Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:57 PM GMT

PDB ID	:	1MTN
Title	:	BOVINE ALPHA-CHYMOTRYPSIN:BPTI CRYSTALLIZATION
Authors	:	Capasso, C.; Rizzi, M.; Menegatti, E.; Ascenzi, P.; Bolognesi, M.
Deposited on	:	1996-03-28
Resolution	:	2.80 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
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:

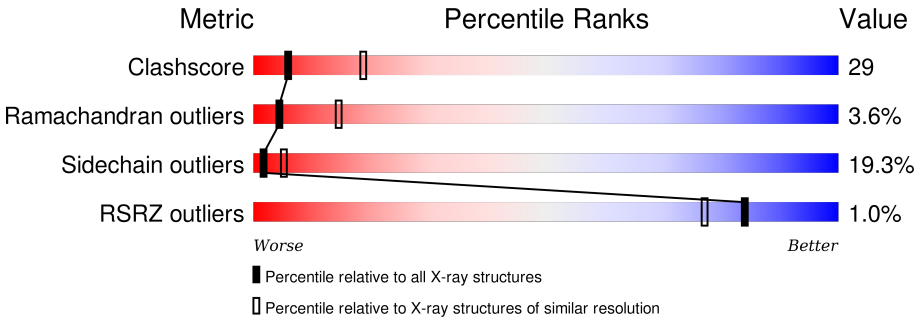
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.80 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))
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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 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	13	8% 54% 23% 8% 15%
1	E	13	38% 38% 8% 15%
2	B	131	48% 41% 10% •
2	F	131	2% 41% 47% 12%
3	C	97	2% 47% 36% 15% •
3	G	97	% 41% 45% 11% •
4	D	58	52% 38% 9% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	H	58	48% 43% 7%

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
5	SO4	D	600	-	-	-	X
5	SO4	D	800	-	-	-	X
5	SO4	H	500	-	-	X	X
5	SO4	H	700	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4520 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 ALPHA-CHYMOTRYPSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	11	Total	C	N	O	S	7	0	0
			74	48	12	13	1			
1	E	11	Total	C	N	O	S	7	0	0
			74	48	12	13	1			

- Molecule 2 is a protein called ALPHA-CHYMOTRYPSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	131	Total	C	N	O	S	79	0	0
			980	618	162	196	4			
2	F	131	Total	C	N	O	S	70	0	0
			980	618	162	196	4			

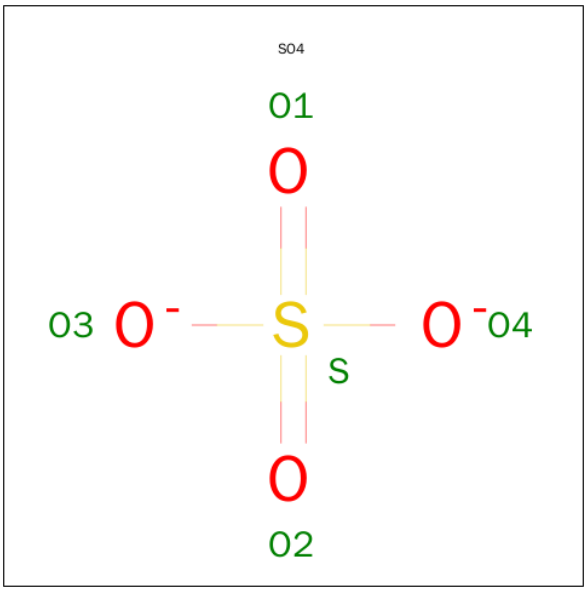
- Molecule 3 is a protein called ALPHA-CHYMOTRYPSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	97	Total	C	N	O	S	43	0	0
			702	436	123	136	7			
3	G	97	Total	C	N	O	S	47	0	0
			702	436	123	136	7			

- Molecule 4 is a protein called BASIC PANCREATIC TRYPSIN INHIBITOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	58	Total	C	N	O	S	25	0	0
			454	284	84	79	7			
4	H	58	Total	C	N	O	S	18	0	0
			454	284	84	79	7			

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 6 is water.

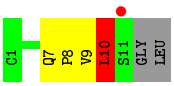
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	16	Total O 16 16	0	0
6	C	14	Total O 14 14	0	0
6	D	11	Total O 11 11	0	0
6	E	2	Total O 2 2	0	0
6	F	12	Total O 12 12	0	0
6	G	10	Total O 10 10	0	0
6	H	15	Total O 15 15	0	0

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.

