Full wwPDB X-ray Structure Validation Report (i)

Sep 5, 2023 – 06:03 PM EDT

PDB ID	:	4DTG
Title	:	Hemostatic effect of a monoclonal antibody mAb 2021 blocking the interaction between FXa and TFPI in a rabbit hemophilia model
Authors	:	Svensson, L.A.; Breinholt, J.; Krogh, B.O.; Hilden, I.
Deposited on	:	2012-02-21
Resolution	:	1.80 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 (i) 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 (i)) were used in the production of this report:

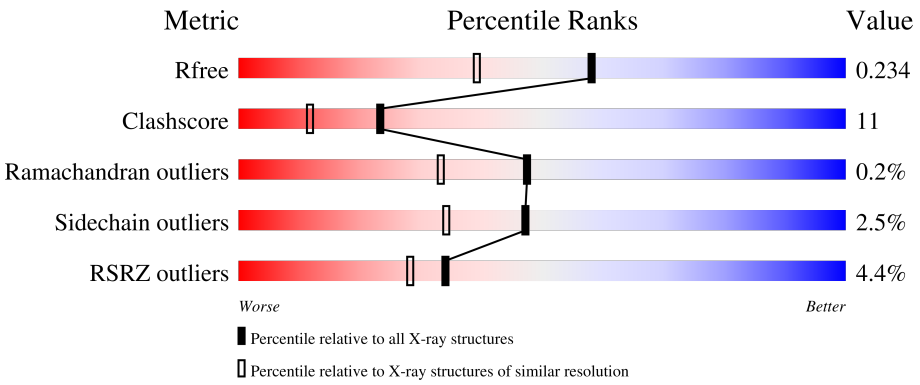
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	L	219	3% 75% 22% •
2	H	222	6% 69% 27% •
3	K	66	3% 62% 26% • 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	H	305	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 4431 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 Humanized recombinant FAB fragment, FAB 2021, of a murine antibody, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	L	219	1712	1077	284	345	6	0	7	0

- Molecule 2 is a protein called Humanized recombinant FAB fragment, FAB 2021, of a murine antibody, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	221	1672	1043	281	338	10	0	5	0

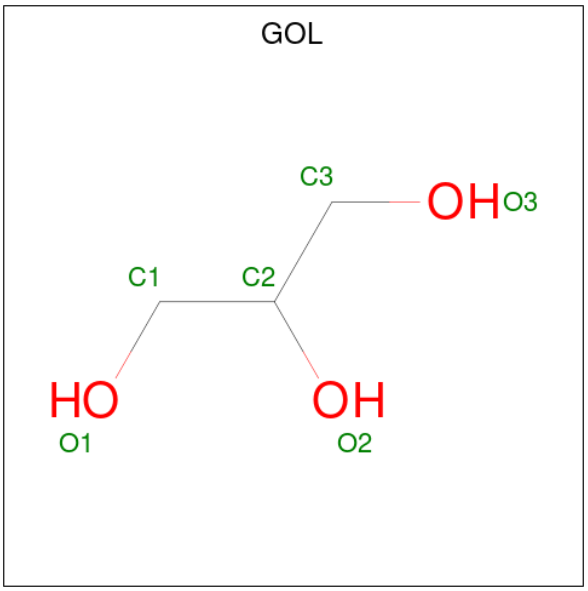
- Molecule 3 is a protein called Tissue factor pathway inhibitor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	K	60	545	340	88	109	8	0	8	0

There are 6 discrepancies between the modelled and reference sequences:

