



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 09:53 am BST

PDB ID : 4D9Q
Title : Inhibiting Alternative Pathway Complement Activation by Targeting the Exosite on Factor D
Authors : Murray, J.M.; Wiesmann, C.
Deposited on : 2012-01-11
Resolution : 2.28 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 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 : 2.11
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) : 2.11

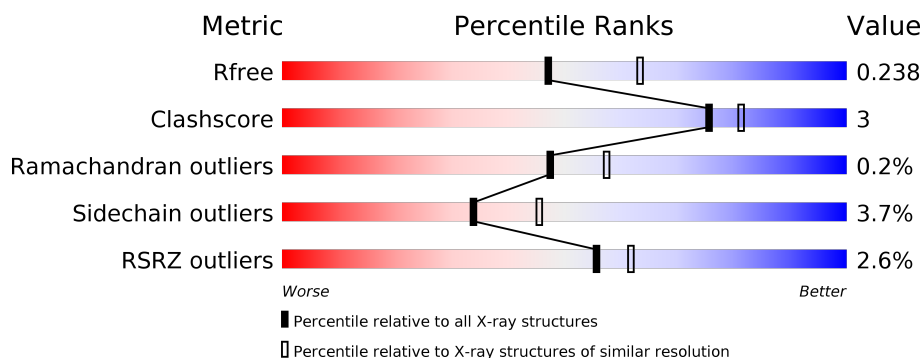
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.28 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	6980 (2.30-2.26)
Clashscore	141614	7711 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)
RSRZ outliers	127900	6849 (2.30-2.26)

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 on 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	228	<div> <div>%</div> <div> <div></div> <div>93%</div> <div>7%</div> <div>.</div> </div> </div>
1	B	228	<div> <div>5%</div> <div> <div></div> <div>87%</div> <div>12%</div> <div>.</div> </div> </div>
2	D	213	<div> <div></div> <div> <div></div> <div>87%</div> <div>13%</div> </div> </div>
2	L	213	<div> <div>4%</div> <div> <div></div> <div>92%</div> <div>8%</div> </div> </div>
3	E	217	<div> <div>%</div> <div> <div></div> <div>88%</div> <div>8%</div> <div>..</div> </div> </div>
3	H	217	<div> <div>3%</div> <div> <div></div> <div>89%</div> <div>10%</div> <div>.</div> </div> </div>

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 10620 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 Factor D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	228	Total	C	N	O	S	0	2	0
			1726	1063	330	322	11			
1	B	228	Total	C	N	O	S	0	2	0
			1726	1063	330	322	11			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	47	VAL	LEU	CONFLICT	UNP F6YBP7
B	47	VAL	LEU	CONFLICT	UNP F6YBP7

- Molecule 2 is a protein called Anti-Factor D, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	213	Total	C	N	O	S	0	0	0
			1624	1011	270	338	5			
2	L	213	Total	C	N	O	S	0	0	0
			1624	1011	270	338	5			

- Molecule 3 is a protein called Anti-Factor D, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	212	Total	C	N	O	S	0	0	0
			1592	1009	260	317	6			
3	H	216	Total	C	N	O	S	0	0	0
			1618	1024	265	323	6			

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	1	Total	Zn	0	0
			1	1		
5	L	2	Total	Zn	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Zn	0	0
			1	1		
5	A	1	Total	Zn	0	0
			1	1		
5	D	2	Total	Zn	0	0
			2	2		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	124	Total	O	0	0
			124	124		
7	B	69	Total	O	0	0
			69	69		
7	D	133	Total	O	0	0
			133	133		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	E	113	Total 113	O 113	0	0
7	H	66	Total 66	O 66	0	0
7	L	123	Total 123	O 123	0	0

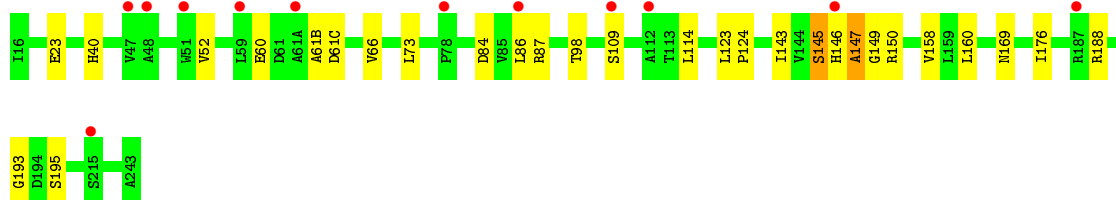
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

