



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 02:15 AM EDT

PDB ID : 8RKS / pdb_00008rks
Title : Structure of VPS29-VPS35 bound to the LF α 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	:	4-5-2 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

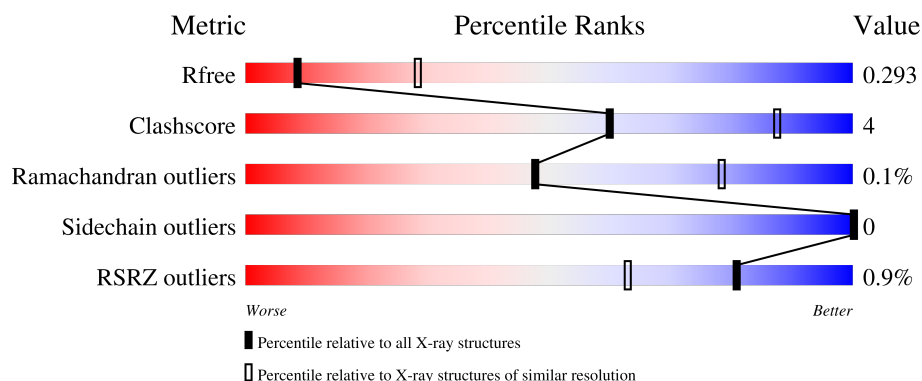
1 Overall quality at a glance

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}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (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 $\leq 5\%$. 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	 91% 9%
1	C	182	 90% 10%
1	E	182	 2% 86% 14%
1	G	182	 91% 9%
2	B	311	 0% 83% 13% 5%

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Mol	Chain	Length	Quality of chain
2	D	311	% 85% 10% 5%
2	F	311	% 86% 10%
2	H	311	% 87% 8% 5%
3	I	7	86% 14%
3	J	7	57% 29% 14%
3	K	7	57% 29% 14%
3	L	7	29% 71%

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:  91% 9%



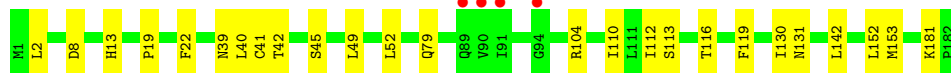
- Molecule 1: Vacuolar protein sorting-associated protein 29

Chain C:  90% 10%



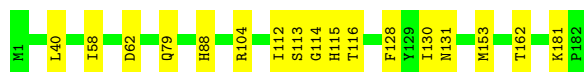
- Molecule 1: Vacuolar protein sorting-associated protein 29

Chain E:  2% 86% 14%



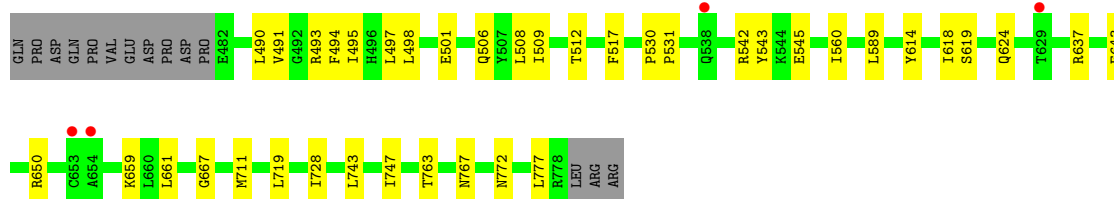
- Molecule 1: Vacuolar protein sorting-associated protein 29

Chain G:  91% 9%



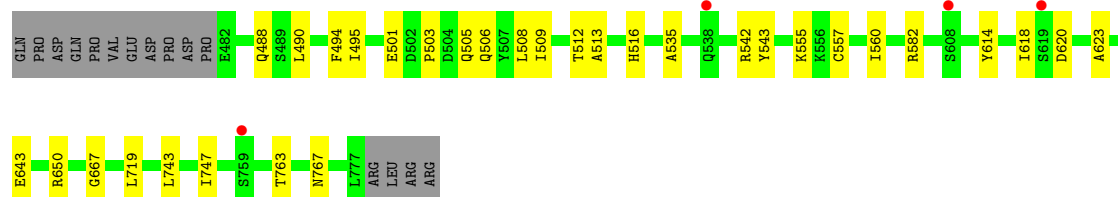
- Molecule 2: Vacuolar protein sorting-associated protein 35

