



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 06:14 am GMT

PDB ID : 3V83
Title : The 2.1 angstrom crystal structure of diferric human transferrin
Authors : Noinaj, N.; Steere, A.; Mason, A.B.; Buchanan, S.K.
Deposited on : 2011-12-22
Resolution : 2.10 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

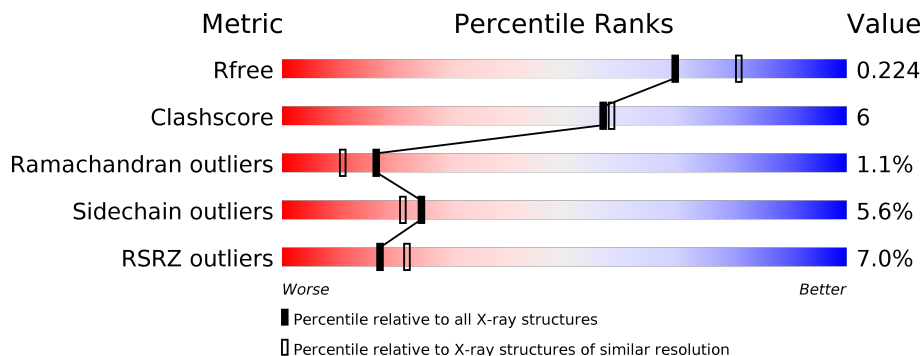
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	100719	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (2.10-2.10)

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 $\leq 5\%$. 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	698	<div> <div>6%</div> <div> <div></div> <div>82%</div> <div>12%</div> <div>• •</div> </div> </div>
1	B	698	<div> <div>5%</div> <div> <div></div> <div>83%</div> <div>12%</div> <div>• •</div> </div> </div>
1	C	698	<div> <div>17%</div> <div> <div></div> <div>78%</div> <div>16%</div> <div>• •</div> </div> </div>
1	D	698	<div> <div>3%</div> <div> <div></div> <div>82%</div> <div>13%</div> <div>• •</div> </div> </div>
1	E	698	<div> <div>5%</div> <div> <div></div> <div>83%</div> <div>11%</div> <div>• •</div> </div> </div>
1	F	698	<div> <div>5%</div> <div> <div></div> <div>81%</div> <div>13%</div> <div>• •</div> </div> </div>

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
2	BCT	C	702	-	-	X	-
2	BCT	D	702	-	-	-	X
2	BCT	E	701	-	-	-	X
2	BCT	F	702	-	-	-	X
3	FE	A	703	-	-	-	X
3	FE	B	703	-	-	-	X
3	FE	B	704	-	-	-	X
3	FE	C	704	-	-	-	X
3	FE	D	703	-	-	-	X
3	FE	D	704	-	-	-	X
3	FE	E	703	-	-	-	X
3	FE	F	703	-	-	-	X
3	FE	F	704	-	-	-	X
4	SO4	A	705	-	-	-	X
4	SO4	A	708	-	-	-	X
4	SO4	C	705	-	-	-	X
4	SO4	F	706	-	-	-	X
5	P6G	A	710	-	-	-	X
5	P6G	A	711	-	-	-	X
5	P6G	B	714	-	-	-	X
5	P6G	C	712	-	-	-	X
5	P6G	D	714	-	-	-	X
5	P6G	D	715	-	-	-	X
5	P6G	E	714	-	-	-	X
5	P6G	E	715	-	-	-	X
5	P6G	F	710	-	-	-	X
5	P6G	F	711	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 33928 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.

