Full wwPDB X-ray Structure Validation Report ⓘ

Apr 20, 2024 – 09:05 am BST

PDB ID	:	8RKS
Title	:	Structure of VPS29-VPS35 bound to the LFa motif R21 of Fam21.
Authors	:	Romano-Moreno, M.; Astorga-Simon, E.N.; Rojas, A.L.; Hierro, A.
Deposited on	:	2023-12-30
Resolution	:	3.10 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:

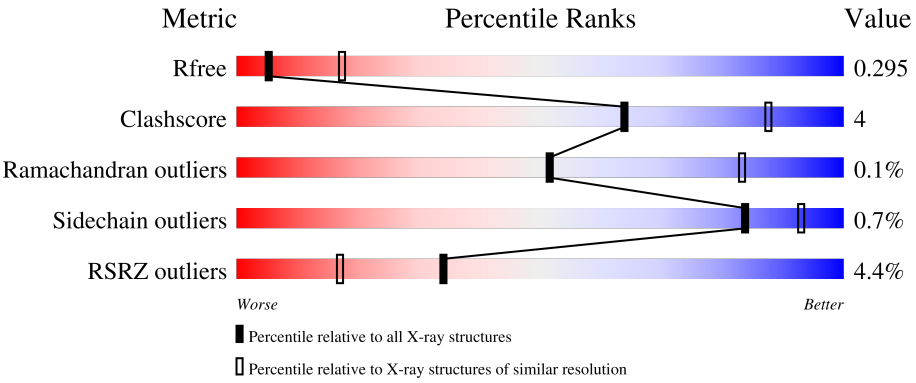
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	90% 10%
1	C	182	90% 10%
1	E	182	87% 13%
1	G	182	91% 9%
2	B	311	5% 82% 13% 5%

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Mol	Chain	Length	Quality of chain
2	D	311	8% 85% 10% 5%
2	F	311	6% 86% 10%
2	H	311	6% 86% 9% 5%
3	I	7	86% 14%
3	J	7	57% 29% 14%
3	K	7	57% 29% 14%
3	L	7	29% 57% 14%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 15571 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	C	182	Total	C	N	O	S	0	0	0
			1447	936	242	263	6			
1	E	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
			1446	936	242	262	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	297	Total	C	N	O	S	0	0	0
			2405	1527	418	450	10			
2	D	296	Total	C	N	O	S	0	0	0
			2394	1521	414	449	10			
2	F	298	Total	C	N	O	S	0	0	0
			2413	1533	419	451	10			
2	H	295	Total	C	N	O	S	0	0	0
			2385	1515	416	444	10			

- Molecule 3 is a protein called WASH complex subunit 2A.

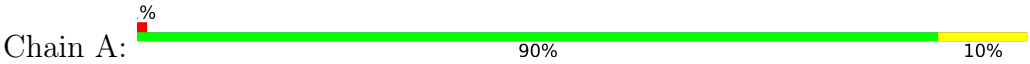
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	K	6	Total	C	N	O	0	0	0
			44	26	7	11			
3	I	6	Total	C	N	O	0	0	0
			44	26	7	11			
3	J	6	Total	C	N	O	0	0	0
			44	26	7	11			
3	L	7	Total	C	N	O	0	0	0
			55	35	8	12			

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.

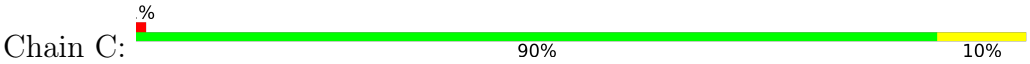
• Molecule 1: Vacuolar protein sorting-associated protein 29

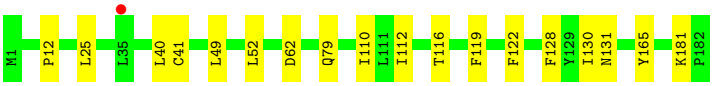
Chain A:



• Molecule 1: Vacuolar protein sorting-associated protein 29

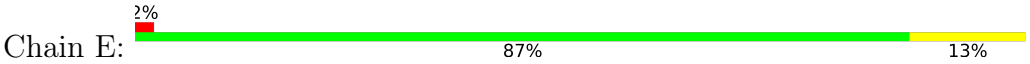
Chain C:

