



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 2, 2025 – 02:12 PM EDT

PDB ID : 9MSP / pdb_00009msp
Title : Crystal structure of MPXV A35R in complex with neutralizing antibody EV35-7
Authors : Yuan, M.; Wilson, I.A.
Deposited on : 2025-01-10
Resolution : 2.19 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:

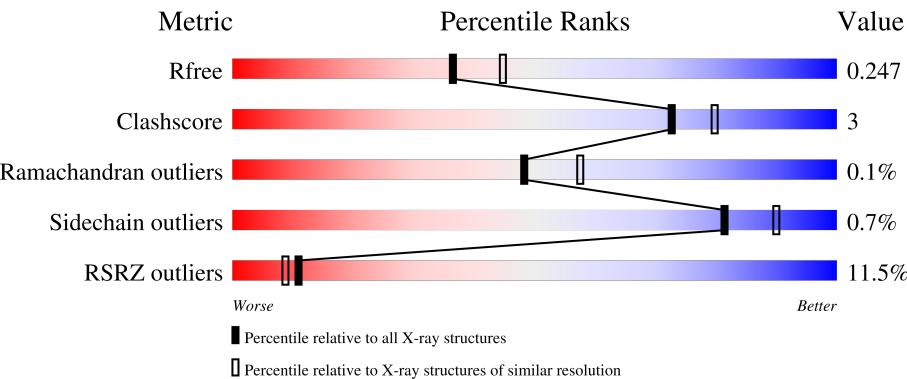
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.45.1

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 2.19 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}	164625	5791 (2.20-2.20)
Clashscore	180529	6634 (2.20-2.20)
Ramachandran outliers	177936	6560 (2.20-2.20)
Sidechain outliers	177891	6561 (2.20-2.20)
RSRZ outliers	164620	5791 (2.20-2.20)

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	100	<div><div>32%</div><div><div></div><div></div><div></div><div></div></div><div>74%</div><div>23%</div></div>
1	B	100	<div><div>15%</div><div><div></div><div></div><div></div><div></div></div><div>73%</div><div>10%</div><div>17%</div></div>
1	E	100	<div><div>11%</div><div><div></div><div></div><div></div><div></div></div><div>76%</div><div>22%</div></div>
1	F	100	<div><div>13%</div><div><div></div><div></div><div></div><div></div></div><div>74%</div><div>5%</div><div>21%</div></div>
2	C	225	<div><div>3%</div><div><div></div><div></div><div></div><div></div></div><div>87%</div><div>12%</div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	H	225	<div><div></div><div>5%</div><div>89%</div><div>8%</div><div></div></div>
3	D	212	<div><div></div><div>8%</div><div>89%</div><div>7%</div><div>5%</div></div>
3	L	212	<div><div></div><div>13%</div><div>85%</div><div>9%</div><div>5%</div></div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9419 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 Protein OPG161.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	78	Total	C	N	O	S	0	0	0
			607	378	96	129	4			
1	F	79	Total	C	N	O	S	0	2	0
			623	390	97	132	4			
1	A	77	Total	C	N	O	S	0	0	0
			601	375	95	127	4			
1	B	83	Total	C	N	O	S	0	0	0
			655	407	102	142	4			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	182	GLY	-	expression tag	UNP A0A7H0DND2
E	183	SER	-	expression tag	UNP A0A7H0DND2
E	184	HIS	-	expression tag	UNP A0A7H0DND2
E	185	HIS	-	expression tag	UNP A0A7H0DND2
E	186	HIS	-	expression tag	UNP A0A7H0DND2
E	187	HIS	-	expression tag	UNP A0A7H0DND2
E	188	HIS	-	expression tag	UNP A0A7H0DND2
E	189	HIS	-	expression tag	UNP A0A7H0DND2
F	182	GLY	-	expression tag	UNP A0A7H0DND2
F	183	SER	-	expression tag	UNP A0A7H0DND2
F	184	HIS	-	expression tag	UNP A0A7H0DND2
F	185	HIS	-	expression tag	UNP A0A7H0DND2
F	186	HIS	-	expression tag	UNP A0A7H0DND2
F	187	HIS	-	expression tag	UNP A0A7H0DND2
F	188	HIS	-	expression tag	UNP A0A7H0DND2
F	189	HIS	-	expression tag	UNP A0A7H0DND2
A	182	GLY	-	expression tag	UNP A0A7H0DND2
A	183	SER	-	expression tag	UNP A0A7H0DND2
A	184	HIS	-	expression tag	UNP A0A7H0DND2
A	185	HIS	-	expression tag	UNP A0A7H0DND2
A	186	HIS	-	expression tag	UNP A0A7H0DND2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	187	HIS	-	expression tag	UNP A0A7H0DND2
A	188	HIS	-	expression tag	UNP A0A7H0DND2
A	189	HIS	-	expression tag	UNP A0A7H0DND2
B	182	GLY	-	expression tag	UNP A0A7H0DND2
B	183	SER	-	expression tag	UNP A0A7H0DND2
B	184	HIS	-	expression tag	UNP A0A7H0DND2
B	185	HIS	-	expression tag	UNP A0A7H0DND2
B	186	HIS	-	expression tag	UNP A0A7H0DND2
B	187	HIS	-	expression tag	UNP A0A7H0DND2
B	188	HIS	-	expression tag	UNP A0A7H0DND2
B	189	HIS	-	expression tag	UNP A0A7H0DND2

