Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:53 AM GMT

PDB ID	:	3CFJ
Title	:	Crystal structure of catalytic elimination antibody 34E4, orthorhombic crystal form
Authors	:	Debler, E.W.; Wilson, I.A.
Deposited on	:	2008-03-04
Resolution	:	2.60 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

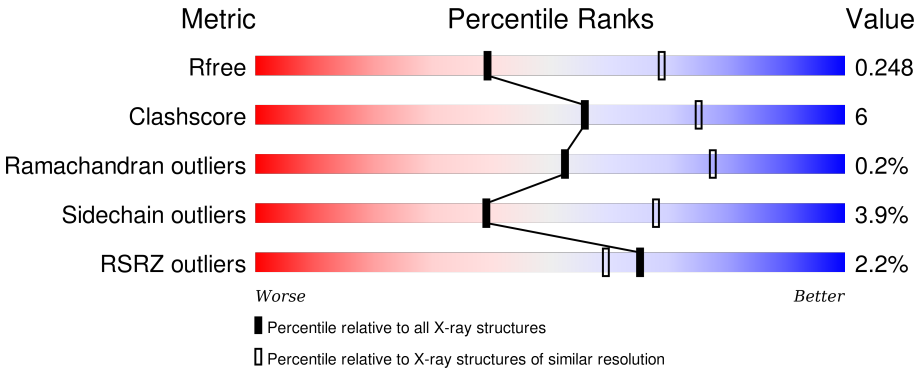
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.60 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}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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. 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	A	216	87% 10%
1	C	216	84% 13%
1	E	216	84% 13%
1	L	216	83% 15%
2	B	227	3% 81% 17%

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Mol	Chain	Length	Quality of chain
2	D	227	4% 86% 11%
2	F	227	5% 81% 16%
2	H	227	% 85% 12%

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	A	703	-	-	-	X
4	GOL	C	702	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13928 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 CATALYTIC ANTIBODY FAB 34E4 LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	215	Total	C	N	O	S	0	0	0
			1628	1016	277	331	4			
1	A	215	Total	C	N	O	S	0	0	0
			1628	1016	277	331	4			
1	C	215	Total	C	N	O	S	0	0	0
			1628	1016	277	331	4			
1	E	215	Total	C	N	O	S	0	0	0
			1628	1016	277	331	4			

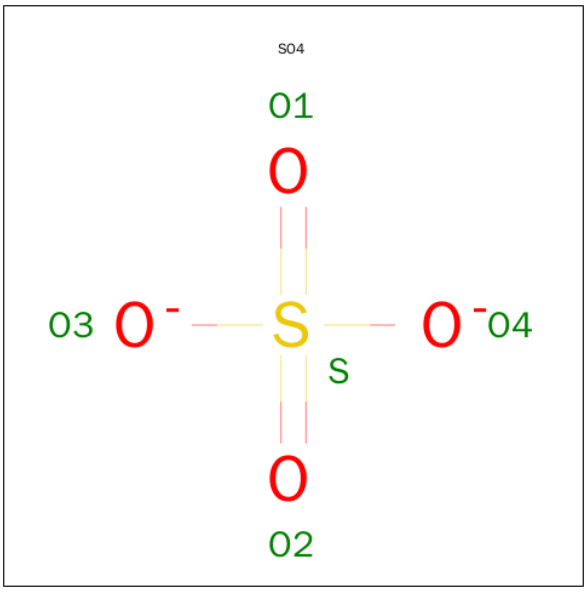
- Molecule 2 is a protein called CATALYTIC ANTIBODY FAB 34E4 HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	224	Total	C	N	O	S	0	0	0
			1718	1093	288	331	6			
2	B	224	Total	C	N	O	S	0	0	0
			1718	1093	288	331	6			
2	D	224	Total	C	N	O	S	0	0	0
			1718	1093	288	331	6			
2	F	224	Total	C	N	O	S	0	0	0
			1711	1087	288	330	6			

There are 4 discrepancies between the modelled and reference sequences:

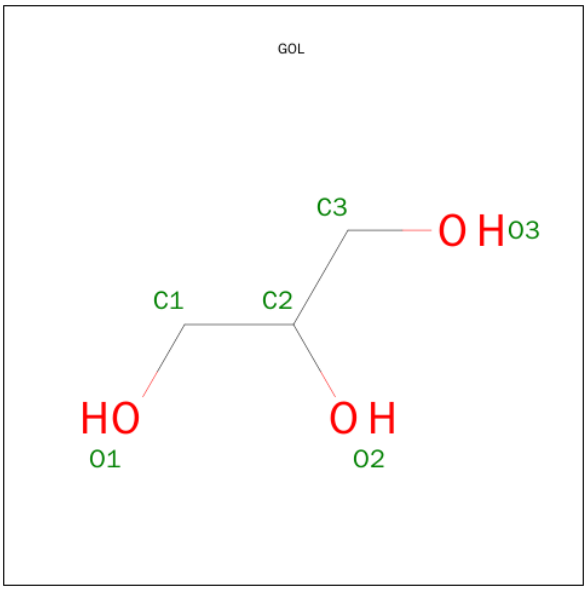
Chain	Residue	Modelled	Actual	Comment	Reference
H	108	SER	THR	ENGINEERED	UNP A8K008
B	108	SER	THR	ENGINEERED	UNP A8K008
D	108	SER	THR	ENGINEERED	UNP A8K008
F	108	SER	THR	ENGINEERED	UNP A8K008

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	H	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0

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



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

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

- Molecule 5 is water.