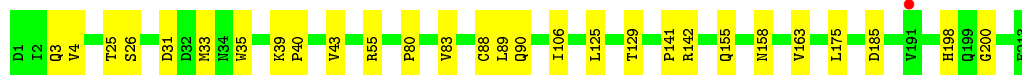
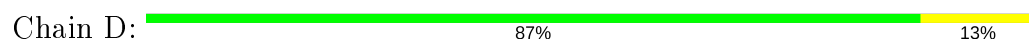
- Molecule 1: Factor D



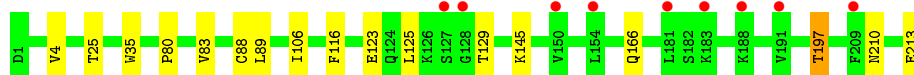
- Molecule 1: Factor D



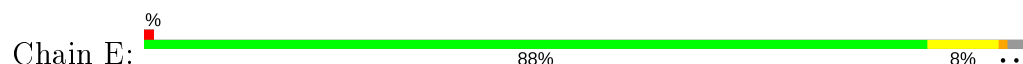
- Molecule 2: Anti-Factor D, light chain



- Molecule 2: Anti-Factor D, light chain

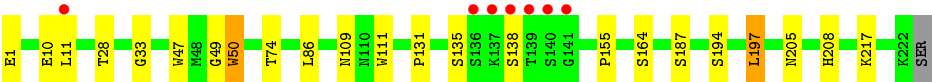
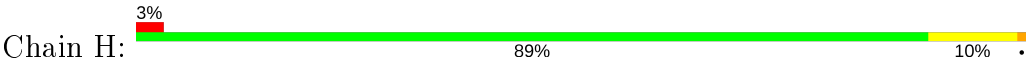


- Molecule 3: Anti-Factor D, heavy chain





● Molecule 3: Anti-Factor D, heavy chain



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	182.33Å 80.76Å 142.63Å 90.00° 107.19° 90.00°	Depositor
Resolution (Å)	33.38 – 2.28 73.27 – 2.28	Depositor EDS
% Data completeness (in resolution range)	99.6 (33.38-2.28) 99.8 (73.27-2.28)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 2.29Å)	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.11.2, BUSTER 2.11.2	Depositor
R, R_{free}	0.189 , 0.230 0.199 , 0.238	Depositor DCC
R_{free} test set	4589 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	37.3	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 55.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10620	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% 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: GOL, ZN, 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	0.58	0/1771	0.68	0/2406
1	B	0.57	0/1771	0.70	0/2406
2	D	0.54	0/1656	0.71	0/2252
2	L	0.53	0/1656	0.70	0/2252
3	E	0.50	0/1631	0.71	0/2224
3	H	0.47	0/1658	0.70	0/2261
All	All	0.53	0/10143	0.70	0/13801

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
1	B	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
1	B	147	ALA	Peptide

