Full wwPDB X-ray Structure Validation Report ⓘ

Sep 2, 2023 – 08:32 PM EDT

PDB ID	:	3QWO
Title	:	Crystal structure of a motavizumab epitope-scaffold bound to motavizumab Fab
Authors	:	McLellan, J.S.; Kwong, P.D.
Deposited on	:	2011-02-28
Resolution	:	1.90 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:

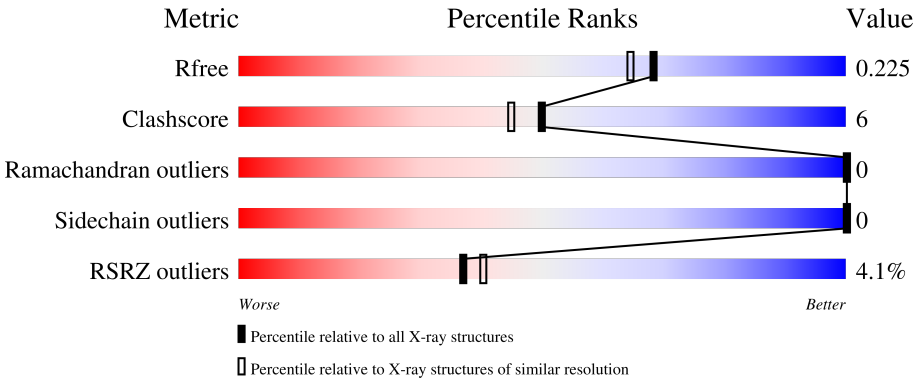
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	B	213	86% 13%
1	L	213	3% 86% 12%
2	A	225	12% 85% 13%
2	H	225	3% 82% 16%
3	C	57	93% 7%

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Mol	Chain	Length	Quality of chain
3	P	57	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 15129 atoms, of which 7231 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 motavizumab light chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	L	210	Total	C	H	N	O	S	0	0	0
			3171	1010	1564	267	324	6			
1	B	210	Total	C	H	N	O	S	0	0	0
			3171	1010	1564	267	324	6			

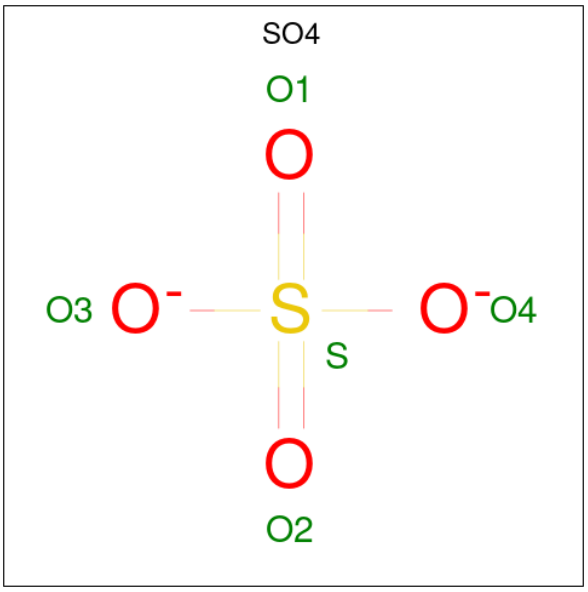
- Molecule 2 is a protein called motavizumab heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	H	220	Total	C	H	N	O	S	0	0	0
			3323	1062	1655	274	325	7			
2	A	220	Total	C	H	N	O	S	0	0	0
			3322	1062	1654	274	325	7			

- Molecule 3 is a protein called motavizumab epitope scaffold.