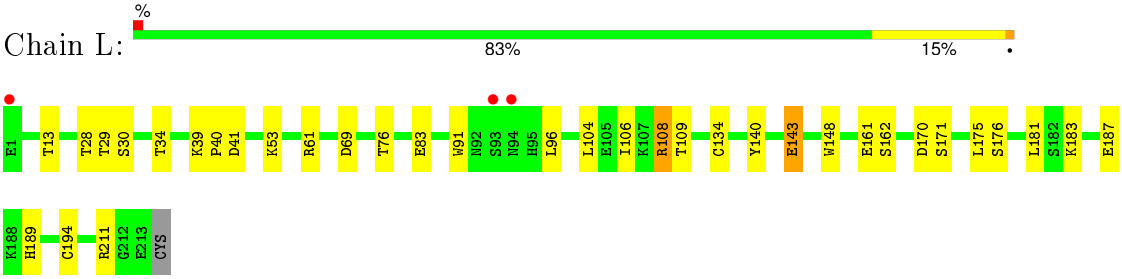
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	66	Total O 66 66	0	0
5	B	52	Total O 52 52	0	0
5	C	69	Total O 69 69	0	0
5	D	53	Total O 53 53	0	0
5	E	59	Total O 59 59	0	0
5	F	48	Total O 48 48	0	0
5	H	59	Total O 59 59	0	0
5	L	112	Total O 112 112	0	0

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 errors 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.

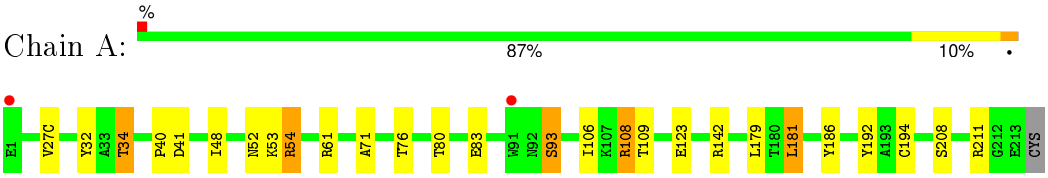
- Molecule 1: CATALYTIC ANTIBODY FAB 34E4 LIGHT CHAIN

Chain L:



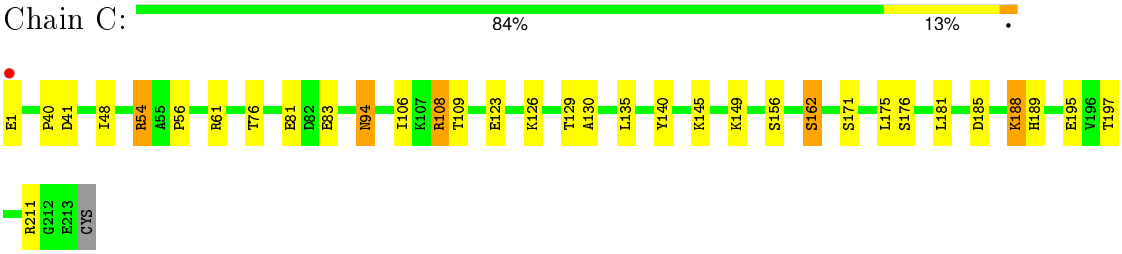
- Molecule 1: CATALYTIC ANTIBODY FAB 34E4 LIGHT CHAIN

Chain A:



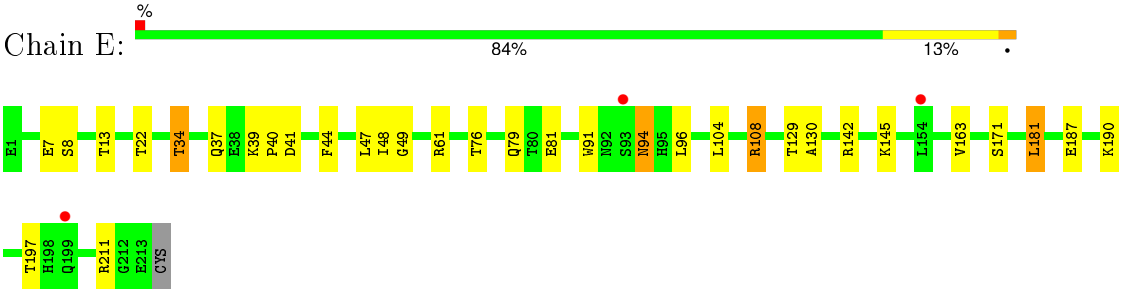
- Molecule 1: CATALYTIC ANTIBODY FAB 34E4 LIGHT CHAIN

