:PHE:O	1:A:397:LEU:HD21	2.12	0.49
1:B:60:LEU:HB3	1:B:61:PRO:CD	2.34	0.49
3:F:185:ARG:HD3	3:F:186:ILE:N	2.27	0.49
1:A:63:ASN:H	1:A:63:ASN:ND2	2.09	0.49
1:B:82:LEU:HG	1:B:106:PRO:HG3	1.94	0.49
1:B:242:ASN:HD22	1:B:265:HIS:H	1.61	0.48
1:B:311:THR:HB	1:B:334:THR:HB	1.94	0.48
2:P:56:CYS:HB3	6:P:203:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:69:ILE:CG2	3:F:82:LEU:O	2.62	0.48
1:A:59:GLU:HG2	1:A:83:PRO:HG2	1.96	0.48
1:A:247:ASP:HB2	6:A:721:HOH:O	2.13	0.48
1:A:432:ASN:OD1	1:A:453:ASN:HB3	2.14	0.48
2:P:61:PHE:CE2	2:P:85:ASP:HB3	2.47	0.48
3:E:190:GLU:O	3:E:191:PRO:O	2.30	0.48
1:A:201:ILE:HG22	1:A:229:CYS:HB2	1.94	0.48
1:A:59:GLU:O	1:A:60:LEU:C	2.51	0.48
1:A:96:ARG:HA	1:A:120:MET:HB2	1.95	0.48
1:B:450:LEU:CD1	1:B:453:ASN:ND2	2.61	0.48
2:P:75:CYS:CB	6:P:203:HOH:O	2.52	0.48
3:F:52:PRO:C	3:F:54:LYS:H	2.16	0.48
1:A:269:ILE:H	1:A:291:ASN:HD22	1.62	0.48
1:A:360:SER:HB3	1:A:361:TYR:CD1	2.48	0.48
1:A:403:LEU:CD1	1:A:403:LEU:C	2.82	0.48
1:B:403:LEU:CD1	1:B:403:LEU:C	2.82	0.48
1:B:459:LEU:HD13	1:B:475:TYR:HB2	1.95	0.48
1:A:171:ASP:HA	1:A:195:LEU:O	2.14	0.48
1:A:322:PRO:HB3	6:A:733:HOH:O	2.12	0.47
1:A:59:GLU:CG	1:A:83:PRO:HG2	2.44	0.47
3:E:97:ASP:HB3	3:E:99:LEU:CD1	2.44	0.47
1:B:403:LEU:HD11	1:B:405:LEU:HG	1.96	0.47
1:A:459:LEU:CD2	1:A:475:TYR:HD1	2.28	0.47
1:B:204:TYR:OH	1:B:228:LYS:HE2	2.15	0.47
1:B:436:SER:HA	1:B:437:PHE:HA	1.80	0.47
1:B:457:GLN:O	1:B:459:LEU:N	2.40	0.47
2:M:69:ILE:HB	3:E:181:LYS:HB2	1.97	0.47
2:P:120:LEU:O	2:P:142:CYS:HA	2.14	0.47
3:F:181:LYS:HA	3:F:182:ALA:CB	2.32	0.47
3:E:175:PHE:CZ	3:E:182:ALA:HB3	2.50	0.47
1:A:55:LEU:O	1:A:56:GLY:C	2.51	0.47
1:A:127:ARG:HD3	6:A:744:HOH:O	2.13	0.47
1:B:400:LEU:C	1:B:400:LEU:HD23	2.35	0.47
3:E:70:ALA:N	6:E:309:HOH:O	2.48	0.47
3:E:182:ALA:O	3:E:184:VAL:HG22	2.15	0.47
1:B:122:GLN:HG3	1:B:144:ARG:HB3	1.97	0.47
3:F:90:LEU:HA	3:F:128:MET:CE	2.45	0.47
1:B:275:LYS:O	1:B:278:VAL:HG22	2.14	0.46
1:A:242:ASN:ND2	1:A:265:HIS:H	2.13	0.46
3:E:140:ASP:C	3:E:140:ASP:OD1	2.52	0.46
3:E:189:LYS:O	3:E:190:GLU:O	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:425:ILE:HG22	1:B:426:LYS:HG2	1.98	0.46
1:A:122:GLN:HG3	1:A:144:ARG:HB3	1.98	0.46
1:A:146:ASP:CB	1:A:170:ASP:HB3	2.44	0.46
1:B:96:ARG:HA	1:B:120:MET:HB2	1.98	0.46
1:B:298:ARG:HE	1:B:320:GLU:HG2	1.81	0.46
