



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:38 AM UTC

PDB ID : 5OSI / pdb_00005osi
Title : Structure of retromer VPS29-VPS35C subunits complexed with RidL harpin loop (163-176)
Authors : Romano-Moreno, M.; Rojas, A.L.; Lucas, M.; Isupov, M.N.; Hierro, A.
Deposited on : 2017-08-17
Resolution : 2.52 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
Mogul : 2022.3.0, CSD as543be (2022)
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

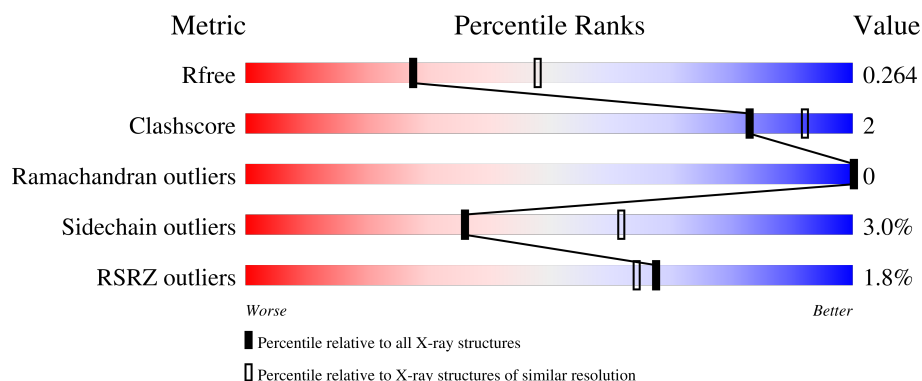
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.52 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	7383 (2.54-2.50)
Clashscore	190562	8079 (2.54-2.50)
Ramachandran outliers	187476	7944 (2.54-2.50)
Sidechain outliers	187428	7946 (2.54-2.50)
RSRZ outliers	180081	7387 (2.54-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	182	92% 8%
1	D	182	90% 10%
1	G	182	2% 91% 8% .
1	J	182	3% 88% 11% .
2	B	311	3% 90% 5% . .

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Mol	Chain	Length	Quality of chain
2	E	311	% 89% 8%
2	H	311	2% 85% 6% 9%
2	K	311	% 87% 7% 6%
3	C	14	14% 71% 7% 7% 14%
3	F	14	79% 21%
3	I	14	7% 86% 14%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 15918 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	1	0
			1452	940	242	263	7			
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	302	Total	C	N	O	S	0	1	0
			2454	1558	429	457	10			
2	H	283	Total	C	N	O	S	0	2	0
			2307	1472	405	420	10			
2	K	293	Total	C	N	O	S	0	1	0
			2389	1519	418	442	10			

- Molecule 3 is a protein called Interaptin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	12	Total	C	N	O	0	0	0
			95	63	13	19			
3	F	11	Total	C	N	O	0	0	0
			87	57	12	18			
3	I	12	Total	C	N	O	0	0	0
			95	63	13	19			

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	G	1	Total	C	O	0	0
			4	2	2		
4	H	1	Total	C	O	0	0
			4	2	2		
4	J	1	Total	C	O	0	0
			4	2	2		
4	J	1	Total	C	O	0	0
			4	2	2		
4	K	1	Total	C	O	0	0
			4	2	2		
4	K	1	Total	C	O	0	0
			4	2	2		
4	K	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	1	Total	Na	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	1	Total 1	Na 1	0	0
5	K	2	Total 2	Na 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	15	Total 15	O 15	0	0
6	B	26	Total 26	O 26	0	0
6	D	22	Total 22	O 22	0	0
6	E	36	Total 36	O 36	0	0
6	G	12	Total 12	O 12	0	0
6	H	17	Total 17	O 17	0	0
6	I	1	Total 1	O 1	0	0
6	J	33	Total 33	O 33	0	0
6	K	64	Total 64	O 64	0	0

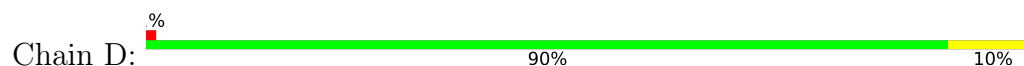
3 Residue-property plots [i](#)

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.