- Molecule 2 is a protein called EV35-7 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	218	Total	C	N	O	S	0	0	0
			1645	1035	285	317	8			
2	C	223	Total	C	N	O	S	0	0	0
			1679	1054	291	326	8			

- Molecule 3 is a protein called EV35-7 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	201	Total	C	N	O	S	0	1	0
			1565	984	259	316	6			
3	D	202	Total	C	N	O	S	0	0	0
			1560	977	258	319	6			

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	E	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	F	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	L	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		

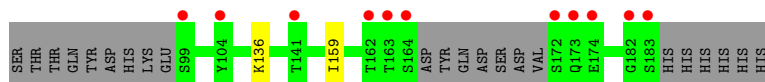
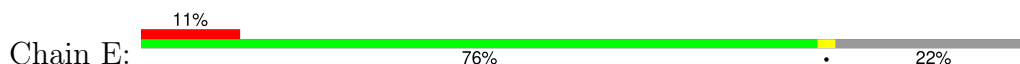
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	E	36	Total	O	0	0
			36	36		
7	F	25	Total	O	0	0
			25	25		
7	H	85	Total	O	0	0
			85	85		
7	L	90	Total	O	0	0
			90	90		
7	A	11	Total	O	0	0
			11	11		
7	B	21	Total	O	0	0
			21	21		
7	C	105	Total	O	0	0
			105	105		
7	D	84	Total	O	0	0
			84	84		

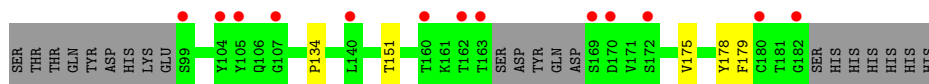
3 Residue-property plots [i](#)

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.

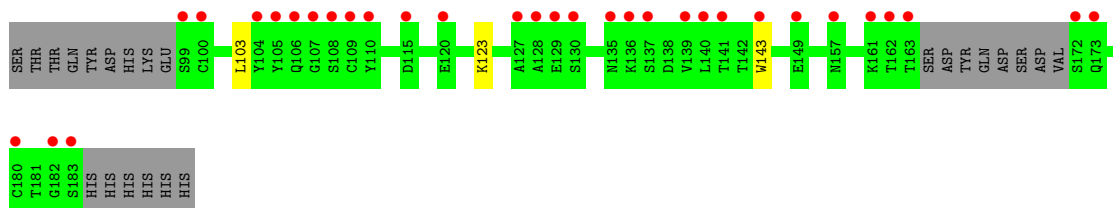
- Molecule 1: Protein OPG161



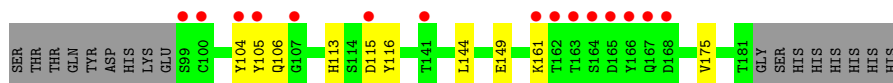
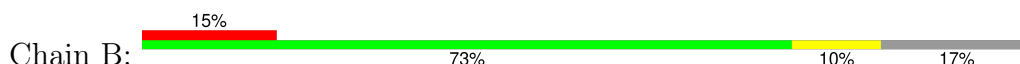
- Molecule 1: Protein OPG161



