



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:47 AM UTC

PDB ID : 5OSH / pdb_00005osh
Title : Structure of retromer VPS29-VPS35C subunits complexed with RidL N-terminal domain (1-236)
Authors : Romano-Moreno, M.; Rojas, A.L.; Lucas, M.; Isupov, M.N.; Hierro, A.
Deposited on : 2017-08-17
Resolution : 4.30 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:

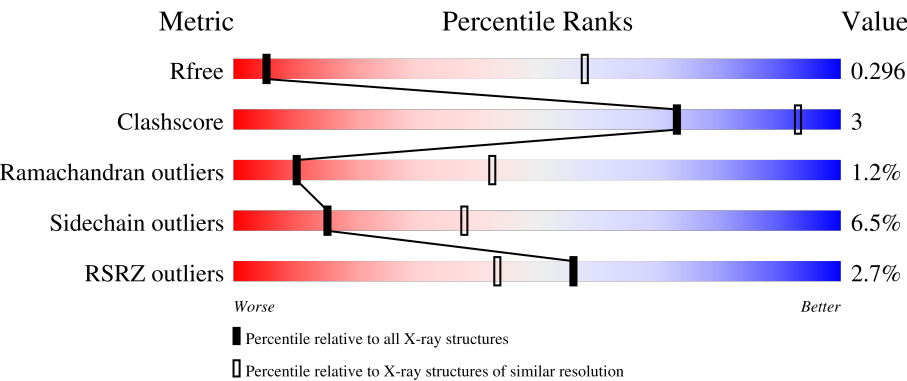
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 4.30 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	1052 (4.70-3.90)
Clashscore	190562	1097 (4.70-3.90)
Ramachandran outliers	187476	1001 (4.70-3.90)
Sidechain outliers	187428	1007 (4.72-3.88)
RSRZ outliers	180081	1049 (4.70-3.90)

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

Mol	Chain	Length	Quality of chain
1	A	182	2% 83% 16% .
1	D	182	% 79% 21%
1	G	182	4% 85% 14% .
1	J	182	10% 92% 8%
2	B	299	% 82% 16% .

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Mol	Chain	Length	Quality of chain
2	E	299	2% 87% 10% ..
2	H	299	3% 87% 9% .
2	K	299	% 86% 10% ..
3	C	223	4% 83% 12% ..
3	F	223	2% 76% 17% ..
3	I	223	2% 85% 13% .
3	L	223	% 81% 11% 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 22276 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 Vacuolar protein sorting-associated protein 29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	182	Total	C	N	O	S	0	0	0
			1447	936	242	263	6			
1	D	182	Total	C	N	O	S	0	0	0
			1447	936	242	263	6			
1	G	182	Total	C	N	O	S	0	0	0
			1447	936	242	263	6			
1	J	182	Total	C	N	O	S	0	0	0
			1447	936	242	263	6			

- Molecule 2 is a protein called Vacuolar protein sorting-associated protein 35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	299	Total	C	N	O	S	0	0	0
			2424	1539	423	452	10			
2	E	294	Total	C	N	O	S	0	0	0
			2383	1514	418	441	10			
2	H	290	Total	C	N	O	S	0	0	0
			2344	1491	408	435	10			
2	K	293	Total	C	N	O	S	0	0	0
			2374	1509	417	438	10			

- Molecule 3 is a protein called Interaptin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	217	Total	C	N	O	S	0	0	0
			1750	1103	299	344	4			
3	F	214	Total	C	N	O	S	0	0	0
			1723	1085	294	340	4			
3	I	223	Total	C	N	O	S	0	0	0
			1802	1135	306	356	5			
3	L	209	Total	C	N	O	S	0	0	0
			1688	1062	288	334	4			

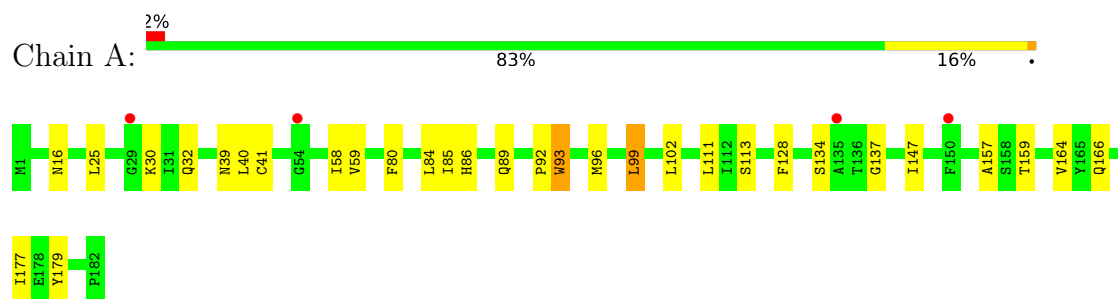
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	MET	-	initiating methionine	UNP G8UZ99
C	2	ALA	-	expression tag	UNP G8UZ99
F	1	MET	-	initiating methionine	UNP G8UZ99
F	2	ALA	-	expression tag	UNP G8UZ99
I	1	MET	-	initiating methionine	UNP G8UZ99
I	2	ALA	-	expression tag	UNP G8UZ99
L	1	MET	-	initiating methionine	UNP G8UZ99
L	2	ALA	-	expression tag	UNP G8UZ99