3:E:49:ARG:NH1	3:E:61:LEU:HB3	2.29	0.46
3:E:70:ALA:CB	3:E:161:VAL:HG22	2.45	0.46
3:F:48:ILE:HB	3:F:65:LEU:HD22	1.96	0.46
1:B:143:LEU:O	1:B:168:TRP:HD1	1.97	0.46
1:B:269:ILE:H	1:B:291:ASN:HD22	1.64	0.46
3:E:90:LEU:HA	3:E:128:MET:CE	2.46	0.46
1:A:336:THR:HG22	1:A:360:SER:HB2	1.98	0.46
1:A:457:GLN:O	1:A:459:LEU:N	2.44	0.46
1:B:61:PRO:HB3	1:B:62:SER:C	2.35	0.46
2:P:48:SER:OG	3:F:110:GLU:OE2	2.23	0.46
1:A:459:LEU:HD23	1:A:475:TYR:HD1	1.81	0.46
2:P:69:ILE:N	2:P:69:ILE:HD13	2.31	0.46
3:E:135:SER:O	3:E:160:PRO:HD2	2.16	0.46
3:F:140:ASP:OD1	3:F:140:ASP:C	2.54	0.46
3:F:177:TYR:C	3:F:177:TYR:CD1	2.90	0.46
1:A:410:ILE:HG23	1:A:433:LEU:H	1.81	0.46
1:A:416:ASN:ND2	1:A:441:GLY:HA3	2.31	0.46
1:B:168:TRP:CD1	1:B:168:TRP:N	2.84	0.46
2:P:99:ILE:HG23	2:P:102:CYS:CB	2.46	0.46
1:B:154:PRO:HA	1:B:155:PRO:HD3	1.83	0.45
1:A:200:HIS:HB3	6:A:712:HOH:O	2.15	0.45
2:M:70:ARG:CG	3:E:181:LYS:HB3	2.45	0.45
2:P:68:ASP:OD2	3:F:178:LYS:HB3	2.16	0.45
1:A:51:ASP:OD1	1:A:53:SER:HB3	2.17	0.45
3:E:93:ALA:O	3:E:94:SER:O	2.34	0.45
1:A:275:LYS:O	1:A:278:VAL:HG22	2.15	0.45
1:A:425:ILE:HG22	1:A:426:LYS:HG2	1.98	0.45
1:A:413:ILE:HG21	1:A:418:PHE:HE2	1.82	0.45
1:A:416:ASN:C	1:A:418:PHE:N	2.69	0.45
1:B:478:GLN:HA	1:B:481:ALA:HB3	1.98	0.45
3:E:72:VAL:HG12	3:E:157:LEU:HD12	1.98	0.45
3:F:184:VAL:CG1	3:F:185:ARG:H	2.30	0.45
1:A:411:ALA:HA	1:A:433:LEU:O	2.17	0.45
3:F:117:ARG:CZ	3:F:117:ARG:HB3	2.47	0.45
1:A:413:ILE:HG21	1:A:418:PHE:CE2	2.52	0.45
1:A:448:LEU:HB3	1:A:471:ILE:CD1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:LEU:N	1:B:83:PRO:CD	2.80	0.45
1:A:199:HIS:HB2	1:A:223:HIS:HE1	1.78	0.45
3:E:190:GLU:HB2	3:E:191:PRO:HD3	1.98	0.45
1:B:85:PRO:C	1:B:86:LEU:HG	2.33	0.44
1:A:403:LEU:HD11	1:A:405:LEU:HG	1.98	0.44
1:A:471:ILE:CG2	1:A:472:GLU:N	2.80	0.44
1:A:459:LEU:HD22	1:A:474:PRO:HG2	2.00	0.44
1:B:106:PRO:HD2	1:B:109:ALA:HB2	1.99	0.44
1:A:341:SER:HA	1:A:363:LEU:O	2.17	0.44
2:M:50:VAL:HG11	3:E:108:LYS:HB2	1.99	0.44
1:A:469:LYS:C	1:A:539:VAL:HG13	2.38	0.44
1:B:242:ASN:HD22	1:B:265:HIS:N	2.16	0.44
1:B:61:PRO:HB3	1:B:62:SER:CA	2.48	0.43
1:B:84:ASN:ND2	1:B:85:PRO:O	2.50	0.43
1:B:456:LEU:HD23	1:B:474:PRO:HG2	1.99	0.43
3:F:54:LYS:CA	3:F:55:MET:CB	2.94	0.43
3:F:56:ASP:N	3:F:56:ASP:OD1	2.50	0.43