- Molecule 1: Protein OPG161

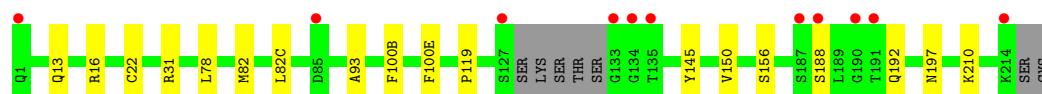


- Molecule 1: Protein OPG161

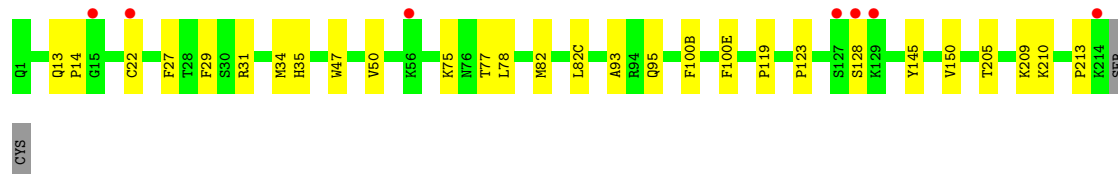
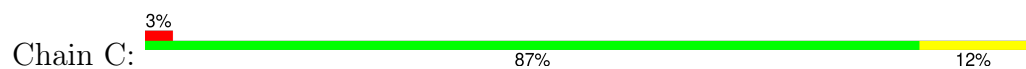


- Molecule 2: EV35-7 heavy chain

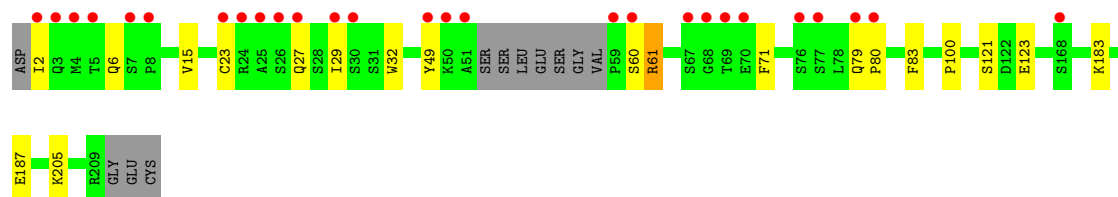
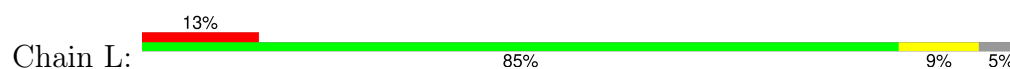




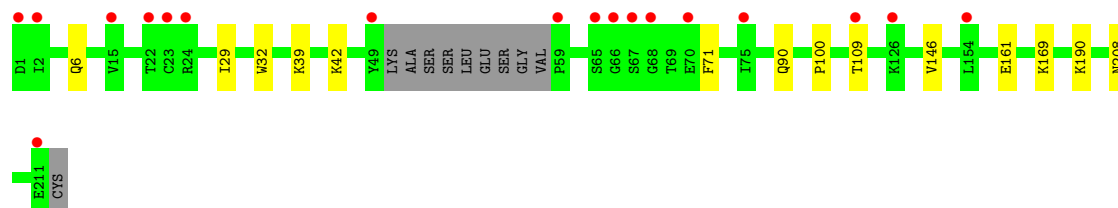
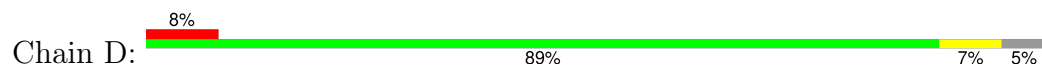
- Molecule 2: EV35-7 heavy chain