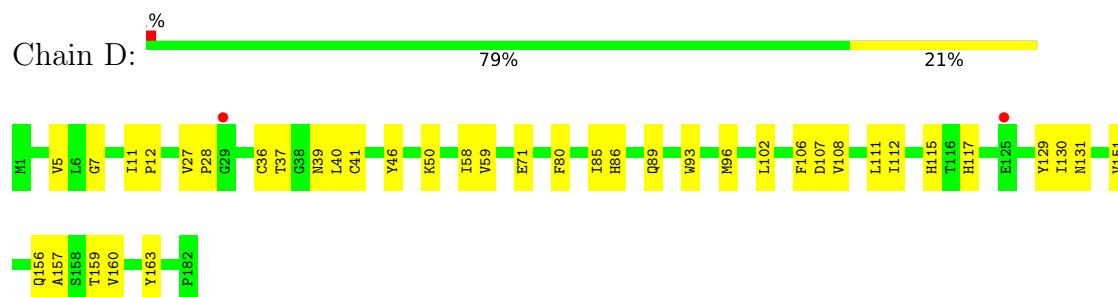
3 Residue-property plots [i](#)

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

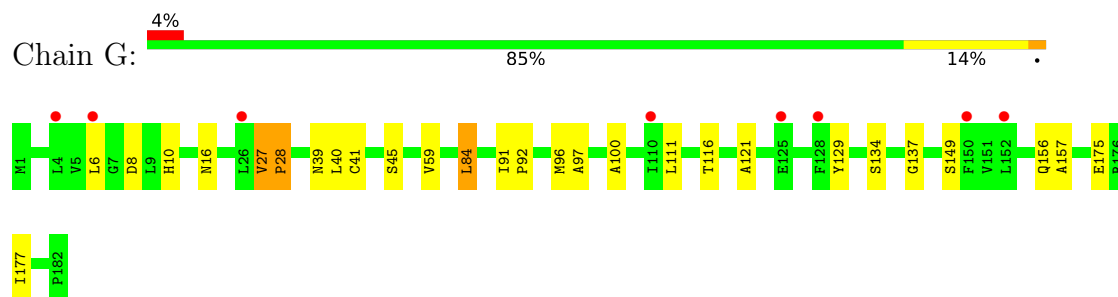
- Molecule 1: Vacuolar protein sorting-associated protein 29



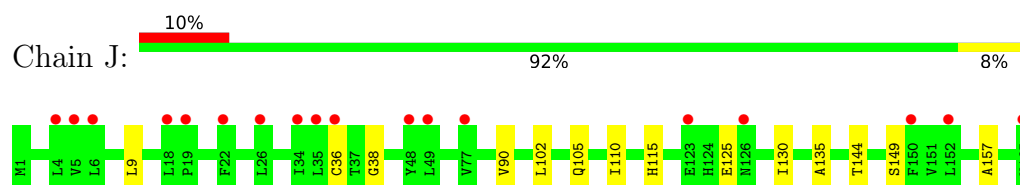
- Molecule 1: Vacuolar protein sorting-associated protein 29



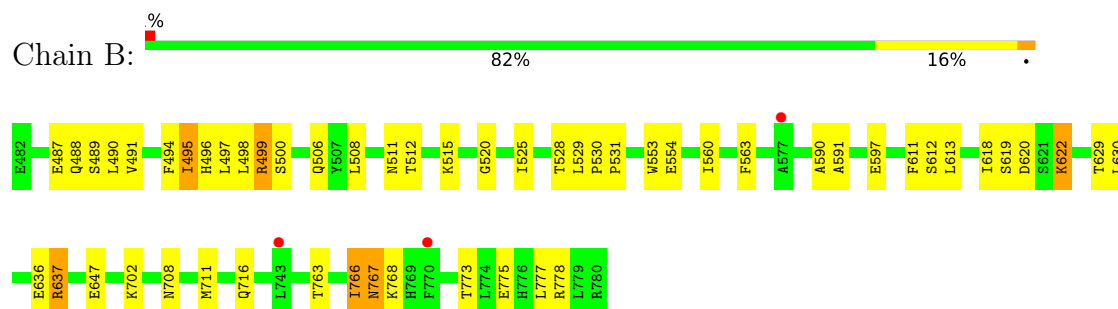
- Molecule 1: Vacuolar protein sorting-associated protein 29



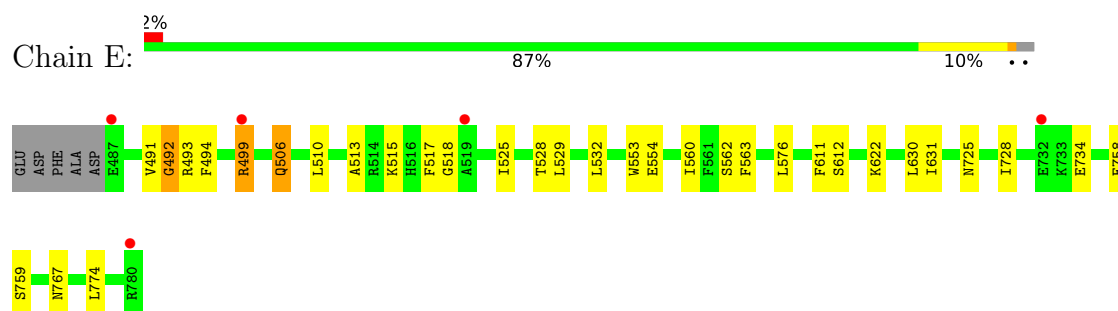
- Molecule 1: Vacuolar protein sorting-associated protein 29



