



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:55 AM GMT

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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) 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

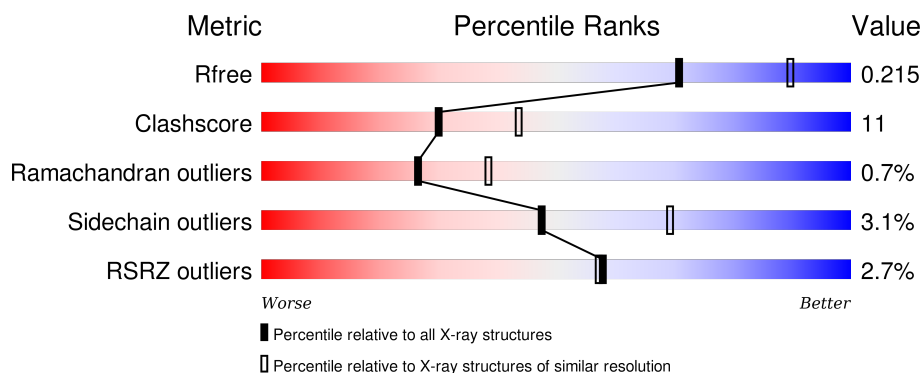
# 1 Overall quality at a glance

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))
$R_{free}$	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	49	<div> <div></div> <div>80%14%6%</div> </div>
1	C	49	<div> <div>2%</div> <div>80%12%6%</div> </div>
1	E	49	<div> <div>2%</div> <div>69%22%6%</div> </div>
2	B	259	<div> <div></div> <div>78%19%..</div> </div>
2	D	259	<div> <div></div> <div>73%21%..</div> </div>

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

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	SO4	A	16	-	-	-	X
4	SO4	B	2	-	-	-	X
4	SO4	D	4	-	-	-	X
4	SO4	D	6	-	-	-	X
4	SO4	E	16	-	-	-	X

## 2 Entry composition

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	UNP P00734
D	195	ALA	SER	ENGINEERED	UNP P00734
F	195	ALA	SER	ENGINEERED	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			

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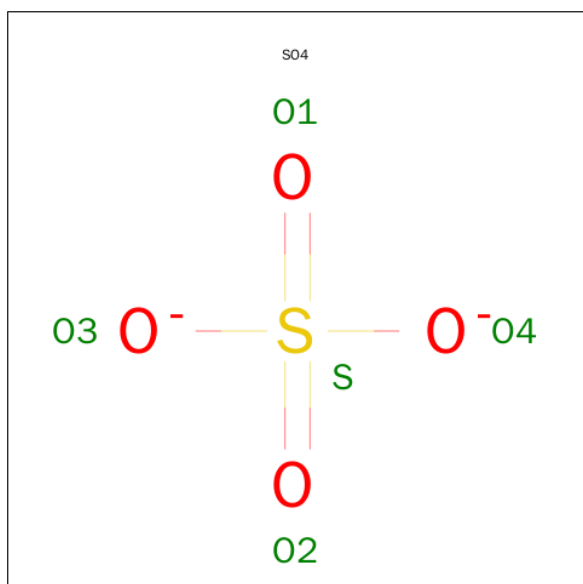
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	Z	112	Total	C	N	O	S	0	0	0
			794	485	127	164	18			

There are 9 discrepancies between the modelled and reference sequences:

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

- Molecule 4 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



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		

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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	Z	1	Total Ca 1 1	0	0
5	Y	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

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

### 3 Residue-property plots


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: Prothrombin

Chain A: 



#### • Molecule 1: Prothrombin

Chain C: 




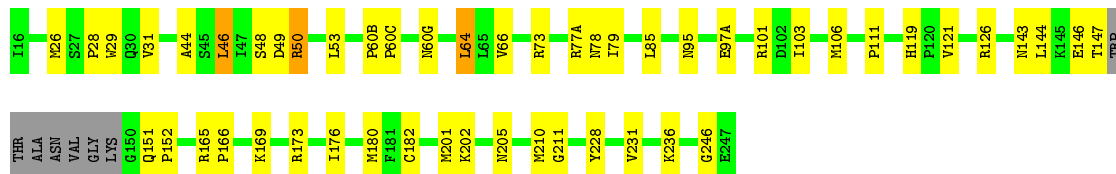
#### • Molecule 1: Prothrombin

Chain E: 



