Full wwPDB X-ray Structure Validation Report (i)

Oct 26, 2023 – 01:21 AM EDT

PDB ID	:	3GIS
Title	:	Crystal Structure of Na-free Thrombin in Complex with Thrombomodulin
Authors	:	Adams, T.E.; Huntington, J.A.
Deposited on	:	2009-03-06
Resolution	:	2.40 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 (1)) were used in the production of this report:

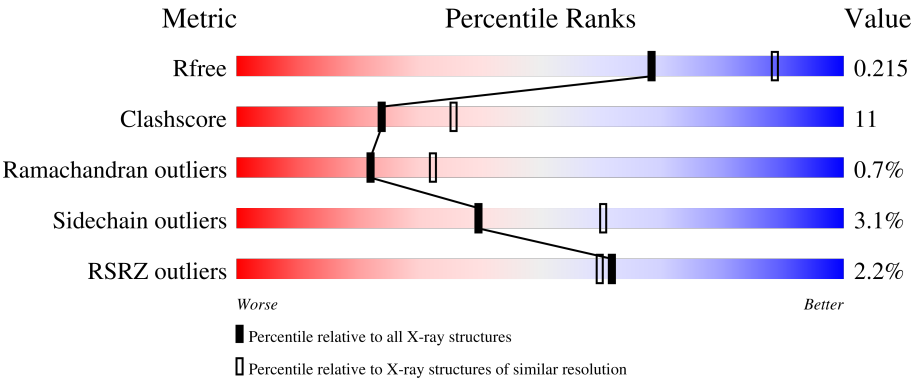
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.40 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.



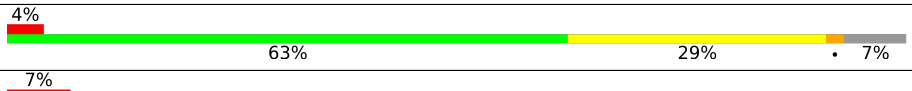
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	A	49	80% 14% 6%
1	C	49	2% 80% 12% • 6%
1	E	49	2% 69% 22% • 6%
2	B	259	78% 19% • •
2	D	259	73% 21% • •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	259	
3	X	121	
3	Y	121	
3	Z	121	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 10192 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 Prothrombin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	46	Total	C	N	O	S	0	0	0
			378	236	63	78	1			
1	C	46	Total	C	N	O	S	0	0	0
			374	234	63	76	1			
1	E	46	Total	C	N	O	S	0	0	0
			367	231	59	76	1			

- Molecule 2 is a protein called Prothrombin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	252	Total	C	N	O	S	0	0	0
			2023	1291	358	360	14			
2	D	252	Total	C	N	O	S	0	0	0
			2016	1287	357	358	14			
2	F	248	Total	C	N	O	S	0	0	0
			1989	1271	350	354	14			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	195	ALA	SER	engineered mutation	UNP P00734
D	195	ALA	SER	engineered mutation	UNP P00734
F	195	ALA	SER	engineered mutation	UNP P00734

- Molecule 3 is a protein called Thrombomodulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	X	113	Total	C	N	O	S	0	0	0
			803	490	131	164	18			
3	Y	113	Total	C	N	O	S	0	0	0
			795	491	129	157	18			

Continued on next page...

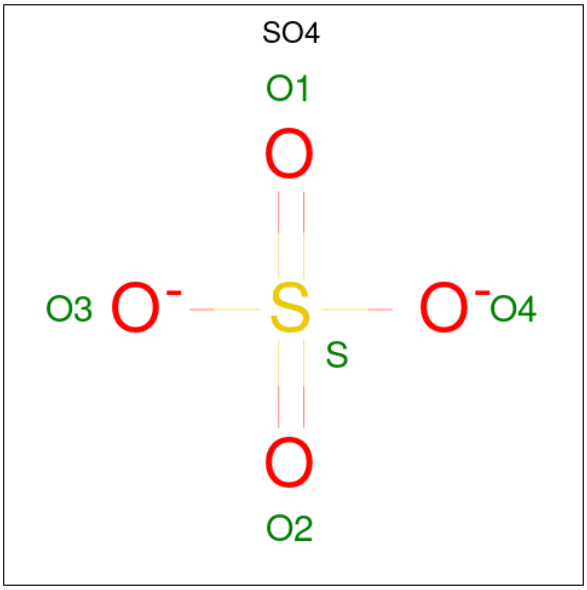
Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	Z	112	Total	C	N	O	S	0	0	0
			794	485	127	164	18			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	388	LEU	MET	engineered mutation	UNP P07204
X	456	GLY	ARG	engineered mutation	UNP P07204
X	457	GLN	HIS	engineered mutation	UNP P07204
Y	388	LEU	MET	engineered mutation	UNP P07204
Y	456	GLY	ARG	engineered mutation	UNP P07204
Y	457	GLN	HIS	engineered mutation	UNP P07204
Z	388	LEU	MET	engineered mutation	UNP P07204
Z	456	GLY	ARG	engineered mutation	UNP P07204
Z	457	GLN	HIS	engineered mutation	UNP P07204

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



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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	E	1	Total O S 5 4 1	0	0
4	F	1	Total O S 5 4 1	0	0
4	F	1	Total O S 5 4 1	0	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	X	1	Total Ca 1 1	0	0
5	Y	1	Total Ca 1 1	0	0
5	Z	1	Total Ca 1 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	31	Total O 31 31	0	0
6	B	152	Total O 152 152	0	0

Continued on next page...