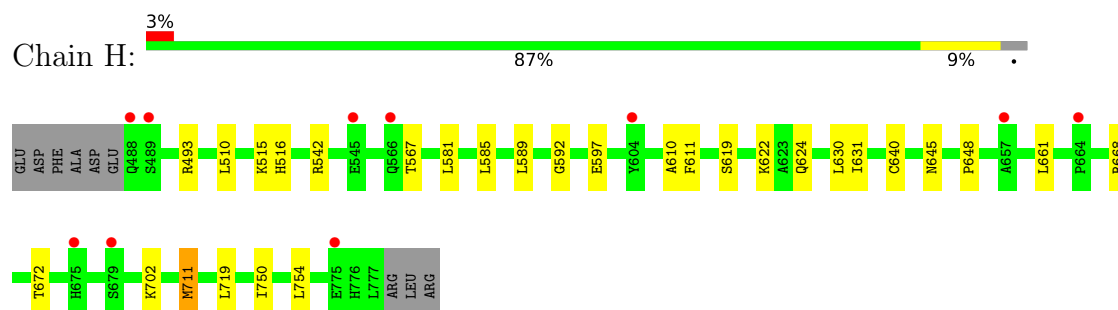
- Molecule 2: Vacuolar protein sorting-associated protein 35



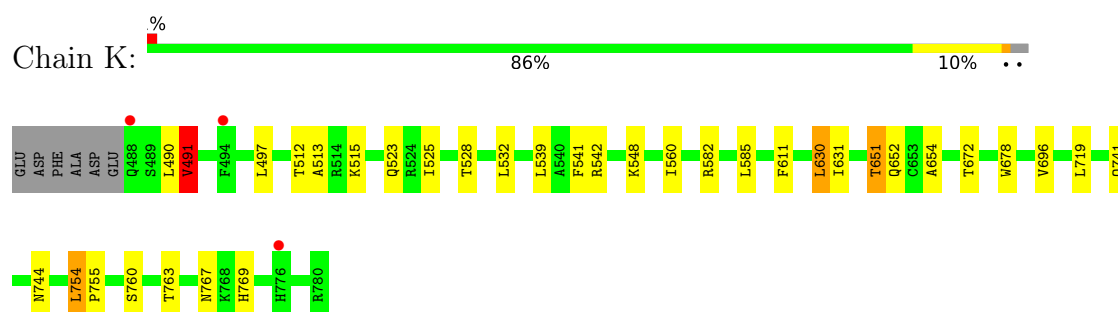
- Molecule 2: Vacuolar protein sorting-associated protein 35



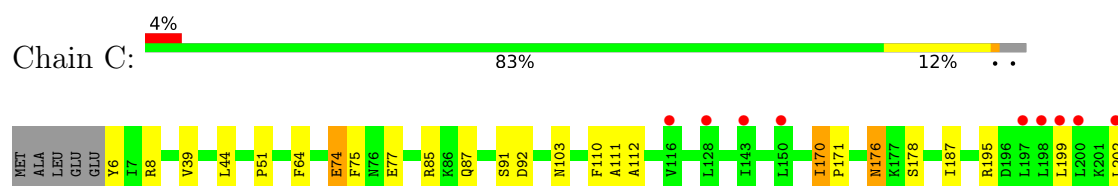
- Molecule 2: Vacuolar protein sorting-associated protein 35

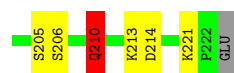


- Molecule 2: Vacuolar protein sorting-associated protein 35

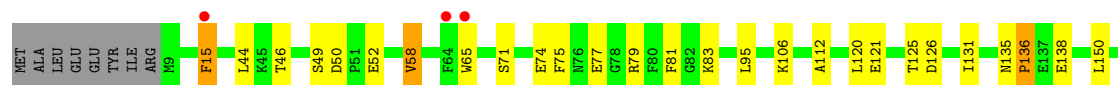
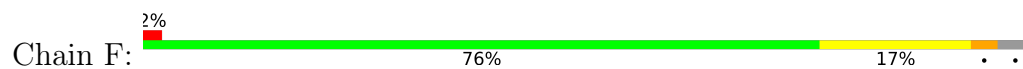


- Molecule 3: Interaptin

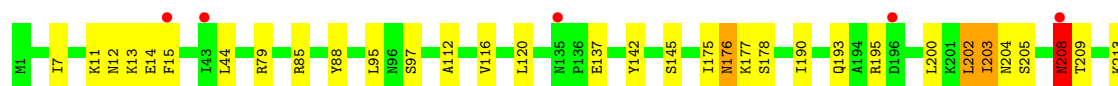
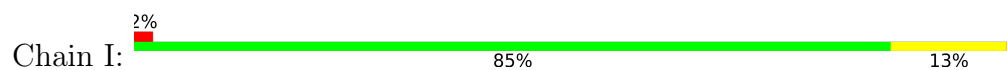




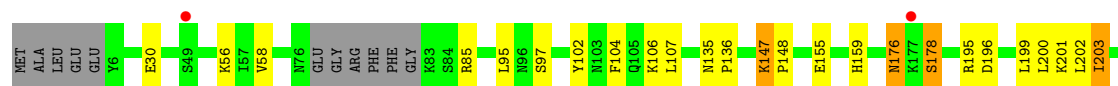
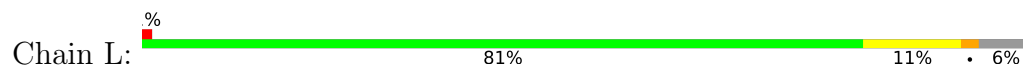
• Molecule 3: Interaptin