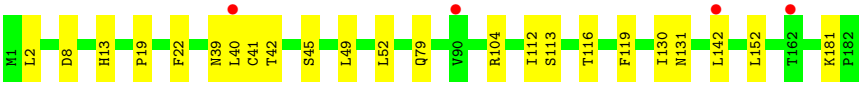




• Molecule 1: Vacuolar protein sorting-associated protein 29

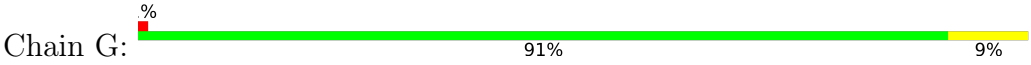
Chain E:

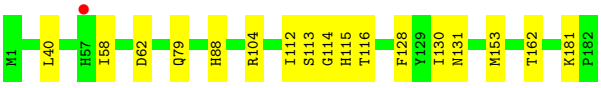




• Molecule 1: Vacuolar protein sorting-associated protein 29

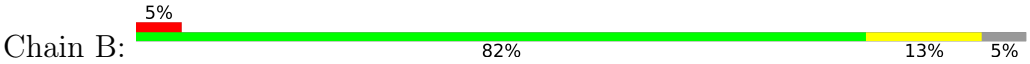
Chain G:

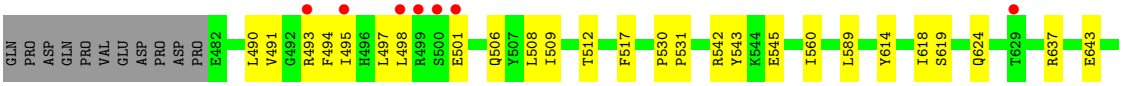


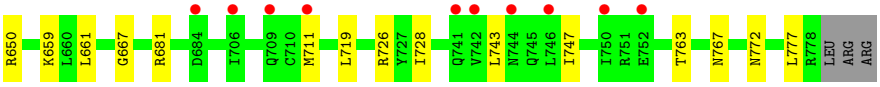


• Molecule 2: Vacuolar protein sorting-associated protein 35

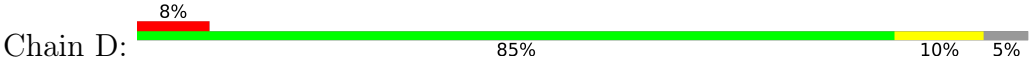
Chain B:

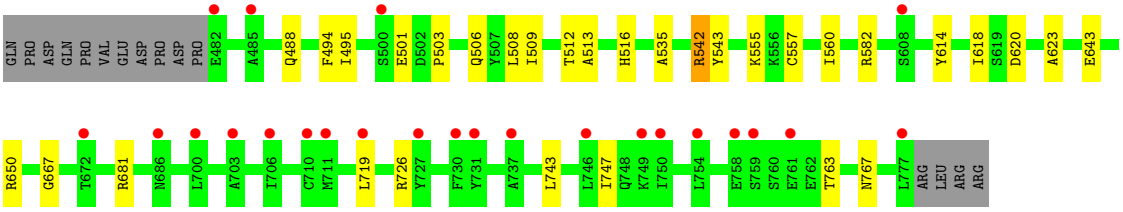




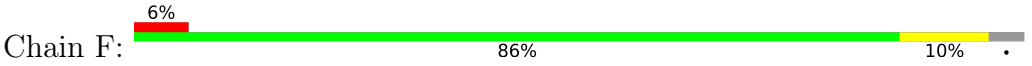


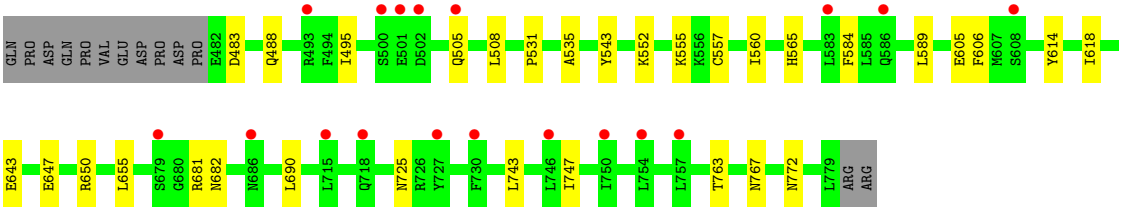
• Molecule 2: Vacuolar protein sorting-associated protein 35