Chain C:



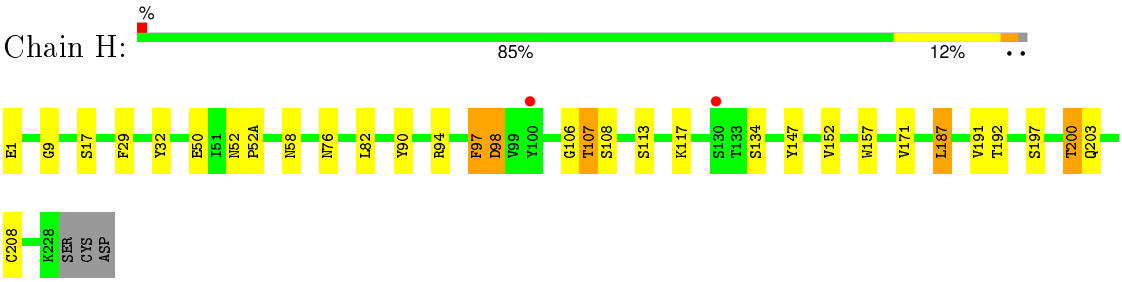
- Molecule 1: CATALYTIC ANTIBODY FAB 34E4 LIGHT CHAIN

Chain E:



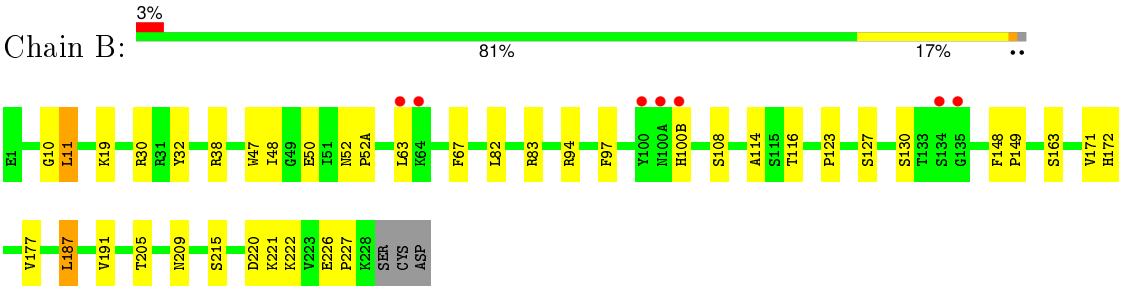
- Molecule 2: CATALYTIC ANTIBODY FAB 34E4 HEAVY CHAIN

Chain H:



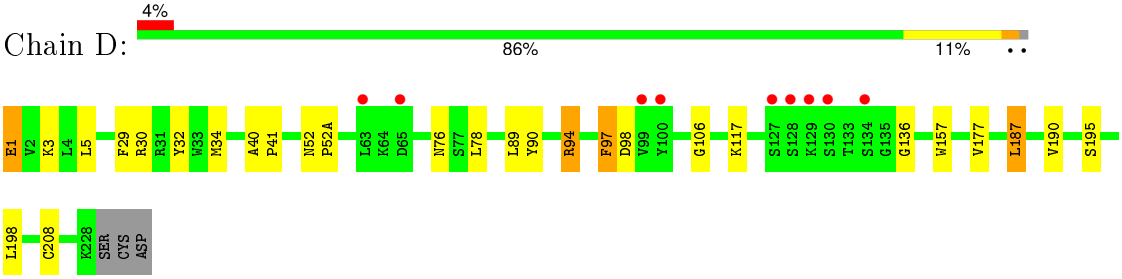
• Molecule 2: CATALYTIC ANTIBODY FAB 34E4 HEAVY CHAIN

Chain B:



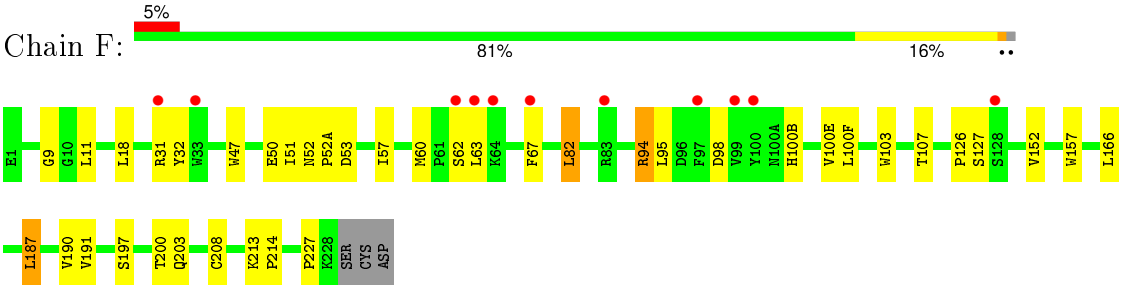
• Molecule 2: CATALYTIC ANTIBODY FAB 34E4 HEAVY CHAIN