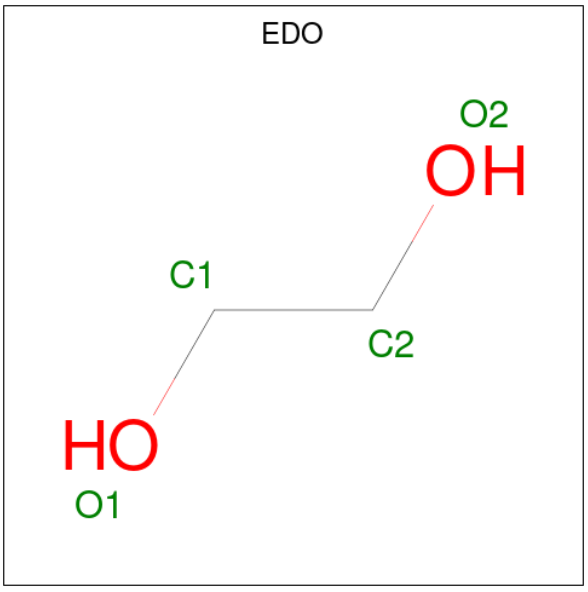
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	53	Total	C	H	N	O	0	0	0
			794	245	388	71	90			
3	P	53	Total	C	H	N	O	0	0	0
			794	245	388	71	90			

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	L	1	Total O S 5 4 1	0	0
4	H	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	H	1	Total C H O 10 2 6 2	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	H	O	0	0
			10	2	6	2		
5	A	1	Total	C	H	O	0	0
			10	2	6	2		

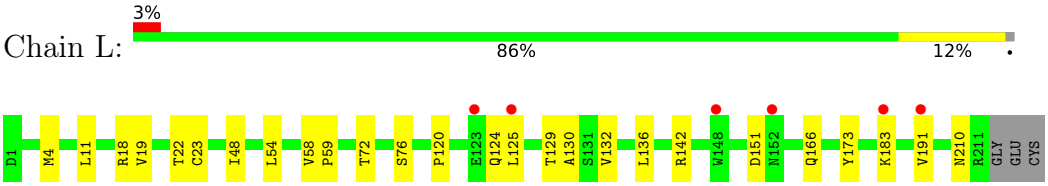
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	L	89	Total	O	0	0
			89	89		
6	H	151	Total	O	0	0
			151	151		
6	B	97	Total	O	0	0
			97	97		
6	A	131	Total	O	0	0
			131	131		
6	C	29	Total	O	0	0
			29	29		
6	P	12	Total	O	0	0
			12	12		

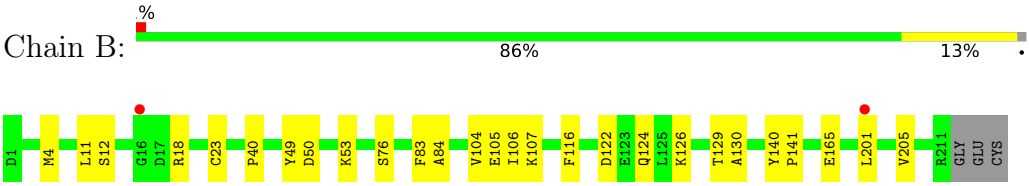
3 Residue-property plots (i)

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.