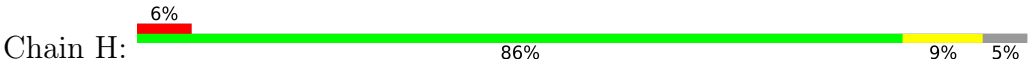


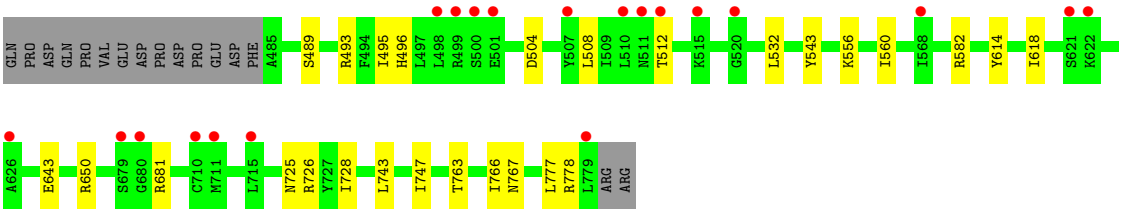
• Molecule 2: Vacuolar protein sorting-associated protein 35



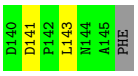


• Molecule 2: Vacuolar protein sorting-associated protein 35

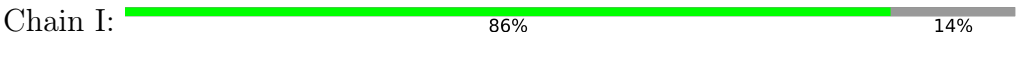




• Molecule 3: WASH complex subunit 2A



• Molecule 3: WASH complex subunit 2A



• Molecule 3: WASH complex subunit 2A

Chain J:

• Molecule 3: WASH complex subunit 2A

Chain L:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	59.27Å 139.09Å 146.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	146.15 – 3.10 146.15 – 2.96	Depositor EDS
% Data completeness (in resolution range)	73.6 (146.15-3.10) 64.5 (146.15-2.96)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.23 (at 2.96Å)	Xtriage
Refinement program	PHENIX 1.19.1	Depositor
R, R_{free}	0.251 , 0.288 0.256 , 0.295	Depositor DCC
R_{free} test set	1613 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	91.5	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 50.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k 0.004 for -h,-l,-k 0.378 for h,-k,-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	15571	wwPDB-VP
Average B, all atoms (Å^2)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.84% 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

5.1 Standard geometry

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	0.24	0/1481	0.47	0/2008
1	C	0.24	0/1481	0.48	0/2008
1	E	0.24	0/1481	0.48	0/2008
1	G	0.24	0/1480	0.50	0/2007
2	B	0.24	0/2452	0.44	0/3302
2	D	0.24	0/2441	0.44	0/3288
2	F	0.24	0/2460	0.44	0/3313
2	H	0.24	0/2431	0.44	0/3274
3	I	0.21	0/44	0.34	0/60
3	J	0.20	0/44	0.33	0/60
3	K	0.23	0/44	0.51	0/60
3	L	0.29	0/56	0.52	0/76
All	All	0.24	0/15895	0.46	0/21464

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

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	12	0
1	C	1447	0	1459	14	0
1	E	1447	0	1459	19	0
1	G	1446	0	1456	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2405	0	2383	30	0
2	D	2394	0	2370	21	0
2	F	2413	0	2394	27	0
2	H	2385	0	2375	16	0
3	I	44	0	36	0	0
3	J	44	0	36	1	0
3	K	44	0	36	3	0
3	L	55	0	45	7	0
All	All	15571	0	15508	130	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 4.