1:B:118:VAL:HG22	1:B:142:SER:HB2	2.00	0.43
3:E:175:PHE:CE2	3:E:182:ALA:HB3	2.53	0.43
1:B:351:LEU:N	1:B:352:PRO:HD2	2.34	0.43
2:P:88:ASN:HB3	2:P:91:MET:O	2.18	0.43
2:M:50:VAL:HG11	3:E:108:LYS:CB	2.49	0.43
1:A:388:GLU:HB3	6:A:738:HOH:O	2.17	0.43
1:A:442:LEU:CD2	1:A:445:LEU:HD13	2.48	0.43
1:B:171:ASP:HA	1:B:195:LEU:O	2.19	0.43
1:B:414:HIS:CG	1:B:415:PRO:HD2	2.54	0.43
1:B:459:LEU:HD12	1:B:474:PRO:HG2	1.99	0.43
1:A:413:ILE:CG2	1:A:439:ILE:HD12	2.48	0.43
1:B:52:CYS:HB2	1:B:73:LEU:HD12	2.00	0.43
1:B:335:LEU:HD23	1:B:335:LEU:O	2.19	0.43
1:B:418:PHE:HD1	1:B:418:PHE:N	2.17	0.43
2:P:99:ILE:HG23	2:P:102:CYS:HB2	2.01	0.42
3:F:177:TYR:C	3:F:177:TYR:HD1	2.22	0.42
1:B:146:ASP:CB	1:B:170:ASP:HB3	2.48	0.42
1:B:442:LEU:HD11	1:B:445:LEU:CD2	2.49	0.42
1:A:343:LEU:C	6:A:735:HOH:O	2.57	0.42
1:B:51:ASP:C	1:B:51:ASP:OD1	2.56	0.42
1:B:84:ASN:ND2	1:B:86:LEU:HD11	2.34	0.42
1:B:435:SER:CB	1:B:455:ALA:HB3	2.50	0.42
1:B:371:SER:N	6:B:745:HOH:O	2.53	0.42
1:B:442:LEU:HD11	1:B:445:LEU:HD22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:CYS:HB2	1:A:73:LEU:HD12	2.01	0.42
1:B:75:MET:CE	1:B:75:MET:HA	2.49	0.42
2:P:69:ILE:HG22	3:F:83:MET:HA	2.01	0.42
1:A:351:LEU:N	1:A:352:PRO:HD2	2.35	0.42
1:B:403:LEU:C	1:B:403:LEU:HD12	2.40	0.42
1:A:265:HIS:HB2	1:A:289:TYR:O	2.20	0.42
1:A:266:SER:HA	1:A:290:ASP:O	2.20	0.42
1:B:265:HIS:HB2	1:B:289:TYR:O	2.20	0.42
2:P:124:ARG:HG3	2:P:126:TYR:CZ	2.55	0.42
1:A:459:LEU:HD11	1:A:473:MET:CE	2.50	0.42
1:B:438:PRO:CB	1:B:439:ILE:HG22	2.36	0.42
3:F:175:PHE:HA	3:F:179:ASN:HD21	1.84	0.42
1:A:82:LEU:HD13	1:A:84:ASN:HB2	2.02	0.41
2:M:42:LYS:HB3	2:M:42:LYS:HE2	1.74	0.41
1:A:123:ASN:HA	1:A:147:ALA:O	2.20	0.41
1:B:457:GLN:C	1:B:459:LEU:N	2.73	0.41
1:A:394:PHE:O	1:A:421:LEU:HD11	2.19	0.41
1:A:400:LEU:HD23	1:A:400:LEU:C	2.40	0.41
1:B:418:PHE:N	1:B:418:PHE:CD1	2.87	0.41
1:B:479:CYS:SG	1:B:542:SER:N	2.93	0.41
1:A:373:CYS:O	1:A:376:LEU:HB2	2.20	0.41
1:A:390:LYS:HA	1:A:414:HIS:CG	2.54	0.41
1:A:409:LYS:HA	6:F:301:HOH:O	2.20	0.41
1:A:459:LEU:HD23	1:A:475:TYR:CD1	2.55	0.41
1:B:299:SER:O	1:B:300:ALA:C	2.57	0.41
2:P:60:LEU:HD22	2:P:77:PRO:HA	2.02	0.41
2:P:116:GLU:HA	2:P:117:GLY:HA2	1.76	0.41
1:A:154:PRO:HA	1:A:155:PRO:HD3	1.83	0.41
1:A:403:LEU:C	1:A:403:LEU:HD12	2.41	0.41
1:B:61:PRO:CB	1:B:62:SER:CA	2.98	0.41