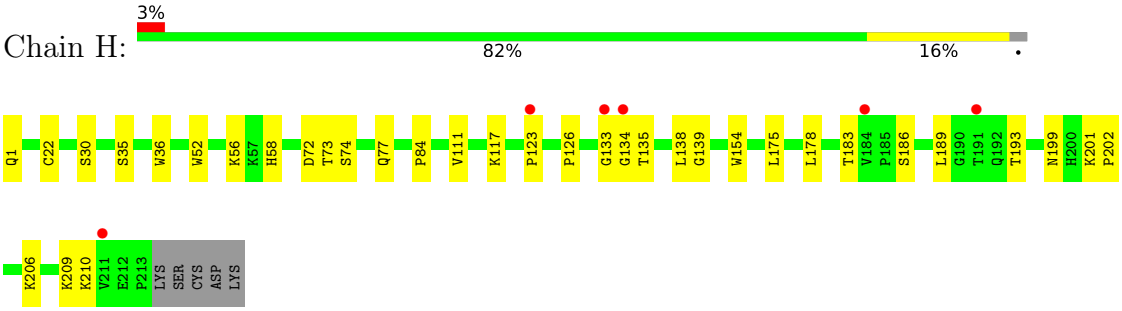
• Molecule 1: motavizumab light chain



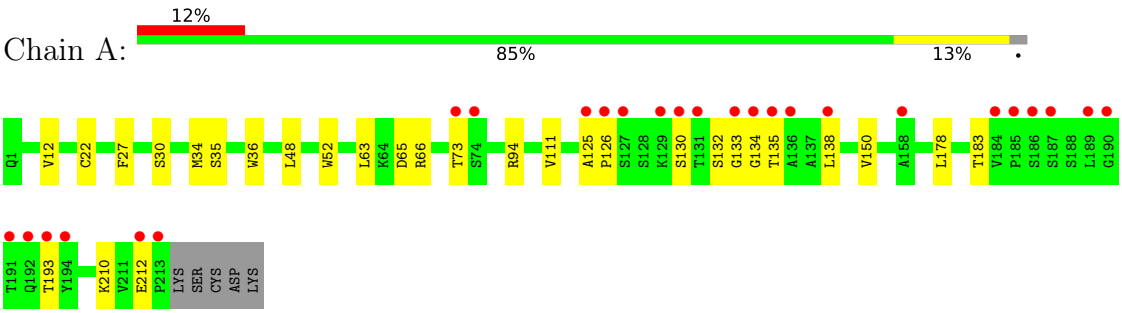
• Molecule 1: motavizumab light chain



• Molecule 2: motavizumab heavy chain

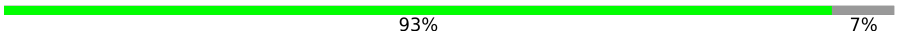


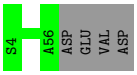
• Molecule 2: motavizumab heavy chain



• Molecule 3: motavizumab epitope scaffold

Chain C:





• Molecule 3: motavizumab epitope scaffold

Chain P:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	75.76Å 74.42Å 86.40Å 90.00° 101.75° 90.00°	Depositor
Resolution (Å)	36.84 – 1.90 36.84 – 1.90	Depositor EDS
% Data completeness (in resolution range)	94.9 (36.84-1.90) 94.7 (36.84-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.06 (at 1.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.188 , 0.231 0.184 , 0.225	Depositor DCC
R_{free} test set	3739 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å^2)	27.0	Xtriage
Anisotropy	0.379	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 46.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	15129	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 77.93 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.6835e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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

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

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	B	0.35	0/1644	0.51	0/2230
1	L	0.32	0/1644	0.51	0/2230
2	A	0.37	0/1712	0.56	0/2341
2	H	0.37	0/1712	0.55	0/2341
3	C	0.33	0/409	0.49	0/552
3	P	0.33	0/409	0.46	0/552
All	All	0.35	0/7530	0.53	0/10246

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	B	1607	1564	1561	15	0
1	L	1607	1564	1561	21	0
2	A	1668	1654	1652	23	0
2	H	1668	1655	1652	23	0
3	C	406	388	388	0	0
3	P	406	388	391	3	0
4	B	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	5	0	0	0	0
4	L	5	0	0	0	0
5	A	4	6	6	0	0
5	B	4	6	6	0	0
5	H	4	6	6	0	0
6	A	131	0	0	2	0
6	B	97	0	0	0	0
6	C	29	0	0	0	1
6	H	151	0	0	1	1
6	L	89	0	0	4	0
6	P	12	0	0	1	0
All	All	7898	7231	7223	84	1

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 6.