- Molecule 3: EV35-7 light chain



- Molecule 3: EV35-7 light chain



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	103.34Å 107.89Å 268.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.74 – 2.19 44.74 – 2.19	Depositor EDS
% Data completeness (in resolution range)	95.5 (44.74-2.19) 95.4 (44.74-2.19)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.87 (at 2.20Å)	Xtriage
Refinement program	PHENIX (1.21.2_5419: ???)	Depositor
R, R_{free}	0.211 , 0.250 0.210 , 0.247	Depositor DCC
R_{free} test set	3661 reflections (4.73%)	wwPDB-VP
Wilson B-factor (Å ²)	29.5	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 35.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.043 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9419	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, ACT, SO4

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	0.14	0/614	0.37	0/833
1	B	0.16	0/670	0.41	0/912
1	E	0.13	0/620	0.34	0/841
1	F	0.13	0/642	0.37	0/872
2	C	0.11	0/1719	0.33	0/2336
2	H	0.12	0/1684	0.32	0/2288
3	D	0.12	0/1593	0.35	0/2161
3	L	0.18	0/1599	0.39	0/2169
All	All	0.14	0/9141	0.36	0/12412

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	L	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	L	61	ARG	Sidechain

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	601	0	549	2	0
1	B	655	0	590	5	0
1	E	607	0	554	1	0
1	F	623	0	576	3	0
2	C	1679	0	1647	16	0
2	H	1645	0	1611	10	0
3	D	1560	0	1513	6	0
3	L	1565	0	1523	13	0
4	E	4	0	3	0	0
5	A	4	0	6	0	0
5	F	4	0	6	0	0
6	C	5	0	0	0	0
6	D	5	0	0	0	0
6	L	5	0	0	0	0
7	A	11	0	0	1	0
7	B	21	0	0	0	0
7	C	105	0	0	1	0
7	D	84	0	0	0	0
7	E	36	0	0	0	0
7	F	25	0	0	0	0
7	H	85	0	0	0	0
7	L	90	0	0	2	0
All	All	9419	0	8578	55	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 (55) 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:H:156:SER:H	2:H:197:ASN:HD21	1.25	0.82
2:C:35:HIS:HD1	2:C:47:TRP:HE1	1.31	0.75
1:E:136:LYS:HE2	1:E:159:ILE:HA	1.71	0.71
3:L:2:ILE:HG12	3:L:27:GLN:HE22	1.56	0.70
3:L:49[B]:TYR:O	3:L:60:SER:HB3	2.00	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:13:GLN:HB2	2:H:16:ARG:HD2	1.84	0.59
2:C:82:MET:HE2	2:C:82(C):LEU:HD21	1.83	0.59
1:B:149:GLU:OE2	1:B:161:LYS:HE3	2.03	0.58
2:H:188:SER:HB3	2:H:192:GLN:HG3	1.85	0.57
2:C:13:GLN:HG3	2:C:14:PRO:HD2	1.86	0.57
3:L:6:GLN:HG3	3:L:100:PRO:HD2	1.87	0.56
