Full wwPDB X-ray Structure Validation Report (i)

Jun 17, 2024 – 07:25 AM EDT

PDB ID	:	5OSH
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 (i) 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 (1)) were used in the production of this report:

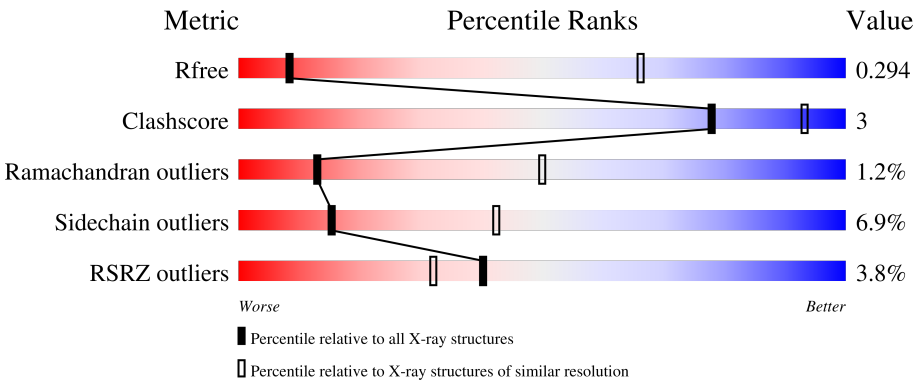
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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}	130704	1014 (4.80-3.80)
Clashscore	141614	1077 (4.80-3.80)
Ramachandran outliers	138981	1029 (4.80-3.80)
Sidechain outliers	138945	1012 (4.80-3.80)
RSRZ outliers	127900	1075 (4.90-3.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	83% 16% •
1	D	182	81% 19%
1	G	182	5% 85% 15% •
1	J	182	10% 92% 8%
2	B	299	2% 85% 13% •

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Mol	Chain	Length	Quality of chain
2	E	299	86% 11%
2	H	299	5% 88% 8%
2	K	299	12% 85% 12%
3	C	223	% 83% 13%
3	F	223	2% 76% 17%
3	I	223	2% 85% 13%
3	L	223	4% 79% 13% 6%

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	182	1447	936	242	263	6	0	0	0
1	D	182	1447	936	242	263	6	0	0	0
1	G	182	1447	936	242	263	6	0	0	0
1	J	182	1447	936	242	263	6	0	0	0

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

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

- Molecule 3 is a protein called Interaptin.

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

There are 8 discrepancies between the modelled and reference sequences:

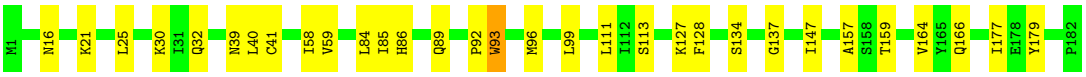
Chain	Residue	Modelled	Actual	Comment	Reference
C	1	MET	-	initiating methionine	UNP G8UZ99
C	2	ALA	-	expression tag	UNP G8UZ99
F	1	MET	-	initiating methionine	UNP G8UZ99
F	2	ALA	-	expression tag	UNP G8UZ99
I	1	MET	-	initiating methionine	UNP G8UZ99
I	2	ALA	-	expression tag	UNP G8UZ99
L	1	MET	-	initiating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

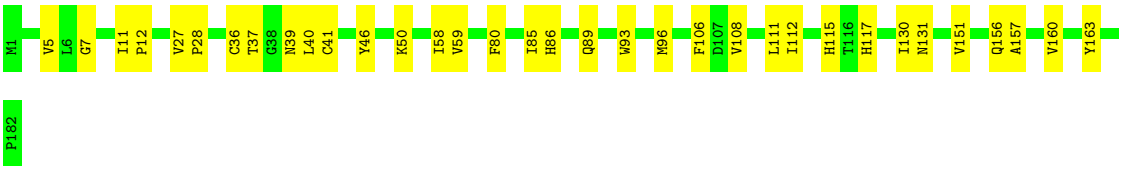
• Molecule 1: Vacuolar protein sorting-associated protein 29

Chain A:



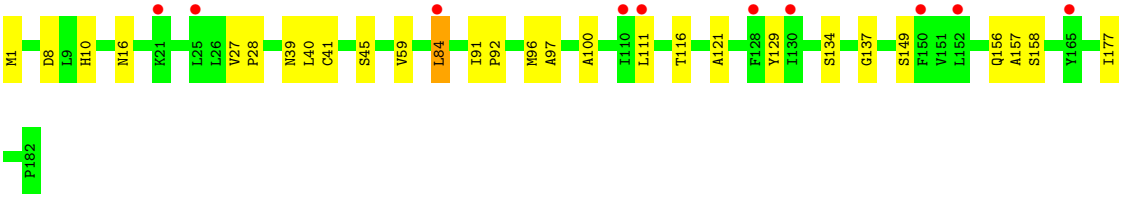
• Molecule 1: Vacuolar protein sorting-associated protein 29

Chain D:



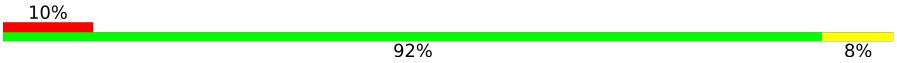
• Molecule 1: Vacuolar protein sorting-associated protein 29

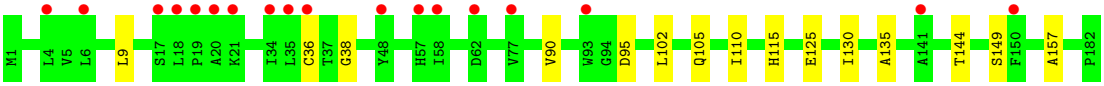
Chain G:



• Molecule 1: Vacuolar protein sorting-associated protein 29

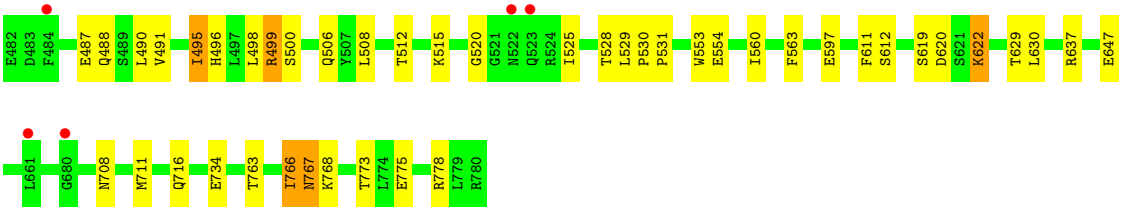
Chain J:





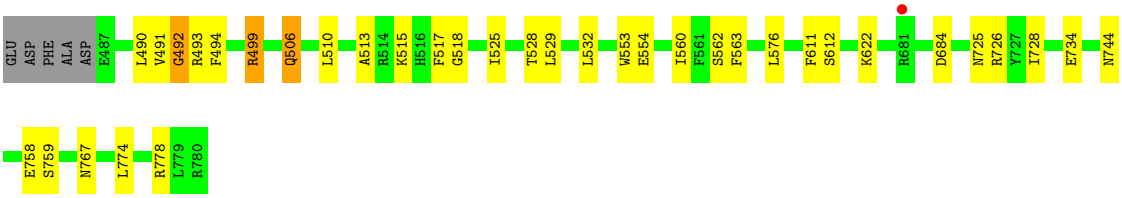
• Molecule 2: Vacuolar protein sorting-associated protein 35

Chain B:



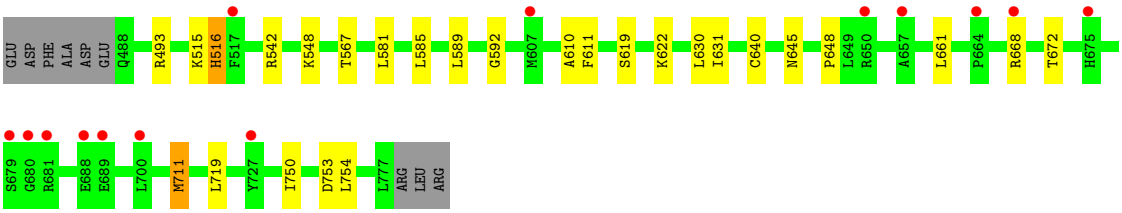
• Molecule 2: Vacuolar protein sorting-associated protein 35

Chain E:



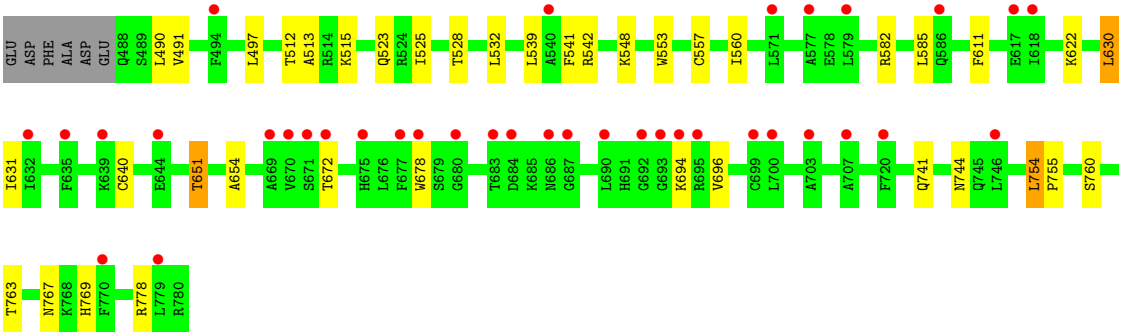
• Molecule 2: Vacuolar protein sorting-associated protein 35

Chain H:



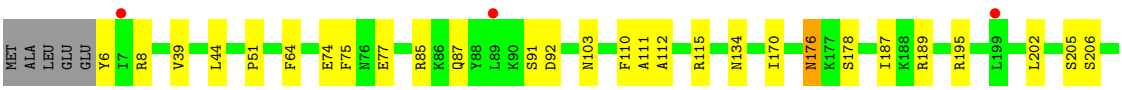
• Molecule 2: Vacuolar protein sorting-associated protein 35

Chain K:



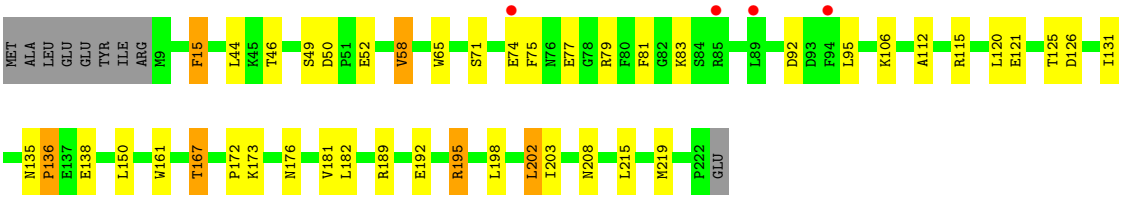
• Molecule 3: Interaptin

Chain C:



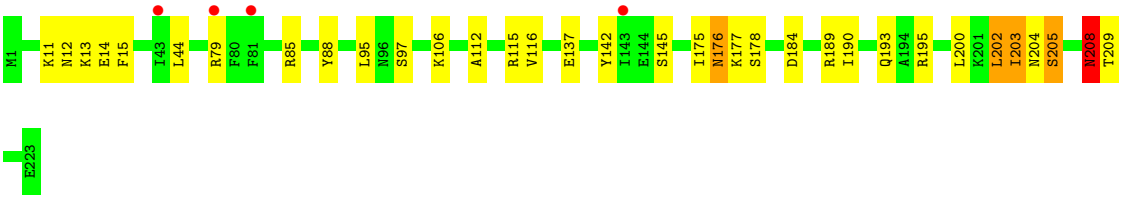
• Molecule 3: Interaptin

Chain F:



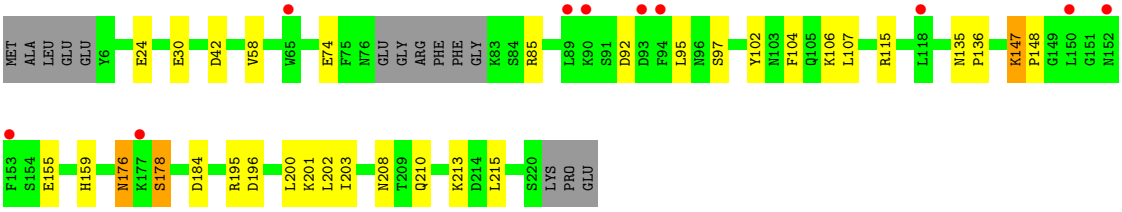
• Molecule 3: Interaptin

Chain I:



• Molecule 3: Interaptin

Chain L:



4 Data and refinement statistics (i)

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 – 4.30 112.79 – 4.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (222.89-4.30) 100.0 (112.79-4.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.24 (at 4.30Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.254 , 0.311 0.249 , 0.294	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)	0.27 , 238.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	0.54	0/1481	0.78	0/2008
1	D	0.56	0/1481	0.77	0/2008
1	G	0.53	0/1481	0.71	0/2008
1	J	0.45	0/1481	0.63	0/2008
2	B	0.56	0/2471	0.69	0/3327
2	E	0.54	0/2429	0.69	0/3270
2	H	0.50	0/2390	0.64	0/3219
2	K	0.54	0/2420	0.64	0/3258
3	C	0.55	0/1783	0.71	0/2401
3	F	0.56	0/1755	0.71	0/2362
3	I	0.57	0/1835	0.70	0/2469
3	L	0.51	0/1717	0.65	0/2311
All	All	0.54	0/22724	0.69	0/30649

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	15	0
1	G	1447	0	1459	10	0
1	J	1447	0	1459	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2424	0	2407	16	0
2	E	2383	0	2379	10	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	16	0
3	I	1802	0	1783	14	0
3	L	1688	0	1673	7	0
All	All	22276	0	22217	131	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 (131) 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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:E:491:VAL:O	2:E:492:GLY:C	2.50	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:215:LEU:HD11	3:F:219:MET:HE3	1.94	0.48
1:A:92:PRO:O	1:A:93:TRP:C	2.52	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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
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
3:F:135:ASN:O	3:F:136:PRO:C	2.56	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: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
2:B:498:LEU:O	2:B:499:ARG:C	2.56	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: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
1:G:91:ILE:HA	1:G:92:PRO:C	2.39	0.42
3:C:87:GLN:O	3:C:91:SER:HB3	2.19	0.42
1:D:130:ILE:HG22	1:D:131:ASN:N	2.35	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:H:589:LEU:O	2:H:592:GLY:N	2.53	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:553:TRP:O	2:K:557:CYS:SG	2.75	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:C:110:PHE:O	3:C:111:ALA:C	2.58	0.40
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
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:F:120:LEU:O	3:F:121:GLU:C	2.59	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%)	9 43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	180/182 (99%)	157 (87%)	21 (12%)	2 (1%)	14	52
1	G	180/182 (99%)	160 (89%)	18 (10%)	2 (1%)	14	52
1	J	180/182 (99%)	157 (87%)	20 (11%)	3 (2%)	9	43
2	B	297/299 (99%)	259 (87%)	34 (11%)	4 (1%)	12	48
2	E	292/299 (98%)	265 (91%)	25 (9%)	2 (1%)	22	62
2	H	288/299 (96%)	265 (92%)	20 (7%)	3 (1%)	15	54
2	K	291/299 (97%)	264 (91%)	25 (9%)	2 (1%)	22	62
3	C	215/223 (96%)	190 (88%)	24 (11%)	1 (0%)	29	68
3	F	212/223 (95%)	182 (86%)	26 (12%)	4 (2%)	8	41
3	I	221/223 (99%)	198 (90%)	19 (9%)	4 (2%)	8	42
3	L	205/223 (92%)	184 (90%)	19 (9%)	2 (1%)	15	54
All	All	2741/2816 (97%)	2441 (89%)	268 (10%)	32 (1%)	13	50

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

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Mol	Chain	Res	Type
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 (i)

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%)	21	48
1	D	160/160 (100%)	157 (98%)	3 (2%)	57	75
1	G	160/160 (100%)	151 (94%)	9 (6%)	21	48
1	J	160/160 (100%)	158 (99%)	2 (1%)	69	82
2	B	260/260 (100%)	240 (92%)	20 (8%)	13	39
2	E	256/260 (98%)	237 (93%)	19 (7%)	13	40
2	H	252/260 (97%)	241 (96%)	11 (4%)	28	54
2	K	255/260 (98%)	237 (93%)	18 (7%)	14	41
3	C	192/198 (97%)	172 (90%)	20 (10%)	7	27
3	F	190/198 (96%)	169 (89%)	21 (11%)	6	25
3	I	198/198 (100%)	184 (93%)	14 (7%)	14	41
3	L	187/198 (94%)	166 (89%)	21 (11%)	6	25
All	All	2430/2472 (98%)	2263 (93%)	167 (7%)	15	42