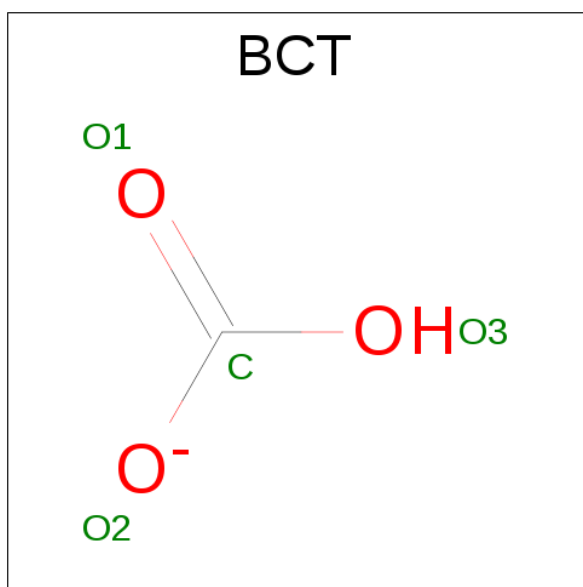
- Molecule 1 is a protein called Serotransferrin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	674	Total	C	N	O	S	0	0	0
			5160	3247	892	974	47			
1	B	677	Total	C	N	O	S	0	0	0
			5179	3260	898	974	47			
1	C	674	Total	C	N	O	S	0	0	0
			5124	3221	888	968	47			
1	D	675	Total	C	N	O	S	0	0	0
			5193	3263	897	986	47			
1	E	674	Total	C	N	O	S	0	0	0
			5202	3267	898	990	47			
1	F	676	Total	C	N	O	S	0	0	0
			5191	3263	900	981	47			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	429	VAL	ILE	VARIANT	UNP P02787
B	429	VAL	ILE	VARIANT	UNP P02787
C	429	VAL	ILE	VARIANT	UNP P02787
D	429	VAL	ILE	VARIANT	UNP P02787
E	429	VAL	ILE	VARIANT	UNP P02787
F	429	VAL	ILE	VARIANT	UNP P02787

- Molecule 2 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).

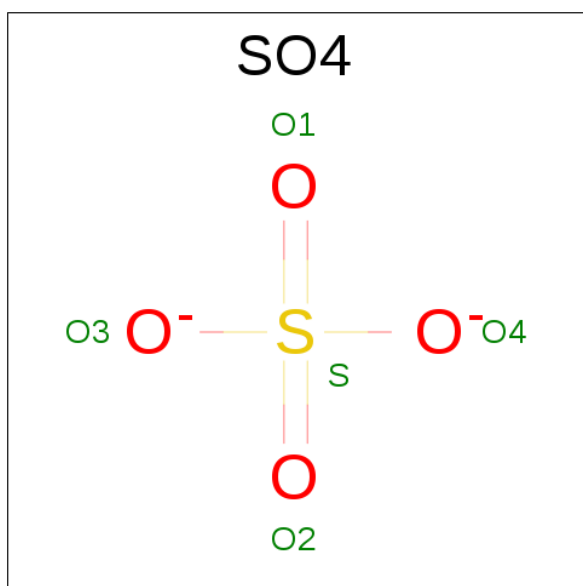


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	1	3		
2	A	1	Total	C	O	0	0
			4	1	3		
2	B	1	Total	C	O	0	0
			4	1	3		
2	B	1	Total	C	O	0	0
			4	1	3		
2	C	1	Total	C	O	0	0
			4	1	3		
2	C	1	Total	C	O	0	0
			4	1	3		
2	D	1	Total	C	O	0	0
			4	1	3		
2	D	1	Total	C	O	0	0
			4	1	3		
2	E	1	Total	C	O	0	0
			4	1	3		
2	E	1	Total	C	O	0	0
			4	1	3		
2	F	1	Total	C	O	0	0
			4	1	3		
2	F	1	Total	C	O	0	0
			4	1	3		

- Molecule 3 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	2	Total Fe 2 2	0	0
3	E	2	Total Fe 2 2	0	0
3	B	2	Total Fe 2 2	0	0
3	C	2	Total Fe 2 2	0	0
3	A	2	Total Fe 2 2	0	0
3	F	2	Total Fe 2 2	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