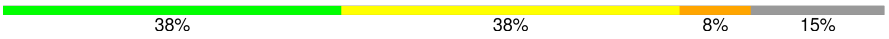
- Molecule 1: ALPHA-CHYMOTRYPSIN

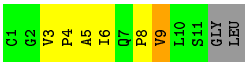
Chain A:



- Molecule 1: ALPHA-CHYMOTRYPSIN

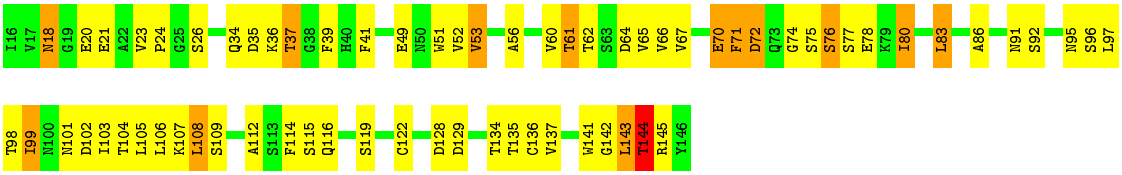
Chain E:





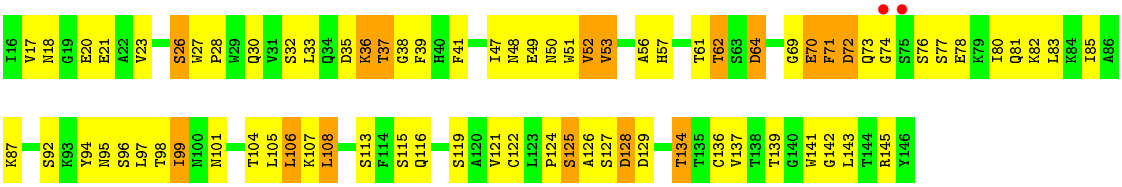
- Molecule 2: ALPHA-CHYMOTRYPSIN

Chain B:



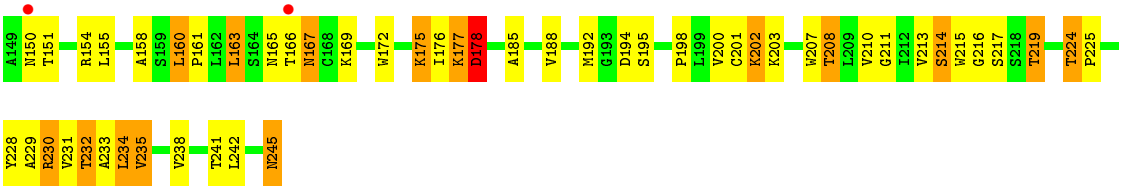
- Molecule 2: ALPHA-CHYMOTRYPSIN

Chain F:



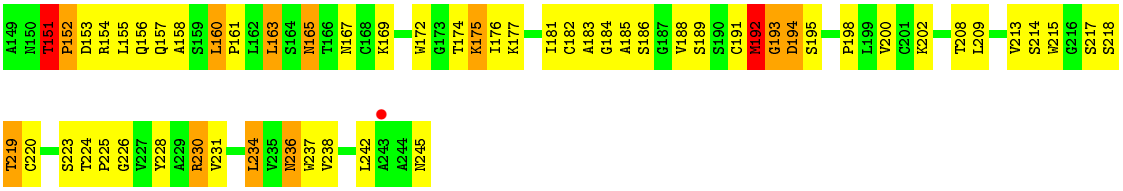
- Molecule 3: ALPHA-CHYMOTRYPSIN

Chain C:



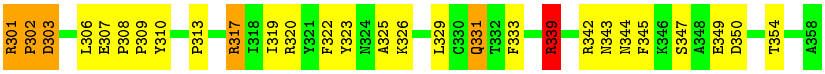
• Molecule 3: ALPHA-CHYMOTRYPSIN

Chain G:



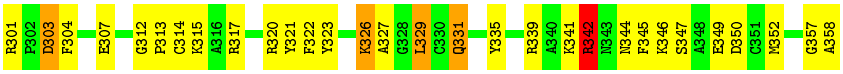
• Molecule 4: BASIC PANCREATIC TRYPSIN INHIBITOR

Chain D:



• Molecule 4: BASIC PANCREATIC TRYPSIN INHIBITOR

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	102.45Å 102.45Å 207.57Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.80 19.56 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.80) 90.2 (19.56-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.38 (at 2.79Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	(Not available) , 0.240 0.178 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	45.1	Xtriage
Anisotropy	0.400	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 126.1	EDS
Estimated twinning fraction	0.048 for h,-h-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 27254 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4520	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% 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, 0.375 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: 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	0.81	0/75	1.42	0/103
1	E	0.79	0/75	1.32	0/103
2	B	0.97	4/1000 (0.4%)	1.41	7/1361 (0.5%)
2	F	0.93	5/1000 (0.5%)	1.37	9/1361 (0.7%)
3	C	0.82	0/715	1.42	4/973 (0.4%)
3	G	0.83	0/715	1.35	5/973 (0.5%)
4	D	1.05	2/465 (0.4%)	1.59	6/622 (1.0%)
4	H	0.99	2/465 (0.4%)	1.57	10/622 (1.6%)
All	All	0.92	13/4510 (0.3%)	1.43	41/6118 (0.7%)

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
4	H	1	0

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	70	GLU	CD-OE1	6.75	1.33	1.25
2	B	21	GLU	CD-OE2	6.60	1.32	1.25
2	B	70	GLU	CD-OE1	6.41	1.32	1.25
2	F	20	GLU	CD-OE1	6.03	1.32	1.25
2	F	49	GLU	CD-OE2	6.00	1.32	1.25
4	H	307	GLU	CD-OE2	5.92	1.32	1.25
2	B	49	GLU	CD-OE1	5.75	1.31	1.25
4	D	307	GLU	CD-OE1	5.58	1.31	1.25
4	H	349	GLU	CD-OE2	5.49	1.31	1.25
2	F	21	GLU	CD-OE1	5.32	1.31	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	349	GLU	CD-OE2	5.31	1.31	1.25
2	B	78	GLU	CD-OE1	5.29	1.31	1.25
2	F	78	GLU	CD-OE2	5.22	1.31	1.25