All (130) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:122:PHE:HB2	2:H:778:ARG:HG2	1.52	0.89
2:B:509:ILE:HG12	2:D:516:HIS:NE2	2.05	0.72
1:G:116:THR:OG1	1:G:131:ASN:ND2	2.28	0.67
1:G:104:ARG:NH1	2:H:725:ASN:OD1	2.29	0.66
1:A:25:LEU:HB3	3:K:143:LEU:HD13	1.78	0.65
1:A:116:THR:OG1	1:A:131:ASN:ND2	2.31	0.64
1:E:42:THR:HB	2:F:488:GLN:HE22	1.63	0.63
1:C:25:LEU:HB3	3:L:143:LEU:HD12	1.82	0.62
1:E:104:ARG:NH1	2:F:725:ASN:OD1	2.33	0.61
2:B:542:ARG:NH1	2:B:545:GLU:OE2	2.30	0.61
2:B:711:MET:HB2	2:F:605:GLU:OE1	2.01	0.60
1:E:116:THR:OG1	1:E:131:ASN:ND2	2.35	0.60
2:D:509:ILE:O	2:D:513:ALA:N	2.33	0.60
1:A:107:ASP:HB2	2:B:772:ASN:HD21	1.66	0.60
2:D:557:CYS:HA	2:D:560:ILE:HD12	1.84	0.59
1:C:110:ILE:HG12	1:C:128:PHE:HB3	1.85	0.59
2:D:503:PRO:HG3	2:D:542:ARG:HG2	1.84	0.59
1:E:142:LEU:HD21	2:F:589:LEU:HD22	1.86	0.58
2:D:643:GLU:OE1	2:D:650:ARG:NH2	2.34	0.57
1:A:142:LEU:HD21	2:B:589:LEU:HD22	1.86	0.57
1:E:13:HIS:HA	2:F:531:PRO:HG3	1.87	0.56
2:B:501:GLU:HB2	2:B:506:GLN:HG2	1.87	0.56
1:A:79:GLN:O	1:A:181:LYS:NZ	2.29	0.56
2:B:643:GLU:OE1	2:B:650:ARG:NH2	2.39	0.56
2:F:682:ASN:HD21	2:F:690:LEU:HD21	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:614:TYR:HA	2:F:618:ILE:HD12	1.88	0.55
2:H:495:ILE:HD11	2:H:532:LEU:HD23	1.88	0.55
2:B:497:LEU:HD13	2:D:494:PHE:CE1	2.42	0.55
1:C:79:GLN:O	1:C:181:LYS:NZ	2.29	0.54
1:G:115:HIS:O	1:G:115:HIS:ND1	2.37	0.54
2:B:493:ARG:HH22	2:D:506:GLN:HA	1.73	0.54
1:G:79:GLN:O	1:G:181:LYS:NZ	2.31	0.54
2:B:763:THR:O	2:B:767:ASN:ND2	2.41	0.53
2:B:498:LEU:HD12	2:B:501:GLU:HG3	1.89	0.53
2:D:763:THR:O	2:D:767:ASN:ND2	2.42	0.53
2:F:505:GLN:NE2	2:F:508:LEU:HD23	2.24	0.52
2:H:614:TYR:HA	2:H:618:ILE:HD12	1.91	0.52
2:H:489:SER:O	2:H:493:ARG:HG3	2.10	0.52
2:F:483:ASP:N	2:F:483:ASP:OD1	2.43	0.52
1:C:40:LEU:N	1:C:41:CYS:HA	2.25	0.52
1:E:40:LEU:N	1:E:41:CYS:HA	2.24	0.52
1:G:40:LEU:HD11	1:G:58:ILE:HD13	1.92	0.52
2:H:643:GLU:OE1	2:H:650:ARG:NH2	2.42	0.52
2:F:505:GLN:HE21	2:F:508:LEU:HD23	1.76	0.51
2:H:496:HIS:ND1	2:H:496:HIS:O	2.43	0.51
2:F:643:GLU:OE1	2:F:650:ARG:NH2	2.38	0.51
2:F:565:HIS:NE2	2:F:605:GLU:OE2	2.43	0.51
2:B:497:LEU:HD13	2:D:494:PHE:HE1	1.78	0.49
1:C:112:ILE:HG22	1:C:130:ILE:HB	1.94	0.49
2:D:667:GLY:HA3	2:D:719:LEU:HD21	1.94	0.49
2:H:504:ASP:OD2	2:H:556:LYS:NZ	2.46	0.49
1:C:116:THR:OG1	1:C:131:ASN:ND2	2.46	0.49
3:L:141:ASP:N	3:L:141:ASP:OD1	2.44	0.49
2:B:508:LEU:O	2:B:512:THR:HG23	2.13	0.48
3:L:143:LEU:H	3:L:143:LEU:HD23	1.78	0.48
1:E:42:THR:CB	2:F:488:GLN:HE22	2.26	0.48
1:G:112:ILE:HD13	1:G:130:ILE:HB	1.95	0.48
1:C:12:PRO:HG3	2:D:488:GLN:HG2	1.96	0.48
1:A:40:LEU:H	1:A:41:CYS:HA	1.79	0.47
2:B:619:SER:HB3	2:F:655:LEU:HD22	1.97	0.47
2:B:659:LYS:HD2	2:F:647:GLU:OE1	2.15	0.47
2:F:584:PHE:O	2:F:606:PHE:HB3	2.15	0.47
1:A:40:LEU:N	1:A:41:CYS:HA	2.29	0.47
1:G:88:HIS:HB3	1:G:115:HIS:CD2	2.49	0.47
2:B:490:LEU:HD23	2:B:517:PHE:HE1	1.80	0.46
2:D:508:LEU:O	2:D:512:THR:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:682:ASN:ND2	2:F:690:LEU:HD21	2.30	0.46
1:E:40:LEU:H	1:E:41:CYS:HA	1.81	0.46
1:E:112:ILE:HG12	1:E:130:ILE:HB	1.97	0.46
2:H:763:THR:HA	2:H:766:ILE:HB	1.98	0.46
2:B:619:SER:HB3	2:F:655:LEU:HB3	1.97	0.46
1:A:174:VAL:HG11	3:K:141:ASP:HB3	1.98	0.45