2:H:156:SER:H	2:H:197:ASN:ND2	2.00	0.56
1:B:116:TYR:HB3	1:B:175:VAL:HG12	1.88	0.55
2:C:95:GLN:NE2	2:C:100(B):PHE:HA	2.20	0.55
3:L:205:LYS:HG2	7:L:470:HOH:O	2.08	0.54
2:H:82:MET:HE2	2:H:82(C):LEU:HD21	1.90	0.53
1:B:105:TYR:HB2	1:B:144:LEU:HD21	1.91	0.53
2:C:128:SER:HB2	2:C:213:PRO:HB3	1.92	0.52
2:C:75:LYS:HB2	2:C:77:THR:HG22	1.93	0.50
3:L:6:GLN:HG2	3:L:23:CYS:HB2	1.94	0.49
2:H:119:PRO:HB3	2:H:145:TYR:HB3	1.94	0.48
3:D:146:VAL:HB	3:D:161:GLU:OE2	2.13	0.48
2:C:50:VAL:HG11	2:C:100(B):PHE:HE1	1.78	0.48
3:L:32:TRP:CD2	3:L:71:PHE:HB2	2.49	0.46
1:A:103:LEU:HD22	1:A:143:TRP:HZ3	1.80	0.46
1:B:104:TYR:HD1	1:B:105:TYR:N	2.13	0.46
2:C:210:LYS:HB2	2:C:210:LYS:HE3	1.86	0.45
3:L:183:LYS:O	3:L:187:GLU:HG2	2.16	0.45
3:L:183:LYS:HB3	7:L:411:HOH:O	2.16	0.45
1:F:151:THR:HB	1:F:178:TYR:HA	2.00	0.44
3:L:79:GLN:HB2	3:L:80:PRO:HD2	1.99	0.44
3:D:190:LYS:HE3	3:D:208:ASN:HB3	1.98	0.44
2:C:119:PRO:HB3	2:C:145:TYR:HB3	1.99	0.44
2:C:22:CYS:HB3	2:C:78:LEU:HB3	1.98	0.44
3:L:29:ILE:HD11	3:L:32:TRP:CE2	2.53	0.43
1:A:123:LYS:HG2	7:A:302:HOH:O	2.18	0.43
3:D:32:TRP:CD2	3:D:71:PHE:HB2	2.53	0.43
1:F:134:PRO:HD3	1:F:179:PHE:O	2.18	0.43
2:C:31:ARG:HA	2:C:31:ARG:HD2	1.74	0.43
2:H:31:ARG:HA	2:H:31:ARG:HD2	1.71	0.43
2:C:205:THR:HG21	7:C:413:HOH:O	2.18	0.43
1:B:113:HIS:HB3	1:B:115:ASP:OD1	2.18	0.43
1:F:175[B]:VAL:CG2	2:H:100(B):PHE:HB2	2.49	0.43
2:C:34:MET:HB3	2:C:78:LEU:HD22	1.99	0.42
2:H:22:CYS:HB3	2:H:78:LEU:HB3	1.99	0.42
3:L:32:TRP:HB3	3:L:71:PHE:CE2	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:123:PRO:HD3	2:C:209:LYS:HE2	2.02	0.42
3:D:6:GLN:HG3	3:D:100:PRO:HD2	2.02	0.42
2:C:93:ALA:HB1	2:C:100(E):PHE:HB3	2.01	0.41
2:H:93:ALA:HB1	2:H:100(E):PHE:HB3	2.01	0.41
2:C:27:PHE:CE2	2:C:29:PHE:HA	2.56	0.41
3:D:29:ILE:HD13	3:D:90:GLN:HB2	2.02	0.41
3:D:39:LYS:HB2	3:D:42:LYS:HD3	2.03	0.40
3:L:80:PRO:HA	3:L:83:PHE:CE2	2.56	0.40
3:L:121:SER:OG	3:L:123:GLU:HG2	2.20	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	73/100 (73%)	71 (97%)	2 (3%)	0	100	100
1	B	81/100 (81%)	75 (93%)	5 (6%)	1 (1%)	11	9
1	E	74/100 (74%)	72 (97%)	2 (3%)	0	100	100
1	F	77/100 (77%)	75 (97%)	2 (3%)	0	100	100
2	C	221/225 (98%)	219 (99%)	2 (1%)	0	100	100
2	H	214/225 (95%)	213 (100%)	1 (0%)	0	100	100
3	D	198/212 (93%)	191 (96%)	7 (4%)	0	100	100
3	L	198/212 (93%)	190 (96%)	8 (4%)	0	100	100
All	All	1136/1274 (89%)	1106 (97%)	29 (3%)	1 (0%)	48	57