Continued from previous page...

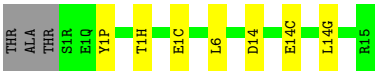
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	37	Total O 37 37	0	0
6	D	136	Total O 136 136	0	0
6	E	19	Total O 19 19	0	0
6	F	105	Total O 105 105	0	0
6	X	45	Total O 45 45	0	0
6	Y	32	Total O 32 32	0	0
6	Z	18	Total O 18 18	0	0

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: Prothrombin

Chain A:

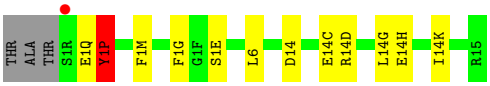


• Molecule 1: Prothrombin

Chain C:

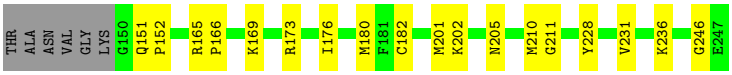
• Molecule 1: Prothrombin

Chain E:



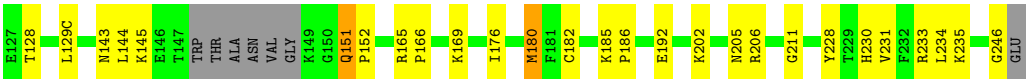
• Molecule 2: Prothrombin

Chain B:

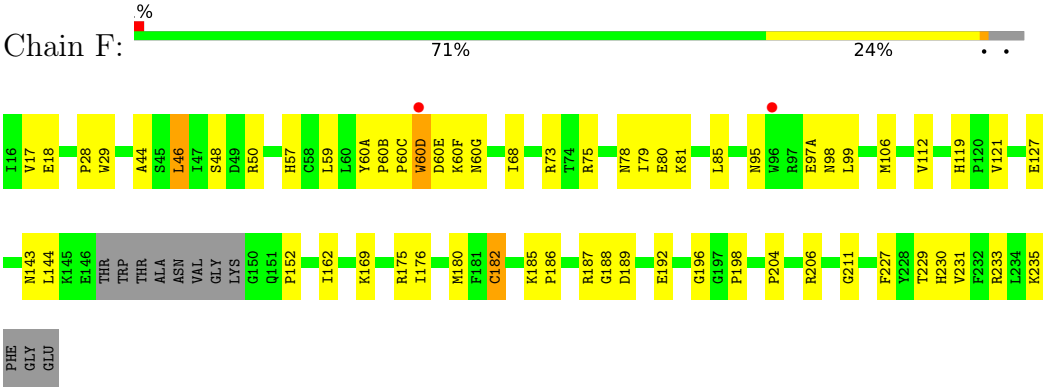


• Molecule 2: Prothrombin

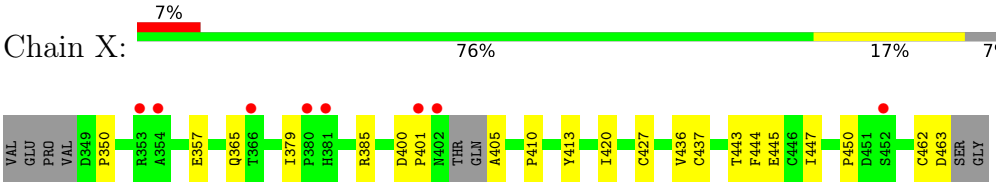
Chain D:



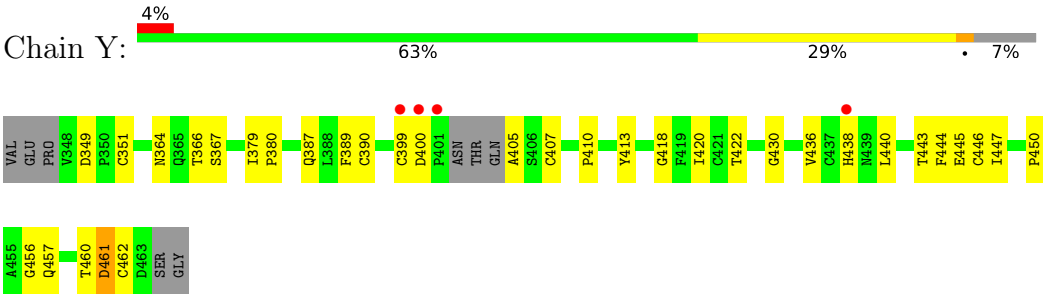
• Molecule 2: Prothrombin



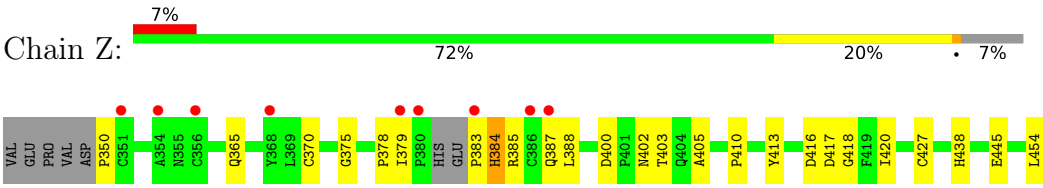
• Molecule 3: Thrombomodulin



• Molecule 3: Thrombomodulin



• Molecule 3: Thrombomodulin



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	66.25Å 100.34Å 229.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.40 40.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	94.5 (40.00-2.40) 93.6 (40.00-2.40)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.57 (at 2.39Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.211 , 0.259 0.215 , 0.215	Depositor DCC
R_{free} test set	2933 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	23.5	Xtriage
Anisotropy	0.341	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 39.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	10192	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.57% 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

5.1 Standard geometry

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

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	0.39	0/385	0.60	0/513
1	C	0.40	0/381	0.64	0/508
1	E	0.39	0/374	0.69	1/500 (0.2%)
2	B	0.34	0/2075	0.63	0/2804
2	D	0.36	0/2068	0.63	1/2796 (0.0%)
2	F	0.36	0/2040	0.64	0/2759
3	X	0.36	0/821	0.60	0/1121
3	Y	0.37	0/815	0.61	0/1114
3	Z	0.33	0/812	0.60	0/1109
All	All	0.36	0/9771	0.63	2/13224 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	79	ILE	N-CA-C	-5.94	94.96	111.00
1	E	1(P)	TYR	N-CA-C	5.04	124.62	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	378	0	357	5	0
1	C	374	0	353	7	0
1	E	367	0	337	12	0
2	B	2023	0	1981	44	0
2	D	2016	0	1974	48	0
2	F	1989	0	1952	48	0
3	X	803	0	680	17	0
3	Y	795	0	665	29	0
3	Z	794	0	668	19	0
4	A	10	0	0	0	0
4	B	25	0	0	2	0
4	C	5	0	0	0	0
4	D	20	0	0	0	0
4	E	5	0	0	1	0
4	F	10	0	0	0	0
5	X	1	0	0	0	0
5	Y	1	0	0	0	0
5	Z	1	0	0	0	0
6	A	31	0	0	0	0
6	B	152	0	0	4	0
6	C	37	0	0	1	0
6	D	136	0	0	2	0
6	E	19	0	0	0	0
6	F	105	0	0	1	0
6	X	45	0	0	1	0
6	Y	32	0	0	1	0
6	Z	18	0	0	0	0
All	All	10192	0	8967	207	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 11.