2:D:543:TYR:CE2	2:D:560:ILE:HD11	2.51	0.45
2:B:493:ARG:CZ	2:D:509:ILE:HD12	2.47	0.45
1:E:113:SER:O	1:E:131:ASN:HA	2.17	0.45
1:E:79:GLN:O	1:E:181:LYS:NZ	2.30	0.45
2:B:491:VAL:O	2:B:495:ILE:HG12	2.17	0.45
2:H:728:ILE:HG12	2:H:777:LEU:HD21	1.99	0.45
2:H:763:THR:O	2:H:767:ASN:ND2	2.49	0.45
3:L:144:ASN:N	3:L:144:ASN:OD1	2.50	0.45
2:B:667:GLY:HA3	2:B:719:LEU:HD21	1.98	0.44
2:D:555:LYS:HD2	2:D:555:LYS:HA	1.84	0.44
2:D:620:ASP:HB3	2:D:623:ALA:HB3	1.99	0.44
1:E:2:LEU:HD12	1:E:152:LEU:HD21	1.99	0.44
1:E:40:LEU:HB3	1:E:45:SER:HB2	1.99	0.44
2:B:543:TYR:CE2	2:B:560:ILE:HD11	2.52	0.44
2:B:624:GLN:OE1	2:B:661:LEU:HD13	2.18	0.44
2:H:489:SER:OG	2:H:493:ARG:NE	2.51	0.44
2:B:493:ARG:HE	2:D:501:GLU:HG3	1.82	0.44
2:D:614:TYR:HA	2:D:618:ILE:HD12	2.00	0.43
2:F:552:LYS:HA	2:F:555:LYS:NZ	2.33	0.43
2:F:543:TYR:CE2	2:F:560:ILE:HD11	2.53	0.43
2:H:508:LEU:O	2:H:512:THR:HG23	2.17	0.43
3:L:141:ASP:OD2	3:L:145:ALA:N	2.49	0.43
1:G:113:SER:O	1:G:131:ASN:HA	2.18	0.43
1:C:62:ASP:O	2:D:582:ARG:HD3	2.19	0.43
1:C:165:TYR:OH	3:L:141:ASP:HB2	2.17	0.43
2:F:763:THR:O	2:F:767:ASN:ND2	2.52	0.43
2:H:543:TYR:CE2	2:H:560:ILE:HD11	2.54	0.43
1:E:49:LEU:HD23	1:E:52:LEU:HD12	2.01	0.42
1:A:118:LYS:HE3	1:A:118:LYS:HB2	1.76	0.42
2:F:495:ILE:HD12	2:F:535:ALA:HB2	2.01	0.42
1:C:119:PHE:HA	1:C:131:ASN:O	2.19	0.42
1:E:119:PHE:HA	1:E:131:ASN:O	2.19	0.42
2:B:494:PHE:O	2:B:498:LEU:HB2	2.19	0.42
2:F:557:CYS:HA	2:F:560:ILE:HD12	2.02	0.42
2:H:743:LEU:O	2:H:747:ILE:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:104:ARG:HG2	2:F:772:ASN:HB3	2.01	0.42
1:G:62:ASP:O	2:H:582:ARG:HD3	2.19	0.42
1:E:8:ASP:HA	1:E:39:ASN:HB2	2.02	0.42
2:F:743:LEU:O	2:F:747:ILE:HG23	2.19	0.42
3:K:143:LEU:HD23	3:K:143:LEU:HA	1.62	0.42
1:G:153:MET:HG2	1:G:162:THR:HG22	2.02	0.42
1:E:19:PRO:HG2	1:E:22:PHE:CG	2.55	0.42
1:G:128:PHE:HE2	1:G:162:THR:HG21	1.85	0.41
2:B:619:SER:CB	2:F:655:LEU:HB3	2.51	0.41
1:C:40:LEU:H	1:C:41:CYS:HA	1.85	0.41
2:D:495:ILE:HD12	2:D:535:ALA:HB2	2.02	0.41
2:B:728:ILE:HG12	2:B:777:LEU:HD21	2.03	0.41
1:A:137:GLY:HA3	1:A:148:PRO:HG3	2.03	0.41
2:B:614:TYR:HA	2:B:618:ILE:HD12	2.03	0.41
1:A:153:MET:HG2	1:A:162:THR:HG22	2.03	0.41
2:B:530:PRO:HB2	2:B:531:PRO:HD3	2.02	0.41
2:B:743:LEU:O	2:B:747:ILE:HG23	2.21	0.41
3:J:141:ASP:OD2	3:J:144:ASN:N	2.54	0.41
1:C:25:LEU:HD21	3:L:145:ALA:HA	2.03	0.41
1:E:42:THR:HG21	2:F:488:GLN:OE1	2.20	0.41
1:C:49:LEU:HD23	1:C:52:LEU:HD12	2.02	0.40
1:A:93:TRP:CE3	2:B:637:ARG:HG3	2.56	0.40
2:D:743:LEU:O	2:D:747:ILE:HG23	2.21	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%)	175 (97%)	5 (3%)	0	100	100
1	C	180/182 (99%)	172 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	E	180/182 (99%)	174 (97%)	6 (3%)	0	100 100
1	G	180/182 (99%)	175 (97%)	4 (2%)	1 (1%)	25 59
2	B	295/311 (95%)	283 (96%)	12 (4%)	0	100 100
2	D	294/311 (94%)	285 (97%)	9 (3%)	0	100 100
2	F	296/311 (95%)	288 (97%)	8 (3%)	0	100 100
2	H	293/311 (94%)	284 (97%)	9 (3%)	0	100 100
3	I	4/7 (57%)	3 (75%)	1 (25%)	0	100 100
3	J	4/7 (57%)	3 (75%)	1 (25%)	0	100 100
3	K	4/7 (57%)	3 (75%)	1 (25%)	0	100 100
3	L	5/7 (71%)	4 (80%)	0	1 (20%)	0 0
All	All	1915/2000 (96%)	1849 (97%)	64 (3%)	2 (0%)	51 83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	L	142	PRO
1	G	114	GLY