All (167) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	21	LYS
1	A	32	GLN
1	A	84	LEU
1	A	111	LEU
1	A	127	LYS
1	A	159	THR
1	A	164	VAL
1	A	177	ILE
2	B	487	GLU
2	B	488	GLN
2	B	490	LEU
2	B	495	ILE
2	B	508	LEU
2	B	515	LYS
2	B	597	GLU
2	B	611	PHE
2	B	612	SER
2	B	622	LYS
2	B	629	THR
2	B	630	LEU
2	B	647	GLU
2	B	711	MET
2	B	734	GLU
2	B	766	ILE
2	B	767	ASN
2	B	773	THR
2	B	775	GLU
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	115	ARG
3	C	134	ASN
3	C	176	ASN
3	C	187	ILE
3	C	189	ARG
3	C	195	ARG

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Mol	Chain	Res	Type
3	C	202	LEU
3	C	205	SER
3	C	206	SER
3	C	210	GLN
3	C	217	ASP
3	C	222	PRO
1	D	59	VAL
1	D	96	MET
1	D	156	GLN
2	E	490	LEU
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
2	E	612	SER
2	E	622	LYS
2	E	684	ASP
2	E	726	ARG
2	E	734	GLU
2	E	744	ASN
2	E	758	GLU
2	E	759	SER
2	E	767	ASN
2	E	774	LEU
2	E	778	ARG
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	92	ASP
3	F	106	LYS
3	F	115	ARG
3	F	126	ASP

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Mol	Chain	Res	Type
3	F	167	THR
3	F	176	ASN
3	F	189	ARG
3	F	195	ARG
3	F	202	LEU
3	F	203	ILE
3	F	208	ASN
1	G	1	MET
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	158	SER
1	G	177	ILE
2	H	515	LYS
2	H	516	HIS
2	H	542	ARG
2	H	548	LYS
2	H	567	THR
2	H	611	PHE
2	H	619	SER
2	H	622	LYS
2	H	711	MET
2	H	719	LEU
2	H	753	ASP
3	I	14	GLU
3	I	79	ARG
3	I	85	ARG
3	I	106	LYS
3	I	115	ARG
3	I	176	ASN
3	I	184	ASP
3	I	189	ARG
3	I	193	GLN
3	I	195	ARG
3	I	202	LEU
3	I	203	ILE
3	I	205	SER
3	I	208	ASN
1	J	95	ASP

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Mol	Chain	Res	Type
1	J	149	SER
2	K	490	LEU
2	K	497	LEU
2	K	515	LYS
2	K	523	GLN
2	K	542	ARG
2	K	548	LYS
2	K	622	LYS
2	K	630	LEU
2	K	640	CYS
2	K	651	THR
2	K	672	THR
2	K	694	LYS
2	K	741	GLN
2	K	744	ASN
2	K	754	LEU
2	K	763	THR
2	K	767	ASN
2	K	778	ARG
3	L	24	GLU
3	L	30	GLU
3	L	42	ASP
3	L	74	GLU
3	L	85	ARG
3	L	92	ASP
3	L	106	LYS
3	L	115	ARG
3	L	155	GLU
3	L	176	ASN
3	L	178	SER
3	L	184	ASP
3	L	195	ARG
3	L	196	ASP
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 (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	166	GLN
2	B	505	GLN
2	B	506	GLN
2	B	624	GLN
2	B	716	GLN
2	B	767	ASN
2	B	769	HIS
3	C	103	ASN
3	C	105	GLN
3	C	134	ASN
3	C	176	ASN
3	C	193	GLN
1	D	10	HIS
1	D	72	GLN
1	D	156	GLN
2	E	506	GLN
2	E	546	ASN
2	E	598	ASN
2	E	744	ASN
3	F	68	HIS
3	F	114	GLN
3	F	176	ASN
3	F	208	ASN
1	G	10	HIS
1	G	79	GLN
1	G	124	HIS
2	H	546	ASN
2	H	772	ASN
3	I	134	ASN
3	I	176	ASN
3	I	193	GLN
3	I	208	ASN
2	K	624	GLN
2	K	769	HIS
2	K	771	HIS
3	L	134	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 monosaccharides 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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	0.21	0	100	100	124, 191, 258, 292	0
1	D	182/182 (100%)	0.07	0	100	100	126, 182, 255, 298	0
1	G	182/182 (100%)	0.29	10 (5%)	25	22	185, 263, 320, 362	0
1	J	182/182 (100%)	0.33	18 (9%)	7	7	219, 314, 372, 462	0
2	B	299/299 (100%)	0.21	5 (1%)	70	61	140, 230, 338, 449	0
2	E	294/299 (98%)	0.13	1 (0%)	94	90	121, 229, 313, 387	0
2	H	290/299 (96%)	0.29	14 (4%)	30	26	165, 275, 377, 435	0
2	K	293/299 (97%)	0.62	37 (12%)	3	5	235, 343, 441, 539	0
3	C	217/223 (97%)	0.04	3 (1%)	75	66	132, 216, 314, 371	0
3	F	214/223 (95%)	0.17	4 (1%)	66	58	148, 226, 334, 438	0
3	I	223/223 (100%)	-0.00	4 (1%)	68	60	210, 307, 384, 453	0
3	L	209/223 (93%)	0.20	10 (4%)	30	26	209, 315, 401, 451	0
All	All	2767/2816 (98%)	0.22	106 (3%)	40	32	121, 261, 385, 539	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	679	SER	9.8
2	H	681	ARG	7.1
2	K	687	GLY	6.1
2	K	694	LYS	5.9
2	K	686	ASN	5.2
2	K	692	GLY	5.0
2	H	689	GLU	4.5
2	K	684	ASP	4.3
2	K	579	LEU	4.3
2	K	695	ARG	4.3
3	F	85	ARG	4.0