All (207) 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:77(A):ARG:HH12	3:Y:422:THR:HG21	1.14	1.08
3:Y:454:LEU:HD23	3:Y:454:LEU:H	1.39	0.85
1:A:1(H):THR:HB	2:B:246:GLY:HA3	1.63	0.81
2:F:187:ARG:HG2	2:F:187:ARG:HH11	1.49	0.77
2:B:143:ASN:HB3	6:B:413:HOH:O	1.86	0.75
2:D:24:ILE:HD11	3:X:420:ILE:HD13	1.67	0.74
2:F:95:ASN:HD21	2:F:98:ASN:H	1.35	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:169:LYS:HA	2:B:176:ILE:HD12	1.70	0.73
2:F:60(B):PRO:HB2	2:F:60(C):PRO:HD3	1.69	0.73
2:B:151:GLN:HG2	6:B:434:HOH:O	1.90	0.71
1:C:14(D):ARG:HG3	6:C:130:HOH:O	1.90	0.71
2:D:46:LEU:HD22	2:D:48:SER:O	1.91	0.69
2:D:126:ARG:HB2	2:D:126:ARG:HH21	1.57	0.69
2:D:59:LEU:HD21	2:D:106:MET:HE3	1.74	0.68
1:C:14(D):ARG:HG3	1:C:14(D):ARG:HH11	1.58	0.68
2:D:77(A):ARG:NH1	3:Y:422:THR:HG21	1.98	0.68
2:B:78:ASN:C	2:B:79:ILE:HD12	2.15	0.67
2:B:46:LEU:HD22	2:B:48:SER:O	1.96	0.66
3:Z:378:PRO:HB3	3:Z:383:PRO:HB3	1.77	0.66
2:F:95:ASN:HD21	2:F:97(A):GLU:HB3	1.60	0.65
3:Y:436:VAL:HB	3:Y:447:ILE:HG13	1.79	0.65
3:X:357:GLU:OE2	3:X:385:ARG:HD2	1.97	0.64
1:C:1(H):THR:HB	2:D:246:GLY:HA3	1.80	0.63
2:F:78:ASN:C	2:F:79:ILE:HD12	2.19	0.63
2:F:169:LYS:HA	2:F:176:ILE:HD12	1.80	0.63
2:B:50:ARG:HH11	2:B:50:ARG:HB3	1.63	0.62
3:Z:410:PRO:HG2	3:Z:413:TYR:CD1	2.36	0.61
3:X:450:PRO:HB3	3:Z:427:CYS:HB3	1.81	0.61
2:F:187:ARG:HG2	2:F:187:ARG:NH1	2.16	0.61
2:F:46:LEU:HD22	2:F:48:SER:O	2.01	0.61
2:F:95:ASN:ND2	2:F:98:ASN:H	1.98	0.61
2:F:59:LEU:HD21	2:F:106:MET:HE3	1.83	0.60
1:E:1(G):PHE:HD1	2:F:242:ILE:HD13	1.66	0.60
2:B:101:ARG:HD3	4:B:2:SO4:O3	2.01	0.60
3:Y:366:THR:O	3:Y:366:THR:HG22	2.02	0.60
2:D:64:LEU:HD12	2:D:64:LEU:H	1.66	0.59
3:Y:450:PRO:C	3:Y:452:SER:H	2.04	0.59
2:F:17:VAL:HG22	2:F:144:LEU:O	2.02	0.59
2:B:64:LEU:HD23	2:B:64:LEU:N	2.18	0.58
2:D:71:HIS:CE1	3:X:420:ILE:HD11	2.39	0.58
2:B:236:LYS:HB2	6:B:385:HOH:O	2.03	0.57
2:B:60(B):PRO:HB2	2:B:60(C):PRO:HD3	1.86	0.57
2:D:128:THR:HG23	2:D:129(C):LEU:HD22	1.87	0.57
3:Z:383:PRO:C	3:Z:385:ARG:H	2.07	0.57
2:B:77(A):ARG:O	2:B:78:ASN:HB2	2.05	0.56
2:F:60(A):TYR:CE2	2:F:60(C):PRO:HB2	2.40	0.56
3:Y:389:PHE:O	3:Y:390:CYS:HB3	2.06	0.56
3:Y:461:ASP:CG	3:Y:462:CYS:H	2.09	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:350:PRO:HG3	3:X:365:GLN:O	2.05	0.56
2:F:130:LEU:HD12	2:F:162:ILE:HD13	1.89	0.55
3:X:410:PRO:HG2	3:X:413:TYR:CD1	2.41	0.55
3:Z:375:GLY:O	3:Z:388:LEU:HD12	2.07	0.55
2:D:98:ASN:N	2:D:98:ASN:HD22	2.06	0.53
1:E:1(E):SER:HB2	4:E:16:SO4:O2	2.08	0.53
2:F:130:LEU:HD12	2:F:162:ILE:CD1	2.38	0.53
1:E:14(D):ARG:O	1:E:14(H):GLU:HG3	2.09	0.52
2:D:103:ILE:HG21	2:D:234:LEU:HD13	1.92	0.52
2:F:17:VAL:O	2:F:188:GLY:HA2	2.09	0.52
3:Z:383:PRO:C	3:Z:385:ARG:N	2.63	0.52
2:F:75:ARG:HB2	3:Z:417:ASP:OD1	2.11	0.51
3:X:445:GLU:OE2	3:X:447:ILE:HD11	2.11	0.51
2:D:98:ASN:HD22	2:D:98:ASN:H	1.59	0.51
2:B:173:ARG:HG2	6:B:415:HOH:O	2.11	0.50
2:D:85:LEU:HD11	2:D:106:MET:HE1	1.93	0.50
2:F:73:ARG:HD3	2:F:152:PRO:O	2.12	0.50
2:D:95:ASN:OD1	2:D:97:ARG:HB2	2.10	0.50
2:D:144:LEU:HD21	2:D:152:PRO:HB3	1.94	0.50
3:Y:440:LEU:HD11	3:Y:445:GLU:HG3	1.94	0.50
2:D:31:VAL:HB	2:D:44:ALA:HB3	1.93	0.49
3:Y:400:ASP:O	3:Y:405:ALA:HB3	2.13	0.49
2:D:211:GLY:HA2	2:D:231:VAL:HG23	1.94	0.49