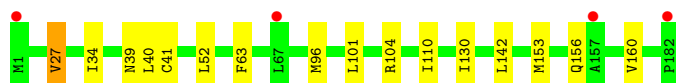
- Molecule 1: Vacuolar protein sorting-associated protein 29



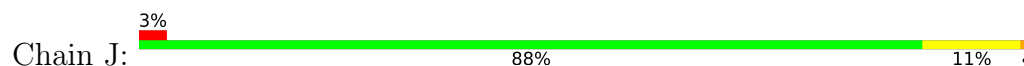
- Molecule 1: Vacuolar protein sorting-associated protein 29



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- Molecule 1: Vacuolar protein sorting-associated protein 29

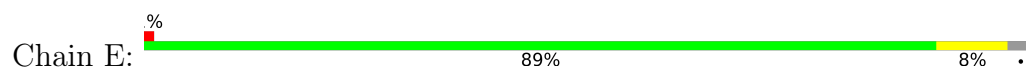


- Molecule 2: Vacuolar protein sorting-associated protein 35

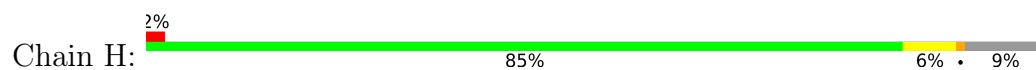




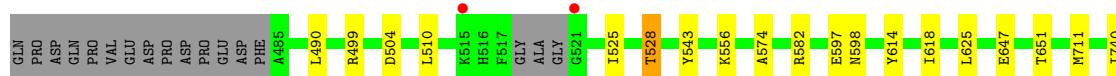
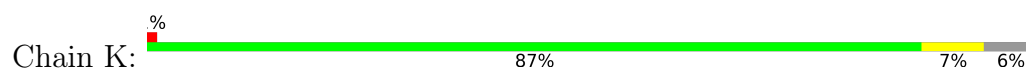
- Molecule 2: Vacuolar protein sorting-associated protein 35



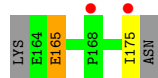
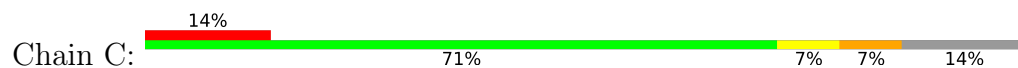
- Molecule 2: Vacuolar protein sorting-associated protein 35



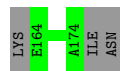
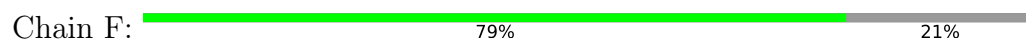
- Molecule 2: Vacuolar protein sorting-associated protein 35



- Molecule 3: Interaptin

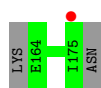


- Molecule 3: Interaptin



- Molecule 3: Interaptin

Chain I: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	58.55Å 138.99Å 126.64Å 90.00° 92.78° 90.00°	Depositor
Resolution (Å)	126.49 – 2.52 126.49 – 2.52	Depositor EDS
% Data completeness (in resolution range)	99.4 (126.49-2.52) 99.4 (126.49-2.52)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 2.52Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.205 , 0.267 0.207 , 0.264	Depositor DCC
R_{free} test set	3453 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	42.1	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 36.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.035 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15918	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, NA

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	0.58	0/1481	0.81	0/2008
1	D	0.60	0/1489	0.80	0/2018
1	G	0.57	0/1481	0.80	1/2008 (0.0%)
1	J	0.57	0/1481	0.81	0/2008
2	B	0.61	0/2471	0.89	1/3327 (0.0%)
2	E	0.61	0/2506	0.88	0/3375
2	H	0.61	0/2358	0.87	0/3174
2	K	0.64	0/2437	0.90	0/3279
3	C	0.64	0/98	0.71	0/135
3	F	0.58	0/90	0.61	0/124
3	I	0.60	0/98	0.61	0/135
All	All	0.60	0/15990	0.85	2/21591 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	27	VAL	CB-CA-C	5.88	115.09	109.33
2	B	560	ILE	CB-CA-C	-5.10	105.18	112.22