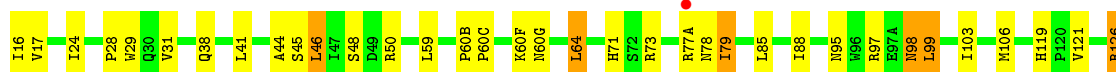
#### • Molecule 2: Prothrombin

Chain B: 

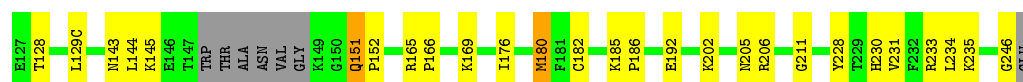


#### • Molecule 2: Prothrombin

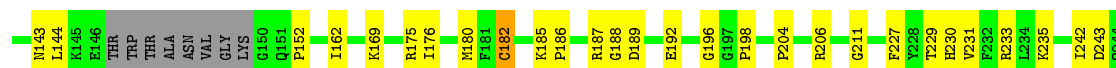
Chain D: 



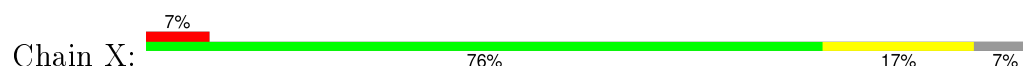




• Molecule 2: Prothrombin



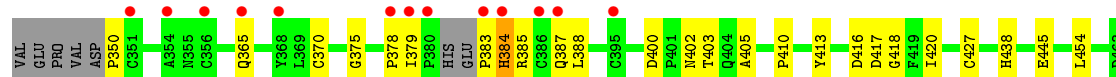
• Molecule 3: Thrombomodulin



• Molecule 3: Thrombomodulin



• Molecule 3: Thrombomodulin



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.97 (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	2884 reflections (5.08%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.4	Xtriage
Anisotropy	0.332	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 39.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	3 of 57861 reflections (0.005%)	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	10192	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.56% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: CA, 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	0.39	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(°)	Ideal(°)
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

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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
2:D:77(A):ARG:NH1	3:Y:422:THR:HG21	1.98	0.68
1:C:14(D):ARG:HH11	1:C:14(D):ARG:HG3	1.58	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:HB3	2:B:50:ARG:HH11	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:NH1	2:F:187:ARG:HG2	2.16	0.61
2:F:95:ASN:ND2	2:F:98:ASN:H	1.98	0.61
2:F:46:LEU:HD22	2:F:48:SER:O	2.01	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:HG22	3:Y:366:THR:O	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:461:ASP:CG	3:Y:462:CYS:H	2.09	0.56
3:Y:389:PHE:O	3:Y:390:CYS:HB3	2.06	0.56

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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:F:17:VAL:O	2:F:188:GLY:HA2	2.09	0.52
2:D:103:ILE:HG21	2:D:234:LEU:HD13	1.92	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:H	2:D:98:ASN:HD22	1.59	0.51
2:D:85:LEU:HD11	2:D:106:MET:HE1	1.93	0.50
2:B:173:ARG:HG2	6:B:415:HOH:O	2.11	0.50
2:F:73:ARG:HD3	2:F:152:PRO:O	2.12	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:95:ASN:OD1	2:D:97:ARG:HB2	2.10	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:F:143:ASN:ND2	2:F:192:GLU:HB3	2.27	0.49
2:D:211:GLY:HA2	2:D:231:VAL:HG23	1.94	0.49
2:F:60(A):TYR:HE2	2:F:60(C):PRO:HB2	1.77	0.49
1:C:14(D):ARG:NH1	1:C:14(D):ARG:HG3	2.27	0.49
3:Y:410:PRO:HG2	3:Y:413:TYR:CD1	2.47	0.49
2:B:50:ARG:CB	2:B:50:ARG:HH11	2.26	0.48
1:E:1(Q):GLU:O	1:E:1(P):TYR:CB	2.61	0.48
2:F:60(E):ASP:O	2:F:60(F):LYS:HG3	2.12	0.48
2:B:31:VAL:HG11	2:B:66:VAL:HG13	1.95	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:D:85:LEU:HD11	2:D:106:MET:CE	2.44	0.47
2:B:64:LEU:HD23	2:B:64:LEU:H	1.79	0.47
3:Y:454:LEU:CD2	3:Y:454:LEU:H	2.17	0.47
2:D:29:TRP:O	2:D:45:SER:HA	2.14	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