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%)	158 (99%)	2 (1%)	69 87
1	C	160/160 (100%)	160 (100%)	0	100 100
1	E	160/160 (100%)	160 (100%)	0	100 100
1	G	159/160 (99%)	159 (100%)	0	100 100
2	B	258/272 (95%)	256 (99%)	2 (1%)	81 92
2	D	257/272 (94%)	254 (99%)	3 (1%)	71 88
2	F	259/272 (95%)	258 (100%)	1 (0%)	91 96
2	H	256/272 (94%)	254 (99%)	2 (1%)	81 92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	I	5/6 (83%)	5 (100%)	0	100 100
3	J	5/6 (83%)	5 (100%)	0	100 100
3	K	5/6 (83%)	5 (100%)	0	100 100
3	L	6/6 (100%)	5 (83%)	1 (17%)	2 9
All	All	1690/1752 (96%)	1679 (99%)	11 (1%)	84 93

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	ASN
1	A	115	HIS
2	B	681	ARG
2	B	726	ARG
2	D	542	ARG
2	D	681	ARG
2	D	726	ARG
2	F	681	ARG
2	H	681	ARG
2	H	726	ARG
3	L	143	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	HIS
1	A	131	ASN
2	B	496	HIS
2	B	523	GLN
1	C	124	HIS
2	D	511	ASN
2	D	599	HIS
1	E	10	HIS
1	E	124	HIS
2	F	488	GLN
2	F	505	GLN
2	F	511	ASN
2	F	682	ASN
1	G	124	HIS
2	H	744	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 monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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%)	-0.03	1 (0%) 91 81	59, 85, 117, 135	0
1	C	182/182 (100%)	-0.02	1 (0%) 91 81	43, 87, 121, 148	0
1	E	182/182 (100%)	0.03	4 (2%) 62 41	56, 87, 128, 159	0
1	G	182/182 (100%)	-0.05	1 (0%) 91 81	51, 88, 120, 151	0
2	B	297/311 (95%)	0.26	17 (5%) 23 11	55, 91, 147, 180	0
2	D	296/311 (95%)	0.47	24 (8%) 12 5	51, 98, 157, 206	0
2	F	298/311 (95%)	0.28	18 (6%) 21 10	63, 96, 139, 189	0
2	H	295/311 (94%)	0.31	20 (6%) 17 7	52, 96, 151, 182	0
3	I	6/7 (85%)	-0.60	0 100 100	86, 89, 117, 119	0
3	J	6/7 (85%)	-0.24	0 100 100	104, 123, 136, 157	0
3	K	6/7 (85%)	-0.34	0 100 100	92, 113, 131, 131	0
3	L	7/7 (100%)	-0.77	0 100 100	96, 104, 111, 112	0
All	All	1939/2000 (96%)	0.19	86 (4%) 34 17	43, 92, 144, 206	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	759	SER	13.5
2	D	750	ILE	8.9
2	H	501	GLU	8.4
2	D	500	SER	8.4
2	B	498	LEU	8.3
2	F	500	SER	6.5
2	H	499	ARG	6.3
2	B	499	ARG	6.2
2	D	758	GLU	6.0
2	B	746	LEU	5.6
2	D	710	CYS	5.4