All (84) 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:30:SER:HB3	2:H:73:THR:HG21	1.67	0.76
1:L:166:GLN:NE2	6:L:415:HOH:O	2.19	0.74
1:L:166:GLN:CD	6:L:415:HOH:O	2.29	0.72
2:A:125:ALA:O	6:A:293:HOH:O	2.09	0.71
2:A:27:PHE:CD1	2:A:34:MET:HE2	2.27	0.68
2:A:126:PRO:HG3	2:A:138:LEU:HB3	1.76	0.68
1:B:18:ARG:HG3	1:B:76:SER:HA	1.78	0.66
2:A:34:MET:HE1	2:A:94:ARG:HH11	1.66	0.61
1:B:4:MET:HG2	1:B:23:CYS:SG	2.41	0.61
2:H:186:SER:HA	2:H:189:LEU:HD13	1.83	0.59
1:B:50:ASP:HB2	1:B:53:LYS:HD2	1.84	0.59
2:H:126:PRO:HG3	2:H:138:LEU:CD2	2.32	0.59
1:B:40:PRO:HB3	1:B:165:GLU:HG3	1.85	0.59
2:H:193:THR:HG23	2:H:210:LYS:HE3	1.84	0.58
2:H:199:ASN:OD1	2:H:206:LYS:HG2	2.03	0.58
2:H:117:LYS:HD2	2:H:175:LEU:HD21	1.87	0.56
2:A:150:VAL:CG2	2:A:178:LEU:HD21	2.36	0.56
2:H:135:THR:CG2	2:H:183:THR:HB	2.36	0.56
2:A:178:LEU:C	2:A:178:LEU:HD12	2.26	0.56
1:B:201:LEU:HD13	1:B:205:VAL:HG23	1.89	0.55
1:L:48:ILE:HD13	1:L:54:LEU:HD23	1.89	0.54
1:B:122:ASP:O	1:B:126:LYS:HG3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:30:SER:HB3	2:A:73:THR:HG21	1.89	0.54
2:H:1:GLN:NE2	6:H:277:HOH:O	2.38	0.54
1:B:12:SER:OG	1:B:107:LYS:HG3	2.08	0.54
2:A:65:ASP:OD2	2:A:66:ARG:HG3	2.08	0.53
2:A:35:SER:HB2	2:A:52:TRP:CE3	2.44	0.52
1:L:11:LEU:HD11	1:L:19:VAL:HG13	1.92	0.52
2:A:193:THR:HG23	2:A:210:LYS:HE3	1.92	0.51
1:L:166:GLN:HG3	1:L:173:TYR:CE1	2.45	0.51
1:L:142:ARG:NE	6:L:267:HOH:O	2.43	0.51
2:H:126:PRO:HG3	2:H:138:LEU:HD22	1.93	0.50
1:B:140:TYR:CG	1:B:141:PRO:HA	2.47	0.50
2:H:35:SER:HB2	2:H:52:TRP:CE3	2.47	0.49
2:H:123:PRO:HG3	2:H:209:LYS:HE2	1.94	0.49
1:L:4:MET:HG2	1:L:23:CYS:SG	2.52	0.49
1:L:191:VAL:HG12	1:L:210:ASN:OD1	2.13	0.49
1:L:48:ILE:CD1	1:L:54:LEU:HD23	2.43	0.49
1:B:116:PHE:CD2	2:A:130:SER:HA	2.48	0.48
2:A:27:PHE:CD1	2:A:34:MET:CE	2.94	0.48
2:A:135:THR:HG21	2:A:183:THR:HB	1.96	0.48
3:P:24:ARG:HD3	6:P:88:HOH:O	2.12	0.48