1:B:341:SER:HA	1:B:363:LEU:O	2.20	0.41
3:E:177:TYR:O	3:E:178:LYS:C	2.58	0.41
1:A:410:ILE:HG23	1:A:410:ILE:O	2.21	0.41
3:F:178:LYS:O	3:F:182:ALA:HB2	2.21	0.41
1:A:144:ARG:HG2	1:A:168:TRP:CE3	2.55	0.41
1:A:415:PRO:O	1:A:439:ILE:CD1	2.69	0.41
1:B:61:PRO:CG	1:B:64:LEU:HD13	2.49	0.41
1:A:414:HIS:HB3	1:A:415:PRO:CD	2.35	0.41
1:A:468:LEU:HD21	1:A:471:ILE:CD1	2.48	0.41
1:B:333:LEU:C	1:B:333:LEU:CD2	2.88	0.41
1:B:373:CYS:O	1:B:376:LEU:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:378:LYS:HG3	1:B:402:SER:HB3	2.02	0.41
2:M:116:GLU:HA	2:M:117:GLY:HA2	1.78	0.41
1:A:63:ASN:ND2	1:A:63:ASN:N	2.69	0.40
1:B:266:SER:HA	1:B:290:ASP:O	2.21	0.40
1:B:459:LEU:HD22	1:B:477:TYR:CE1	2.56	0.40
1:A:145:LEU:HB2	1:A:169:LEU:HD13	2.04	0.40
1:A:461:SER:O	1:A:478:GLN:NE2	2.54	0.40
1:B:192:THR:CG2	1:B:216:HIS:HB2	2.44	0.40
1:A:82:LEU:HD13	1:A:84:ASN:CB	2.52	0.40
1:A:134:LEU:O	1:A:161:LEU:HD21	2.21	0.40
2:P:50:VAL:O	2:P:70:ARG:NH1	2.52	0.40
3:E:69:PHE:CZ	3:E:188:LEU:HD21	2.56	0.40
1:B:340:ILE:H	1:B:362:ASN:HD22	1.70	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	458/531 (86%)	389 (85%)	58 (13%)	11 (2%)	5	8
1	B	459/531 (86%)	392 (85%)	56 (12%)	11 (2%)	5	8
2	M	94/115 (82%)	82 (87%)	10 (11%)	2 (2%)	5	10
2	P	91/115 (79%)	80 (88%)	8 (9%)	3 (3%)	3	4
3	E	147/160 (92%)	120 (82%)	19 (13%)	8 (5%)	1	1
3	F	146/160 (91%)	119 (82%)	19 (13%)	8 (6%)	1	1
All	All	1395/1612 (86%)	1182 (85%)	170 (12%)	43 (3%)	3	5

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	410	ILE
1	A	430	SER
1	B	84	ASN
1	B	430	SER
1	B	438	PRO
2	M	142	CYS
3	E	94	SER
3	E	166	GLY
3	E	190	GLU
3	F	55	MET
3	F	166	GLY
1	A	53	SER
1	A	170	ASP
1	B	458	SER
3	E	59	GLY
3	E	75	ILE
3	F	181	LYS
1	A	31	PRO
1	A	417	ALA
1	A	458	SER
1	B	170	ASP
1	B	435	SER
1	B	463	GLU
2	P	100	GLU
3	E	191	PRO
1	A	83	PRO
1	A	437	PHE
1	A	451	THR
1	B	543	PRO
2	M	100	GLU
2	P	68	ASP
3	E	178	LYS
3	F	133	GLY
1	A	415	PRO
1	B	37	HIS
2	P	42	LYS
3	F	53	LEU
3	F	60	LYS
3	F	178	LYS
1	B	85	PRO
1	B	439	ILE
3	F	156	GLY
3	E	156	GLY

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	418/476 (88%)	356 (85%)	62 (15%)	2	4
1	B	419/476 (88%)	354 (84%)	65 (16%)	2	4
2	M	87/95 (92%)	77 (88%)	10 (12%)	4	9
2	P	83/95 (87%)	72 (87%)	11 (13%)	3	6
3	E	124/130 (95%)	106 (86%)	18 (14%)	2	5