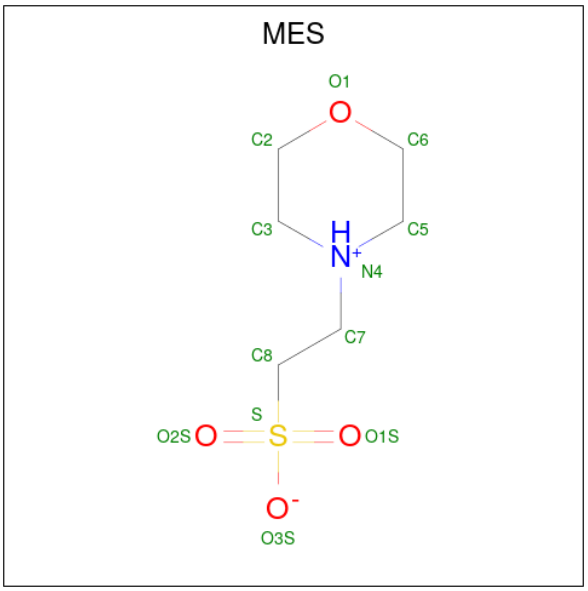
Chain	Residue	Modelled	Actual	Comment	Reference
K	61	HIS	-	expression tag	UNP P10646
K	62	HIS	-	expression tag	UNP P10646
K	63	HIS	-	expression tag	UNP P10646
K	64	HIS	-	expression tag	UNP P10646
K	65	HIS	-	expression tag	UNP P10646
K	66	HIS	-	expression tag	UNP P10646

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



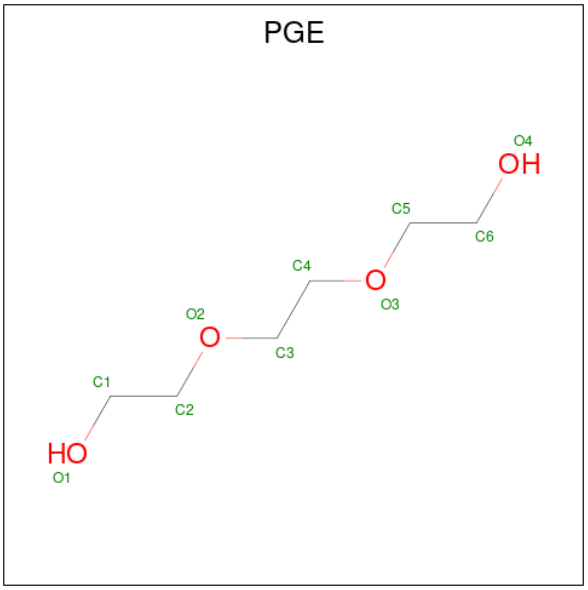
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	L	1	6	3	3	0	0
4	L	1	6	3	3	0	0
4	L	1	6	3	3	0	0
4	L	1	6	3	3	0	0
4	L	1	6	3	3	0	0
4	L	1	6	3	3	0	0
4	L	1	6	3	3	0	0
4	H	1	6	3	3	0	0
4	H	1	6	3	3	0	0
4	H	1	6	3	3	0	0

- Molecule 5 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
5	H	1	12	6	1	4	1	0	0

- Molecule 6 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
6	H	1	10	6	4		0	0
			Total	C	O			
6	H	1	10	6	4		0	0
			Total	C	O			
6	H	1	10	6	4		0	0

- Molecule 7 is water.

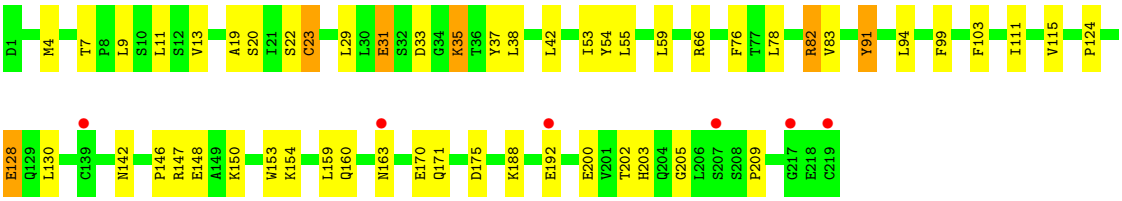
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	L	182	182	182	0	0
			Total	O		
7	H	147	147	147	0	0
			Total	O		
7	K	71	71	71	0	0

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.