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	6	0
1	D	1452	0	1468	9	0
1	G	1447	0	1459	9	0
1	J	1447	0	1459	10	0
2	B	2424	0	2407	11	0
2	E	2454	0	2439	17	0
2	H	2307	0	2318	8	0
2	K	2389	0	2389	9	0
3	C	95	0	95	1	0
3	F	87	0	84	0	0
3	I	95	0	95	0	0
4	A	4	0	6	0	0
4	B	4	0	6	0	0
4	D	8	0	12	0	0
4	G	4	0	6	0	0
4	H	4	0	6	0	0
4	J	8	0	12	0	0
4	K	12	0	18	0	0
5	E	1	0	0	0	0
5	H	1	0	0	0	0
5	K	2	0	0	0	0
6	A	15	0	0	0	0
6	B	26	0	0	0	0
6	D	22	0	0	0	0
6	E	36	0	0	0	0
6	G	12	0	0	0	0
6	H	17	0	0	0	0
6	I	1	0	0	0	0
6	J	33	0	0	0	0
6	K	64	0	0	1	0
All	All	15918	0	15738	74	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 2.

All (74) 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)
2:E:514[A]:ARG:HH11	2:E:514[A]:ARG:CG	1.74	1.01
2:E:514[A]:ARG:HH11	2:E:514[A]:ARG:HG2	1.31	0.94
2:E:514[A]:ARG:HG2	2:E:514[A]:ARG:NH1	2.03	0.74
2:E:498:LEU:HD13	2:E:509:ILE:HD11	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:153:MET:HE2	1:G:160:VAL:HG21	1.72	0.71
2:E:514[A]:ARG:CG	2:E:514[A]:ARG:NH1	2.46	0.70
2:E:514[A]:ARG:HH11	2:E:514[A]:ARG:HG3	1.62	0.62
1:A:8:ASP:OD2	1:A:114:GLY:O	2.18	0.61
1:G:39:ASN:HD21	1:G:63:PHE:H	1.50	0.58
1:G:104:ARG:NH1	2:H:725:ASN:OD1	2.38	0.57
1:D:142:LEU:HD21	2:E:589:LEU:HD22	1.87	0.56
2:H:584:PHE:CZ	2:H:609:GLN:HG2	2.40	0.56
1:D:96[B]:MET:HE1	1:D:129:TYR:CG	2.41	0.55
1:G:110:ILE:HD13	1:G:153:MET:HE1	1.88	0.55
1:J:9:LEU:CD2	1:J:135:ALA:HB3	2.37	0.54
2:K:614:TYR:CD1	2:K:618:ILE:HD11	2.43	0.54
2:E:741:GLN:HE21	2:E:745:GLN:HE21	1.57	0.53
2:E:625:LEU:O	2:E:629:THR:HG23	2.09	0.52
1:D:85:ILE:O	1:D:113:SER:HA	2.10	0.52
2:K:525:ILE:HA	2:K:528:THR:HG22	1.90	0.52
2:B:584:PHE:CZ	2:B:609:GLN:HG2	2.45	0.51
2:K:525:ILE:HD11	2:K:574:ALA:HB2	1.94	0.50
1:J:119:PHE:CE2	1:J:164:VAL:HG11	2.46	0.50
2:B:543:TYR:CE2	2:B:560:ILE:HD11	2.47	0.49
2:K:647:GLU:O	2:K:651:THR:HG23	2.12	0.49
2:B:667:GLY:HA3	2:B:719:LEU:HD21	1.94	0.49
2:B:557:CYS:HA	2:B:560:ILE:HD12	1.94	0.48
2:E:498:LEU:CD1	2:E:509:ILE:HD11	2.41	0.48
1:J:7:GLY:HA3	1:J:37:THR:HG22	1.96	0.47
2:K:582:ARG:NH2	6:K:901:HOH:O	2.47	0.47
2:H:581:LEU:C	2:H:581:LEU:HD23	2.39	0.47
1:A:142:LEU:HD21	2:B:589:LEU:HD22	1.97	0.47
1:D:12:PRO:HA	1:D:15:CYS:O	2.14	0.47
1:J:153:MET:HG2	1:J:162:THR:HG22	1.96	0.47
2:K:525:ILE:HD11	2:K:574:ALA:CB	2.44	0.47