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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:50:ARG:NH1	2:B:50:ARG:HB3	2.29	0.47
2:B:31:VAL:HB	2:B:44:ALA:HB3	1.96	0.47
2:F:233:ARG:HH21	2:F:233:ARG:HG3	1.79	0.47
2:F:68:ILE:HD12	2:F:112:VAL:HG11	1.97	0.47
2:F:185:LYS:CG	2:F:186:PRO:HD2	2.45	0.47
3:Y:447:ILE:HA	3:Y:456:GLY:HA3	1.96	0.47
3:X:379:ILE:HD12	3:X:385:ARG:HB2	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:Z:400:ASP:OD2	3:Z:402:ASN:HB2	2.16	0.46
3:X:443:THR:OG1	3:X:444:PHE:N	2.48	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:ND1	3:Z:384:HIS:O	2.49	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: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
3:Y:430:GLY:HA2	6:Y:92:HOH:O	2.15	0.45
2:F:28:PRO:HB2	2:F:119:HIS:HB3	1.98	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
1:E:14:ASP:OD1	1:E:14(C):GLU:HB2	2.17	0.45
2:B:201:MET:SD	2:B:210:MET:HG3	2.57	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:211:GLY:HA2	2:B:231:VAL:HG23	1.99	0.45
1:E:1(G):PHE:CD1	2:F:242:ILE:HD13	2.48	0.44
2:D:64:LEU:N	2:D:64:LEU:HD12	2.30	0.44
2:B:95:ASN:ND2	2:B:97(A):GLU:HG2	2.32	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:F:79:ILE:N	2:F:79:ILE:HD12	2.33	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

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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:F:85:LEU:HD22	2:F:106:MET:HB3	2.00	0.44
2:D:16:ILE:N	6:D:312:HOH:O	2.51	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:CD2	2:B:64:LEU:N	2.81	0.43
2:F:211:GLY:HA2	2:F:229:THR:O	2.18	0.43
2:D:143:ASN:ND2	2:D:192:GLU:HB3	2.33	0.43
2:D:24:ILE:HD11	3:X:420:ILE:CD1	2.43	0.43
3:Y:450:PRO:C	3:Y:452:SER:N	2.70	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
2:D:71:HIS:CE1	3:X:420:ILE:CD1	3.01	0.43
2:B:173:ARG:NH1	2:B:173:ARG:HB3	2.33	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
3:Z:403:THR:C	3:Z:405:ALA:H	2.22	0.42
2:B:85:LEU:HD11	2:B:106:MET:HE1	2.01	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
1:C:1(M):PHE:CE2	2:D:235:LYS:HE2	2.54	0.42
2:B:146:GLU:O	2:B:147:THR:CB	2.67	0.42
3:Z:403:THR:HG22	3:Z:405:ALA:H	1.85	0.42
1:A:1(P):TYR:HE2	1:A:1(C):GLU:HG2	1.84	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:N	2:B:79:ILE:HD12	2.35	0.42
3:Y:418:GLY:O	3:Y:420:ILE:HG23	2.20	0.42
2:D:41:LEU:HD23	2:D:64:LEU:HD23	2.02	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