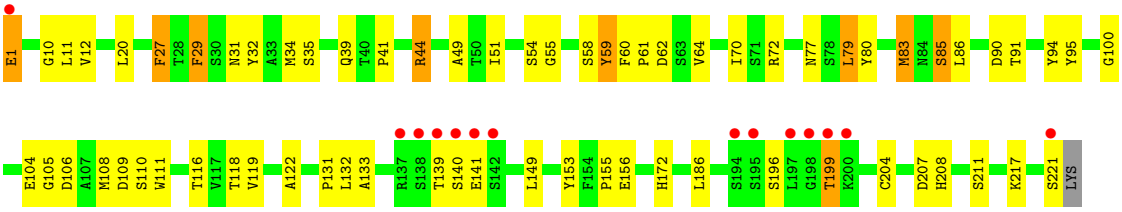
• Molecule 1: Humanized recombinant FAB fragment, FAB 2021, of a murine antibody, light chain

Chain L:



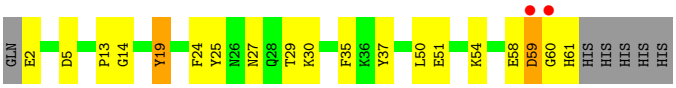
• Molecule 2: Humanized recombinant FAB fragment, FAB 2021, of a murine antibody, heavy chain

Chain H:



• Molecule 3: Tissue factor pathway inhibitor

Chain K:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	65.01Å 125.64Å 202.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.10 – 1.80 29.10 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.4 (29.10-1.80) 98.4 (29.10-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	3.20 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.6.0119	Depositor
R, R_{free}	0.196 , 0.236 0.195 , 0.234	Depositor DCC
R_{free} test set	3817 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	30.3	Xtriage
Anisotropy	0.360	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 51.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	4431	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% of the height of the origin peak. No significant pseudotranslation is detected.*

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, PGE, MES

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	L	1.39	12/1768 (0.7%)	1.25	10/2402 (0.4%)
2	H	1.54	19/1724 (1.1%)	1.38	13/2345 (0.6%)
3	K	1.69	7/571 (1.2%)	1.55	4/762 (0.5%)
All	All	1.50	38/4063 (0.9%)	1.35	27/5509 (0.5%)

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	K	0	1

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	19	TYR	CE1-CZ	12.61	1.54	1.38
1	L	91	TYR	CE1-CZ	7.85	1.48	1.38
3	K	25	TYR	CG-CD1	7.37	1.48	1.39
2	H	54	SER	CB-OG	7.32	1.51	1.42
1	L	23	CYS	C-O	7.12	1.36	1.23
2	H	111	TRP	CG-CD1	7.08	1.46	1.36
2	H	106	ASP	N-CA	7.03	1.60	1.46
2	H	29	PHE	CG-CD2	6.99	1.49	1.38
2	H	51	ILE	C-O	6.85	1.36	1.23
2	H	110	SER	CB-OG	6.80	1.51	1.42
1	L	153	TRP	CD2-CE2	6.67	1.49	1.41
2	H	94	TYR	CE2-CZ	6.63	1.47	1.38
2	H	10	GLY	N-CA	6.61	1.55	1.46
1	L	37	TYR	CG-CD1	6.41	1.47	1.39
3	K	35	PHE	CG-CD1	6.34	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	95	TYR	CB-CG	-6.32	1.42	1.51
1	L	103	PHE	CE1-CZ	6.24	1.49	1.37
1	L	37	TYR	CB-CG	-6.24	1.42	1.51
1	L	54	TYR	C-O	6.22	1.35	1.23
1	L	76	PHE	CG-CD1	5.86	1.47	1.38
2	H	35	SER	C-O	5.76	1.34	1.23
2	H	58	SER	CB-OG	5.74	1.49	1.42
2	H	111	TRP	N-CA	5.71	1.57	1.46
3	K	14	GLY	N-CA	5.65	1.54	1.46
3	K	51[A]	GLU	CD-OE1	5.63	1.31	1.25
3	K	51[B]	GLU	CD-OE1	5.63	1.31	1.25
3	K	24	PHE	CG-CD2	5.52	1.47	1.38
2	H	111	TRP	CD2-CE2	5.42	1.47	1.41
1	L	99	PHE	CG-CD1	5.26	1.46	1.38
2	H	55	GLY	N-CA	5.26	1.53	1.46
1	L	54	TYR	CB-CG	5.22	1.59	1.51
2	H	153	TYR	CG-CD2	5.22	1.46	1.39
2	H	109	ASP	CB-CG	5.11	1.62	1.51
2	H	72	ARG	CZ-NH2	5.10	1.39	1.33
2	H	62	ASP	C-O	5.08	1.33	1.23
2	H	100	GLY	C-O	5.04	1.31	1.23
1	L	31	GLU	CG-CD	5.03	1.59	1.51
1	L	76	PHE	CE2-CZ	5.01	1.46	1.37