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	1726	0	1709	8	0
1	B	1726	0	1709	10	0
2	D	1624	0	1582	16	0
2	L	1624	0	1582	10	0
3	E	1592	0	1550	10	0
3	H	1618	0	1579	12	0
4	A	12	0	16	0	0
4	B	18	0	24	0	0
4	D	12	0	16	1	0
4	E	12	0	16	0	0
4	H	6	0	8	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	D	2	0	0	0	0
5	H	1	0	0	0	0
5	L	2	0	0	0	0
6	A	10	0	0	0	0
6	B	5	0	0	0	0
7	A	124	0	0	1	0
7	B	69	0	0	0	0
7	D	133	0	0	2	0
7	E	113	0	0	1	0
7	H	66	0	0	0	0
7	L	123	0	0	0	0
All	All	10620	0	9791	62	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 (62) 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:D:155:GLN:HE21	2:D:158:ASN:HD21	1.31	0.75
1:B:169:ASN:HD21	1:B:176:ILE:H	1.36	0.73
1:A:77:GLU:HG3	7:A:522:HOH:O	1.90	0.71
3:E:109:ASN:HD21	3:E:111:TRP:HE1	1.41	0.69
1:A:123:LEU:HD12	1:A:124:PRO:HD2	1.76	0.68
3:E:55:THR:OG1	3:E:57:GLU:HG2	1.93	0.68
1:B:123:LEU:HD12	1:B:124:PRO:HD2	1.77	0.67
2:L:145:LYS:HB3	2:L:197:THR:HG23	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:109:ASN:HD21	3:H:111:TRP:HE1	1.41	0.65
3:H:135:SER:H	3:H:138:SER:HB3	1.61	0.65
3:H:164:SER:H	3:H:205:ASN:HD21	1.46	0.64
2:L:83:VAL:HG23	2:L:106:ILE:HD12	1.86	0.58
1:B:143:ILE:HD12	1:B:146:HIS:O	2.06	0.56
1:A:86:LEU:HD13	1:A:109:SER:HA	1.89	0.55
2:D:83:VAL:HG13	2:D:106:ILE:HD12	1.87	0.55
1:A:52:VAL:HG21	1:A:66:VAL:HG11	1.89	0.55
3:H:138:SER:HA	2:L:116:PHE:HD1	1.72	0.54
1:B:52:VAL:HG21	1:B:66:VAL:HG11	1.89	0.53
3:E:33:GLY:HA3	3:E:50:TRP:CZ3	2.44	0.52
2:D:31:ASP:OD1	4:D:301:GOL:O1	2.27	0.52
1:B:158:VAL:HG21	1:B:188:ARG:HG3	1.90	0.51
3:E:152:ASP:HB3	3:E:183:LEU:HD23	1.93	0.51
1:B:146:HIS:CG	1:B:147:ALA:N	2.79	0.51
3:H:11:LEU:HB2	3:H:155:PRO:HG3	1.91	0.51
1:B:160:LEU:CD2	1:B:188:ARG:HB3	2.41	0.51
2:D:55:ARG:NH1	7:D:402:HOH:O	2.33	0.51
2:D:141:PRO:O	2:D:198:HIS:HE1	1.94	0.51
3:H:47:TRP:CZ3	3:H:49:GLY:HA2	2.47	0.50
2:D:198:HIS:CD2	2:D:200:GLY:H	2.31	0.49
3:H:33:GLY:HA3	3:H:50:TRP:CZ3	2.47	0.49
2:L:80:PRO:HA	2:L:106:ILE:CD1	2.44	0.48
2:L:83:VAL:HG11	2:L:166:GLN:HB3	1.94	0.48
2:D:80:PRO:HA	2:D:106:ILE:CD1	2.44	0.48
1:A:172:HIS:CE1	1:A:227:ILE:HD11	2.49	0.48
3:H:194:SER:O	3:H:197:LEU:HD22	2.14	0.47
2:L:80:PRO:HA	2:L:106:ILE:HD13	1.97	0.47
3:E:47:TRP:CZ3	3:E:49:GLY:HA2	2.50	0.47
3:E:11:LEU:HB2	3:E:155:PRO:HG3	1.97	0.46
3:H:131:PRO:HD3	3:H:217:LYS:HE2	1.98	0.46
2:L:35:TRP:CZ3	2:L:88:CYS:HB3	2.51	0.45
1:B:146:HIS:CD2	1:B:147:ALA:N	2.85	0.44
2:D:80:PRO:HA	2:D:106:ILE:HD13	2.00	0.44
2:L:4:VAL:HG22	2:L:25:THR:HG22	1.98	0.43
3:E:131:PRO:HD3	3:E:217:LYS:HE2	2.00	0.43
2:D:142:ARG:HD2	2:D:163:VAL:HG11	2.00	0.43
1:A:40:HIS:HE1	1:A:193:GLY:O	2.02	0.43
2:D:163:VAL:HG22	2:D:175:LEU:HD12	2.01	0.43
2:D:3:GLN:HB3	2:D:26:SER:HB3	2.00	0.43
1:B:145:SER:O	1:B:149:GLY:HA3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:33:MET:SD	2:D:88:CYS:HB2	2.60	0.42
2:L:210:ASN:HB2	2:L:213:GLU:HB2	2.02	0.42
2:D:39:LYS:NZ	7:D:423:HOH:O	2.53	0.42
3:H:155:PRO:O	3:H:208:HIS:HE1	2.03	0.42
2:D:35:TRP:CZ3	2:D:88:CYS:HB3	2.55	0.41
3:E:155:PRO:O	3:E:208:HIS:HE1	2.04	0.41
1:A:178:GLN:HE22	3:H:28:THR:HG21	1.86	0.41
3:E:23:LYS:NZ	7:E:469:HOH:O	2.53	0.41
1:B:40:HIS:HE1	1:B:193:GLY:O	2.04	0.41
3:H:217:LYS:NZ	2:L:123:GLU:OE2	2.51	0.41
2:D:43:VAL:HG22	3:E:95:TYR:HE1	1.86	0.40
1:A:179:ARG:HD2	1:A:233[A]:SER:HB3	2.03	0.40
2:D:4:VAL:HG22	2:D:25:THR:HG22	2.03	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	228/228 (100%)	222 (97%)	6 (3%)	0	100	100
1	B	228/228 (100%)	217 (95%)	10 (4%)	1 (0%)	34	40
2	D	211/213 (99%)	204 (97%)	6 (3%)	1 (0%)	29	34
2	L	211/213 (99%)	205 (97%)	6 (3%)	0	100	100
3	E	208/217 (96%)	201 (97%)	7 (3%)	0	100	100
3	H	214/217 (99%)	205 (96%)	9 (4%)	0	100	100
All	All	1300/1316 (99%)	1254 (96%)	44 (3%)	2 (0%)	47	57