• Molecule 3: Interaptin



• Molecule 3: Interaptin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	90.20Å 173.24Å 445.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	222.89 – 4.30 222.89 – 4.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (222.89-4.30) 99.9 (222.89-4.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 4.30Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.254 , 0.311 0.249 , 0.296	Depositor DCC
R_{free} test set	2460 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	216.4	Xtriage
Anisotropy	0.285	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 405.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	22276	wwPDB-VP
Average B, all atoms (Å ²)	266.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.70	0/1481	0.95	1/2008 (0.0%)
1	D	0.76	1/1481 (0.1%)	1.02	0/2008
1	G	0.74	0/1481	0.93	2/2008 (0.1%)
1	J	0.65	0/1481	0.80	0/2008
2	B	0.76	0/2471	0.97	1/3327 (0.0%)
2	E	0.75	0/2429	0.94	0/3270
2	H	0.69	0/2390	0.95	0/3219
2	K	0.81	0/2420	0.89	0/3258
3	C	0.73	0/1783	1.00	5/2401 (0.2%)
3	F	0.77	0/1755	1.00	0/2362
3	I	0.83	0/1835	1.03	0/2469
3	L	0.75	0/1717	0.93	1/2311 (0.0%)
All	All	0.75	1/22724 (0.0%)	0.95	10/30649 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	159	THR	CA-CB	5.35	1.57	1.53

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	28	PRO	N-CA-C	6.47	121.40	111.11
3	C	171	PRO	N-CA-C	-6.21	103.13	110.70
1	G	27	VAL	CB-CA-C	6.13	115.34	109.33
3	L	203	ILE	CB-CA-C	-5.81	104.87	111.55
3	C	74	GLU	N-CA-C	5.76	118.42	110.35
3	C	170	ILE	CA-C-N	-5.53	114.68	120.38
3	C	170	ILE	C-N-CA	-5.53	114.68	120.38
2	B	618	ILE	N-CA-C	5.27	115.37	107.51
3	C	210	GLN	N-CA-C	5.22	119.28	113.01
1	A	80	PHE	N-CA-C	5.05	118.18	110.20

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	1447	0	1459	13	0
1	D	1447	0	1459	17	0
1	G	1447	0	1459	10	0
1	J	1447	0	1459	7	0
2	B	2424	0	2407	21	0
2	E	2383	0	2379	11	0
2	H	2344	0	2336	9	0
2	K	2374	0	2373	18	0
3	C	1750	0	1726	8	0
3	F	1723	0	1704	21	0
3	I	1802	0	1783	15	0
3	L	1688	0	1673	7	0
All	All	22276	0	22217	141	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 3.