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	44	ARG	NE-CZ-NH1	6.95	123.78	120.30
2	H	109	ASP	CB-CG-OD1	6.93	124.53	118.30
2	H	27	PHE	CB-CG-CD1	-6.85	116.01	120.80
1	L	66	ARG	NE-CZ-NH1	-6.81	116.89	120.30
2	H	44	ARG	NE-CZ-NH2	-6.63	116.98	120.30
3	K	5	ASP	CB-CG-OD1	6.56	124.20	118.30
1	L	38	LEU	CA-CB-CG	6.40	130.02	115.30
3	K	35	PHE	CZ-CE2-CD2	6.36	127.73	120.10
2	H	59	TYR	CZ-CE2-CD2	-6.28	114.14	119.80
3	K	19	TYR	CD1-CE1-CZ	-6.04	114.37	119.80
3	K	50	LEU	CB-CG-CD2	-6.01	100.77	111.00
2	H	79	LEU	CB-CG-CD1	-5.98	100.83	111.00
1	L	33	ASP	CB-CG-OD1	5.89	123.60	118.30
1	L	11	LEU	CA-CB-CG	5.83	128.72	115.30
1	L	175	ASP	CB-CG-OD1	5.77	123.49	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	37	TYR	CD1-CE1-CZ	-5.69	114.68	119.80
2	H	85	SER	N-CA-CB	5.55	118.82	110.50
1	L	78	LEU	CB-CG-CD1	-5.53	101.61	111.00
2	H	32	TYR	CB-CG-CD1	-5.49	117.70	121.00
1	L	94	LEU	CB-CG-CD2	-5.49	101.66	111.00
1	L	29	LEU	CB-CG-CD2	-5.45	101.74	111.00
2	H	90	ASP	CB-CG-OD2	5.42	123.18	118.30
2	H	34	MET	CB-CG-SD	-5.38	96.26	112.40
1	L	35	LYS	CD-CE-NZ	-5.25	99.62	111.70
2	H	83	MET	CG-SD-CE	5.21	108.53	100.20
2	H	34	MET	CA-CB-CG	5.13	122.02	113.30
2	H	49	ALA	CB-CA-C	-5.00	102.59	110.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	K	13	PRO	Mainchain

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	L	1712	0	1699	34	0
2	H	1672	0	1626	35	0
3	K	545	0	496	17	0
4	H	18	0	24	6	0
4	L	42	0	56	1	0
5	H	12	0	13	0	0
6	H	30	0	42	10	0
7	H	147	0	0	9	1
7	K	71	0	0	9	0
7	L	182	0	0	7	0
All	All	4431	0	3956	90	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 11.