2:F:143:ASN:ND2	2:F:192:GLU:HB3	2.27	0.49
1:C:14(D):ARG:HG3	1:C:14(D):ARG:NH1	2.27	0.49
2:F:60(A):TYR:HE2	2:F:60(C):PRO:HB2	1.77	0.49
3:Y:410:PRO:HG2	3:Y:413:TYR:CD1	2.47	0.49
2:B:50:ARG:HH11	2:B:50:ARG:CB	2.26	0.48
1:E:1(Q):GLU:O	1:E:1(P):TYR:CB	2.61	0.48
2:B:31:VAL:HG11	2:B:66:VAL:HG13	1.95	0.48
2:F:60(E):ASP:O	2:F:60(F):LYS:HG3	2.12	0.48
3:Y:349:ASP:O	3:Y:351:CYS:N	2.47	0.48
3:X:405:ALA:N	6:X:554:HOH:O	2.46	0.48
2:D:230:HIS:CG	2:D:233:ARG:HG3	2.49	0.48
2:B:78:ASN:O	2:B:79:ILE:HD12	2.13	0.47
2:B:64:LEU:HD23	2:B:64:LEU:H	1.79	0.47
2:D:85:LEU:HD11	2:D:106:MET:CE	2.44	0.47
2:D:29:TRP:O	2:D:45:SER:HA	2.14	0.47
3:Y:454:LEU:H	3:Y:454:LEU:CD2	2.17	0.47
3:X:400:ASP:OD1	3:X:401:PRO:HD2	2.14	0.47
2:B:73:ARG:HD3	2:B:152:PRO:O	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1(H):THR:CB	2:B:246:GLY:HA3	2.41	0.47
3:X:379:ILE:HD12	3:X:385:ARG:CB	2.45	0.47
2:B:31:VAL:HB	2:B:44:ALA:HB3	1.96	0.47
2:B:50:ARG:HB3	2:B:50:ARG:NH1	2.29	0.47
2:F:68:ILE:HD12	2:F:112:VAL:HG11	1.97	0.47
2:F:233:ARG:HH21	2:F:233:ARG:HG3	1.79	0.47
2:F:185:LYS:CG	2:F:186:PRO:HD2	2.45	0.47
3:X:379:ILE:HD12	3:X:385:ARG:HB2	1.96	0.47
3:Y:447:ILE:HA	3:Y:456:GLY:HA3	1.96	0.47
2:D:28:PRO:HB2	2:D:119:HIS:HB3	1.97	0.47
3:Z:350:PRO:HG3	3:Z:365:GLN:O	2.15	0.46
2:F:59:LEU:CD2	2:F:106:MET:HE3	2.44	0.46
3:X:443:THR:OG1	3:X:444:PHE:N	2.48	0.46
3:Z:400:ASP:OD2	3:Z:402:ASN:HB2	2.16	0.46
2:B:79:ILE:CD1	3:Y:418:GLY:HA3	2.45	0.46
3:Z:403:THR:HG22	3:Z:405:ALA:HB3	1.96	0.46
3:Z:438:HIS:HB3	3:Z:445:GLU:HB3	1.98	0.46
3:Y:349:ASP:OD1	3:Y:351:CYS:HB2	2.16	0.46
2:F:230:HIS:CE1	2:F:233:ARG:HG2	2.51	0.45
3:Z:384:HIS:O	3:Z:384:HIS:ND1	2.49	0.45
2:B:79:ILE:HD11	3:Y:418:GLY:CA	2.45	0.45
2:B:202:LYS:HE2	2:B:205:ASN:OD1	2.17	0.45
2:F:18:GLU:HG3	2:F:187:ARG:HB2	1.97	0.45
2:F:57:HIS:CD2	2:F:60(D):TRP:HZ3	2.33	0.45
2:F:28:PRO:HB2	2:F:119:HIS:HB3	1.98	0.45
3:Y:430:GLY:HA2	6:Y:92:HOH:O	2.15	0.45
2:F:185:LYS:HG2	2:F:186:PRO:HD2	1.99	0.45
2:F:60(A):TYR:CE2	2:F:60(D):TRP:CE2	3.04	0.45
2:B:201:MET:SD	2:B:210:MET:HG3	2.57	0.45
1:E:14:ASP:OD1	1:E:14(C):GLU:HB2	2.17	0.45
2:B:211:GLY:HA2	2:B:231:VAL:HG23	1.99	0.45
2:D:17:VAL:HG22	2:D:144:LEU:O	2.17	0.45
1:E:1(Q):GLU:HA	6:F:556:HOH:O	2.17	0.45
2:B:95:ASN:ND2	2:B:97(A):GLU:HG2	2.32	0.44
2:D:64:LEU:HD12	2:D:64:LEU:N	2.30	0.44
1:E:1(G):PHE:CD1	2:F:242:ILE:HD13	2.48	0.44
2:F:29:TRP:CG	2:F:121:VAL:HB	2.52	0.44
3:Y:364:ASN:ND2	3:Y:367:SER:OG	2.50	0.44
2:B:29:TRP:CG	2:B:121:VAL:HB	2.52	0.44
2:D:202:LYS:HE2	2:D:205:ASN:OD1	2.18	0.44
2:F:79:ILE:HD12	2:F:79:ILE:N	2.33	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:49:ASP:O	2:B:111:PRO:HA	2.17	0.44
2:D:16:ILE:N	6:D:312:HOH:O	2.51	0.44
2:F:85:LEU:HD22	2:F:106:MET:HB3	2.00	0.44
1:A:14:ASP:HB2	2:B:26:MET:HE3	2.00	0.44
3:Y:457:GLN:HG3	3:Y:460:THR:OG1	2.18	0.44
1:C:1:CYS:O	2:D:206:ARG:HD3	2.18	0.44
2:F:182:CYS:HB3	2:F:227:PHE:CE2	2.53	0.44
1:C:1(K):ASN:HD21	1:C:1(I):ARG:NH1	2.16	0.43
3:Y:399:CYS:HA	3:Y:407:CYS:HA	1.99	0.43
2:B:64:LEU:N	2:B:64:LEU:CD2	2.81	0.43
2:D:143:ASN:ND2	2:D:192:GLU:HB3	2.33	0.43
2:F:211:GLY:HA2	2:F:229:THR:O	2.18	0.43
2:D:24:ILE:HD11	3:X:420:ILE:CD1	2.43	0.43
2:D:169:LYS:HA	2:D:176:ILE:HD12	1.99	0.43
2:D:180:MET:HA	2:D:228:TYR:O	2.19	0.43