2:H:178:LEU:C	2:H:178:LEU:HD12	2.35	0.47
1:L:191:VAL:HG23	6:L:399:HOH:O	2.14	0.47
2:H:56:LYS:HE3	2:H:58:HIS:NE2	2.30	0.47
2:H:72:ASP:OD1	2:H:74:SER:HB3	2.15	0.47
1:B:11:LEU:HD11	1:B:104:VAL:HG13	1.98	0.46
1:L:22:THR:HG22	1:L:72:THR:HG22	1.98	0.46
1:L:54:LEU:HD22	1:L:58:VAL:CG1	2.46	0.45
1:L:125:LEU:O	1:L:183:LYS:HD2	2.15	0.45
1:L:151:ASP:HA	1:L:191:VAL:HG22	1.99	0.44
2:H:133:GLY:HA3	2:H:134:GLY:HA3	1.79	0.44
2:A:150:VAL:HG23	2:A:178:LEU:HD21	2.00	0.44
1:L:120:PRO:HD3	1:L:132:VAL:HG22	1.98	0.44
1:L:124:GLN:HG2	1:L:129:THR:O	2.18	0.44
2:A:22:CYS:HB2	2:A:36:TRP:CZ2	2.52	0.44
2:H:139:GLY:HA2	2:H:154:TRP:CH2	2.53	0.44
2:H:126:PRO:HG3	2:H:138:LEU:HD23	1.99	0.43
2:A:132:SER:O	2:A:135:THR:N	2.52	0.43
2:A:133:GLY:HA3	2:A:134:GLY:HA3	1.79	0.43
2:A:34:MET:CE	2:A:94:ARG:HD3	2.48	0.43
2:A:12:VAL:CG2	2:A:111:VAL:HG22	2.48	0.43
2:H:201:LYS:N	2:H:202:PRO:CD	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:18:ARG:HG3	1:L:76:SER:HA	2.00	0.43
1:B:105:GLU:HG2	1:B:106:ILE:N	2.34	0.43
2:A:135:THR:CG2	2:A:183:THR:HB	2.48	0.43
2:H:139:GLY:HA2	2:H:154:TRP:CZ2	2.53	0.42
2:H:22:CYS:O	2:H:77:GLN:HA	2.19	0.42
2:H:84:PRO:HA	2:H:111:VAL:HB	2.01	0.42
3:P:38:SER:O	3:P:42:LEU:HG	2.19	0.42
1:B:129:THR:HG22	1:B:130:ALA:N	2.34	0.42
2:H:22:CYS:HB2	2:H:36:TRP:CZ2	2.54	0.41
2:A:48:LEU:HD22	2:A:63:LEU:HD12	2.02	0.41
2:A:210:LYS:HE2	2:A:212:GLU:CD	2.41	0.41
2:H:209:LYS:HE3	2:H:210:LYS:O	2.21	0.41
1:B:83:PHE:O	1:B:84:ALA:HB2	2.21	0.41
3:P:27:PHE:HE2	3:P:48:LEU:HD23	1.86	0.41
1:L:129:THR:CG2	1:L:130:ALA:N	2.84	0.41
1:L:136:LEU:HD12	1:L:136:LEU:N	2.35	0.40
1:B:49:TYR:CE1	1:B:53:LYS:HD2	2.56	0.40
1:B:124:GLN:HG2	1:B:129:THR:O	2.22	0.40
1:L:129:THR:HG22	1:L:130:ALA:N	2.36	0.40
2:A:73:THR:HG23	6:A:235:HOH:O	2.21	0.40
1:L:58:VAL:HA	1:L:59:PRO:HD3	1.93	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:241:HOH:O	6:C:442:HOH:O[1_656]	2.15	0.05