1:A:67:LEU:HD23	1:A:67:LEU:O	2.15	0.46
1:D:153:MET:HG2	1:D:162:THR:HG22	1.97	0.46
1:D:28:PRO:HG3	1:D:51:THR:HG22	1.97	0.46
2:B:682:ASN:C	2:B:682:ASN:HD22	2.24	0.45
2:B:743:LEU:O	2:B:747:ILE:HG23	2.16	0.45
2:B:543:TYR:CD2	2:B:560:ILE:HD11	2.52	0.45
2:K:750:ILE:HG21	2:K:770:PHE:CD1	2.52	0.45
1:J:3:VAL:HG11	1:J:35:LEU:HD12	1.98	0.45
1:J:40:LEU:N	1:J:41:CYS:HA	2.32	0.45
2:K:543:TYR:CE1	2:K:556:LYS:HD3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:536:ALA:HB1	2:B:560:ILE:HG22	1.99	0.44
1:D:9:LEU:CD2	1:D:135:ALA:HB3	2.48	0.44
2:H:495:ILE:HD13	2:H:535:ALA:HB2	2.00	0.43
2:B:526:ARG:HG3	2:B:576:LEU:HD11	2.01	0.43
2:B:763:THR:O	2:B:767:ASN:ND2	2.51	0.43
1:D:101:LEU:C	1:D:101:LEU:HD23	2.44	0.43
2:H:650:ARG:HD3	2:H:677:PHE:CE2	2.53	0.43
1:J:9:LEU:HD23	1:J:135:ALA:HB3	2.01	0.43
1:J:14:ARG:O	2:K:499:ARG:NH2	2.52	0.43
1:A:59:VAL:HG13	1:A:84:LEU:HD23	2.01	0.43
1:A:85:ILE:O	1:A:113:SER:HA	2.19	0.42
1:G:34:ILE:HD11	1:G:52:LEU:HB2	2.01	0.42
1:G:40:LEU:N	1:G:41:CYS:HA	2.33	0.42
1:G:101:LEU:HD23	1:G:101:LEU:C	2.43	0.42
2:E:581:LEU:C	2:E:581:LEU:HD23	2.44	0.42
1:A:9:LEU:CD2	1:A:135:ALA:HB3	2.49	0.42
1:J:1:MET:HE3	1:J:155:ILE:O	2.19	0.42
2:H:614:TYR:HA	2:H:618:ILE:HD12	2.01	0.42
2:E:707:ALA:HA	2:E:719:LEU:HD23	2.02	0.41
2:E:732:GLU:OE2	2:E:776:HIS:NE2	2.49	0.41
1:G:130:ILE:HD11	1:G:153:MET:HE3	2.02	0.41
1:D:104:ARG:NH1	2:E:725:ASN:OD1	2.53	0.41
2:H:724:LEU:HD12	2:H:773:THR:HG21	2.01	0.41
2:E:666:GLN:HG3	2:E:706:ILE:HD13	2.02	0.41
2:E:741:GLN:HE21	2:E:745:GLN:NE2	2.17	0.41
2:E:750:ILE:HG21	2:E:770:PHE:CD1	2.56	0.41
1:J:28:PRO:HG3	1:J:51:THR:HG22	2.02	0.41
3:C:165:GLU:HB3	3:C:175:ILE:HD12	2.03	0.40
1:G:142:LEU:HD21	2:H:589:LEU:HD11	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	D	181/182 (100%)	176 (97%)	5 (3%)	0	100	100
1	G	180/182 (99%)	173 (96%)	7 (4%)	0	100	100
1	J	180/182 (99%)	172 (96%)	8 (4%)	0	100	100
2	B	297/311 (96%)	287 (97%)	10 (3%)	0	100	100
2	E	301/311 (97%)	293 (97%)	8 (3%)	0	100	100
2	H	281/311 (90%)	274 (98%)	7 (2%)	0	100	100
2	K	290/311 (93%)	281 (97%)	9 (3%)	0	100	100
3	C	10/14 (71%)	10 (100%)	0	0	100	100
3	F	9/14 (64%)	8 (89%)	1 (11%)	0	100	100
3	I	10/14 (71%)	10 (100%)	0	0	100	100
All	All	1919/2014 (95%)	1859 (97%)	60 (3%)	0	100	100

There are no Ramachandran outliers to report.