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	339	ARG	NE-CZ-NH1	8.46	124.53	120.30
3	C	194	ASP	CB-CG-OD1	-8.44	110.71	118.30
2	F	64	ASP	CB-CG-OD1	-8.34	110.80	118.30
4	D	350	ASP	CB-CG-OD2	-8.22	110.90	118.30
2	B	64	ASP	CB-CG-OD1	-7.88	111.20	118.30
4	D	317	ARG	NE-CZ-NH2	-7.71	116.45	120.30
4	H	350	ASP	CB-CG-OD2	-7.59	111.47	118.30
3	C	194	ASP	CB-CG-OD2	7.50	125.05	118.30
4	H	342	ARG	NE-CZ-NH2	-7.39	116.60	120.30
2	F	64	ASP	CB-CG-OD2	7.04	124.63	118.30
3	G	194	ASP	CB-CG-OD2	6.78	124.41	118.30
2	B	144	THR	CA-CB-CG2	-6.73	102.97	112.40
4	H	339	ARG	NE-CZ-NH2	-6.71	116.94	120.30
2	B	128	ASP	CB-CG-OD2	-6.47	112.48	118.30
2	B	64	ASP	CB-CG-OD2	6.42	124.08	118.30
4	D	303	ASP	CB-CG-OD2	-6.41	112.53	118.30
4	D	339	ARG	CA-CB-CG	6.27	127.20	113.40
4	H	303	ASP	CB-CA-C	6.19	122.78	110.40
3	C	178	ASP	CB-CG-OD2	-6.14	112.77	118.30
4	H	350	ASP	CB-CG-OD1	6.08	123.77	118.30
2	F	72	ASP	CB-CG-OD1	-6.06	112.84	118.30
4	H	339	ARG	NE-CZ-NH1	5.92	123.26	120.30
3	G	153	ASP	CB-CG-OD1	-5.80	113.08	118.30
2	F	134	THR	CA-CB-CG2	-5.79	104.29	112.40
2	F	129	ASP	CB-CG-OD1	-5.78	113.10	118.30
4	H	303	ASP	CB-CG-OD2	-5.78	113.10	118.30
2	B	108	LEU	CA-CB-CG	-5.76	102.06	115.30
3	G	151	THR	C-N-CD	-5.62	108.23	120.60
2	F	129	ASP	CB-CG-OD2	5.60	123.34	118.30
4	H	335	TYR	CB-CG-CD2	-5.51	117.69	121.00
3	C	178	ASP	CB-CG-OD1	5.49	123.24	118.30
2	B	72	ASP	CB-CG-OD1	-5.47	113.38	118.30
4	D	350	ASP	CB-CG-OD1	5.45	123.21	118.30
2	F	128	ASP	CB-CG-OD2	-5.33	113.50	118.30
3	G	194	ASP	CB-CG-OD1	-5.33	113.50	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	153	ASP	CB-CG-OD2	5.26	123.04	118.30
2	F	72	ASP	CB-CG-OD2	5.24	123.01	118.30
2	B	129	ASP	CB-CG-OD1	-5.23	113.59	118.30
4	H	323	TYR	CB-CG-CD1	-5.22	117.87	121.00
2	F	52	VAL	CB-CA-C	-5.11	101.69	111.40
4	H	303	ASP	CB-CG-OD1	5.09	122.88	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	H	303	ASP	CA

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	74	0	81	6	0
1	E	74	0	81	8	0
2	B	980	0	951	51	0
2	F	980	0	951	63	0
3	C	702	0	698	50	0
3	G	702	0	698	58	0
4	D	454	0	435	22	1
4	H	454	0	435	25	0
5	D	10	0	0	0	0
5	H	10	0	0	3	0
6	B	16	0	0	1	0
6	C	14	0	0	4	0
6	D	11	0	0	1	0
6	E	2	0	0	0	0
6	F	12	0	0	1	0
6	G	10	0	0	0	0
6	H	15	0	0	4	1
All	All	4520	0	4330	232	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 29.