Chain D:



• Molecule 2: CATALYTIC ANTIBODY FAB 34E4 HEAVY CHAIN

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	81.14Å 114.47Å 212.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.34 – 2.60 48.32 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.34-2.60) 99.8 (48.32-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	2.29 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.199 , 0.253 0.197 , 0.248	Depositor DCC
R_{free} test set	3094 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	42.9	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 42.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	2 of 61433 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	13928	wwPDB-VP
Average B, all atoms (Å^2)	38.0	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 22.34 % 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 5.8168e-03.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, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, 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	0.74	1/1660 (0.1%)	0.73	0/2258
1	C	0.73	3/1660 (0.2%)	0.66	0/2258
1	E	0.62	0/1660	0.67	1/2258 (0.0%)
1	L	0.72	1/1660 (0.1%)	0.75	0/2258
2	B	0.65	1/1762 (0.1%)	0.71	2/2397 (0.1%)
2	D	0.63	0/1762	0.70	1/2397 (0.0%)
2	F	0.66	2/1754 (0.1%)	0.72	1/2386 (0.0%)
2	H	0.70	0/1762	0.71	0/2397
All	All	0.68	8/13680 (0.1%)	0.70	5/18609 (0.0%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	188	LYS	CD-CE	10.47	1.77	1.51
2	F	31	ARG	CZ-NH1	9.48	1.45	1.33
2	B	83	ARG	CZ-NH1	5.96	1.40	1.33
1	C	1	GLU	CG-CD	5.93	1.60	1.51
1	A	194	CYS	CB-SG	-5.87	1.72	1.81
1	L	194	CYS	CB-SG	-5.82	1.72	1.81
1	C	1	GLU	CD-OE2	5.55	1.31	1.25
2	F	31	ARG	CZ-NH2	5.30	1.40	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	31	ARG	NE-CZ-NH2	-7.76	116.42	120.30
2	B	83	ARG	NE-CZ-NH2	-5.86	117.37	120.30
2	D	187	LEU	CA-CB-CG	5.73	128.48	115.30
1	E	181	LEU	CA-CB-CG	5.71	128.43	115.30
2	B	187	LEU	CA-CB-CG	5.43	127.80	115.30

There are no chirality outliers.

There are no planarity outliers.

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	1628	0	1590	15	0
1	C	1628	0	1590	31	0
1	E	1628	0	1590	21	0
1	L	1628	0	1590	22	0
2	B	1718	0	1693	27	0
2	D	1718	0	1693	15	0
2	F	1711	0	1686	26	0
2	H	1718	0	1693	16	0
3	D	10	0	0	0	0
3	H	5	0	0	0	0
4	A	6	0	8	0	0
4	C	6	0	8	1	0
4	L	6	0	8	0	0
5	A	66	0	0	0	0
5	B	52	0	0	5	0
5	C	69	0	0	0	0
5	D	53	0	0	2	0
5	E	59	0	0	0	0
5	F	48	0	0	2	0
5	H	59	0	0	1	0
5	L	112	0	0	0	0
All	All	13928	0	13149	165	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 6.