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%)	155 (97%)	5 (3%)	35	60
1	D	161/160 (101%)	158 (98%)	3 (2%)	50	74
1	G	160/160 (100%)	157 (98%)	3 (2%)	50	74
1	J	160/160 (100%)	153 (96%)	7 (4%)	25	47
2	B	260/272 (96%)	256 (98%)	4 (2%)	57	79
2	E	264/272 (97%)	255 (97%)	9 (3%)	32	57
2	H	248/272 (91%)	239 (96%)	9 (4%)	31	55
2	K	258/272 (95%)	247 (96%)	11 (4%)	26	49
3	C	11/13 (85%)	10 (91%)	1 (9%)	9	17
3	F	10/13 (77%)	10 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	I	11/13 (85%)	11 (100%)	0	100	100
All	All	1703/1767 (96%)	1651 (97%)	52 (3%)	36	60

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LYS
1	A	45	SER
1	A	68	ASN
1	A	72	GLN
1	A	145	ASN
2	B	542	ARG
2	B	555	LYS
2	B	673	CYS
2	B	682	ASN
3	C	165	GLU
1	D	43	LYS
1	D	75	VAL
1	D	181	LYS
2	E	514[A]	ARG
2	E	514[B]	ARG
2	E	608	SER
2	E	611	PHE
2	E	652	GLN
2	E	726	ARG
2	E	748	GLN
2	E	757	LEU
2	E	761	GLU
1	G	27	VAL
1	G	96	MET
1	G	156	GLN
2	H	493	ARG
2	H	511	ASN
2	H	528	THR
2	H	559	LYS
2	H	582	ARG
2	H	609	GLN
2	H	719	LEU
2	H	724	LEU
2	H	734	GLU
1	J	6	LEU
1	J	37	THR

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Mol	Chain	Res	Type
1	J	65	GLU
1	J	75	VAL
1	J	164	VAL
1	J	170	ASP
1	J	171	ASP
2	K	490	LEU
2	K	504	ASP
2	K	510	LEU
2	K	528	THR
2	K	597	GLU
2	K	598	ASN
2	K	625	LEU
2	K	711	MET
2	K	740	ILE
2	K	747	ILE
2	K	767	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	ASN
1	A	124	HIS
2	B	511	ASN
2	B	523	GLN
2	B	609	GLN
2	B	624	GLN
2	B	682	ASN
2	B	772	ASN
1	D	115	HIS
1	D	124	HIS
1	D	145	ASN
1	D	156	GLN
2	E	566	GLN
2	E	586	GLN
2	E	609	GLN
2	E	624	GLN
2	E	666	GLN
2	E	716	GLN
2	E	745	GLN
1	G	39	ASN
1	G	156	GLN
2	H	599	HIS

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Mol	Chain	Res	Type
2	H	609	GLN
2	H	765	GLN
2	H	776	HIS
1	J	57	HIS
1	J	68	ASN
1	J	79	GLN
1	J	115	HIS
2	K	505	GLN
2	K	523	GLN
2	K	538	GLN
2	K	769	HIS

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](#)