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	106	GLN

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	68/91 (75%)	68 (100%)	0	100	100
1	B	75/91 (82%)	75 (100%)	0	100	100
1	E	69/91 (76%)	69 (100%)	0	100	100
1	F	72/91 (79%)	72 (100%)	0	100	100
2	C	190/192 (99%)	189 (100%)	1 (0%)	86	93
2	H	185/192 (96%)	183 (99%)	2 (1%)	70	82
3	D	179/187 (96%)	177 (99%)	2 (1%)	70	82
3	L	179/187 (96%)	177 (99%)	2 (1%)	70	82
All	All	1017/1122 (91%)	1010 (99%)	7 (1%)	81	90

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	150	VAL
2	H	210	LYS
3	L	15	VAL
3	L	61	ARG
2	C	150	VAL
3	D	109	THR
3	D	169	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	135	ASN
2	H	3	GLN
2	H	197	ASN
3	L	27	GLN
3	L	147	GLN
1	A	125	ASN
1	A	157	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	167	GLN
1	B	173	GLN
2	C	13	GLN
2	C	39	GLN
2	C	81	GLN
2	C	82(A)	ASN
2	C	95	GLN
2	C	164	HIS
3	D	38	GLN
3	D	137	ASN
3	D	138	ASN
3	D	147	GLN
3	D	160	GLN
3	D	189	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](#)

6 ligands are modelled in this entry.

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
6	SO4	L	301	-	4,4,4	0.67	0	6,6,6	0.09	0
6	SO4	C	301	-	4,4,4	0.67	0	6,6,6	0.09	0
5	EDO	A	201	-	3,3,3	0.25	0	2,2,2	0.34	0
6	SO4	D	301	-	4,4,4	0.67	0	6,6,6	0.10	0
5	EDO	F	201	-	3,3,3	0.26	0	2,2,2	0.35	0
4	ACT	E	201	-	3,3,3	1.12	0	3,3,3	1.21	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
5	EDO	F	201	-	-	0/1/1/1	-
5	EDO	A	201	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	201	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	77/100 (77%)	1.76	32 (41%)	1 0	32, 53, 89, 115	0
1	B	83/100 (83%)	1.28	15 (18%)	4 4	23, 38, 81, 96	0
1	E	78/100 (78%)	0.65	11 (14%)	7 6	18, 31, 78, 98	0
1	F	79/100 (79%)	0.88	13 (16%)	5 4	14, 34, 68, 100	2 (2%)
2	C	223/225 (99%)	0.15	7 (3%)	51 48	13, 29, 49, 83	0
2	H	218/225 (96%)	0.25	11 (5%)	35 32	15, 27, 51, 73	0
3	D	202/212 (95%)	0.65	18 (8%)	17 14	17, 35, 64, 90	0
3	L	201/212 (94%)	0.71	27 (13%)	8 6	17, 33, 73, 94	1 (0%)
All	All	1161/1274 (91%)	0.62	134 (11%)	11 9	13, 33, 72, 115	3 (0%)