All (90) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:160:GLN:HB3	1:L:163[B]:ASN:ND2	1.44	1.29
1:L:9:LEU:HD23	7:L:561:HOH:O	1.43	1.17
2:H:1:GLU:HA	2:H:1:GLU:OE2	1.47	1.11
1:L:147[B]:ARG:NH1	7:L:574:HOH:O	1.83	1.10
1:L:160:GLN:CB	1:L:163[B]:ASN:HD21	1.63	1.09
3:K:58[B]:GLU:O	7:K:171:HOH:O	1.72	1.06
2:H:91:THR:OG1	7:H:503:HOH:O	1.79	1.01
3:K:61:HIS:C	7:K:132:HOH:O	1.98	1.00
3:K:59[B]:ASP:HB2	7:K:171:HOH:O	1.64	0.96
2:H:156:GLU:HB2	4:H:305:GOL:H32	1.49	0.94
6:H:304:PGE:H32	7:K:118:HOH:O	1.69	0.93
1:L:203:HIS:HD2	1:L:205:GLY:H	1.21	0.89
1:L:203:HIS:CD2	1:L:205:GLY:H	1.91	0.87
2:H:1:GLU:OE2	2:H:1:GLU:CA	2.24	0.86
6:H:303:PGE:H52	7:H:402:HOH:O	1.75	0.84
3:K:58[B]:GLU:O	3:K:59[B]:ASP:HB2	1.75	0.84
1:L:7[B]:THR:HG22	7:L:410:HOH:O	1.78	0.82
1:L:35:LYS:HE3	7:H:448:HOH:O	1.79	0.81
1:L:142:ASN:HD21	2:H:172:HIS:HD2	1.29	0.80
6:H:302:PGE:H2	4:H:305:GOL:O1	1.83	0.78
3:K:54[B]:LYS:HG2	3:K:58[B]:GLU:OE1	1.85	0.75
1:L:142:ASN:HD21	2:H:172:HIS:CD2	2.07	0.72
6:H:303:PGE:H12	7:K:113:HOH:O	1.90	0.71
2:H:41:PRO:HG3	4:H:305:GOL:H11	1.74	0.70
3:K:59[B]:ASP:OD1	3:K:59[B]:ASP:C	2.30	0.69
3:K:58[B]:GLU:O	3:K:59[B]:ASP:CB	2.39	0.69
1:L:160:GLN:HB3	1:L:163[B]:ASN:HD21	0.69	0.67
2:H:208:HIS:HD2	2:H:211:SER:OG	1.79	0.65
1:L:128:GLU:HB2	7:L:522:HOH:O	1.97	0.65
6:H:304:PGE:H6	3:K:29:THR:HG22	1.77	0.64
2:H:155:PRO:O	2:H:208:HIS:HE1	1.82	0.63
6:H:304:PGE:H3	7:K:115:HOH:O	1.98	0.63
6:H:304:PGE:H6	3:K:29:THR:CG2	2.29	0.63
3:K:59[B]:ASP:OD1	3:K:59[B]:ASP:O	2.16	0.62
6:H:303:PGE:O1	7:H:492:HOH:O	1.84	0.61
3:K:27:ASN:O	3:K:30:LYS:HE3	2.01	0.60
2:H:116:THR:OG1	4:H:307:GOL:H32	2.03	0.59
3:K:58[B]:GLU:OE2	7:K:126:HOH:O	2.17	0.59
2:H:118:THR:HG1	4:H:305:GOL:HO3	1.54	0.56
6:H:303:PGE:H5	7:H:475:HOH:O	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:61:PRO:HD2	2:H:64:VAL:HG22	1.89	0.55
1:L:200:GLU:OE2	1:L:209:PRO:HB2	2.07	0.54
1:L:203:HIS:HD2	1:L:205:GLY:N	1.99	0.54
2:H:11:LEU:HD21	2:H:122:ALA:O	2.06	0.54
1:L:4:MET:CE	1:L:23:CYS:SG	2.96	0.53