3	F	123/130 (95%)	98 (80%)	25 (20%)	1	2
All	All	1254/1402 (89%)	1063 (85%)	191 (15%)	2	4

All (191) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	ARG
1	A	34	CYS
1	A	37	HIS
1	A	45	ARG
1	A	53	SER
1	A	55	LEU
1	A	58	SER
1	A	63	ASN
1	A	73	LEU
1	A	81	LEU
1	A	82	LEU
1	A	113	LEU
1	A	122	GLN
1	A	127	ARG
1	A	146	ASP
1	A	169	LEU
1	A	176	GLU
1	A	192	THR
1	A	221	ARG
1	A	235	SER
1	A	246	LEU
1	A	247	ASP

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Mol	Chain	Res	Type
1	A	251	THR
1	A	255	THR
1	A	256	LEU
1	A	278	VAL
1	A	285	THR
1	A	299	SER
1	A	304	LEU
1	A	307	LEU
1	A	310	LEU
1	A	311	THR
1	A	313	ASN
1	A	316	SER
1	A	319	THR
1	A	330	LEU
1	A	335	LEU
1	A	365	GLU
1	A	367	LEU
1	A	389	ILE
1	A	390	LYS
1	A	392	ASP
1	A	398	LEU
1	A	403	LEU
1	A	425	ILE
1	A	427	LEU
1	A	429	LEU
1	A	435	SER
1	A	442	LEU
1	A	443	HIS
1	A	445	LEU
1	A	448	LEU
1	A	449	LYS
1	A	454	HIS
1	A	456	LEU
1	A	457	GLN
1	A	459	LEU
1	A	463	GLU
1	A	464	ASN
1	A	468	LEU
1	A	479	CYS
1	A	541	CYS
1	B	55	LEU
1	B	59	GLU

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Mol	Chain	Res	Type
1	B	62	SER
1	B	64	LEU
1	B	73	LEU
1	B	75	MET
1	B	77	ASN
1	B	81	LEU
1	B	86	LEU
1	B	92	LEU
1	B	113	LEU
1	B	122	GLN
1	B	127	ARG
1	B	146	ASP
1	B	168	TRP
1	B	192	THR
1	B	195	LEU
1	B	221	ARG
1	B	227	LYS
1	B	228	LYS
1	B	235	SER
1	B	246	LEU
1	B	251	THR
1	B	255	THR
1	B	256	LEU
1	B	266	SER
1	B	278	VAL
1	B	285	THR
1	B	304	LEU
1	B	307	LEU
1	B	310	LEU
1	B	311	THR
1	B	316	SER
1	B	319	THR
1	B	330	LEU
1	B	363	LEU
1	B	367	LEU
1	B	389	ILE
1	B	390	LYS
1	B	391	VAL
1	B	392	ASP
1	B	398	LEU
1	B	403	LEU
1	B	412	ILE

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Mol	Chain	Res	Type
1	B	421	LEU
1	B	425	ILE
1	B	427	LEU
1	B	429	LEU
1	B	432	ASN
1	B	436	SER
1	B	440	THR
1	B	442	LEU
1	B	445	LEU
1	B	449	LYS
1	B	450	LEU
1	B	454	HIS
1	B	456	LEU
1	B	457	GLN
1	B	462	SER
1	B	463	GLU
1	B	464	ASN
1	B	468	LEU
1	B	469	LYS
1	B	479	CYS
1	B	482	PHE
2	M	40	CYS
2	M	42	LYS
2	M	76	LEU
2	M	81	PRO
2	M	85	ASP
2	M	100	GLU
2	M	112	THR
2	M	115	LYS
2	M	124	ARG
2	M	131	GLU
2	P	40	CYS
2	P	69	ILE
2	P	76	LEU
2	P	81	PRO
2	P	85	ASP
2	P	88	ASN
2	P	100	GLU
2	P	112	THR
2	P	115	LYS
2	P	124	ARG
2	P	131	GLU

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Mol	Chain	Res	Type
3	E	56	ASP
3	E	63	LEU
3	E	66	GLU