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	B	208/213 (98%)	203 (98%)	5 (2%)	0	100	100
1	L	208/213 (98%)	202 (97%)	6 (3%)	0	100	100
2	A	218/225 (97%)	212 (97%)	6 (3%)	0	100	100
2	H	218/225 (97%)	213 (98%)	5 (2%)	0	100	100
3	C	51/57 (90%)	51 (100%)	0	0	100	100
3	P	51/57 (90%)	51 (100%)	0	0	100	100
All	All	954/990 (96%)	932 (98%)	22 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	B	183/185 (99%)	183 (100%)	0	100	100
1	L	183/185 (99%)	183 (100%)	0	100	100
2	A	192/197 (98%)	192 (100%)	0	100	100
2	H	192/197 (98%)	192 (100%)	0	100	100
3	C	45/49 (92%)	45 (100%)	0	100	100
3	P	45/49 (92%)	45 (100%)	0	100	100
All	All	840/862 (97%)	840 (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 (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	166	GLN
2	H	164	HIS

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

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	$\#\|Z\| > 2$
4	SO4	H	219	-	4,4,4	0.13	0	6,6,6	0.09	0
4	SO4	L	215	-	4,4,4	0.13	0	6,6,6	0.07	0
5	EDO	A	219	-	3,3,3	0.51	0	2,2,2	0.16	0
4	SO4	B	215	-	4,4,4	0.15	0	6,6,6	0.05	0
5	EDO	H	220	-	3,3,3	0.48	0	2,2,2	0.25	0
5	EDO	B	216	-	3,3,3	0.53	0	2,2,2	0.13	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	H	220	-	-	0/1/1/1	-
5	EDO	B	216	-	-	1/1/1/1	-
5	EDO	A	219	-	-	0/1/1/1	-

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	B	216	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, 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	B	210/213 (98%)	-0.10	2 (0%) 82 84	18, 40, 59, 75	0
1	L	210/213 (98%)	0.21	6 (2%) 51 54	20, 46, 92, 129	0
2	A	220/225 (97%)	0.49	26 (11%) 4 5	18, 34, 97, 162	0
2	H	220/225 (97%)	0.19	6 (2%) 54 57	18, 34, 76, 107	0
3	C	53/57 (92%)	-0.12	0 100 100	22, 38, 61, 65	0
3	P	53/57 (92%)	0.15	0 100 100	29, 46, 75, 97	0
All	All	966/990 (97%)	0.18	40 (4%) 37 40	18, 40, 82, 162	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	189	LEU	6.3
2	A	134	GLY	5.7
2	A	133	GLY	5.5
2	A	131	THR	4.7
1	L	125	LEU	4.3
2	H	133	GLY	4.2
2	A	74	SER	4.2
2	A	129	LYS	4.1
2	A	136	ALA	4.0
2	A	135	THR	3.9
2	A	191	THR	3.8
2	A	186	SER	3.7
2	A	127	SER	3.7
2	A	213	PRO	3.6
2	A	190	GLY	3.6
2	A	212	GLU	3.4
2	A	187	SER	3.2
2	A	184	VAL	3.2
2	A	185	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
1	L	183	LYS	3.1
2	A	73	THR	3.0
2	H	211	VAL	3.0
2	A	130	SER	2.9
1	L	191	VAL	2.8
2	H	134	GLY	2.8
2	A	193	THR	2.7
1	L	152	ASN	2.5
1	B	16	GLY	2.5
2	H	191	THR	2.4
1	L	123	GLU	2.4
2	A	125	ALA	2.3
1	L	148	TRP	2.3
2	A	126	PRO	2.3
2	H	184	VAL	2.2
2	A	194	TYR	2.1
2	A	138	LEU	2.1
2	A	158	ALA	2.1
1	B	201	LEU	2.1
2	H	123	PRO	2.1
2	A	192	GLN	2.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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, 95^{th} 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
5	EDO	B	216	4/4	0.85	0.15	38,49,58,59	0
5	EDO	H	220	4/4	0.87	0.17	40,49,59,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SO4	H	219	5/5	0.92	0.23	114,114,115,115	0
5	EDO	A	219	4/4	0.93	0.20	36,43,51,51	0
4	SO4	B	215	5/5	0.95	0.14	87,89,93,95	0
4	SO4	L	215	5/5	0.96	0.13	80,81,84,87	0

6.5 Other polymers (i)

There are no such residues in this entry.