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	L	49[A]	TYR	6.7
3	L	2	ILE	5.8
1	B	166	TYR	5.7
2	H	133	GLY	5.3
1	F	162	THR	5.2
1	A	163	THR	5.1
1	E	173	GLN	5.0
3	D	68	GLY	5.0
3	L	7	SER	4.7
1	A	105	TYR	4.6
3	D	49	TYR	4.6
3	L	68	GLY	4.6
3	L	4	MET	4.5
1	E	172	SER	4.4
1	F	163	THR	4.4
1	A	104	TYR	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	141	THR	4.2
3	L	8	PRO	4.2
1	B	141	THR	4.1
1	A	140	LEU	4.1
3	D	66	GLY	4.0
1	A	120	GLU	4.0
3	L	67	SER	3.9
3	L	25	ALA	3.9
1	E	163	THR	3.9
1	E	174	GLU	3.9
2	C	214	LYS	3.9
2	H	134	GLY	3.9
3	D	23	CYS	3.9
1	B	107	GLY	3.9
3	L	59	PRO	3.8
1	B	99	SER	3.8
3	L	23	CYS	3.8
3	L	76	SER	3.8
3	L	29	ILE	3.7
2	H	127	SER	3.7
1	B	115	ASP	3.7
1	A	108	SER	3.7
1	A	183	SER	3.7
2	C	127	SER	3.7
3	L	30	SER	3.7
1	B	165	ASP	3.7
1	E	182	GLY	3.6
3	D	154	LEU	3.6
1	B	104	TYR	3.6
1	F	169	SER	3.6
2	H	188	SER	3.6
1	B	163	THR	3.5
1	B	162	THR	3.5
3	L	5	THR	3.5
1	E	99	SER	3.4
1	A	182	GLY	3.4
1	A	172	SER	3.4
1	F	104	TYR	3.4
1	F	99	SER	3.3
1	A	161	LYS	3.3
1	F	107	GLY	3.3
1	A	109	CYS	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	167	GLN	3.2
3	D	59	PRO	3.2
3	D	70	GLU	3.1
1	A	162	THR	3.1
3	D	2	ILE	3.0
1	B	164	SER	3.0
3	L	80	PRO	3.0
1	A	106	GLN	3.0
1	B	105	TYR	3.0
2	C	129	LYS	3.0
2	H	187	SER	3.0
1	F	160	THR	3.0
3	L	69	THR	2.9
1	F	182	GLY	2.9
1	A	107	GLY	2.9
3	D	67	SER	2.9
1	E	183	SER	2.9
3	L	24	ARG	2.9
2	H	214	LYS	2.8
1	E	141	THR	2.8
3	D	24	ARG	2.8
1	A	136	LYS	2.7
1	A	128	ALA	2.7
2	H	135	THR	2.7
2	H	191	THR	2.7
1	E	164	SER	2.7
1	A	143	TRP	2.7
1	A	137	SER	2.7
3	D	15	VAL	2.6
1	A	127	ALA	2.6
2	H	190	GLY	2.6
3	D	75	ILE	2.6
1	B	100	CYS	2.6
1	F	140	LEU	2.6
3	D	211	GLU	2.6
2	C	56	LYS	2.5
1	A	115	ASP	2.5
3	D	22	THR	2.5
3	L	70	GLU	2.5
1	A	139	VAL	2.5
3	L	51	ALA	2.5
3	D	109	THR	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	180	CYS	2.4
1	E	162	THR	2.4
3	L	60	SER	2.4
3	L	168	SER	2.4
3	D	65	SER	2.4
1	F	105	TYR	2.4
3	L	3	GLN	2.4
1	A	180	CYS	2.4
3	L	27	GLN	2.4
2	H	1	GLN	2.3
1	F	172	SER	2.3
1	F	170	ASP	2.3
3	D	1	ASP	2.3
3	L	50	LYS	2.2
1	E	104	TYR	2.2
3	L	26	SER	2.2
3	L	77	SER	2.2
1	A	100	CYS	2.2
1	A	135	ASN	2.2
2	H	85	ASP	2.2
3	D	126	LYS	2.2
1	A	110	TYR	2.2
3	L	79	GLN	2.2
1	A	173	GLN	2.1
1	A	129	GLU	2.1
2	C	22	CYS	2.1
2	C	15	GLY	2.1
1	A	149	GLU	2.1
1	A	130	SER	2.1
2	C	128	SER	2.1
1	A	157	ASN	2.0
1	A	99	SER	2.0
1	B	161	LYS	2.0
1	B	168	ASP	2.0

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

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(\AA^2)	Q<0.9
6	SO4	C	301	5/5	0.78	0.10	64,73,88,91	0
5	EDO	A	201	4/4	0.80	0.18	44,48,51,53	0
6	SO4	D	301	5/5	0.82	0.10	58,65,76,79	0
5	EDO	F	201	4/4	0.87	0.16	38,40,43,51	0
4	ACT	E	201	4/4	0.87	0.13	49,50,51,51	0
6	SO4	L	301	5/5	0.88	0.11	56,63,70,74	0

6.5 Other polymers [i](#)

There are no such residues in this entry.