All (232) 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:F:52:VAL:HB	2:F:106:LEU:HD12	1.32	1.11
3:C:207:TRP:HA	6:C:460:HOH:O	1.54	1.08
3:C:202:LYS:HA	6:C:460:HOH:O	1.68	0.91
3:G:160:LEU:HB2	3:G:161:PRO:HD2	1.56	0.87
4:D:339:ARG:CZ	4:H:342:ARG:HD3	2.03	0.87
3:C:224:THR:HG23	3:C:225:PRO:HD2	1.59	0.85
4:D:339:ARG:NH1	4:H:342:ARG:HD3	1.91	0.85
2:B:83:LEU:H	2:B:83:LEU:HD12	1.44	0.81
2:F:52:VAL:HB	2:F:106:LEU:CD1	2.09	0.80
2:F:53:VAL:HG23	2:F:105:LEU:CD2	2.12	0.79
2:F:53:VAL:HG23	2:F:105:LEU:HD23	1.65	0.79
2:F:35:ASP:OD1	2:F:37:THR:HG22	1.83	0.78
2:F:139:THR:HG22	3:G:157:GLN:HB3	1.64	0.78
1:E:9:VAL:CG1	2:F:23:VAL:HG21	2.15	0.77
3:C:195:SER:HA	3:C:213:VAL:HG12	1.67	0.76
3:G:172:TRP:O	3:G:175:LYS:HB2	1.85	0.76
3:C:160:LEU:HB2	3:C:161:PRO:HD2	1.69	0.74
2:F:71:PHE:O	3:G:154:ARG:HA	1.87	0.74
4:H:331:GLN:NE2	6:H:457:HOH:O	2.17	0.74
3:G:236:ASN:ND2	3:G:236:ASN:H	1.85	0.74
2:F:139:THR:HG22	3:G:157:GLN:CB	2.18	0.72
4:H:329:LEU:N	4:H:329:LEU:HD12	2.04	0.72
4:D:339:ARG:HG3	4:D:339:ARG:HH11	1.55	0.72
3:C:202:LYS:HG3	6:C:460:HOH:O	1.91	0.70
2:B:115:SER:OG	2:B:116:GLN:N	2.21	0.70
6:B:416:HOH:O	3:C:178:ASP:HB2	1.91	0.69
3:C:202:LYS:HD2	3:C:207:TRP:CZ2	2.28	0.69
3:C:195:SER:HA	3:C:213:VAL:CG1	2.22	0.69
2:F:105:LEU:HD11	3:G:238:VAL:HG13	1.75	0.69
4:H:329:LEU:H	4:H:329:LEU:HD12	1.60	0.67
4:D:342:ARG:NE	5:H:500:SO4:O2	2.27	0.66
2:B:66:VAL:O	2:B:83:LEU:HD12	1.94	0.66
2:B:112:ALA:HB3	2:B:114:PHE:HE1	1.60	0.66
3:C:241:THR:O	3:C:245:ASN:ND2	2.28	0.66
2:B:83:LEU:HD12	2:B:83:LEU:N	2.12	0.65
2:B:18:ASN:HB3	3:C:188:VAL:HG12	1.76	0.65
2:F:136:CYS:HB3	3:G:200:VAL:O	1.97	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:326:LYS:HD3	4:H:326:LYS:N	2.11	0.65
2:F:47:ILE:HG12	2:F:51:TRP:O	1.96	0.65
4:D:339:ARG:CG	4:D:339:ARG:HH11	2.10	0.65
1:A:9:VAL:HG12	2:B:23:VAL:HG21	1.78	0.64
3:G:217:SER:O	3:G:219:THR:N	2.30	0.64
1:A:9:VAL:CG1	2:B:23:VAL:HG21	2.27	0.64
2:B:143:LEU:HA	3:C:150:ASN:O	1.98	0.64
3:C:230:ARG:HG3	3:C:230:ARG:O	1.98	0.63
1:E:9:VAL:HG13	2:F:23:VAL:HG21	1.81	0.63
2:B:53:VAL:HG23	2:B:105:LEU:CD2	2.28	0.63
4:H:352:MET:HG3	6:H:435:HOH:O	1.99	0.62
3:C:202:LYS:HD2	3:C:207:TRP:CE2	2.35	0.62
2:F:125:SER:N	2:F:128:ASP:OD2	2.32	0.62
1:E:5:ALA:HB1	2:F:116:GLN:HG2	1.82	0.61
2:F:125:SER:HB3	2:F:128:ASP:OD2	2.00	0.61
2:B:136:CYS:HB3	3:C:200:VAL:O	2.00	0.61
4:D:342:ARG:N	5:H:500:SO4:O4	2.34	0.61
2:B:86:ALA:HB3	2:B:107:LYS:O	2.02	0.60
2:B:71:PHE:O	3:C:154:ARG:HA	2.02	0.60
2:F:52:VAL:HG12	2:F:53:VAL:N	2.16	0.59
3:G:160:LEU:HB2	3:G:161:PRO:CD	2.31	0.59
2:B:112:ALA:HB3	2:B:114:PHE:CE1	2.37	0.59
1:E:9:VAL:HG13	2:F:23:VAL:CG2	2.32	0.59
2:F:30:GLN:O	2:F:30:GLN:HG3	2.02	0.59
3:G:224:THR:HG23	3:G:225:PRO:HD2	1.85	0.58
2:B:53:VAL:HG23	2:B:105:LEU:HD21	1.85	0.58
4:H:345:PHE:CD1	4:H:345:PHE:N	2.70	0.58
2:F:50:ASN:HA	2:F:108:LEU:HD12	1.85	0.57
3:C:185:ALA:HB2	3:C:225:PRO:N	2.20	0.57
3:G:191:CYS:O	3:G:192:MET:O	2.23	0.57
2:B:99:ILE:HG22	2:B:99:ILE:O	2.05	0.57
1:E:5:ALA:CB	2:F:116:GLN:HG2	2.35	0.56
2:F:142:GLY:HA3	3:G:192:MET:O	2.06	0.56
3:G:217:SER:C	3:G:219:THR:H	2.07	0.56
3:C:224:THR:HG23	3:C:225:PRO:CD	2.35	0.55
4:H:322:PHE:CE1	4:H:331:GLN:HB2	2.41	0.55
3:G:234:LEU:O	3:G:237:TRP:HB3	2.06	0.55
2:F:56:ALA:HA	2:F:104:THR:OG1	2.07	0.55
4:H:357:GLY:O	4:H:358:ALA:C	2.44	0.55
2:B:52:VAL:HB	2:B:106:LEU:HB2	1.89	0.55