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	61(B)	ALA
2	D	40	PRO

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	186/184 (101%)	181 (97%)	5 (3%)	44	59
1	B	186/184 (101%)	173 (93%)	13 (7%)	15	18
2	D	190/190 (100%)	185 (97%)	5 (3%)	46	60
2	L	190/190 (100%)	186 (98%)	4 (2%)	53	68
3	E	179/183 (98%)	172 (96%)	7 (4%)	32	43
3	H	182/183 (100%)	175 (96%)	7 (4%)	33	44
All	All	1113/1114 (100%)	1072 (96%)	41 (4%)	34	45

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61(C)	ASP
1	A	87	ARG
1	A	114	LEU
1	A	178	GLN
1	A	179	ARG
1	B	23	GLU
1	B	60	GLU
1	B	61(C)	ASP
1	B	73	LEU
1	B	84	ASP
1	B	86	LEU
1	B	87	ARG
1	B	98	THR
1	B	109	SER
1	B	114	LEU
1	B	145	SER
1	B	150	ARG

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Mol	Chain	Res	Type
1	B	195	SER
2	D	89	LEU
2	D	90	GLN
2	D	125	LEU
2	D	129	THR
2	D	185	ASP
3	E	1	GLU
3	E	23	LYS
3	E	50	TRP
3	E	57	GLU
3	E	86	LEU
3	E	214	LYS
3	E	222	LYS
3	H	1	GLU
3	H	10	GLU
3	H	50	TRP
3	H	74	THR
3	H	86	LEU
3	H	187	SER
3	H	197	LEU
2	L	89	LEU
2	L	125	LEU
2	L	129	THR
2	L	197	THR

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

Mol	Chain	Res	Type
1	A	40	HIS
1	A	157	HIS
1	A	178	GLN
1	B	40	HIS
1	B	146	HIS
1	B	157	HIS
1	B	169	ASN
2	D	52	ASN
2	D	90	GLN
2	D	155	GLN
2	D	198	HIS
3	E	109	ASN
3	E	179	GLN
3	E	208	HIS

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Mol	Chain	Res	Type
3	H	109	ASN
3	H	179	GLN
3	H	205	ASN
3	H	208	HIS
2	L	52	ASN
2	L	152	ASN
2	L	210	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 20 ligands modelled in this entry, 7 are monoatomic - leaving 13 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	$\# Z > 2$
6	SO4	A	304	-	4,4,4	0.24	0	6,6,6	0.23	0
4	GOL	B	302	-	5,5,5	0.16	0	5,5,5	0.29	0
6	SO4	A	305	-	4,4,4	0.17	0	6,6,6	0.12	0
6	SO4	B	305	-	4,4,4	0.14	0	6,6,6	0.23	0
4	GOL	B	303	-	5,5,5	0.12	0	5,5,5	0.49	0
4	GOL	E	302	-	5,5,5	0.12	0	5,5,5	0.26	0
4	GOL	A	302	-	5,5,5	0.08	0	5,5,5	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	H	301	-	5,5,5	0.15	0	5,5,5	0.45	0
4	GOL	E	301	-	5,5,5	0.17	0	5,5,5	0.54	0
4	GOL	D	301	-	5,5,5	0.24	0	5,5,5	0.86	0
4	GOL	A	301	-	5,5,5	0.25	0	5,5,5	0.48	0
4	GOL	B	301	-	5,5,5	0.11	0	5,5,5	0.25	0
4	GOL	D	302	-	5,5,5	0.23	0	5,5,5	0.53	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	GOL	B	302	-	-	0/4/4/4	-
4	GOL	B	303	-	-	1/4/4/4	-
4	GOL	E	302	-	-	1/4/4/4	-
4	GOL	A	302	-	-	1/4/4/4	-
4	GOL	H	301	-	-	2/4/4/4	-
4	GOL	E	301	-	-	4/4/4/4	-
4	GOL	D	301	-	-	4/4/4/4	-
4	GOL	A	301	-	-	1/4/4/4	-
4	GOL	B	301	-	-	0/4/4/4	-
4	GOL	D	302	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	301	GOL	C1-C2-C3-O3
4	D	301	GOL	C1-C2-C3-O3
4	B	303	GOL	O1-C1-C2-C3
4	E	301	GOL	C1-C2-C3-O3
4	H	301	GOL	O2-C2-C3-O3
4	D	301	GOL	O2-C2-C3-O3
4	E	301	GOL	O2-C2-C3-O3
4	D	301	GOL	O1-C1-C2-O2
4	E	302	GOL	O1-C1-C2-O2
4	E	301	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	E	301	GOL	O1-C1-C2-C3
4	A	301	GOL	O1-C1-C2-C3
4	D	301	GOL	O1-C1-C2-C3
4	D	302	GOL	C1-C2-C3-O3
4	A	302	GOL	C1-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	301	GOL	1	0