Chain B:  83% 13% 5%



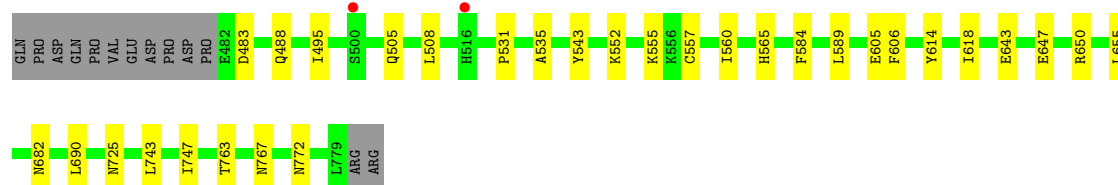
- Molecule 2: Vacuolar protein sorting-associated protein 35

Chain D: 



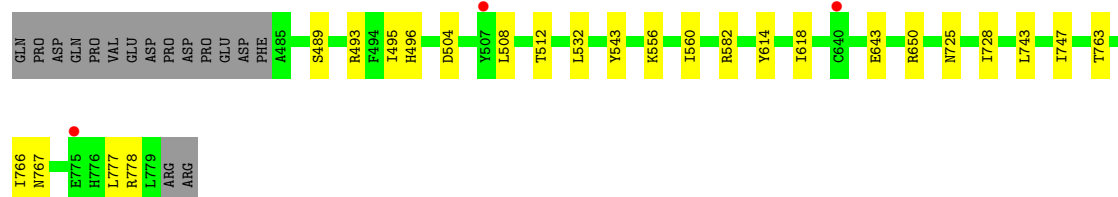
- Molecule 2: Vacuolar protein sorting-associated protein 35

Chain F: 



- Molecule 2: Vacuolar protein sorting-associated protein 35

Chain H: 



- Molecule 3: WASH complex subunit 2A

Chain K: 



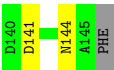
- Molecule 3: WASH complex subunit 2A

Chain I: 

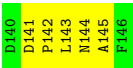


- Molecule 3: WASH complex subunit 2A

Chain J: 



- Molecule 3: WASH complex subunit 2A



4 Data and refinement statistics

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 – 3.10	Depositor EDS
% Data completeness (in resolution range)	73.6 (146.15-3.10) 73.5 (146.15-3.10)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.23 (at 2.96Å)	Xtriage
Refinement program	PHENIX 1.19.1	Depositor
R, R_{free}	0.251 , 0.288 0.255 , 0.293	Depositor DCC
R_{free} test set	1613 reflections (3.26%)	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 , 134.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	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	0.94	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.*