2:F:62:THR:HG23	2:F:62:THR:O	2.06	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:137:VAL:HA	3:G:158:ALA:O	2.07	0.54
3:C:166:THR:HG22	3:C:167:ASN:N	2.22	0.54
2:B:35:ASP:OD1	2:B:37:THR:N	2.40	0.54
2:B:144:THR:N	3:C:150:ASN:O	2.39	0.54
3:C:175:LYS:NZ	4:H:342:ARG:O	2.40	0.54
3:C:235:VAL:O	3:C:238:VAL:HB	2.08	0.53
3:C:160:LEU:HB2	3:C:161:PRO:CD	2.36	0.53
2:F:99:ILE:HG21	3:G:215:TRP:CD1	2.44	0.53
2:F:95:ASN:HB3	2:F:98:THR:OG1	2.09	0.53
2:B:137:VAL:HA	3:C:158:ALA:O	2.09	0.53
3:C:232:THR:HG22	3:C:233:ALA:N	2.24	0.52
4:H:312:GLY:HA3	6:H:405:HOH:O	2.09	0.52
2:B:95:ASN:OD1	2:B:97:LEU:N	2.41	0.52
4:D:345:PHE:N	4:D:345:PHE:CD1	2.77	0.52
3:C:215:TRP:HB2	4:D:313:PRO:O	2.09	0.52
3:G:184:GLY:O	3:G:185:ALA:HB3	2.08	0.52
2:F:69:GLY:C	2:F:80:ILE:HG22	2.31	0.52
3:G:236:ASN:N	3:G:236:ASN:ND2	2.57	0.52
2:B:56:ALA:HA	2:B:104:THR:OG1	2.10	0.52
2:F:53:VAL:HG23	2:F:105:LEU:HD21	1.90	0.51
2:F:48:ASN:OD1	2:F:50:ASN:N	2.33	0.51
1:E:4:PRO:HB2	1:E:6:ILE:O	2.10	0.51
2:F:23:VAL:O	2:F:26:SER:OG	2.29	0.51
3:G:217:SER:C	3:G:219:THR:N	2.64	0.51
4:D:308:PRO:CB	4:D:309:PRO:HD2	2.40	0.51
4:D:310:TYR:HB3	6:D:447:HOH:O	2.10	0.51
4:H:327:ALA:HB1	4:H:329:LEU:CD1	2.41	0.51
3:C:217:SER:C	3:C:219:THR:H	2.14	0.50
1:E:8:PRO:HA	6:F:434:HOH:O	2.10	0.50
2:F:95:ASN:O	2:F:99:ILE:N	2.40	0.50
2:F:99:ILE:O	2:F:99:ILE:HG22	2.10	0.50
2:F:57:HIS:CD2	4:H:314:CYS:HB3	2.47	0.50
3:C:211:GLY:HA2	3:C:229:ALA:O	2.12	0.49
2:B:53:VAL:HG23	2:B:105:LEU:HD23	1.94	0.49
4:D:301:ARG:O	4:D:302:PRO:C	2.46	0.49
2:F:121:VAL:HG22	2:F:122:CYS:N	2.27	0.49
3:C:224:THR:HG22	6:C:453:HOH:O	2.11	0.49
2:B:65:VAL:HG12	2:B:66:VAL:N	2.27	0.49
3:C:200:VAL:HA	3:C:208:THR:O	2.12	0.49
4:H:321:TYR:HA	4:H:331:GLN:O	2.12	0.49
2:B:95:ASN:HB3	2:B:98:THR:OG1	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:17:VAL:O	2:F:18:ASN:HB2	2.13	0.48
2:B:102:ASP:OD2	3:C:214:SER:OG	2.30	0.48
3:C:163:LEU:N	3:C:163:LEU:HD13	2.28	0.48
3:G:181:ILE:HG23	3:G:228:TYR:HB2	1.95	0.48
4:D:320:ARG:O	4:D:333:PHE:N	2.45	0.48
3:G:230:ARG:HG3	3:G:230:ARG:O	2.11	0.48
3:C:228:TYR:N	3:C:228:TYR:CD1	2.81	0.48
2:B:72:ASP:OD1	2:B:74:GLY:N	2.47	0.48
2:B:142:GLY:O	2:B:143:LEU:C	2.51	0.48
3:G:163:LEU:HD22	3:G:183:ALA:HA	1.96	0.48
2:F:17:VAL:N	3:G:189:SER:O	2.34	0.48
2:F:139:THR:HG22	3:G:157:GLN:CA	2.44	0.48
3:G:191:CYS:HA	4:H:315:LYS:HD2	1.96	0.47
3:G:160:LEU:HD23	3:G:160:LEU:O	2.13	0.47
3:G:236:ASN:H	3:G:236:ASN:HD22	1.59	0.47
3:G:234:LEU:O	3:G:238:VAL:HG23	2.13	0.47
2:F:136:CYS:N	3:G:160:LEU:O	2.30	0.47
2:F:70:GLU:N	2:F:80:ILE:HG22	2.29	0.47
2:B:23:VAL:O	2:B:24:PRO:C	2.52	0.47
2:F:52:VAL:CG1	2:F:53:VAL:N	2.78	0.47
3:G:182:CYS:HA	3:G:226:GLY:O	2.15	0.47
3:G:165:ASN:O	3:G:169:LYS:HG3	2.14	0.47
3:C:216:GLY:O	3:C:217:SER:C	2.53	0.47
2:B:34:GLN:HA	2:B:39:PHE:O	2.15	0.47
3:G:160:LEU:CB	3:G:161:PRO:CD	2.88	0.47
2:B:83:LEU:CD1	2:B:83:LEU:N	2.72	0.47
3:C:163:LEU:HA	3:C:163:LEU:HD12	1.49	0.47
3:G:245:ASN:N	3:G:245:ASN:ND2	2.64	0.46
2:F:70:GLU:N	2:F:80:ILE:CG2	2.78	0.46
4:H:341:LYS:HE2	6:H:477:HOH:O	2.15	0.46
2:F:26:SER:C	2:F:28:PRO:HD3	2.35	0.46
4:H:326:LYS:CD	4:H:326:LYS:N	2.77	0.46
2:F:47:ILE:HD11	2:F:51:TRP:HB3	1.96	0.46
3:C:201:CYS:SG	3:C:210:VAL:HG21	2.55	0.46
2:B:108:LEU:HD23	2:B:108:LEU:HA	1.28	0.46
2:F:35:ASP:O	2:F:38:GLY:N	2.43	0.45
2:F:94:TYR:HB2	2:F:101:ASN:O	2.16	0.45
2:B:66:VAL:CG1	2:B:67:VAL:N	2.79	0.45