All (141) 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:I:11:LYS:NZ	3:I:88:TYR:OH	2.19	0.75
3:L:176:ASN:ND2	3:L:178:SER:OG	2.26	0.69
1:A:134:SER:OG	1:A:137:GLY:N	2.30	0.64
1:G:27:VAL:HG22	1:G:28:PRO:HD2	1.84	0.60
3:L:58:VAL:HG21	3:L:95:LEU:HD11	1.83	0.59
1:A:25:LEU:O	3:C:170:ILE:HD11	2.03	0.58
3:I:202:LEU:HD22	2:K:512:THR:HG21	1.85	0.58
3:I:202:LEU:HD22	2:K:512:THR:CG2	2.34	0.57
1:D:106:PHE:HB3	1:D:108:VAL:HG13	1.87	0.57
2:B:499:ARG:HA	2:B:506:GLN:HE22	1.71	0.55
2:K:525:ILE:HA	2:K:528:THR:HG22	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:131:ILE:HD11	3:F:150:LEU:HD11	1.87	0.55
1:D:80:PHE:CE2	1:D:160:VAL:HB	2.43	0.54
3:I:11:LYS:O	3:I:13:LYS:N	2.41	0.54
2:E:525:ILE:HA	2:E:528:THR:HG22	1.90	0.54
2:E:491:VAL:O	2:E:492:GLY:C	2.50	0.53
1:A:92:PRO:O	1:A:93:TRP:C	2.52	0.53
1:A:39:ASN:OD1	1:A:86:HIS:NE2	2.41	0.52
2:K:585:LEU:HD13	2:K:630:LEU:HD22	1.91	0.52
2:B:525:ILE:HA	2:B:528:THR:HG22	1.90	0.52
2:K:611:PHE:CZ	2:K:631:ILE:HG21	2.44	0.52
3:C:44:LEU:HD21	3:C:112:ALA:N	2.25	0.51
1:J:90:VAL:HG22	1:J:102:LEU:CD1	2.41	0.51
3:C:176:ASN:ND2	3:C:178:SER:OG	2.44	0.51
3:I:176:ASN:HD22	3:I:177:LYS:N	2.09	0.51
2:E:510:LEU:O	2:E:513:ALA:HB3	2.10	0.51
2:H:581:LEU:HD21	2:H:631:ILE:HD11	1.93	0.51
1:A:147:ILE:HG21	1:A:166:GLN:HE21	1.76	0.51
3:F:58:VAL:HG21	3:F:95:LEU:HD11	1.93	0.51
2:H:581:LEU:HD23	2:H:610:ALA:HB1	1.91	0.50
1:D:163:TYR:CE1	3:F:172:PRO:HG2	2.47	0.50
2:K:585:LEU:CD1	2:K:630:LEU:HD22	2.41	0.50
2:B:497:LEU:CD2	3:F:219:MET:HE2	2.43	0.49
2:E:517:PHE:O	2:E:528:THR:HG21	2.13	0.49
1:D:111:LEU:HD23	1:D:112:ILE:N	2.28	0.49
1:G:59:VAL:HG13	1:G:84:LEU:HD13	1.95	0.48
1:J:110:ILE:HG21	1:J:130:ILE:HD12	1.94	0.48
3:F:135:ASN:O	3:F:136:PRO:C	2.56	0.48
3:C:210:GLN:O	3:C:214:ASP:HB2	2.12	0.48
1:D:46:TYR:CZ	1:D:50:LYS:HE3	2.48	0.48
3:F:125:THR:HG23	3:F:198:LEU:HD11	1.95	0.48
2:E:529:LEU:O	2:E:532:LEU:N	2.46	0.48
2:B:529:LEU:N	2:B:530:PRO:CD	2.77	0.47
3:I:205:SER:HB3	3:I:208:ASN:HA	1.97	0.47
1:J:9:LEU:CD1	1:J:135:ALA:HB3	2.43	0.47
2:B:763:THR:HA	2:B:766:ILE:HD11	1.96	0.47
3:F:135:ASN:ND2	3:F:138:GLU:OE2	2.47	0.47
3:L:102:TYR:HB3	3:L:107:LEU:HD21	1.96	0.47
2:B:498:LEU:O	2:B:499:ARG:C	2.56	0.47
3:F:167:THR:OG1	3:F:173:LYS:N	2.48	0.47
1:D:5:VAL:HB	1:D:151:VAL:HB	1.96	0.47
3:I:200:LEU:O	3:I:204:ASN:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:91:ILE:HA	1:G:92:PRO:C	2.39	0.47
2:K:678:TRP:HB2	2:K:696:VAL:HG21	1.96	0.47
2:B:500:SER:OG	3:F:195:ARG:NH2	2.48	0.46
1:J:9:LEU:HD11	1:J:135:ALA:HB3	1.97	0.46
2:B:560:ILE:O	2:B:563:PHE:HB3	2.15	0.46
3:I:116:VAL:HG11	3:I:190:ILE:HG21	1.97	0.46
1:D:40:LEU:N	1:D:41:CYS:HA	2.31	0.46
1:A:85:ILE:HD11	1:A:89:GLN:HB2	1.97	0.46
2:H:750:ILE:O	2:H:754:LEU:N	2.48	0.46
1:J:144:THR:HG21	2:K:541:PHE:CD1	2.51	0.46
3:L:97:SER:HA	3:L:104:PHE:CD1	2.51	0.46
1:J:36:CYS:SG	1:J:38:GLY:N	2.89	0.46
2:B:525:ILE:HA	2:B:528:THR:CG2	2.46	0.45
2:E:499:ARG:HB2	2:E:506:GLN:HE22	1.80	0.45
3:F:215:LEU:HD11	3:F:219:MET:HE3	1.97	0.45
3:C:110:PHE:O	3:C:111:ALA:C	2.58	0.45
2:E:553:TRP:CE2	2:E:554:GLU:HG3	2.52	0.45
1:A:99:LEU:HD21	1:A:113:SER:HB3	1.99	0.45
2:B:619:SER:OG	2:B:620:ASP:N	2.48	0.45
2:H:585:LEU:HD13	2:H:630:LEU:HD22	1.99	0.45
2:B:491:VAL:O	2:B:495:ILE:HG22	2.17	0.45
3:F:120:LEU:O	3:F:121:GLU:C	2.59	0.45
2:B:590:ALA:O	2:B:591:ALA:C	2.59	0.45
1:G:8:ASP:HA	1:G:39:ASN:HB2	1.99	0.45
2:K:513:ALA:HB3	2:K:532:LEU:HD21	1.99	0.45
2:B:494:PHE:HD2	3:F:219:MET:HE1	1.82	0.44
2:E:518:GLY:HA2	2:E:525:ILE:HG22	1.99	0.44
1:D:39:ASN:OD1	1:D:86:HIS:NE2	2.50	0.44
3:I:219:MET:HE2	2:K:491:VAL:CG1	2.47	0.44
2:B:497:LEU:HD23	3:F:219:MET:HE2	2.00	0.44
2:B:636:GLU:CD	2:B:636:GLU:C	2.86	0.44
1:D:27:VAL:HG22	1:D:28:PRO:HD2	2.00	0.44
2:H:668:ARG:O	2:H:672:THR:OG1	2.32	0.44
2:K:513:ALA:HB3	2:K:532:LEU:HD11	1.99	0.44
3:C:39:VAL:HG21	3:C:64:PHE:CD2	2.53	0.43
2:K:651:THR:HG22	2:K:654:ALA:HB3	2.00	0.43
1:J:105:GLN:HA	2:K:769:HIS:CD2	2.53	0.43
2:E:560:ILE:O	2:E:563:PHE:HB3	2.18	0.43
1:G:40:LEU:N	1:G:41:CYS:HA	2.32	0.43
2:H:645:ASN:O	2:H:648:PRO:HG2	2.18	0.43
1:D:107:ASP:O	1:D:107:ASP:CG	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:10:HIS:HA	1:G:41:CYS:SG	2.58	0.43
1:D:85:ILE:HD11	1:D:89:GLN:HB2	2.01	0.43
3:I:176:ASN:ND2	3:I:178:SER:OG	2.52	0.43
2:B:767:ASN:HD22	2:B:768:LYS:N	2.16	0.43
2:K:513:ALA:CB	2:K:532:LEU:HD11	2.48	0.43
1:D:36:CYS:HB3	1:D:58:ILE:HD13	2.01	0.43
2:K:539:LEU:HD23	2:K:560:ILE:HD12	2.01	0.43
1:A:40:LEU:N	1:A:41:CYS:HA	2.32	0.42
2:E:725:ASN:HA	2:E:728:ILE:HD12	2.00	0.42
3:F:15:PHE:HE1	3:F:65:TRP:CD2	2.37	0.42
3:F:125:THR:O	3:F:126:ASP:C	2.62	0.42
3:F:192:GLU:O	3:F:195:ARG:HG3	2.19	0.42
1:A:128:PHE:HB2	1:A:179:TYR:CE2	2.54	0.42
3:F:44:LEU:HD11	3:F:112:ALA:HA	2.02	0.42
3:C:87:GLN:O	3:C:91:SER:HB3	2.19	0.42
3:I:44:LEU:HD21	3:I:112:ALA:CA	2.49	0.42
1:A:58:ILE:HG22	1:A:59:VAL:N	2.35	0.42
2:K:754:LEU:HB2	2:K:755:PRO:HD3	2.01	0.42
2:E:630:LEU:O	2:E:631:ILE:C	2.63	0.41
2:H:589:LEU:O	2:H:592:GLY:N	2.53	0.41
1:D:130:ILE:HG22	1:D:131:ASN:N	2.35	0.41
1:A:59:VAL:HG21	1:A:86:HIS:N	2.36	0.41
2:B:708:ASN:HA	2:B:716:GLN:HE21	1.85	0.41
1:D:129:TYR:C	1:D:130:ILE:HG13	2.45	0.41
3:F:191:LYS:O	3:F:192:GLU:C	2.64	0.41
1:A:30:LYS:CD	3:C:170:ILE:HD12	2.51	0.41
3:F:181:VAL:HG22	3:F:182:LEU:HG	2.02	0.41
2:B:512:THR:HG21	3:F:202:LEU:HB3	2.03	0.41
3:I:15:PHE:CD2	3:I:95:LEU:HD21	2.56	0.41
3:I:203:ILE:HG22	2:K:512:THR:CG2	2.51	0.41
3:L:147:LYS:HA	3:L:148:PRO:HA	1.86	0.41
1:A:93:TRP:HB2	2:B:637:ARG:HD2	2.02	0.41
1:D:11:ILE:HA	1:D:12:PRO:HA	1.85	0.41
1:D:93:TRP:CZ3	1:D:115:HIS:NE2	2.87	0.41
1:G:40:LEU:HB3	1:G:45:SER:HB2	2.03	0.41
3:I:142:TYR:HA	3:I:145:SER:OG	2.21	0.41
2:K:582:ARG:HG2	2:K:630:LEU:HD13	2.03	0.41
3:F:161:TRP:CE3	3:F:181:VAL:HG11	2.56	0.40
1:D:7:GLY:HA3	1:D:37:THR:OG1	2.21	0.40
1:G:97:ALA:HA	1:G:100:ALA:HB3	2.04	0.40
2:B:530:PRO:N	2:B:531:PRO:HD2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:121:ALA:HA	1:G:129:TYR:O	2.22	0.40
1:G:134:SER:OG	1:G:137:GLY:N	2.53	0.40
2:H:516:HIS:NE2	3:L:202:LEU:O	2.54	0.40
2:H:711:MET:SD	2:H:711:MET:N	2.94	0.40
3:I:137:GLU:HB3	3:I:175:ILE:HB	2.03	0.40
2:B:553:TRP:CE2	2:B:554:GLU:HG3	2.56	0.40
3:L:135:ASN:HB2	3:L:136:PRO:HD2	2.02	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	180/182 (99%)	160 (89%)	17 (9%)	3 (2%)	7	35
1	D	180/182 (99%)	157 (87%)	21 (12%)	2 (1%)	11	45
1	G	180/182 (99%)	160 (89%)	18 (10%)	2 (1%)	11	45
1	J	180/182 (99%)	157 (87%)	20 (11%)	3 (2%)	7	35
2	B	297/299 (99%)	259 (87%)	34 (11%)	4 (1%)	9	41
2	E	292/299 (98%)	265 (91%)	25 (9%)	2 (1%)	18	55
2	H	288/299 (96%)	265 (92%)	20 (7%)	3 (1%)	12	47
2	K	291/299 (97%)	264 (91%)	25 (9%)	2 (1%)	18	55
3	C	215/223 (96%)	190 (88%)	24 (11%)	1 (0%)	24	62
3	F	212/223 (95%)	182 (86%)	26 (12%)	4 (2%)	6	32
3	I	221/223 (99%)	198 (90%)	19 (9%)	4 (2%)	6	33
3	L	205/223 (92%)	184 (90%)	19 (9%)	2 (1%)	12	47
All	All	2741/2816 (97%)	2441 (89%)	268 (10%)	32 (1%)	10	42