3	E	76	THR
3	E	99	LEU
3	E	113	ARG
3	E	114	ARG
3	E	145	ARG
3	E	155	LEU
3	E	158	THR
3	E	164	ILE
3	E	165	TRP
3	E	167	ASN
3	E	180	GLN
3	E	181	LYS
3	E	184	VAL
3	E	185	ARG
3	E	189	LYS
3	F	44	GLN
3	F	55	MET
3	F	56	ASP
3	F	61	LEU
3	F	63	LEU
3	F	65	LEU
3	F	66	GLU
3	F	72	VAL
3	F	84	GLN
3	F	92	ASN
3	F	99	LEU
3	F	113	ARG
3	F	114	ARG
3	F	117	ARG
3	F	155	LEU
3	F	158	THR
3	F	161	VAL
3	F	164	ILE
3	F	167	ASN
3	F	176	VAL
3	F	177	TYR
3	F	178	LYS
3	F	183	HIS
3	F	185	ARG

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Mol	Chain	Res	Type
3	F	190	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
1	A	76	ASN
1	A	141	GLN
1	A	166	HIS
1	A	200	HIS
1	A	218	HIS
1	A	223	HIS
1	A	242	ASN
1	A	258	ASN
1	A	265	HIS
1	A	291	ASN
1	A	302	GLN
1	A	350	GLN
1	A	355	GLN
1	A	362	ASN
1	A	478	GLN
1	B	84	ASN
1	B	141	GLN
1	B	166	HIS
1	B	199	HIS
1	B	200	HIS
1	B	218	HIS
1	B	223	HIS
1	B	242	ASN
1	B	258	ASN
1	B	265	HIS
1	B	291	ASN
1	B	302	GLN
1	B	313	ASN
1	B	350	GLN
1	B	355	GLN
1	B	362	ASN
1	B	416	ASN
1	B	540	GLN
2	M	51	ASN
2	P	51	ASN
2	P	88	ASN

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Mol	Chain	Res	Type
3	E	167	ASN
3	F	179	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	$\# Z > 2$
4	NAG	B	602	1	14,14,15	0.88	0	17,19,21	1.93	5 (29%)
4	NAG	A	601	1	14,14,15	0.79	1 (7%)	17,19,21	2.12	5 (29%)

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
4	NAG	B	602	1	-	0/6/23/26	0/1/1/1
4	NAG	A	601	1	-	3/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	601	NAG	C1-C2	2.41	1.55	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	601	NAG	C4-C3-C2	-5.33	103.20	111.02
4	B	602	NAG	C1-O5-C5	-4.71	105.87	112.19
4	A	601	NAG	C1-C2-N2	4.12	116.93	110.43
4	A	601	NAG	C1-O5-C5	3.67	117.10	112.19
4	B	602	NAG	O5-C5-C6	2.90	113.32	107.66
4	B	602	NAG	C6-C5-C4	2.89	120.11	113.02
4	B	602	NAG	O5-C1-C2	-2.47	107.47	111.29
4	B	602	NAG	O7-C7-N2	2.11	125.70	121.98
4	A	601	NAG	O3-C3-C2	2.09	113.74	109.40
4	A	601	NAG	O4-C4-C5	2.01	114.28	109.32

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	601	NAG	C1-C2-N2-C7
4	A	601	NAG	C4-C5-C6-O6
4	A	601	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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	461/531 (86%)	0.56	58 (12%)	9 9	18, 66, 145, 192	1 (0%)