3:Y:450:PRO:C	3:Y:452:SER:N	2.70	0.43
2:B:173:ARG:HB3	2:B:173:ARG:NH1	2.33	0.43
2:D:71:HIS:CE1	3:X:420:ILE:CD1	3.01	0.43
3:Y:379:ILE:HD11	3:Y:387:GLN:HB3	2.00	0.43
2:D:41:LEU:CD2	2:D:64:LEU:HD23	2.49	0.43
2:D:151:GLN:H	2:D:151:GLN:HG2	1.49	0.43
2:F:44:ALA:HA	2:F:196:GLY:O	2.19	0.43
1:E:1(Q):GLU:O	1:E:1(P):TYR:HB3	2.19	0.43
2:B:85:LEU:HD11	2:B:106:MET:HE1	2.01	0.42
3:Z:403:THR:C	3:Z:405:ALA:H	2.22	0.42
2:D:85:LEU:HD22	2:D:106:MET:HB3	2.01	0.42
2:D:144:LEU:O	2:D:145:LYS:HG2	2.19	0.42
2:B:146:GLU:O	2:B:147:THR:CB	2.67	0.42
1:C:1(M):PHE:CE2	2:D:235:LYS:HE2	2.54	0.42
1:A:1(P):TYR:HE2	1:A:1(C):GLU:HG2	1.84	0.42
3:Z:403:THR:HG22	3:Z:405:ALA:H	1.85	0.42
2:D:41:LEU:CD1	2:D:60(F):LYS:HE3	2.49	0.42
2:D:50:ARG:HD2	6:D:442:HOH:O	2.18	0.42
1:E:1(P):TYR:HB2	2:F:206:ARG:NE	2.34	0.42
3:Z:379:ILE:HG12	3:Z:387:GLN:HG2	2.01	0.42
2:B:79:ILE:HD12	2:B:79:ILE:N	2.35	0.42
2:D:41:LEU:HD23	2:D:64:LEU:HD23	2.02	0.42
3:Y:418:GLY:O	3:Y:420:ILE:HG23	2.20	0.42
2:B:79:ILE:HD11	3:Y:418:GLY:HA3	2.02	0.42
3:Z:370:CYS:SG	3:Z:384:HIS:HA	2.60	0.42
2:B:151:GLN:HB3	2:B:152:PRO:HD2	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1(M):PHE:CD2	2:F:235:LYS:HE2	2.55	0.42
3:Z:418:GLY:O	3:Z:420:ILE:HG13	2.20	0.41
2:B:53:LEU:HD11	2:B:103:ILE:HD11	2.03	0.41
1:E:14(K):ILE:O	1:E:14(K):ILE:HG23	2.20	0.41
2:F:211:GLY:HA2	2:F:231:VAL:HG23	2.02	0.41
2:F:230:HIS:ND1	2:F:233:ARG:HG2	2.35	0.41
2:B:28:PRO:HB2	2:B:119:HIS:HB3	2.00	0.41
2:F:128:THR:HG23	2:F:129(C):LEU:HD22	2.01	0.41
2:F:80:GLU:O	2:F:81:LYS:HD2	2.21	0.41
2:B:126:ARG:HG3	4:B:1:SO4:O4	2.21	0.41
2:D:98:ASN:N	2:D:98:ASN:ND2	2.68	0.41
2:F:50:ARG:HE	2:F:50:ARG:HB3	1.77	0.41
3:X:427:CYS:SG	3:X:437:CYS:C	2.99	0.41
2:D:60(B):PRO:HB2	2:D:60(C):PRO:HD3	2.03	0.41
2:D:165:ARG:N	2:D:166:PRO:HD2	2.35	0.41
1:A:14:ASP:OD1	1:A:14(C):GLU:HB2	2.20	0.41
2:F:129(C):LEU:HD11	2:F:204:PRO:HD2	2.03	0.41
2:F:188:GLY:O	2:F:189:ASP:HB2	2.21	0.41
3:X:436:VAL:HG13	3:Z:454:LEU:HD21	2.03	0.41
3:Y:349:ASP:C	3:Y:351:CYS:N	2.72	0.41
3:Y:443:THR:OG1	3:Y:444:PHE:N	2.50	0.41
3:Z:416:ASP:OD2	3:Z:417:ASP:N	2.48	0.41
3:Y:446:CYS:O	3:Y:456:GLY:HA3	2.21	0.41
2:B:31:VAL:CG1	2:B:66:VAL:HG13	2.51	0.40
2:D:73:ARG:HD3	2:D:152:PRO:O	2.21	0.40
2:D:99:LEU:HD12	2:D:99:LEU:HA	1.86	0.40
3:X:462:CYS:O	3:X:463:ASP:HB2	2.21	0.40
2:B:144:LEU:HD21	2:B:152:PRO:HB3	2.02	0.40
2:B:165:ARG:N	2:B:166:PRO:HD2	2.37	0.40
2:B:228:TYR:CD1	2:B:228:TYR:N	2.89	0.40
2:D:185:LYS:HG2	2:D:186:PRO:HD2	2.02	0.40
3:Y:438:HIS:HB3	3:Y:445:GLU:HB2	2.03	0.40
2:D:59:LEU:HD13	2:D:88:ILE:CG2	2.52	0.40
2:F:60(B):PRO:CB	2:F:60(C):PRO:HD3	2.47	0.40
2:D:29:TRP:CG	2:D:121:VAL:HB	2.56	0.40
1:E:14(G):LEU:N	1:E:14(G):LEU:CD1	2.85	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	44/49 (90%)	43 (98%)	1 (2%)	0	100 100
1	C	44/49 (90%)	41 (93%)	3 (7%)	0	100 100
1	E	44/49 (90%)	39 (89%)	4 (9%)	1 (2%)	6 7
2	B	248/259 (96%)	238 (96%)	10 (4%)	0	100 100
2	D	248/259 (96%)	236 (95%)	9 (4%)	3 (1%)	13 19
2	F	244/259 (94%)	227 (93%)	16 (7%)	1 (0%)	34 48
3	X	109/121 (90%)	99 (91%)	10 (9%)	0	100 100
3	Y	109/121 (90%)	91 (84%)	15 (14%)	3 (3%)	5 4
3	Z	108/121 (89%)	98 (91%)	10 (9%)	0	100 100
All	All	1198/1287 (93%)	1112 (93%)	78 (6%)	8 (1%)	22 32