4:D:354:THR:OG1	3:G:174:THR:HG23	2.16	0.45
3:G:195:SER:HA	3:G:213:VAL:HG12	1.98	0.45
4:D:323:TYR:CE2	4:D:325:ALA:HA	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:73:GLN:HG3	2:F:141:TRP:NE1	2.32	0.45
3:G:224:THR:HG22	3:G:225:PRO:O	2.17	0.45
3:G:192:MET:O	3:G:194:ASP:N	2.49	0.45
2:B:51:TRP:CD2	3:C:242:LEU:CD2	3.00	0.45
2:B:122:CYS:HB2	3:C:207:TRP:O	2.17	0.45
2:F:139:THR:CG2	3:G:157:GLN:HB3	2.41	0.45
3:G:242:LEU:HA	3:G:242:LEU:HD23	1.84	0.44
2:F:82:LYS:C	2:F:83:LEU:HG	2.36	0.44
3:G:175:LYS:HD2	3:G:175:LYS:HA	1.61	0.44
3:C:219:THR:HG23	3:C:219:THR:O	2.16	0.44
3:C:165:ASN:O	3:C:169:LYS:HG3	2.18	0.44
2:F:35:ASP:OD2	2:F:39:PHE:HB3	2.17	0.44
3:C:224:THR:HG22	3:C:224:THR:O	2.15	0.44
2:F:64:ASP:O	2:F:85:ILE:HD12	2.17	0.44
2:F:134:THR:HG22	2:F:136:CYS:SG	2.57	0.44
3:C:224:THR:HA	3:C:225:PRO:HD3	1.67	0.44
3:G:219:THR:O	3:G:220:CYS:HB2	2.18	0.44
2:B:39:PHE:CE2	4:D:319:ILE:HD11	2.53	0.44
3:G:194:ASP:O	3:G:195:SER:C	2.55	0.44
2:B:103:ILE:HG21	3:C:234:LEU:HG	1.99	0.44
4:H:304:PHE:CD1	4:H:342:ARG:HB3	2.53	0.44
3:G:172:TRP:CB	3:G:176:ILE:HD11	2.48	0.44
3:G:230:ARG:CG	3:G:230:ARG:O	2.64	0.44
2:F:41:PHE:CD1	2:F:41:PHE:C	2.90	0.44
2:B:141:TRP:CZ2	3:C:155:LEU:HD13	2.53	0.43
3:G:163:LEU:HA	3:G:163:LEU:HD12	1.78	0.43
4:H:327:ALA:HB1	4:H:329:LEU:HD11	1.99	0.43
1:A:9:VAL:CG1	2:B:23:VAL:CG2	2.97	0.43
2:F:18:ASN:HB3	3:G:188:VAL:HG12	1.99	0.43
1:A:8:PRO:CA	2:B:26:SER:HB2	2.48	0.43
2:B:66:VAL:HG12	2:B:67:VAL:N	2.31	0.43
2:F:72:ASP:OD1	2:F:74:GLY:N	2.47	0.43
1:A:8:PRO:HA	2:B:26:SER:CB	2.48	0.43
1:E:8:PRO:HB3	2:F:27:TRP:CZ2	2.53	0.43
4:H:320:ARG:NH1	4:H:344:ASN:OD1	2.49	0.43
2:F:33:LEU:HD23	2:F:33:LEU:N	2.33	0.43
2:F:124:PRO:CG	3:G:231:VAL:HG12	2.48	0.42
2:F:142:GLY:CA	3:G:192:MET:O	2.66	0.42
4:H:326:LYS:HD3	4:H:326:LYS:H	1.82	0.42
2:B:95:ASN:O	2:B:99:ILE:N	2.47	0.42
2:B:108:LEU:HD23	2:B:108:LEU:N	2.25	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:184:GLY:C	3:G:186:SER:H	2.21	0.42
3:G:209:LEU:HG	3:G:231:VAL:HG21	2.00	0.42
2:B:41:PHE:HB2	4:D:317:ARG:O	2.19	0.42
2:B:60:VAL:HG12	2:B:61:THR:N	2.34	0.42
3:C:231:VAL:O	3:C:232:THR:C	2.57	0.42
4:D:320:ARG:NH1	4:D:344:ASN:OD1	2.52	0.42
3:G:155:LEU:HG	3:G:156:GLN:N	2.35	0.41
3:C:154:ARG:O	3:C:155:LEU:C	2.59	0.41
3:C:211:GLY:HA2	3:C:231:VAL:HG23	2.01	0.41
2:B:134:THR:HG22	2:B:135:THR:N	2.35	0.41
2:B:86:ALA:HB2	2:B:109:SER:HA	2.01	0.41
3:G:151:THR:HA	3:G:152:PRO:HD3	1.76	0.41
4:D:322:PHE:CE1	4:D:331:GLN:HB2	2.56	0.41
2:B:80:ILE:O	2:B:80:ILE:HG12	2.19	0.41
2:B:106:LEU:HD23	2:B:106:LEU:HA	1.82	0.41
4:H:304:PHE:CG	4:H:342:ARG:HB3	2.55	0.41
4:D:342:ARG:HB2	5:H:500:SO4:O4	2.21	0.41
3:G:191:CYS:O	3:G:192:MET:C	2.59	0.41
4:D:343:ASN:O	4:D:344:ASN:HB2	2.20	0.41
3:C:177:LYS:HA	3:C:177:LYS:HD2	1.77	0.41
3:C:172:TRP:CB	3:C:176:ILE:HD11	2.51	0.41
3:C:234:LEU:HD12	3:C:234:LEU:HA	1.72	0.41
1:A:10:LEU:HD23	2:B:20:GLU:OE1	2.21	0.41
4:D:339:ARG:CG	4:D:339:ARG:NH1	2.77	0.40
4:D:339:ARG:NH2	4:H:341:LYS:HA	2.35	0.40
2:F:95:ASN:ND2	2:F:96:SER:N	2.68	0.40
2:F:139:THR:HG22	3:G:157:GLN:HA	2.02	0.40
3:G:193:GLY:N	4:H:317:ARG:HG3	2.36	0.40
3:G:191:CYS:C	3:G:192:MET:O	2.60	0.40
2:F:51:TRP:CD2	3:G:242:LEU:CD2	3.04	0.40
2:F:35:ASP:C	2:F:35:ASP:OD1	2.60	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)
4:D:331:GLN:NE2	6:H:457:HOH:O[5_564]	2.19	0.01