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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:F:230:HIS:ND1	2:F:233:ARG:HG2	2.35	0.41
2:F:211:GLY:HA2	2:F:231:VAL:HG23	2.02	0.41
1:E:14(K):ILE:HG23	1:E:14(K):ILE:O	2.20	0.41
2:B:53:LEU:HD11	2:B:103:ILE:HD11	2.03	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:D:98:ASN:N	2:D:98:ASN:ND2	2.68	0.41
2:B:126:ARG:HG3	4:B:1:SO4:O4	2.21	0.41
3:X:427:CYS:SG	3:X:437:CYS:C	2.99	0.41
2:F:50:ARG:HB3	2:F:50:ARG:HE	1.77	0.41
2:D:165:ARG:N	2:D:166:PRO:HD2	2.35	0.41
2:D:60(B):PRO:HB2	2:D:60(C):PRO:HD3	2.03	0.41
2:F:188:GLY:O	2:F:189:ASP:HB2	2.21	0.41
3:Z:416:ASP:OD2	3:Z:417:ASP:N	2.48	0.41
3:Y:349:ASP:C	3:Y:351:CYS:N	2.72	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
3:X:436:VAL:HG13	3:Z:454:LEU:HD21	2.03	0.41
3:Y:443:THR:OG1	3:Y:444:PHE:N	2.50	0.41
3:Y:446:CYS:O	3:Y:456:GLY:HA3	2.21	0.41
2:D:73:ARG:HD3	2:D:152:PRO:O	2.21	0.40
2:B:31:VAL:CG1	2:B:66:VAL:HG13	2.51	0.40
2:D:99:LEU:HA	2:D:99:LEU:HD12	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
3:Y:438:HIS:HB3	3:Y:445:GLU:HB2	2.03	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
2:B:165:ARG:N	2:B:166:PRO:HD2	2.37	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:CD1	1:E:14(G):LEU:N	2.85	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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%)	8	8
2	B	248/259 (96%)	238 (96%)	10 (4%)	0	100	100
2	D	248/259 (96%)	236 (95%)	9 (4%)	3 (1%)	16	23
2	F	244/259 (94%)	227 (93%)	16 (7%)	1 (0%)	39	56
3	X	109/121 (90%)	99 (91%)	10 (9%)	0	100	100
3	Y	109/121 (90%)	91 (84%)	15 (14%)	3 (3%)	6	5
3	Z	108/121 (89%)	98 (91%)	10 (9%)	0	100	100
All	All	1198/1287 (93%)	1112 (93%)	78 (6%)	8 (1%)	26	38

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

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%)	31	48
1	C	40/43 (93%)	38 (95%)	2 (5%)	30	48
1	E	38/43 (88%)	37 (97%)	1 (3%)	54	74
2	B	214/224 (96%)	208 (97%)	6 (3%)	51	72
2	D	213/224 (95%)	204 (96%)	9 (4%)	36	56
2	F	211/224 (94%)	202 (96%)	9 (4%)	35	55
3	X	87/102 (85%)	87 (100%)	0	100	100
3	Y	83/102 (81%)	82 (99%)	1 (1%)	78	90
3	Z	86/102 (84%)	85 (99%)	1 (1%)	78	90
All	All	1013/1107 (92%)	982 (97%)	31 (3%)	47	69

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

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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

Some 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

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

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	A	16	-	4,4,4	0.26	0	6,6,6	0.14	0
4	SO4	A	17	-	4,4,4	0.24	0	6,6,6	0.07	0
4	SO4	B	1	-	4,4,4	0.23	0	6,6,6	0.09	0
4	SO4	B	11	-	4,4,4	0.22	0	6,6,6	0.06	0
4	SO4	B	13	-	4,4,4	0.24	0	6,6,6	0.07	0
4	SO4	B	14	-	4,4,4	0.24	0	6,6,6	0.09	0
4	SO4	B	2	-	4,4,4	0.21	0	6,6,6	0.11	0
4	SO4	C	16	-	4,4,4	0.21	0	6,6,6	0.12	0
4	SO4	D	3	-	4,4,4	0.21	0	6,6,6	0.11	0
4	SO4	D	4	-	4,4,4	0.20	0	6,6,6	0.11	0
4	SO4	D	5	-	4,4,4	0.24	0	6,6,6	0.08	0
4	SO4	D	6	-	4,4,4	0.23	0	6,6,6	0.07	0
4	SO4	E	16	-	4,4,4	0.20	0	6,6,6	0.10	0
4	SO4	F	12	-	4,4,4	0.22	0	6,6,6	0.08	0
4	SO4	F	7	-	4,4,4	0.24	0	6,6,6	0.10	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	SO4	A	16	-	-	0/0/0/0	0/0/0/0
4	SO4	A	17	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1	-	-	0/0/0/0	0/0/0/0
4	SO4	B	11	-	-	0/0/0/0	0/0/0/0
4	SO4	B	13	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SO4	B	14	-	-	0/0/0/0	0/0/0/0
4	SO4	B	2	-	-	0/0/0/0	0/0/0/0
4	SO4	C	16	-	-	0/0/0/0	0/0/0/0
4	SO4	D	3	-	-	0/0/0/0	0/0/0/0
4	SO4	D	4	-	-	0/0/0/0	0/0/0/0
4	SO4	D	5	-	-	0/0/0/0	0/0/0/0
4	SO4	D	6	-	-	0/0/0/0	0/0/0/0
4	SO4	E	16	-	-	0/0/0/0	0/0/0/0
4	SO4	F	12	-	-	0/0/0/0	0/0/0/0
4	SO4	F	7	-	-	0/0/0/0	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.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1	SO4	1	0
4	B	2	SO4	1	0
4	E	16	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	46/49 (93%)	-0.18	0 100 100	15, 23, 37, 53	0
1	C	46/49 (93%)	-0.30	1 (2%) 65 64	10, 22, 38, 50	0
1	E	46/49 (93%)	-0.42	1 (2%) 65 64	16, 24, 35, 56	0
2	B	252/259 (97%)	-0.34	0 100 100	8, 20, 33, 50	0
2	D	252/259 (97%)	-0.29	1 (0%) 93 93	7, 21, 41, 47	0
2	F	248/259 (95%)	-0.39	2 (0%) 87 87	9, 22, 41, 61	0
3	X	113/121 (93%)	0.28	9 (7%) 15 15	16, 37, 61, 64	0
3	Y	113/121 (93%)	0.43	6 (5%) 30 30	22, 44, 60, 66	0
3	Z	112/121 (92%)	0.66	13 (11%) 6 6	22, 45, 67, 80	0
All	All	1228/1287 (95%)	-0.12	33 (2%) 58 57	7, 25, 56, 80	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Z	351	CYS	5.6
3	X	381	HIS	4.8
3	Y	453	ALA	3.6
3	X	402	ASN	3.2
3	Z	356	CYS	3.2
3	Z	383	PRO	3.2
3	Z	354	ALA	3.0
3	Y	400	ASP	2.9
3	X	354	ALA	2.9
1	E	1(R)	SER	2.9
3	X	401	PRO	2.8
3	Z	380	PRO	2.8
3	X	380	PRO	2.7
1	C	1(S)	SER	2.6
2	F	60(D)	TRP	2.6