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	228/228 (100%)	0.11	2 (0%) 84 87	28, 40, 73, 99	0
1	B	228/228 (100%)	0.59	12 (5%) 26 31	24, 53, 86, 98	0
2	D	213/213 (100%)	0.27	1 (0%) 91 93	22, 40, 71, 105	0
2	L	213/213 (100%)	0.37	9 (4%) 36 41	25, 42, 75, 114	0
3	E	212/217 (97%)	0.13	3 (1%) 75 79	24, 43, 74, 109	0
3	H	216/217 (99%)	0.32	7 (3%) 47 53	25, 51, 80, 114	0
All	All	1310/1316 (99%)	0.30	34 (2%) 56 62	22, 46, 79, 114	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	61(A)	ALA	8.9
3	H	138	SER	8.9
3	H	140	SER	6.7
3	H	137	LYS	6.1
1	B	78	PRO	5.7
3	H	139	THR	4.7
1	B	109	SER	3.7
1	B	187	ARG	3.6
1	B	215	SER	3.5
1	B	146	HIS	3.5
3	H	136	SER	3.4
1	B	86	LEU	3.4
2	L	154	LEU	3.3
3	H	141	GLY	3.2
2	L	183	LYS	3.0
2	L	150	VAL	3.0
1	B	59	LEU	2.9
2	L	181	LEU	2.8
1	B	48	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
2	D	191	VAL	2.5
3	H	11	LEU	2.3
1	A	242	LEU	2.3
1	A	243	ALA	2.3
2	L	127	SER	2.2
2	L	191	VAL	2.2
3	E	199	THR	2.2
1	B	47	VAL	2.2
2	L	209	PHE	2.2
3	E	200	GLN	2.2
1	B	51	TRP	2.2
1	B	112	ALA	2.1
2	L	188	LYS	2.0
3	E	222	LYS	2.0
2	L	128	GLY	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 carbohydrates 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	GOL	A	302	6/6	0.76	0.32	76,77,78,79	0
4	GOL	H	301	6/6	0.76	0.33	59,62,63,64	0
4	GOL	D	302	6/6	0.76	0.26	55,62,66,69	0
4	GOL	E	301	6/6	0.83	0.23	44,60,65,65	0
4	GOL	B	303	6/6	0.83	0.25	64,69,70,73	0
6	SO4	A	305	5/5	0.84	0.26	127,127,128,129	0
4	GOL	D	301	6/6	0.87	0.22	38,51,52,54	0
4	GOL	B	302	6/6	0.87	0.17	58,64,68,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	GOL	E	302	6/6	0.89	0.22	49,57,60,62	0
5	ZN	D	304	1/1	0.94	0.13	83,83,83,83	0
5	ZN	A	303	1/1	0.94	0.18	124,124,124,124	0
5	ZN	L	302	1/1	0.94	0.10	96,96,96,96	0
6	SO4	B	305	5/5	0.95	0.11	82,84,84,87	0
5	ZN	H	302	1/1	0.95	0.14	73,73,73,73	0
4	GOL	B	301	6/6	0.97	0.15	30,31,34,35	0
4	GOL	A	301	6/6	0.98	0.12	32,32,33,34	0
5	ZN	L	301	1/1	0.98	0.24	41,41,41,41	0
5	ZN	D	303	1/1	0.98	0.23	33,33,33,33	0
5	ZN	B	304	1/1	0.98	0.17	36,36,36,36	0
6	SO4	A	304	5/5	0.99	0.11	53,53,53,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.