Of 15 ligands modelled in this entry, 4 are monoatomic - leaving 11 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	EDO	D	201	-	3,3,3	0.45	0	2,2,2	0.27	0
4	EDO	G	201	-	3,3,3	0.44	0	2,2,2	0.37	0
4	EDO	K	802	-	3,3,3	0.44	0	2,2,2	0.12	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	K	801	-	3,3,3	0.38	0	2,2,2	0.27	0
4	EDO	K	803	-	3,3,3	0.51	0	2,2,2	0.21	0
4	EDO	J	202	-	3,3,3	0.46	0	2,2,2	0.28	0
4	EDO	D	202	-	3,3,3	0.44	0	2,2,2	0.25	0
4	EDO	J	201	-	3,3,3	0.50	0	2,2,2	0.25	0
4	EDO	B	801	-	3,3,3	0.40	0	2,2,2	0.55	0
4	EDO	A	201	-	3,3,3	0.48	0	2,2,2	0.19	0
4	EDO	H	801	-	3,3,3	0.44	0	2,2,2	0.37	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	D	201	-	-	0/1/1/1	-
4	EDO	G	201	-	-	0/1/1/1	-
4	EDO	K	802	-	-	1/1/1/1	-
4	EDO	K	801	-	-	1/1/1/1	-
4	EDO	K	803	-	-	1/1/1/1	-
4	EDO	J	202	-	-	1/1/1/1	-
4	EDO	D	202	-	-	1/1/1/1	-
4	EDO	J	201	-	-	0/1/1/1	-
4	EDO	B	801	-	-	0/1/1/1	-
4	EDO	A	201	-	-	1/1/1/1	-
4	EDO	H	801	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	202	EDO	O1-C1-C2-O2
4	J	202	EDO	O1-C1-C2-O2
4	A	201	EDO	O1-C1-C2-O2
4	K	801	EDO	O1-C1-C2-O2
4	K	803	EDO	O1-C1-C2-O2
4	K	802	EDO	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	182/182 (100%)	0.24	1 (0%) 87 85	31, 53, 87, 97	0
1	D	182/182 (100%)	0.13	1 (0%) 87 85	23, 48, 75, 109	1 (0%)
1	G	182/182 (100%)	0.26	4 (2%) 62 59	35, 56, 83, 99	0
1	J	182/182 (100%)	0.19	5 (2%) 56 52	23, 50, 81, 98	0
2	B	299/311 (96%)	0.32	8 (2%) 56 52	28, 58, 93, 112	0
2	E	302/311 (97%)	-0.02	3 (0%) 79 77	20, 45, 83, 112	1 (0%)
2	H	283/311 (90%)	0.35	6 (2%) 63 60	32, 58, 91, 116	2 (0%)
2	K	293/311 (94%)	-0.12	3 (1%) 79 77	17, 37, 72, 103	1 (0%)
3	C	12/14 (85%)	0.97	2 (16%) 4 3	71, 78, 86, 88	0
3	F	11/14 (78%)	0.60	0 100 100	48, 59, 86, 107	0
3	I	12/14 (85%)	1.44	1 (8%) 17 15	71, 91, 102, 103	0
All	All	1940/2014 (96%)	0.17	34 (1%) 67 64	17, 51, 87, 116	5 (0%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	479	PRO	3.5
2	K	759	SER	3.0
1	J	1	MET	2.8
3	I	175	ILE	2.8
2	E	779	LEU	2.8
2	H	680	GLY	2.8
2	K	521	GLY	2.8
1	G	157	ALA	2.7
2	H	490	LEU	2.6
2	H	514[A]	ARG	2.6
2	H	779	LEU	2.6
2	B	549	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
3	C	175	ILE	2.5
2	B	711	MET	2.5
2	E	485	ALA	2.4
1	D	182	PRO	2.3
2	B	517	PHE	2.3
1	G	182	PRO	2.3
1	J	172	VAL	2.3
1	J	182	PRO	2.3
2	H	692	GLY	2.2
2	B	512	THR	2.2
3	C	168	PRO	2.2
1	J	174	VAL	2.2
2	B	779	LEU	2.2
2	B	684	ASP	2.2
1	G	1	MET	2.1
2	K	515	LYS	2.1
2	B	710	CYS	2.1
1	J	159	THR	2.1
1	G	67	LEU	2.0
2	B	738	VAL	2.0
1	A	29	GLY	2.0
2	H	683	THR	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	EDO	J	201	4/4	0.67	0.23	61,64,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	J	202	4/4	0.68	0.22	64,64,65,65	0
5	NA	E	801	1/1	0.69	0.31	68,68,68,68	0
4	EDO	D	202	4/4	0.75	0.16	82,84,85,87	0
4	EDO	K	803	4/4	0.81	0.17	61,64,66,66	0
4	EDO	H	801	4/4	0.84	0.20	62,62,63,63	0
4	EDO	K	802	4/4	0.86	0.13	63,64,64,66	0
5	NA	K	805	1/1	0.87	0.25	56,56,56,56	0
4	EDO	A	201	4/4	0.88	0.17	71,71,72,73	0
5	NA	K	804	1/1	0.88	0.21	47,47,47,47	0
4	EDO	B	801	4/4	0.88	0.12	53,53,54,55	0
4	EDO	K	801	4/4	0.89	0.16	44,44,44,45	0
4	EDO	D	201	4/4	0.91	0.10	43,45,46,46	0
4	EDO	G	201	4/4	0.93	0.12	54,54,55,55	0
5	NA	H	802	1/1	0.93	0.17	58,58,58,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.