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	157	ALA
2	B	496	HIS
1	D	157	ALA
3	F	50	ASP
3	F	71	SER
1	G	157	ALA
2	H	640	CYS
3	I	12	ASN
2	B	499	ARG
2	B	520	GLY
1	G	96	MET
2	H	493	ARG
3	I	208	ASN
1	J	157	ALA
2	E	492	GLY
3	I	209	THR
2	K	760	SER
3	L	159	HIS
1	A	96	MET
1	D	117	HIS
3	F	79	ARG
3	F	136	PRO
2	H	661	LEU
3	I	97	SER
1	A	93	TRP
2	E	493	ARG
1	J	115	HIS
1	J	125	GLU
3	L	147	LYS
2	B	622	LYS
3	C	51	PRO
2	K	491	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	160/160 (100%)	151 (94%)	9 (6%)	19	42
1	D	160/160 (100%)	155 (97%)	5 (3%)	35	56
1	G	160/160 (100%)	151 (94%)	9 (6%)	19	42
1	J	160/160 (100%)	159 (99%)	1 (1%)	78	80
2	B	260/260 (100%)	235 (90%)	25 (10%)	8	26
2	E	256/260 (98%)	242 (94%)	14 (6%)	19	43
2	H	252/260 (97%)	240 (95%)	12 (5%)	23	45
2	K	255/260 (98%)	238 (93%)	17 (7%)	15	37
3	C	192/198 (97%)	174 (91%)	18 (9%)	8	27
3	F	190/198 (96%)	171 (90%)	19 (10%)	7	24
3	I	198/198 (100%)	186 (94%)	12 (6%)	17	39
3	L	187/198 (94%)	170 (91%)	17 (9%)	9	28
All	All	2430/2472 (98%)	2272 (94%)	158 (6%)	15	38