All (165) 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:C:188:LYS:CE	1:C:188:LYS:CD	1.77	1.58
2:B:19:LYS:HE3	5:B:238:HOH:O	1.66	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:83:GLU:HG2	1:C:106:ILE:HG12	1.53	0.90
1:C:145:LYS:HB3	1:C:197:THR:CG2	2.01	0.89
1:C:83:GLU:CG	1:C:106:ILE:HG12	2.04	0.87
1:C:145:LYS:HB3	1:C:197:THR:HG22	1.55	0.86
1:C:188:LYS:CE	1:C:188:LYS:CG	2.54	0.85
2:H:117:LYS:HE2	5:H:631:HOH:O	1.75	0.85
1:C:135:LEU:HD22	2:D:190:VAL:HG11	1.67	0.77
1:L:83:GLU:HG3	1:L:106:ILE:HG12	1.68	0.75
1:E:145:LYS:HB3	1:E:197:THR:CG2	2.18	0.74
2:F:9:GLY:HA3	2:F:107:THR:CG2	2.17	0.74
2:D:136:GLY:HA2	5:D:614:HOH:O	1.89	0.72
2:F:9:GLY:HA3	2:F:107:THR:HG22	1.70	0.72
2:H:32:TYR:CD2	2:H:94:ARG:HD2	2.26	0.71
1:A:40:PRO:O	1:A:41:ASP:HB2	1.89	0.70
1:L:40:PRO:O	1:L:41:ASP:HB2	1.90	0.70
2:F:9:GLY:H	2:F:107:THR:HG21	1.58	0.69
1:C:83:GLU:CG	1:C:106:ILE:CG1	2.72	0.67
1:L:28:THR:HG22	1:L:30:SER:H	1.58	0.67
1:C:40:PRO:O	1:C:41:ASP:HB2	1.93	0.67
2:D:30:ARG:NH2	5:D:638:HOH:O	2.27	0.67
1:C:83:GLU:HG3	1:C:106:ILE:CG1	2.26	0.66
1:L:108:ARG:HD3	1:L:109:THR:O	1.95	0.66
2:H:97:PHE:O	2:H:98:ASP:HB2	1.94	0.66
2:F:9:GLY:N	2:F:107:THR:HG21	2.11	0.65
2:F:47:TRP:HZ2	2:F:50:GLU:HG3	1.62	0.65
1:C:188:LYS:NZ	1:C:188:LYS:CD	2.59	0.65
2:D:3:LYS:NZ	2:D:5:LEU:HD21	2.12	0.65
1:E:40:PRO:O	1:E:41:ASP:HB2	1.98	0.63
2:H:171:VAL:HG22	2:H:191:VAL:HG22	1.80	0.63
1:L:83:GLU:CG	1:L:106:ILE:HG12	2.29	0.62
2:B:116:THR:HG22	2:B:215:SER:HB3	1.83	0.61
1:C:83:GLU:OE2	1:C:106:ILE:HB	2.01	0.61
1:L:83:GLU:HG3	1:L:106:ILE:CG1	2.30	0.61
2:B:63:LEU:HB3	2:B:67:PHE:CD1	2.36	0.60
1:A:61:ARG:HG3	1:A:76:THR:O	2.02	0.59
2:H:192:THR:O	2:D:3:LYS:HE3	2.03	0.58
2:H:200:THR:HG22	2:H:203:GLN:HG2	1.83	0.58
1:L:108:ARG:HD2	1:L:140:TYR:CB	2.33	0.58
1:C:108:ARG:HD3	1:C:109:THR:O	2.04	0.58
2:B:47:TRP:CZ2	2:B:50:GLU:HG2	2.39	0.58
2:F:126:PRO:HG2	2:F:227:PRO:HA	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:TYR:CE1	2:B:100(B):HIS:HB3	2.39	0.57
1:L:61:ARG:HG3	1:L:76:THR:O	2.05	0.57
1:C:83:GLU:HG3	1:C:106:ILE:HG12	1.80	0.56
1:E:13:THR:HG22	1:E:104:LEU:HD11	1.85	0.56
1:E:108:ARG:HG2	1:E:171:SER:HB2	1.86	0.56
1:E:145:LYS:HB3	1:E:197:THR:HG22	1.87	0.56
1:L:28:THR:HG22	1:L:29:THR:N	2.21	0.56
1:E:7:GLU:OE2	1:E:22:THR:OG1	2.22	0.56
1:C:185:ASP:HA	1:C:188:LYS:HD2	1.88	0.56
1:A:108:ARG:HD3	1:A:109:THR:O	2.06	0.56
2:B:209:ASN:ND2	2:B:220:ASP:OD1	2.26	0.55
1:C:48:ILE:HD13	1:C:54:ARG:HA	1.89	0.55
2:F:200:THR:HG22	2:F:203:GLN:HG3	1.88	0.55
1:A:83:GLU:HG2	1:A:106:ILE:HG12	1.89	0.54
2:D:32:TYR:CD2	2:D:94:ARG:HD2	2.42	0.54
1:L:143:GLU:H	1:L:143:GLU:CD	2.12	0.54
1:L:183:LYS:O	1:L:187:GLU:HG2	2.08	0.53
1:C:135:LEU:CD2	2:D:190:VAL:HG11	2.37	0.53
1:L:39:LYS:HE3	1:L:83:GLU:O	2.09	0.53
1:L:108:ARG:HD2	1:L:140:TYR:HB3	1.91	0.53
2:B:116:THR:CG2	2:B:215:SER:HB3	2.39	0.52
2:F:63:LEU:HD13	2:F:67:PHE:CE2	2.44	0.52
1:C:83:GLU:HG3	1:C:106:ILE:HG13	1.90	0.52
2:F:32:TYR:CD2	2:F:94:ARG:HD2	2.44	0.52
1:A:32:TYR:HE1	2:B:100(B):HIS:HB3	1.74	0.52
1:E:39:LYS:HE2	1:E:81:GLU:O	2.10	0.52
1:E:49:GLY:HA3	2:F:100(E):VAL:CG2	2.38	0.52
2:B:47:TRP:HZ2	2:B:50:GLU:HG2	1.75	0.52
1:A:34:THR:HG22	1:A:48:ILE:O	2.10	0.51
1:E:145:LYS:HB3	1:E:197:THR:HG23	1.92	0.51
2:B:11:LEU:HD12	2:B:149:PRO:HG3	1.92	0.51
1:L:91:TRP:CE2	1:L:96:LEU:HD13	2.46	0.51
2:B:205:THR:HG23	2:B:222:LYS:HE3	1.92	0.51
2:F:166:LEU:HD21	2:F:191:VAL:HG11	1.93	0.50
1:L:161:GLU:HG3	1:L:175:LEU:HD21	1.92	0.50
2:B:32:TYR:CD2	2:B:94:ARG:HD2	2.46	0.50
1:A:186:TYR:CZ	1:A:211:ARG:HG3	2.47	0.50
1:L:170:ASP:OD2	2:D:1:GLU:HB2	2.12	0.50
2:F:95:LEU:HD13	2:F:100(F):LEU:HD23	1.94	0.49
1:L:189:HIS:O	1:L:211:ARG:NH1	2.40	0.49
2:H:9:GLY:H	2:H:107:THR:HG21	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:47:TRP:CZ2	2:F:50:GLU:HG3	2.46	0.49
2:F:52:ASN:OD1	2:F:52(A):PRO:HD2	2.13	0.49