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	9/13 (69%)	8 (89%)	0	1 (11%)	0 1
1	E	9/13 (69%)	8 (89%)	1 (11%)	0	100 100
2	B	129/131 (98%)	115 (89%)	9 (7%)	5 (4%)	4 12
2	F	129/131 (98%)	109 (84%)	13 (10%)	7 (5%)	2 7
3	C	95/97 (98%)	84 (88%)	10 (10%)	1 (1%)	17 50
3	G	95/97 (98%)	79 (83%)	11 (12%)	5 (5%)	2 7
4	D	56/58 (97%)	53 (95%)	2 (4%)	1 (2%)	11 34
4	H	56/58 (97%)	48 (86%)	7 (12%)	1 (2%)	11 34
All	All	578/598 (97%)	504 (87%)	53 (9%)	21 (4%)	4 14

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	198	PRO
3	G	192	MET
1	A	10	LEU
2	B	76	SER
2	B	99	ILE
2	B	143	LEU
2	F	76	SER
3	G	193	GLY
2	B	62	THR
2	B	71	PHE
2	F	126	ALA
2	F	143	LEU
3	G	152	PRO
3	G	218	SER
2	F	36	LYS
2	F	71	PHE
3	G	198	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	37	THR
2	F	99	ILE
4	H	313	PRO
4	D	302	PRO