2:H:207:ASP:OD1	7:H:506:HOH:O	2.19	0.51
1:L:130:LEU:O	1:L:188:LYS:HD2	2.10	0.50
1:L:82[B]:ARG:NH1	7:L:569:HOH:O	2.43	0.50
2:H:83:MET:HB3	2:H:86:LEU:HD21	1.93	0.49
3:K:54[B]:LYS:HG2	3:K:58[B]:GLU:CD	2.32	0.49
1:L:154:LYS:HE2	1:L:159:LEU:CD2	2.43	0.49
1:L:53:ILE:HG12	1:L:59:LEU:HD23	1.96	0.48
2:H:208:HIS:CD2	2:H:211:SER:OG	2.65	0.47
2:H:60:PHE:HZ	2:H:70:ILE:HG22	1.80	0.47
2:H:132:LEU:HD21	2:H:149:LEU:HB2	1.97	0.46
2:H:141:GLU:OE2	2:H:141:GLU:HA	2.15	0.46
2:H:29:PHE:CD2	2:H:77:ASN:HA	2.51	0.45
2:H:131:PRO:HD3	2:H:217:LYS:HE2	1.99	0.45
3:K:2:GLU:N	7:K:146:HOH:O	2.49	0.45
2:H:204[A]:CYS:SG	2:H:217:LYS:HB3	2.56	0.45
1:L:150:LYS:HB3	1:L:202:THR:HB	1.98	0.45
1:L:142:ASN:ND2	2:H:172:HIS:CD2	2.82	0.45
1:L:42:LEU:HD13	1:L:91:TYR:CZ	2.52	0.44
7:L:467:HOH:O	2:H:108:MET:HG3	2.17	0.44
1:L:31:GLU:HB3	1:L:35:LYS:O	2.18	0.44
1:L:55:LEU:HG	2:H:105:GLY:HA3	1.99	0.44
1:L:170:GLU:O	1:L:171:GLN:C	2.54	0.44
3:K:54[B]:LYS:NZ	3:K:58[B]:GLU:OE1	2.50	0.44
2:H:59:TYR:N	2:H:59:TYR:CD1	2.85	0.43
1:L:124:PRO:HD2	2:H:133:ALA:O	2.18	0.43
4:H:307:GOL:H12	7:H:446:HOH:O	2.18	0.43
1:L:82[B]:ARG:CG	1:L:82[B]:ARG:HH11	2.31	0.43
2:H:139:THR:HA	2:H:140:SER:HA	1.72	0.43
2:H:196:SER:HA	2:H:199:THR:HG23	2.01	0.43
2:H:31:ASN:ND2	7:H:428:HOH:O	2.51	0.43
1:L:115:VAL:HG23	7:L:549:HOH:O	2.19	0.43
2:H:27:PHE:CE2	2:H:29:PHE:HA	2.54	0.43
1:L:7[B]:THR:HG23	1:L:22[B]:SER:HB2	2.01	0.42
2:H:104:GLU:O	2:H:104:GLU:HG2	2.19	0.42
6:H:304:PGE:H62	7:K:115:HOH:O	2.18	0.42
1:L:13:VAL:HG21	1:L:19:ALA:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:154:LYS:HE2	1:L:159:LEU:HD23	2.01	0.42
3:K:2:GLU:O	3:K:60[A]:GLY:HA2	2.21	0.41
2:H:119:VAL:N	7:H:503:HOH:O	2.45	0.41
1:L:146:PRO:O	1:L:203:HIS:HE1	2.03	0.41
1:L:83:VAL:HG12	1:L:111:ILE:HD12	2.01	0.41
1:L:148:GLU:HB3	4:L:306:GOL:H32	2.02	0.41
2:H:20:LEU:O	2:H:80:TYR:HA	2.21	0.41
2:H:39:GLN:HA	2:H:44:ARG:O	2.22	0.40
3:K:19:TYR:HA	3:K:37:TYR:O	2.21	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)
7:H:403:HOH:O	7:H:490:HOH:O[8_555]	1.93	0.27