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	79	ILE
2	D	78	ASN
2	D	38	GLN
2	F	60(G)	ASN
3	Y	461	ASP
1	E	1(P)	TYR
3	Y	451	ASP
3	Y	380	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	41/43 (95%)	39 (95%)	2 (5%)	25	40
1	C	40/43 (93%)	38 (95%)	2 (5%)	24	40
1	E	38/43 (88%)	37 (97%)	1 (3%)	46	66
2	B	214/224 (96%)	208 (97%)	6 (3%)	43	63
2	D	213/224 (95%)	204 (96%)	9 (4%)	30	47
2	F	211/224 (94%)	202 (96%)	9 (4%)	29	46
3	X	87/102 (85%)	87 (100%)	0	100	100
3	Y	83/102 (81%)	82 (99%)	1 (1%)	71	85
3	Z	86/102 (84%)	85 (99%)	1 (1%)	71	85
All	All	1013/1107 (92%)	982 (97%)	31 (3%)	40	60

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	14(G)	LEU
2	B	46	LEU
2	B	50	ARG
2	B	60(G)	ASN
2	B	64	LEU
2	B	180	MET
2	B	182	CYS
1	C	6	LEU
1	C	14(D)	ARG
2	D	46	LEU
2	D	60(G)	ASN
2	D	64	LEU
2	D	98	ASN
2	D	99	LEU
2	D	126	ARG
2	D	151	GLN
2	D	180	MET
2	D	182	CYS
1	E	6	LEU
2	F	46	LEU
2	F	60(D)	TRP
2	F	99	LEU
2	F	127	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	175	ARG
2	F	180	MET
2	F	182	CYS
2	F	198	PRO
2	F	243	ASP
3	Y	454	LEU
3	Z	384	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	60(G)	ASN
2	B	62	ASN
2	B	131	GLN
2	B	244	GLN
2	D	60(G)	ASN
2	D	71	HIS
2	D	98	ASN
2	D	131	GLN
2	D	143	ASN
2	F	62	ASN
2	F	95	ASN
2	F	131	GLN
2	F	143	ASN
3	X	392	GLN
3	Y	387	GLN
3	Y	438	HIS
3	Z	387	GLN
3	Z	457	GLN