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Mol	Chain	Res	Type	RSRZ
3	Y	399	CYS	2.5
3	Z	368	TYR	2.5
3	Z	379	ILE	2.4
3	Y	438	HIS	2.4
3	Y	401	PRO	2.3
2	F	96	TRP	2.3
3	Z	386	CYS	2.3
3	X	353	ARG	2.3
3	Z	387	GLN	2.2
3	X	452	SER	2.2
3	X	366	THR	2.2
2	D	77(A)	ARG	2.2
3	Z	395	CYS	2.1
3	Z	384	HIS	2.1
3	Z	365	GLN	2.1
3	Y	390	CYS	2.0
3	X	382	GLU	2.0
3	Z	378	PRO	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	SO4	E	16	5/5	0.85	0.24	12.01	79,79,81,81	0
4	SO4	D	4	5/5	0.83	0.27	4.83	107,107,107,108	0
4	SO4	A	16	5/5	0.86	0.21	3.42	61,61,62,63	0

*Continued on next page...*



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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	SO4	D	6	5/5	0.94	0.30	2.90	77,78,78,78	0
4	SO4	B	2	5/5	0.84	0.21	2.25	77,77,79,79	0
4	SO4	F	7	5/5	0.88	0.20	1.65	69,70,71,72	0
4	SO4	D	3	5/5	0.90	0.25	1.24	86,86,86,86	0
4	SO4	B	1	5/5	0.95	0.13	-0.34	73,74,74,74	0
5	CA	X	1001	1/1	0.99	0.09	-1.29	15,15,15,15	0
5	CA	Y	1002	1/1	0.96	0.09	-1.78	27,27,27,27	0
5	CA	Z	1003	1/1	0.97	0.04	-4.45	32,32,32,32	0
4	SO4	D	5	5/5	0.86	0.27	-	63,65,66,66	0
4	SO4	B	13	5/5	0.82	0.38	-	89,90,90,91	0
4	SO4	C	16	5/5	0.92	0.24	-	73,74,74,74	0
4	SO4	B	14	5/5	0.81	0.39	-	98,98,98,99	0
4	SO4	A	17	5/5	0.84	0.26	-	92,92,93,93	0
4	SO4	F	12	5/5	0.78	0.40	-	124,124,124,124	0
4	SO4	B	11	5/5	0.94	0.25	-	82,82,83,83	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.