1	B	463/531 (87%)	0.27	38 (8%)	19 18	23, 52, 120, 159	0
2	M	98/115 (85%)	0.57	16 (16%)	5 5	32, 59, 110, 123	0
2	P	94/115 (81%)	1.13	21 (22%)	3 3	31, 83, 113, 125	0
3	E	149/160 (93%)	0.84	23 (15%)	6 6	40, 79, 132, 151	0
3	F	148/160 (92%)	1.92	64 (43%)	1 1	78, 133, 169, 200	0
All	All	1413/1612 (87%)	0.68	220 (15%)	6 6	18, 68, 148, 200	1 (0%)

All (220) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	82	LEU	9.4
1	B	81	LEU	9.1
1	B	437	PHE	6.3
3	F	176	VAL	5.7
3	F	61	LEU	5.3
3	F	53	LEU	5.3
1	A	60	LEU	5.3
3	F	175	PHE	5.2
3	E	191	PRO	5.2
1	B	84	ASN	5.0
3	E	192	PRO	4.9
2	P	132	GLY	4.9
2	P	50	VAL	4.8
2	M	117	GLY	4.5
1	A	477	TYR	4.5
3	F	63	LEU	4.2
2	P	119	TYR	4.2
1	A	453	ASN	4.1
2	M	100	GLU	4.1

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Mol	Chain	Res	Type	RSRZ
3	F	129	ALA	4.0
3	E	61	LEU	3.9
2	M	143	SER	3.9
3	F	178	LYS	3.9
3	F	85	SER	3.8
1	A	394	PHE	3.8
1	A	415	PRO	3.8
3	F	51	ILE	3.8
3	F	47	ILE	3.7
3	F	161	VAL	3.7
3	E	178	LYS	3.6
3	F	164	ILE	3.6
1	B	439	ILE	3.6
2	P	130	PRO	3.6
1	A	86	LEU	3.6
3	F	55	MET	3.6
2	M	130	PRO	3.5
1	B	61	PRO	3.5
3	F	191	PRO	3.5
1	B	59	GLU	3.5
3	F	158	THR	3.5
1	A	411	ALA	3.4
1	A	370	PHE	3.4
1	B	539	VAL	3.4
3	E	57	PRO	3.4
3	F	165	TRP	3.4
3	E	184	VAL	3.4
1	B	440	THR	3.4
1	A	432	ASN	3.3
1	A	429	LEU	3.3
1	A	455	ALA	3.3
3	F	155	LEU	3.3
1	A	410	ILE	3.3
3	F	138	LEU	3.3
2	P	117	GLY	3.3
1	A	460	ILE	3.2
3	E	181	LYS	3.2
2	M	140	MET	3.2
3	F	136	ALA	3.2
3	F	159	TRP	3.2
1	B	436	SER	3.2
2	P	114	CYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	539	VAL	3.2
1	A	437	PHE	3.2
1	B	441	GLY	3.2
3	F	188	LEU	3.1
2	P	43	GLY	3.1
1	B	482	PHE	3.1
3	F	139	PHE	3.1
1	B	465	PHE	3.1
3	F	169	ALA	3.1
1	B	459	LEU	3.0
1	B	476	ALA	3.0
3	F	46	ALA	3.0
1	A	456	LEU	3.0
1	B	443	HIS	3.0
3	F	173	MET	3.0
1	A	417	ALA	3.0
1	A	364	LEU	2.9
3	F	74	GLU	2.9
3	F	58	THR	2.9
3	F	93	ALA	2.9
1	A	442	LEU	2.9
1	B	433	LEU	2.9
1	B	543	PRO	2.9
3	F	183	HIS	2.9
1	A	393	THR	2.9
1	A	412	ILE	2.8
3	E	47	ILE	2.8
1	B	546	GLY	2.8
1	A	438	PRO	2.8
1	B	62	SER	2.8
2	M	141	GLU	2.8
3	F	108	LYS	2.8
1	A	45	ARG	2.8
1	B	480	CYS	2.8
3	E	44	GLN	2.8
2	M	139	THR	2.8
3	F	163	LEU	2.8
3	F	141	ILE	2.8
2	P	142	CYS	2.8
3	F	186	ILE	2.8
3	F	105	SER	2.8
3	F	171	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	480	CYS	2.8
1	A	391	VAL	2.8