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	L	224/219 (102%)	219 (98%)	5 (2%)	0	100	100
2	H	224/222 (101%)	220 (98%)	4 (2%)	0	100	100
3	K	66/66 (100%)	61 (92%)	3 (4%)	2 (3%)	4	0
All	All	514/507 (101%)	500 (97%)	12 (2%)	2 (0%)	47	21

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	K	59[A]	ASP
3	K	59[B]	ASP

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	L	201/194 (104%)	196 (98%)	5 (2%)	47	34
2	H	192/188 (102%)	185 (96%)	7 (4%)	35	20
3	K	61/60 (102%)	61 (100%)	0	100	100
All	All	454/442 (103%)	442 (97%)	12 (3%)	47	32

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	20	SER
1	L	82[A]	ARG
1	L	82[B]	ARG
1	L	128	GLU
1	L	192	GLU
2	H	1	GLU
2	H	12	VAL
2	H	79	LEU
2	H	85	SER
2	H	186	LEU
2	H	199	THR
2	H	221	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	27	GLN
1	L	142	ASN
1	L	203	HIS
1	L	215	ASN
2	H	31	ASN
2	H	82	GLN
2	H	208	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

14 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	PGE	H	303	-	9,9,9	1.26	0	8,8,8	1.80	2 (25%)
4	GOL	H	307	-	5,5,5	0.54	0	5,5,5	0.69	0
6	PGE	H	304	-	9,9,9	0.71	0	8,8,8	0.52	0
4	GOL	L	304	-	5,5,5	0.34	0	5,5,5	0.26	0
4	GOL	H	305	-	5,5,5	0.49	0	5,5,5	0.91	0
4	GOL	H	306	-	5,5,5	0.83	0	5,5,5	0.69	0
4	GOL	L	302	-	5,5,5	0.48	0	5,5,5	1.00	0
4	GOL	L	307	-	5,5,5	0.31	0	5,5,5	0.44	0
6	PGE	H	302	-	9,9,9	0.68	0	8,8,8	0.77	0
5	MES	H	301	-	12,12,12	2.09	1 (8%)	14,16,16	2.97	6 (42%)
4	GOL	L	306	-	5,5,5	0.42	0	5,5,5	0.39	0
4	GOL	L	305	-	5,5,5	0.32	0	5,5,5	0.51	0
4	GOL	L	301	-	5,5,5	0.62	0	5,5,5	1.02	0
4	GOL	L	303	-	5,5,5	0.46	0	5,5,5	0.61	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
6	PGE	H	303	-	-	6/7/7/7	-
4	GOL	H	307	-	-	2/4/4/4	-
6	PGE	H	304	-	-	3/7/7/7	-
4	GOL	L	304	-	-	2/4/4/4	-
4	GOL	H	305	-	-	4/4/4/4	-
4	GOL	H	306	-	-	2/4/4/4	-
4	GOL	L	302	-	-	4/4/4/4	-
4	GOL	L	307	-	-	3/4/4/4	-
6	PGE	H	302	-	-	1/7/7/7	-
5	MES	H	301	-	-	3/6/14/14	0/1/1/1
4	GOL	L	306	-	-	2/4/4/4	-
4	GOL	L	305	-	-	4/4/4/4	-
4	GOL	L	301	-	-	1/4/4/4	-
4	GOL	L	303	-	-	4/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	301	MES	C8-S	-6.54	1.68	1.77

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	H	301	MES	O1S-S-C8	7.16	115.54	106.92
5	H	301	MES	O2S-S-C8	4.60	112.45	106.92
5	H	301	MES	O2S-S-O1S	-4.03	99.99	113.95
6	H	303	PGE	O3-C5-C6	3.52	125.52	110.07
6	H	303	PGE	O2-C3-C4	3.09	124.31	110.39
5	H	301	MES	C7-N4-C3	2.96	118.79	111.23
5	H	301	MES	O3S-S-O2S	-2.65	104.79	111.27
5	H	301	MES	O3S-S-C8	2.65	110.06	105.77