All (158) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	32	GLN
1	A	84	LEU
1	A	99	LEU
1	A	102	LEU
1	A	111	LEU
1	A	159	THR
1	A	164	VAL
1	A	177	ILE
2	B	487	GLU
2	B	488	GLN
2	B	489	SER
2	B	490	LEU
2	B	495	ILE
2	B	508	LEU
2	B	511	ASN
2	B	515	LYS
2	B	597	GLU
2	B	611	PHE
2	B	612	SER
2	B	613	LEU
2	B	622	LYS

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Mol	Chain	Res	Type
2	B	629	THR
2	B	630	LEU
2	B	637	ARG
2	B	647	GLU
2	B	702	LYS
2	B	711	MET
2	B	766	ILE
2	B	767	ASN
2	B	773	THR
2	B	775	GLU
2	B	777	LEU
2	B	778	ARG
3	C	6	TYR
3	C	8	ARG
3	C	74	GLU
3	C	75	PHE
3	C	77	GLU
3	C	85	ARG
3	C	92	ASP
3	C	103	ASN
3	C	176	ASN
3	C	187	ILE
3	C	195	ARG
3	C	199	LEU
3	C	202	LEU
3	C	205	SER
3	C	206	SER
3	C	210	GLN
3	C	213	LYS
3	C	221	LYS
1	D	59	VAL
1	D	71	GLU
1	D	96	MET
1	D	102	LEU
1	D	156	GLN
2	E	494	PHE
2	E	499	ARG
2	E	506	GLN
2	E	515	LYS
2	E	562	SER
2	E	576	LEU
2	E	611	PHE

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Mol	Chain	Res	Type
2	E	612	SER
2	E	622	LYS
2	E	734	GLU
2	E	758	GLU
2	E	759	SER
2	E	767	ASN
2	E	774	LEU
3	F	15	PHE
3	F	46	THR
3	F	49	SER
3	F	52	GLU
3	F	58	VAL
3	F	74	GLU
3	F	75	PHE
3	F	77	GLU
3	F	81	PHE
3	F	83	LYS
3	F	106	LYS
3	F	167	THR
3	F	170	ILE
3	F	176	ASN
3	F	187	ILE
3	F	195	ARG
3	F	197	LEU
3	F	202	LEU
3	F	203	ILE
1	G	6	LEU
1	G	16	ASN
1	G	84	LEU
1	G	111	LEU
1	G	116	THR
1	G	149	SER
1	G	156	GLN
1	G	175	GLU
1	G	177	ILE
2	H	510	LEU
2	H	515	LYS
2	H	542	ARG
2	H	567	THR
2	H	597	GLU
2	H	611	PHE
2	H	619	SER

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Mol	Chain	Res	Type
2	H	622	LYS
2	H	624	GLN
2	H	702	LYS
2	H	711	MET
2	H	719	LEU
3	I	7	ILE
3	I	14	GLU
3	I	79	ARG
3	I	85	ARG
3	I	120	LEU
3	I	176	ASN
3	I	193	GLN
3	I	195	ARG
3	I	202	LEU
3	I	203	ILE
3	I	208	ASN
3	I	213	LYS
1	J	149	SER
2	K	490	LEU
2	K	491	VAL
2	K	497	LEU
2	K	515	LYS
2	K	523	GLN
2	K	542	ARG
2	K	548	LYS
2	K	630	LEU
2	K	651	THR
2	K	652	GLN
2	K	672	THR
2	K	719	LEU
2	K	741	GLN
2	K	744	ASN
2	K	754	LEU
2	K	763	THR
2	K	767	ASN
3	L	30	GLU
3	L	56	LYS
3	L	85	ARG
3	L	106	LYS
3	L	155	GLU
3	L	176	ASN
3	L	178	SER

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Mol	Chain	Res	Type
3	L	195	ARG
3	L	196	ASP
3	L	199	LEU
3	L	200	LEU
3	L	201	LYS
3	L	203	ILE
3	L	208	ASN
3	L	210	GLN
3	L	213	LYS
3	L	215	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	HIS
1	A	124	HIS
1	A	166	GLN
2	B	505	GLN
2	B	506	GLN
2	B	624	GLN
2	B	645	ASN
2	B	716	GLN
2	B	735	ASN
2	B	744	ASN
2	B	767	ASN
2	B	769	HIS
3	C	68	HIS
3	C	103	ASN
3	C	105	GLN
3	C	134	ASN
3	C	152	ASN
3	C	176	ASN
3	C	210	GLN
1	D	10	HIS
1	D	72	GLN
1	D	79	GLN
1	D	105	GLN
1	D	156	GLN
2	E	506	GLN
2	E	511	ASN
2	E	546	ASN
2	E	666	GLN