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Mol	Chain	Res	Type	RSRZ
3	L	153	PHE	3.9
2	K	677	PHE	3.9
3	I	81	PHE	3.8
2	K	683	THR	3.8
2	K	779	LEU	3.8
2	K	617	GLU	3.7
3	L	152	ASN	3.6
3	I	79	ARG	3.5
1	J	93	TRP	3.5
2	K	635	PHE	3.5
2	H	688	GLU	3.4
2	H	675	HIS	3.4
1	J	35	LEU	3.4
2	K	693	GLY	3.2
1	J	58	ILE	3.2
3	L	90	LYS	3.1
3	C	89	LEU	3.1
2	K	700	LEU	2.9
1	J	18	LEU	2.9
2	H	680	GLY	2.8
1	J	6	LEU	2.8
2	K	639	LYS	2.8
1	G	84	LEU	2.8
1	J	17	SER	2.8
1	G	110	ILE	2.7
2	K	669	ALA	2.7
3	C	7	ILE	2.7
2	K	675	HIS	2.7
2	H	700	LEU	2.6
3	L	65	TRP	2.6
3	L	150	LEU	2.6
2	K	672	THR	2.6
2	K	577	ALA	2.6
2	B	522	ASN	2.6
3	L	89	LEU	2.6
1	J	21	LYS	2.5
2	H	607	MET	2.5
3	F	74	GLU	2.5
1	J	77	VAL	2.5
3	F	89	LEU	2.5
2	H	668	ARG	2.5
2	K	571	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	661	LEU	2.5
2	H	517	PHE	2.5
2	K	670	VAL	2.5
3	L	94	PHE	2.5
2	B	680	GLY	2.4
2	B	523	GLN	2.4
1	J	150	PHE	2.4
2	K	699	CYS	2.4
1	J	36	CYS	2.4
3	L	177	LYS	2.4
1	G	130	ILE	2.4
2	K	746	LEU	2.3
2	K	586	GLN	2.3
2	K	680	GLY	2.3
2	K	770	PHE	2.3
1	G	150	PHE	2.3
2	K	644	GLU	2.3
2	H	664	PRO	2.2
1	G	165	TYR	2.2
2	H	727	TYR	2.2
1	J	19	PRO	2.2
1	J	34	ILE	2.2
1	J	48	TYR	2.2
3	I	143	ILE	2.2
1	G	111	LEU	2.2
2	K	632	ILE	2.2
2	K	671	SER	2.2
2	K	703	ALA	2.2
1	G	128	PHE	2.2
2	H	657	ALA	2.2
3	I	43	ILE	2.2
1	G	21	LYS	2.1
2	K	707	ALA	2.1
1	J	62	ASP	2.1
2	K	678	TRP	2.1
2	K	690	LEU	2.1
1	G	25	LEU	2.1
2	K	720	PHE	2.1
1	G	152	LEU	2.1
2	K	618	ILE	2.1
2	H	650	ARG	2.1
2	K	540	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	J	4	LEU	2.1
1	J	141	ALA	2.1
2	K	494	PHE	2.1
1	J	20	ALA	2.0
2	E	681	ARG	2.0
3	C	199	LEU	2.0
3	L	93	ASP	2.0
1	J	57	HIS	2.0
3	F	94	PHE	2.0
2	B	484	PHE	2.0
3	L	118	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides 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.