1:E:142:ARG:NH2	1:E:163:VAL:HG11	2.28	0.49
2:F:51:ILE:HG13	2:F:57:ILE:HG12	1.94	0.49
2:B:171:VAL:HG22	2:B:191:VAL:HG22	1.94	0.49
1:E:37:GLN:HB2	1:E:47:LEU:HD11	1.95	0.49
1:C:108:ARG:HD2	1:C:140:TYR:CB	2.43	0.49
1:C:129:THR:HG22	1:C:130:ALA:N	2.28	0.48
1:C:108:ARG:HG2	1:C:171:SER:HB2	1.94	0.48
2:B:123:PRO:HD3	2:B:221:LYS:HE2	1.95	0.48
1:E:44:PHE:HB2	2:F:103:TRP:CG	2.48	0.48
2:B:63:LEU:HB3	2:B:67:PHE:CE1	2.49	0.47
2:D:34:MET:HB3	2:D:78:LEU:HD22	1.95	0.47
2:B:11:LEU:HD11	2:B:148:PHE:CE2	2.48	0.47
1:L:175:LEU:HD23	1:L:176:SER:N	2.29	0.47
1:C:175:LEU:HD23	1:C:176:SER:N	2.28	0.47
1:E:61:ARG:HB2	1:E:76:THR:O	2.15	0.47
2:H:197:SER:O	2:H:200:THR:HB	2.14	0.47
2:B:11:LEU:HD21	2:B:114:ALA:O	2.14	0.47
1:L:28:THR:CG2	1:L:29:THR:N	2.77	0.47
2:H:147:TYR:CE2	2:H:152:VAL:HG13	2.49	0.47
1:C:162:SER:HB2	4:C:702:GOL:H11	1.97	0.47
1:L:13:THR:HG22	1:L:104:LEU:HD11	1.97	0.46
2:F:197:SER:O	2:F:200:THR:HB	2.15	0.46
1:E:129:THR:CG2	1:E:130:ALA:N	2.78	0.46
1:A:80:THR:O	1:A:83:GLU:HG3	2.15	0.46
2:H:29:PHE:CD2	2:H:76:ASN:HA	2.50	0.46
2:D:40:ALA:HB1	2:D:41:PRO:HD2	1.97	0.46
1:E:79:GLN:HB3	1:E:81:GLU:OE2	2.15	0.46
2:B:10:GLY:HA2	5:B:260:HOH:O	2.15	0.46
1:A:179:LEU:HG	1:A:181:LEU:CD2	2.45	0.46
2:B:127:SER:HB3	2:B:130:SER:HB2	1.97	0.46
1:C:149:LYS:HE3	1:C:195:GLU:OE1	2.16	0.46
2:F:157:TRP:CH2	2:F:208:CYS:HB3	2.51	0.46
2:B:177:VAL:HG13	5:B:237:HOH:O	2.15	0.46
1:C:189:HIS:O	1:C:211:ARG:NH1	2.48	0.45
1:E:34:THR:HG22	1:E:48:ILE:O	2.17	0.45
2:F:9:GLY:CA	2:F:107:THR:HG21	2.46	0.45
2:D:29:PHE:CD2	2:D:76:ASN:HA	2.51	0.45
1:A:48:ILE:HD13	1:A:54:ARG:HA	1.98	0.45
1:E:34:THR:CG2	5:F:240:HOH:O	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:52:ASN:HB2	2:B:52(A):PRO:HD2	1.98	0.45
2:F:52:ASN:ND2	2:F:53:ASP:OD1	2.50	0.45
1:L:134:CYS:HB2	1:L:148:TRP:CZ2	2.52	0.45
2:F:9:GLY:CA	2:F:107:THR:CG2	2.92	0.44
1:E:34:THR:HG21	5:F:240:HOH:O	2.17	0.44
1:E:190:LYS:HE3	1:E:211:ARG:O	2.17	0.44
2:F:213:LYS:HB2	2:F:214:PRO:HD3	2.00	0.44
1:A:192:TYR:O	1:A:208:SER:HB2	2.17	0.44
2:B:30:ARG:O	2:B:52(A):PRO:HB3	2.16	0.44
2:H:157:TRP:CH2	2:H:208:CYS:HB3	2.53	0.44
2:F:18:LEU:HB3	2:F:82:LEU:HD12	1.99	0.44
2:F:60:MET:HE2	2:F:62:SER:HB3	2.00	0.44
2:H:17:SER:HB2	2:H:82:LEU:O	2.18	0.43
2:F:63:LEU:HD13	2:F:67:PHE:CD2	2.53	0.43
1:E:94:ASN:OD1	1:E:94:ASN:N	2.45	0.43
2:B:38:ARG:HB3	2:B:48:ILE:HD11	2.00	0.43
1:A:40:PRO:O	1:A:41:ASP:CB	2.62	0.43
2:B:11:LEU:HD21	5:B:263:HOH:O	2.19	0.43
1:C:94:ASN:N	1:C:94:ASN:OD1	2.52	0.43
2:H:52:ASN:HB2	2:H:52(A):PRO:HD2	2.00	0.42
2:H:187:LEU:C	2:H:187:LEU:HD12	2.40	0.42
2:F:187:LEU:HD12	2:F:187:LEU:C	2.40	0.42
1:C:61:ARG:HB2	1:C:76:THR:O	2.20	0.42
1:A:52:ASN:OD1	1:A:53:LYS:HD3	2.18	0.42
2:B:11:LEU:HD11	2:B:148:PHE:HE2	1.83	0.42
2:D:52:ASN:HB2	2:D:52(A):PRO:HD2	2.01	0.42
2:H:90:TYR:O	2:H:106:GLY:HA2	2.19	0.42
2:H:50:GLU:HG2	2:H:58:ASN:HB2	2.01	0.42
1:C:123:GLU:O	1:C:126:LYS:HB2	2.20	0.42
1:L:108:ARG:HG2	1:L:171:SER:HB2	2.02	0.41
1:A:27(C):VAL:HG11	1:A:71:ALA:HB2	2.02	0.41
2:D:97:PHE:O	2:D:98:ASP:HB2	2.21	0.41
1:E:91:TRP:CE2	1:E:96:LEU:HD13	2.55	0.41
2:B:172:HIS:HD2	5:B:264:HOH:O	2.02	0.41
2:D:157:TRP:CH2	2:D:208:CYS:HB3	2.56	0.41
1:C:108:ARG:HD2	1:C:140:TYR:HB3	2.02	0.41
1:C:145:LYS:HB3	1:C:197:THR:HG23	1.96	0.41
2:D:90:TYR:O	2:D:106:GLY:HA2	2.21	0.41
1:C:188:LYS:CE	1:C:188:LYS:HG2	2.46	0.40
2:B:226:GLU:HA	2:B:227:PRO:HD3	1.98	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	213/216 (99%)	206 (97%)	6 (3%)	1 (0%)	34	60
1	C	213/216 (99%)	206 (97%)	7 (3%)	0	100	100
1	E	213/216 (99%)	206 (97%)	7 (3%)	0	100	100
1	L	213/216 (99%)	209 (98%)	4 (2%)	0	100	100
2	B	222/227 (98%)	218 (98%)	4 (2%)	0	100	100
2	D	222/227 (98%)	219 (99%)	3 (1%)	0	100	100
2	F	222/227 (98%)	215 (97%)	6 (3%)	1 (0%)	34	60
2	H	222/227 (98%)	215 (97%)	6 (3%)	1 (0%)	34	60
All	All	1740/1772 (98%)	1694 (97%)	43 (2%)	3 (0%)	52	77