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L	302	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	L	303	GOL	O1-C1-C2-C3
4	L	303	GOL	C1-C2-C3-O3
4	L	305	GOL	O1-C1-C2-O2
4	L	305	GOL	O1-C1-C2-C3
4	L	306	GOL	O1-C1-C2-C3
4	H	306	GOL	C1-C2-C3-O3
4	H	307	GOL	O1-C1-C2-C3
5	H	301	MES	C8-C7-N4-C3
5	H	301	MES	C7-C8-S-O1S
4	L	302	GOL	O2-C2-C3-O3
4	L	307	GOL	O1-C1-C2-O2
6	H	303	PGE	O2-C3-C4-O3
6	H	303	PGE	O1-C1-C2-O2
6	H	303	PGE	O3-C5-C6-O4
4	L	301	GOL	C1-C2-C3-O3
4	L	305	GOL	C1-C2-C3-O3
4	L	307	GOL	O1-C1-C2-C3
4	H	305	GOL	O1-C1-C2-C3
4	H	305	GOL	C1-C2-C3-O3
4	L	303	GOL	O1-C1-C2-O2
4	L	303	GOL	O2-C2-C3-O3
4	H	306	GOL	O2-C2-C3-O3
4	H	307	GOL	O1-C1-C2-O2
6	H	304	PGE	O2-C3-C4-O3
4	L	306	GOL	O1-C1-C2-O2
4	L	305	GOL	O2-C2-C3-O3
4	H	305	GOL	O1-C1-C2-O2
4	H	305	GOL	O2-C2-C3-O3
6	H	303	PGE	C3-C4-O3-C5
4	L	302	GOL	O1-C1-C2-O2
4	L	304	GOL	O2-C2-C3-O3
6	H	302	PGE	O1-C1-C2-O2
6	H	303	PGE	C1-C2-O2-C3
6	H	303	PGE	C4-C3-O2-C2
6	H	304	PGE	C3-C4-O3-C5
6	H	304	PGE	O1-C1-C2-O2
5	H	301	MES	C8-C7-N4-C5
4	L	307	GOL	O2-C2-C3-O3
4	L	302	GOL	O1-C1-C2-C3
4	L	304	GOL	C1-C2-C3-O3

There are no ring outliers.

6 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	H	303	PGE	4	0
4	H	307	GOL	2	0
6	H	304	PGE	5	0
4	H	305	GOL	4	0
6	H	302	PGE	1	0
4	L	306	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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	L	219/219 (100%)	0.04	6 (2%)	54	49	22, 38, 57, 77	0
2	H	221/222 (99%)	0.18	14 (6%)	20	15	21, 38, 70, 117	0
3	K	60/66 (90%)	-0.17	2 (3%)	46	40	24, 31, 52, 65	0
All	All	500/507 (98%)	0.08	22 (4%)	34	28	21, 36, 59, 117	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	139	THR	9.4
1	L	217	GLY	5.8
1	L	219	CYS	5.4
2	H	140	SER	5.1
2	H	199	THR	4.4
1	L	207	SER	3.4
2	H	142	SER	3.2
2	H	138	SER	3.1
2	H	221	SER	3.0
2	H	195	SER	2.9
3	K	60[A]	GLY	2.7
2	H	197	LEU	2.7
2	H	198	GLY	2.6
2	H	137	ARG	2.5
2	H	141	GLU	2.5
1	L	192	GLU	2.5
1	L	163[A]	ASN	2.4
3	K	59[A]	ASP	2.4
2	H	194	SER	2.3
2	H	1	GLU	2.3
1	L	139	CYS	2.3
2	H	200	LYS	2.2

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, 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	H	306	6/6	0.76	0.19	48,55,63,72	0
4	GOL	H	305	6/6	0.77	0.29	68,71,73,80	0
4	GOL	L	306	6/6	0.81	0.43	62,74,83,84	0
4	GOL	L	307	6/6	0.81	0.22	64,80,82,94	0
6	PGE	H	304	10/10	0.81	0.17	40,52,61,63	0
4	GOL	H	307	6/6	0.85	0.14	38,53,64,68	0
6	PGE	H	303	10/10	0.86	0.32	38,43,52,52	0
4	GOL	L	304	6/6	0.87	0.18	58,64,70,80	0
6	PGE	H	302	10/10	0.88	0.17	48,52,83,92	0
4	GOL	L	303	6/6	0.90	0.26	57,62,67,78	0
4	GOL	L	305	6/6	0.91	0.21	70,72,76,80	0
4	GOL	L	302	6/6	0.92	0.16	53,54,66,66	0
4	GOL	L	301	6/6	0.95	0.11	39,41,44,49	0
5	MES	H	301	12/12	0.97	0.08	42,47,54,55	0

6.5 Other polymers (i)

There are no such residues in this entry.