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Mol	Chain	Res	Type	RSRZ
2	D	777	LEU	5.1
2	D	686	ASN	5.0
2	F	754	LEU	4.8
2	B	752	GLU	4.3
2	B	684	ASP	4.0
2	H	498	LEU	3.8
2	B	741	GLN	3.8
2	H	621	SER	3.7
2	H	500	SER	3.6
2	H	510	LEU	3.6
2	B	495	ILE	3.5
2	D	700	LEU	3.3
2	H	679	SER	3.3
2	D	727	TYR	3.3
2	F	718	GLN	3.2
2	H	680	GLY	3.2
2	D	754	LEU	3.2
2	H	711	MET	3.2
2	D	730	PHE	3.2
2	F	715	LEU	3.1
2	H	622	LYS	3.1
2	F	686	ASN	3.0
2	H	507	TYR	3.0
2	D	749	LYS	3.0
2	B	706	ILE	2.9
2	D	746	LEU	2.8
2	F	750	ILE	2.8
2	B	629	THR	2.8
2	F	586	GLN	2.8
2	F	727	TYR	2.8
1	C	35	LEU	2.6
2	H	779	LEU	2.6
2	B	742	VAL	2.6
2	B	750	ILE	2.6
2	B	744	ASN	2.6
2	D	608	SER	2.6
2	H	511	ASN	2.6
2	D	719	LEU	2.6
2	F	679	SER	2.6
2	D	703	ALA	2.5
2	D	761	GLU	2.5
2	H	710	CYS	2.5

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Mol	Chain	Res	Type	RSRZ
2	H	512	THR	2.5
2	F	501	GLU	2.5
2	F	746	LEU	2.5
2	F	730	PHE	2.4
2	F	505	GLN	2.4
2	B	711	MET	2.4
1	E	40	LEU	2.4
2	D	731	TYR	2.3
1	E	90	VAL	2.3
2	D	672	THR	2.3
2	F	583	LEU	2.3
2	H	515	LYS	2.3
1	E	162	THR	2.3
2	D	482	GLU	2.3
2	D	706	ILE	2.3
2	B	500	SER	2.3
2	F	493	ARG	2.2
2	F	502	ASP	2.2
2	H	568	ILE	2.2
1	G	57	HIS	2.2
2	D	485	ALA	2.2
2	D	711	MET	2.2
1	A	73	LYS	2.1
2	F	608	SER	2.1
2	H	520	GLY	2.1
2	F	757	LEU	2.1
2	H	715	LEU	2.1
2	H	626	ALA	2.1
2	B	493	ARG	2.1
2	B	709	GLN	2.1
2	B	501	GLU	2.0
2	D	737	ALA	2.0
1	E	142	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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.