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	0.10	0/1481	0.30	0/2008
1	C	0.10	0/1481	0.31	0/2008
1	E	0.10	0/1481	0.32	0/2008
1	G	0.10	0/1480	0.32	0/2007
2	B	0.11	0/2452	0.26	0/3302
2	D	0.10	0/2441	0.26	0/3288
2	F	0.10	0/2460	0.25	0/3313
2	H	0.09	0/2431	0.25	0/3274
3	I	0.10	0/44	0.27	0/60
3	J	0.09	0/44	0.27	0/60
3	K	0.18	0/44	0.42	0/60
3	L	0.19	0/56	0.40	0/76
All	All	0.10	0/15895	0.28	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 [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	C	1447	0	1459	14	0
1	E	1447	0	1459	20	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	32	0
2	D	2394	0	2370	23	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	134	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 (134) 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
1:G:79:GLN:O	1:G:181:LYS:NZ	2.31	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:79:GLN:O	1:C:181:LYS:NZ	2.29	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
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
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
1:A:110:ILE:HG21	1:A:153:MET:HE1	1.96	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:E:110:ILE:HG21	1:E:153:MET:HE1	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:508:LEU:O	2:D:512:THR:HG23	2.15	0.46
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
3:L:141:ASP:OD1	3:L:141:ASP:N	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:B:501:GLU:CD	2:D:490:LEU:HD11	2.45	0.41
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:B:493:ARG:HH12	2:D:505:GLN:C	2.28	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
1	E	180/182 (99%)	174 (97%)	6 (3%)	0	100	100
1	G	180/182 (99%)	175 (97%)	4 (2%)	1 (1%)	21	52
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%)	48	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	L	142	PRO
1	G	114	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	160/160 (100%)	160 (100%)	0	100	100
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%)	258 (100%)	0	100	100
2	D	257/272 (94%)	257 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	259/272 (95%)	259 (100%)	0	100	100
2	H	256/272 (94%)	256 (100%)	0	100	100
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%)	6 (100%)	0	100	100
All	All	1690/1752 (96%)	1690 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	HIS
1	A	16	ASN
1	A	39	ASN
1	A	72	GLN
1	A	124	HIS
2	B	496	HIS
2	B	516	HIS
2	B	599	HIS
2	B	609	GLN
2	B	666	GLN
2	B	744	ASN
2	B	772	ASN
1	C	10	HIS
1	C	124	HIS
2	D	511	ASN
2	D	599	HIS
2	D	675	HIS
2	D	744	ASN
1	E	10	HIS
1	E	39	ASN
1	E	124	HIS
1	E	156	GLN
2	F	488	GLN
2	F	505	GLN
2	F	511	ASN
2	F	516	HIS
2	F	523	GLN

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Mol	Chain	Res	Type
2	F	599	HIS
2	F	682	ASN
2	F	744	ASN
1	G	124	HIS
2	H	511	ASN
2	H	516	HIS
2	H	599	HIS
2	H	609	GLN
2	H	744	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 [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%)	-0.93	0 100 100	59, 85, 117, 135	0
1	C	182/182 (100%)	-0.96	0 100 100	43, 87, 121, 148	0
1	E	182/182 (100%)	-0.76	4 (2%) 62 41	56, 87, 128, 159	0
1	G	182/182 (100%)	-0.93	0 100 100	51, 88, 120, 151	0
2	B	297/311 (95%)	-0.78	4 (1%) 75 56	55, 91, 147, 180	0
2	D	296/311 (95%)	-0.74	4 (1%) 73 53	51, 98, 157, 206	0
2	F	298/311 (95%)	-0.84	2 (0%) 84 68	63, 96, 139, 189	0
2	H	295/311 (94%)	-0.73	3 (1%) 79 61	52, 96, 151, 182	0
3	I	6/7 (85%)	-1.17	0 100 100	86, 89, 117, 119	0
3	J	6/7 (85%)	-0.92	0 100 100	104, 123, 136, 157	0
3	K	6/7 (85%)	-1.33	0 100 100	92, 113, 131, 131	0
3	L	7/7 (100%)	-1.42	0 100 100	96, 104, 111, 112	0
All	All	1939/2000 (96%)	-0.82	17 (0%) 81 63	43, 92, 144, 206	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	654	ALA	4.6
2	D	538	GLN	3.3
2	H	640	CYS	3.2
1	E	91	ILE	3.0
1	E	90	VAL	2.9
2	F	500	SER	2.9
2	H	775	GLU	2.7
2	B	629	THR	2.7
2	D	619	SER	2.7
2	D	759	SER	2.5
2	H	507	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	94	GLY	2.4
2	F	516	HIS	2.4
2	B	538	GLN	2.1
2	B	653	CYS	2.1
2	D	608	SER	2.0
1	E	89	GLN	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.