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	98	ASP
1	A	93	SER
2	F	98	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	A	182/183 (100%)	175 (96%)	7 (4%)	40	68
1	C	182/183 (100%)	174 (96%)	8 (4%)	35	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	E	182/183 (100%)	176 (97%)	6 (3%)	45 73
1	L	182/183 (100%)	175 (96%)	7 (4%)	40 68
2	B	193/196 (98%)	187 (97%)	6 (3%)	47 76
2	D	193/196 (98%)	184 (95%)	9 (5%)	32 59
2	F	192/196 (98%)	184 (96%)	8 (4%)	36 65
2	H	193/196 (98%)	185 (96%)	8 (4%)	37 66
All	All	1499/1516 (99%)	1440 (96%)	59 (4%)	39 68

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	34	THR
1	L	53	LYS
1	L	69	ASP
1	L	108	ARG
1	L	143	GLU
1	L	162	SER
1	L	181	LEU
2	H	1	GLU
2	H	97	PHE
2	H	107	THR
2	H	108	SER
2	H	113	SER
2	H	134	SER
2	H	187	LEU
2	H	200	THR
1	A	34	THR
1	A	54	ARG
1	A	93	SER
1	A	108	ARG
1	A	123	GLU
1	A	142	ARG
1	A	181	LEU
2	B	11	LEU
2	B	82	LEU
2	B	97	PHE
2	B	108	SER
2	B	163	SER
2	B	187	LEU
1	C	54	ARG