2	M	118	LEU	2.7
1	A	443	HIS	2.7
3	E	59	GLY	2.7
3	E	190	GLU	2.7
3	F	62	ASN	2.7
2	M	132	GLY	2.7
3	F	189	LYS	2.7
1	B	475	TYR	2.7
1	A	365	GLU	2.7
2	M	142	CYS	2.7
1	A	59	GLU	2.7
3	F	166	GLY	2.7
3	F	190	GLU	2.7
2	M	127	PRO	2.6
3	E	179	ASN	2.6
1	B	458	SER	2.6
1	B	545	PRO	2.6
2	P	74	VAL	2.6
2	P	59	LYS	2.6
3	F	110	GLU	2.6
2	P	71	GLN	2.6
3	F	99	LEU	2.6
1	A	82	LEU	2.5
1	B	442	LEU	2.5
3	E	60	LYS	2.5
3	E	165	TRP	2.5
3	F	75	ILE	2.5
1	A	450	LEU	2.5
1	A	31	PRO	2.5
1	A	30	GLY	2.5
1	B	419	SER	2.4
1	A	457	GLN	2.4
3	F	76	THR	2.4
1	B	450	LEU	2.4
2	M	131	GLU	2.4
1	B	462	SER	2.4
1	A	452	GLY	2.4
3	F	102	GLY	2.4
3	E	183	HIS	2.4
1	A	459	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	418	PHE	2.4
3	E	62	ASN	2.4
3	E	175	PHE	2.4
3	E	70	ALA	2.4
3	F	59	GLY	2.4
3	F	80	GLY	2.4
1	A	448	LEU	2.3
3	F	172	LEU	2.3
2	P	109	ASN	2.3
3	F	179	ASN	2.3
2	P	69	ILE	2.3
2	P	128	ALA	2.3
1	B	60	LEU	2.3
2	P	98	LYS	2.3
1	B	391	VAL	2.3
3	F	79	GLU	2.3
1	A	78	ILE	2.3
2	M	128	ALA	2.3
3	F	81	LYS	2.3
3	F	57	PRO	2.3
3	F	101	PRO	2.3
1	A	389	ILE	2.3
1	A	481	ALA	2.3
2	P	127	PRO	2.3
3	E	164	ILE	2.3
1	A	483	GLY	2.2
3	F	83	MET	2.2
3	F	160	PRO	2.2
1	A	476	ALA	2.2
1	A	414	HIS	2.2
1	A	444	GLY	2.2
2	P	54	LEU	2.2
2	M	115	LYS	2.2
1	A	368	PRO	2.2
3	F	177	TYR	2.2
1	A	537	HIS	2.2
1	B	537	HIS	2.2
1	A	405	LEU	2.2
3	E	53	LEU	2.2
1	A	33	GLY	2.2
3	E	64	THR	2.2
1	A	85	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
2	P	72	VAL	2.2
3	F	137	VAL	2.2
1	A	39	HIS	2.2
1	A	409	LYS	2.2
1	A	458	SER	2.2
3	E	69	PHE	2.2
3	F	135	SER	2.2
1	B	456	LEU	2.1
2	P	70	ARG	2.1
1	A	446	THR	2.1
1	B	79	SER	2.1
1	B	31	PRO	2.1
3	F	50	VAL	2.1
1	A	367	LEU	2.1
2	M	119	TYR	2.1
1	B	83	PRO	2.1
1	A	395	GLN	2.1
2	P	115	LYS	2.1
3	F	107	VAL	2.1
1	B	58	SER	2.1
1	A	386	ILE	2.1
1	A	447	HIS	2.1
1	A	343	LEU	2.1
1	B	448	LEU	2.1
3	F	65	LEU	2.1
3	F	109	LEU	2.1
3	F	126	ALA	2.1
2	M	68	ASP	2.1
1	B	418	PHE	2.0
3	F	111	SER	2.0
2	P	118	LEU	2.0
3	F	181	LYS	2.0
3	E	152	GLN	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 ⓘ

There are no monosaccharides 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(\AA^2)	Q<0.9
4	NAG	A	601	14/15	0.79	0.12	66,82,88,95	0
4	NAG	B	602	14/15	0.86	0.10	54,60,66,67	0
5	NI	B	601	1/1	0.99	0.02	44,44,44,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.