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 (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 3 are monoatomic - leaving 15 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	$\#\|Z\| > 2$
4	SO4	F	7	-	4,4,4	0.28	0	6,6,6	0.11	0
4	SO4	B	11	-	4,4,4	0.27	0	6,6,6	0.04	0
4	SO4	D	6	-	4,4,4	0.27	0	6,6,6	0.08	0
4	SO4	B	14	-	4,4,4	0.26	0	6,6,6	0.07	0
4	SO4	E	16	-	4,4,4	0.25	0	6,6,6	0.11	0
4	SO4	F	12	-	4,4,4	0.26	0	6,6,6	0.05	0
4	SO4	B	13	-	4,4,4	0.27	0	6,6,6	0.05	0
4	SO4	A	16	-	4,4,4	0.27	0	6,6,6	0.12	0
4	SO4	A	17	-	4,4,4	0.27	0	6,6,6	0.05	0
4	SO4	B	1	-	4,4,4	0.28	0	6,6,6	0.06	0
4	SO4	D	3	-	4,4,4	0.25	0	6,6,6	0.07	0
4	SO4	D	4	-	4,4,4	0.26	0	6,6,6	0.08	0
4	SO4	C	16	-	4,4,4	0.26	0	6,6,6	0.10	0
4	SO4	B	2	-	4,4,4	0.26	0	6,6,6	0.10	0
4	SO4	D	5	-	4,4,4	0.26	0	6,6,6	0.11	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.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	16	SO4	1	0
4	B	1	SO4	1	0
4	B	2	SO4	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, 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	46/49 (93%)	-0.23	0 100 100	15, 23, 37, 53	0
1	C	46/49 (93%)	-0.35	1 (2%) 62 60	10, 22, 38, 50	0
1	E	46/49 (93%)	-0.46	1 (2%) 62 60	16, 24, 35, 56	0
2	B	252/259 (97%)	-0.38	0 100 100	8, 20, 33, 50	0
2	D	252/259 (97%)	-0.33	1 (0%) 92 91	7, 21, 41, 47	0
2	F	248/259 (95%)	-0.44	2 (0%) 86 84	9, 22, 41, 61	0
3	X	113/121 (93%)	0.22	8 (7%) 16 14	16, 37, 61, 64	0
3	Y	113/121 (93%)	0.36	5 (4%) 34 33	22, 44, 60, 66	0
3	Z	112/121 (92%)	0.59	9 (8%) 12 11	22, 45, 67, 80	0
All	All	1228/1287 (95%)	-0.17	27 (2%) 62 60	7, 25, 56, 80	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Z	351	CYS	5.3
3	X	381	HIS	4.6
3	Y	453	ALA	3.4
3	X	402	ASN	3.1
3	Z	356	CYS	3.0
3	Z	383	PRO	3.0
3	Z	354	ALA	2.8
3	Y	400	ASP	2.8
3	X	354	ALA	2.8
1	E	1(R)	SER	2.7
3	X	401	PRO	2.6
3	Z	380	PRO	2.6
3	X	380	PRO	2.6
1	C	1(S)	SER	2.5
2	F	60(D)	TRP	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	Z	368	TYR	2.4
3	Y	399	CYS	2.4
3	Z	379	ILE	2.3
3	Y	438	HIS	2.3
3	Y	401	PRO	2.2
2	F	96	TRP	2.2
3	Z	386	CYS	2.2
3	X	353	ARG	2.1
3	Z	387	GLN	2.1
3	X	366	THR	2.1
3	X	452	SER	2.1
2	D	77(A)	ARG	2.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SO4	F	12	5/5	0.78	0.40	124,124,124,124	0
4	SO4	B	14	5/5	0.81	0.39	98,98,98,99	0
4	SO4	B	13	5/5	0.82	0.38	89,90,90,91	0
4	SO4	D	4	5/5	0.83	0.27	107,107,107,108	0
4	SO4	A	17	5/5	0.84	0.26	92,92,93,93	0
4	SO4	B	2	5/5	0.84	0.21	77,77,79,79	0
4	SO4	E	16	5/5	0.85	0.24	79,79,81,81	0
4	SO4	A	16	5/5	0.86	0.21	61,61,62,63	0
4	SO4	D	5	5/5	0.86	0.27	63,65,66,66	0
4	SO4	F	7	5/5	0.88	0.20	69,70,71,72	0
4	SO4	D	3	5/5	0.90	0.25	86,86,86,86	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SO4	C	16	5/5	0.92	0.24	73,74,74,74	0
4	SO4	D	6	5/5	0.94	0.31	77,78,78,78	0
4	SO4	B	11	5/5	0.94	0.25	82,82,83,83	0
4	SO4	B	1	5/5	0.95	0.13	73,74,74,74	0
5	CA	Y	1002	1/1	0.96	0.09	27,27,27,27	0
5	CA	Z	1003	1/1	0.97	0.04	32,32,32,32	0
5	CA	X	1001	1/1	0.99	0.09	15,15,15,15	0

6.5 Other polymers (i)

There are no such residues in this entry.