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Mol	Chain	Res	Type
1	C	56	PRO
1	C	81	GLU
1	C	94	ASN
1	C	108	ARG
1	C	156	SER
1	C	162	SER
1	C	181	LEU
2	D	1	GLU
2	D	89	LEU
2	D	94	ARG
2	D	97	PHE
2	D	117	LYS
2	D	177	VAL
2	D	187	LEU
2	D	195	SER
2	D	198	LEU
1	E	8	SER
1	E	34	THR
1	E	94	ASN
1	E	108	ARG
1	E	181	LEU
1	E	187	GLU
2	F	11	LEU
2	F	82	LEU
2	F	94	ARG
2	F	100(B)	HIS
2	F	127	SER
2	F	152	VAL
2	F	187	LEU
2	F	190	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	137	ASN
2	D	100(A)	ASN
2	D	172	HIS

5.3.3 RNA

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 carbohydrates 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	$\#\|Z\| > 2$
4	GOL	A	703	-	5,5,5	0.22	0	5,5,5	0.49	0
4	GOL	C	702	-	5,5,5	0.34	0	5,5,5	0.40	0
3	SO4	D	601	-	4,4,4	0.40	0	6,6,6	0.11	0
3	SO4	D	603	-	4,4,4	0.28	0	6,6,6	0.17	0
3	SO4	H	602	-	4,4,4	0.12	0	6,6,6	0.31	0
4	GOL	L	701	-	5,5,5	0.47	0	5,5,5	0.93	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	A	703	-	-	0/4/4/4	0/0/0/0
4	GOL	C	702	-	-	0/4/4/4	0/0/0/0
3	SO4	D	601	-	-	0/0/0/0	0/0/0/0
3	SO4	D	603	-	-	0/0/0/0	0/0/0/0
3	SO4	H	602	-	-	0/0/0/0	0/0/0/0
4	GOL	L	701	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	702	GOL	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	A	215/216 (99%)	0.09	2 (0%)	85	83	29, 38, 44, 54	0
1	C	215/216 (99%)	0.10	1 (0%)	91	90	30, 37, 44, 53	0
1	E	215/216 (99%)	0.11	3 (1%)	78	74	31, 37, 44, 51	0
1	L	215/216 (99%)	0.07	3 (1%)	78	74	30, 37, 44, 55	0
2	B	224/227 (98%)	0.27	7 (3%)	52	45	30, 37, 48, 52	0
2	D	224/227 (98%)	0.28	9 (4%)	42	34	30, 37, 47, 62	0
2	F	224/227 (98%)	0.40	11 (4%)	33	26	31, 38, 48, 52	0
2	H	224/227 (98%)	0.13	2 (0%)	85	83	30, 37, 47, 59	0
All	All	1756/1772 (99%)	0.18	38 (2%)	65	59	29, 37, 46, 62	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	100	TYR	7.3
2	D	65	ASP	4.8
2	B	63	LEU	4.7
2	B	64	LYS	4.5
1	L	1	GLU	4.1
2	D	128	SER	4.0
2	B	100	TYR	3.9
1	C	1	GLU	3.8
2	F	64	LYS	3.7
2	H	100	TYR	3.6
2	F	63	LEU	3.3
1	A	1	GLU	3.3
2	D	134	SER	3.3
2	F	97	PHE	3.2
2	D	127	SER	3.2
2	F	99	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
2	B	100(B)	HIS	2.8
1	E	154	LEU	2.7
2	F	31	ARG	2.6
2	F	128	SER	2.5
1	L	94	ASN	2.5
2	F	100	TYR	2.5
2	D	129	LYS	2.5
2	B	100(A)	ASN	2.5
1	L	93	SER	2.4
1	E	93	SER	2.4
2	H	130	SER	2.4
1	E	199	GLN	2.3
2	F	67	PHE	2.3
2	F	62	SER	2.3
2	D	63	LEU	2.2
2	B	134	SER	2.2
1	A	91	TRP	2.2
2	F	83	ARG	2.1
2	B	135	GLY	2.1
2	D	99	VAL	2.1
2	F	33	TRP	2.1
2	D	130	SER	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 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
4	GOL	A	703	6/6	0.90	0.29	4.89	38,41,42,46	0
4	GOL	C	702	6/6	0.94	0.21	2.51	43,47,48,51	0
4	GOL	L	701	6/6	0.91	0.20	1.66	40,43,45,45	0
3	SO4	D	601	5/5	0.97	0.31	1.12	55,56,57,57	0
3	SO4	D	603	5/5	0.95	0.29	0.85	78,79,79,79	0
3	SO4	H	602	5/5	0.99	0.19	-	52,53,54,54	0

6.5 Other polymers (i)

There are no such residues in this entry.