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Mol	Chain	Res	Type
3	F	68	HIS
3	F	96	ASN
3	F	114	GLN
3	F	134	ASN
3	F	176	ASN
3	F	208	ASN
1	G	10	HIS
1	G	16	ASN
1	G	124	HIS
1	G	145	ASN
2	H	496	HIS
2	H	538	GLN
2	H	546	ASN
2	H	598	ASN
2	H	652	GLN
2	H	718	GLN
2	H	744	ASN
2	H	771	HIS
2	H	772	ASN
3	I	61	HIS
3	I	96	ASN
3	I	134	ASN
3	I	152	ASN
3	I	176	ASN
3	I	193	GLN
3	I	208	ASN
1	J	79	GLN
1	J	140	ASN
2	K	505	GLN
2	K	522	ASN
2	K	566	GLN
2	K	769	HIS
2	K	771	HIS
2	K	772	ASN
3	L	96	ASN
3	L	134	ASN
3	L	135	ASN
3	L	157	ASN
3	L	176	ASN
3	L	208	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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](#)

There are no ligands in this entry.

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	182/182 (100%)	0.08	4 (2%) 62 48	124, 191, 258, 292	0
1	D	182/182 (100%)	-0.15	2 (1%) 78 62	126, 182, 255, 298	0
1	G	182/182 (100%)	0.31	8 (4%) 39 34	185, 263, 320, 362	0
1	J	182/182 (100%)	0.44	19 (10%) 11 15	219, 314, 372, 462	0
2	B	299/299 (100%)	0.05	3 (1%) 79 64	140, 230, 338, 449	0
2	E	294/299 (98%)	-0.01	5 (1%) 69 54	121, 229, 313, 387	0
2	H	290/299 (96%)	0.18	10 (3%) 48 38	165, 275, 377, 435	0
2	K	293/299 (97%)	-0.05	3 (1%) 79 64	235, 343, 441, 539	0
3	C	217/223 (97%)	0.07	9 (4%) 41 35	132, 216, 314, 371	0
3	F	214/223 (95%)	0.08	4 (1%) 66 51	148, 226, 334, 438	0
3	I	223/223 (100%)	0.03	5 (2%) 62 48	210, 307, 384, 453	0
3	L	209/223 (93%)	0.07	3 (1%) 73 58	209, 315, 401, 451	0
All	All	2767/2816 (98%)	0.08	75 (2%) 56 43	121, 261, 385, 539	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	4	LEU	4.9
1	J	22	PHE	4.8
3	C	199	LEU	4.8
1	J	150	PHE	4.7
1	J	6	LEU	4.6
3	L	177	LYS	4.1
1	J	49	LEU	4.0
1	J	19	PRO	3.8
1	J	26	LEU	3.8
2	H	664	PRO	3.7
3	L	220	SER	3.7

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Mol	Chain	Res	Type	RSRZ
3	C	198	LEU	3.7
1	J	165	TYR	3.4
1	J	35	LEU	3.4
1	J	34	ILE	3.3
3	C	200	LEU	3.2
1	J	36	CYS	3.1
1	J	77	VAL	3.1
3	C	150	LEU	3.1
3	F	65	TRP	3.1
2	H	489	SER	3.0
3	F	222	PRO	3.0
1	A	135	ALA	3.0
1	D	125	GLU	3.0
1	A	150	PHE	2.9
3	F	15	PHE	2.9
2	B	770	PHE	2.9
1	J	48	TYR	2.8
3	I	43	ILE	2.8
1	D	29	GLY	2.8
2	H	488	GLN	2.8
2	E	519	ALA	2.8
2	E	732	GLU	2.7
1	A	29	GLY	2.7
1	G	6	LEU	2.6
2	H	679	SER	2.6
1	G	150	PHE	2.6
1	J	5	VAL	2.6
2	K	494	PHE	2.6
1	G	110	ILE	2.6
1	A	54	GLY	2.5
1	G	26	LEU	2.5
3	C	116	VAL	2.5
2	E	487	GLU	2.5
1	G	128	PHE	2.5
2	H	657	ALA	2.5
1	J	126	ASN	2.5
2	H	604	TYR	2.5
1	G	4	LEU	2.4
3	I	196	ASP	2.4
1	J	18	LEU	2.4
2	H	775	GLU	2.3
3	I	208	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
3	L	49	SER	2.3
2	K	488	GLN	2.3
3	C	143	ILE	2.3
2	K	776	HIS	2.2
2	H	675	HIS	2.2
3	C	128	LEU	2.2
3	I	15	PHE	2.2
3	I	135	ASN	2.2
1	J	168	ILE	2.2
2	B	743	LEU	2.2
2	H	545	GLU	2.2
3	C	197	LEU	2.1
3	C	202	LEU	2.1
1	J	152	LEU	2.1
1	G	125	GLU	2.0
2	E	780	ARG	2.0
3	F	64	PHE	2.0
2	B	577	ALA	2.0
2	H	566	GLN	2.0
2	E	499	ARG	2.0
1	G	152	LEU	2.0
1	J	123	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.