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	9/10 (90%)	7 (78%)	2 (22%)	1 3
1	E	9/10 (90%)	7 (78%)	2 (22%)	1 3
2	B	109/109 (100%)	91 (84%)	18 (16%)	3 8
2	F	109/109 (100%)	89 (82%)	20 (18%)	2 6
3	C	77/77 (100%)	58 (75%)	19 (25%)	1 2
3	G	77/77 (100%)	61 (79%)	16 (21%)	1 4
4	D	46/46 (100%)	38 (83%)	8 (17%)	2 7
4	H	46/46 (100%)	38 (83%)	8 (17%)	2 7
All	All	482/484 (100%)	389 (81%)	93 (19%)	2 5

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	10	LEU
2	B	18	ASN
2	B	36	LYS
2	B	37	THR
2	B	53	VAL
2	B	61	THR
2	B	70	GLU
2	B	75	SER
2	B	76	SER
2	B	77	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	80	ILE
2	B	83	LEU
2	B	91	ASN
2	B	92	SER
2	B	96	SER
2	B	101	ASN
2	B	119	SER
2	B	144	THR
2	B	145	ARG
3	C	151	THR
3	C	160	LEU
3	C	163	LEU
3	C	167	ASN
3	C	175	LYS
3	C	177	LYS
3	C	178	ASP
3	C	192	MET
3	C	202	LYS
3	C	203	LYS
3	C	208	THR
3	C	214	SER
3	C	219	THR
3	C	224	THR
3	C	230	ARG
3	C	232	THR
3	C	234	LEU
3	C	235	VAL
3	C	245	ASN
4	D	301	ARG
4	D	303	ASP
4	D	306	LEU
4	D	326	LYS
4	D	329	LEU
4	D	331	GLN
4	D	339	ARG
4	D	347	SER
1	E	3	VAL
1	E	9	VAL
2	F	26	SER
2	F	32	SER
2	F	36	LYS
2	F	53	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	61	THR
2	F	62	THR
2	F	77	SER
2	F	81	GLN
2	F	87	LYS
2	F	92	SER
2	F	97	LEU
2	F	106	LEU
2	F	107	LYS
2	F	108	LEU
2	F	113	SER
2	F	115	SER
2	F	119	SER
2	F	125	SER
2	F	127	SER
2	F	145	ARG
3	G	151	THR
3	G	160	LEU
3	G	163	LEU
3	G	165	ASN
3	G	167	ASN
3	G	175	LYS
3	G	177	LYS
3	G	192	MET
3	G	202	LYS
3	G	208	THR
3	G	214	SER
3	G	219	THR
3	G	223	SER
3	G	230	ARG
3	G	234	LEU
3	G	236	ASN
4	H	301	ARG
4	H	303	ASP
4	H	326	LYS
4	H	329	LEU
4	H	331	GLN
4	H	342	ARG
4	H	346	LYS
4	H	347	SER

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

Mol	Chain	Res	Type
2	B	95	ASN
3	C	165	ASN
3	G	236	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

4 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	$\#\|Z\| > 2$
5	SO4	D	600	-	4,4,4	1.28	1 (25%)	6,6,6	0.31	0
5	SO4	D	800	-	4,4,4	1.10	1 (25%)	6,6,6	0.28	0
5	SO4	H	500	-	4,4,4	1.49	1 (25%)	6,6,6	0.15	0
5	SO4	H	700	-	4,4,4	1.87	3 (75%)	6,6,6	0.22	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	SO4	D	600	-	-	0/0/0/0	0/0/0/0
5	SO4	D	800	-	-	0/0/0/0	0/0/0/0
5	SO4	H	500	-	-	0/0/0/0	0/0/0/0
5	SO4	H	700	-	-	0/0/0/0	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	700	SO4	O1-S	-2.06	1.40	1.47
5	H	700	SO4	O3-S	2.07	1.54	1.47
5	D	800	SO4	O4-S	2.16	1.55	1.47
5	H	700	SO4	O2-S	2.23	1.54	1.47
5	D	600	SO4	O4-S	2.49	1.56	1.47
5	H	500	SO4	O1-S	2.60	1.56	1.47

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 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	500	SO4	3	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, 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	11/13 (84%)	-0.21	1 (9%) 11 6	35, 41, 74, 92	2 (18%)
1	E	11/13 (84%)	-0.54	0 100 100	32, 46, 72, 75	2 (18%)
2	B	128/131 (97%)	-0.66	0 100 100	20, 42, 65, 92	21 (16%)
2	F	129/131 (98%)	-0.62	2 (1%) 74 66	20, 41, 66, 100	19 (14%)
3	C	96/97 (98%)	-0.61	2 (2%) 67 56	15, 40, 69, 90	12 (12%)
3	G	95/97 (97%)	-0.56	1 (1%) 82 74	22, 40, 69, 76	11 (11%)
4	D	58/58 (100%)	-0.87	0 100 100	17, 29, 50, 60	7 (12%)
4	H	58/58 (100%)	-0.94	0 100 100	16, 30, 55, 72	6 (10%)
All	All	586/598 (97%)	-0.67	6 (1%) 84 77	15, 39, 69, 100	80 (13%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	150	ASN	4.3
1	A	11	SER	4.0
3	G	243	ALA	2.7
2	F	74	GLY	2.5
2	F	75	SER	2.2
3	C	166	THR	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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
5	SO4	D	600	5/5	0.95	0.28	13.74	80,80,80,80	0
5	SO4	H	500	5/5	0.87	0.32	12.97	80,80,80,80	0
5	SO4	D	800	5/5	0.93	0.44	11.94	80,80,80,80	5
5	SO4	H	700	5/5	0.89	0.41	8.45	80,80,80,80	5

6.5 Other polymers

There are no such residues in this entry.