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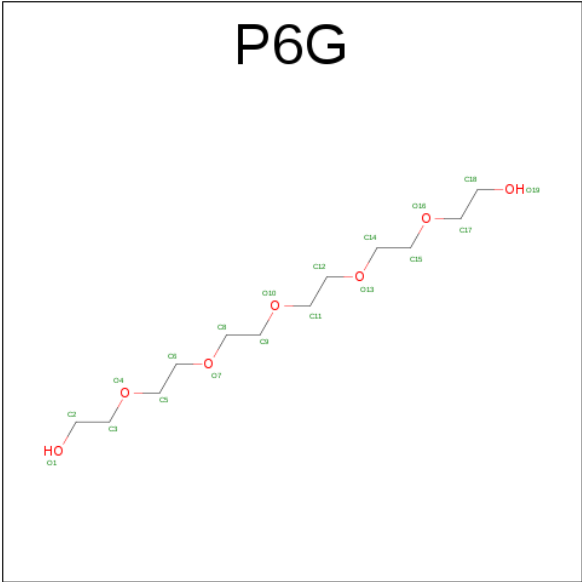
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total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

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

- Molecule 5 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: C₁₂H₂₆O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			19	12	7		
5	A	1	Total	C	O	0	0
			19	12	7		
5	A	1	Total	C	O	0	0
			19	12	7		
5	B	1	Total	C	O	0	0
			19	12	7		
5	B	1	Total	C	O	0	0
			19	12	7		
5	C	1	Total	C	O	0	0
			19	12	7		
5	C	1	Total	C	O	0	0
			19	12	7		
5	C	1	Total	C	O	0	0
			19	12	7		
5	D	1	Total	C	O	0	0
			19	12	7		
5	D	1	Total	C	O	0	0
			19	12	7		
5	E	1	Total	C	O	0	0
			19	12	7		
5	E	1	Total	C	O	0	0
			19	12	7		
5	F	1	Total	C	O	0	0
			19	12	7		
5	F	1	Total	C	O	0	0
			19	12	7		

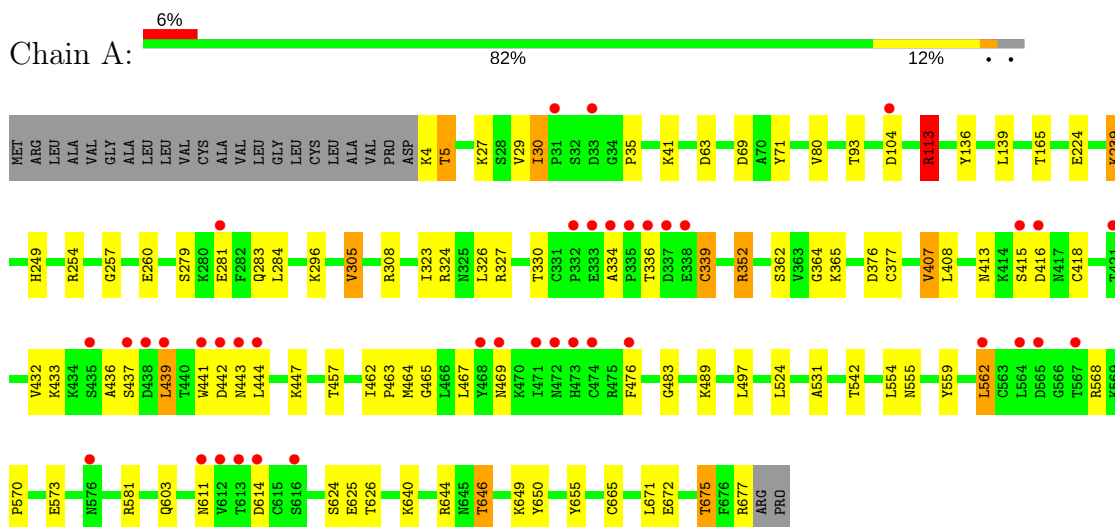
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	352	Total 352	O 352	0	0
6	B	454	Total 454	O 454	0	0
6	C	305	Total 305	O 305	0	0
6	D	398	Total 398	O 398	0	0
6	E	431	Total 431	O 431	0	0
6	F	393	Total 393	O 393	0	0

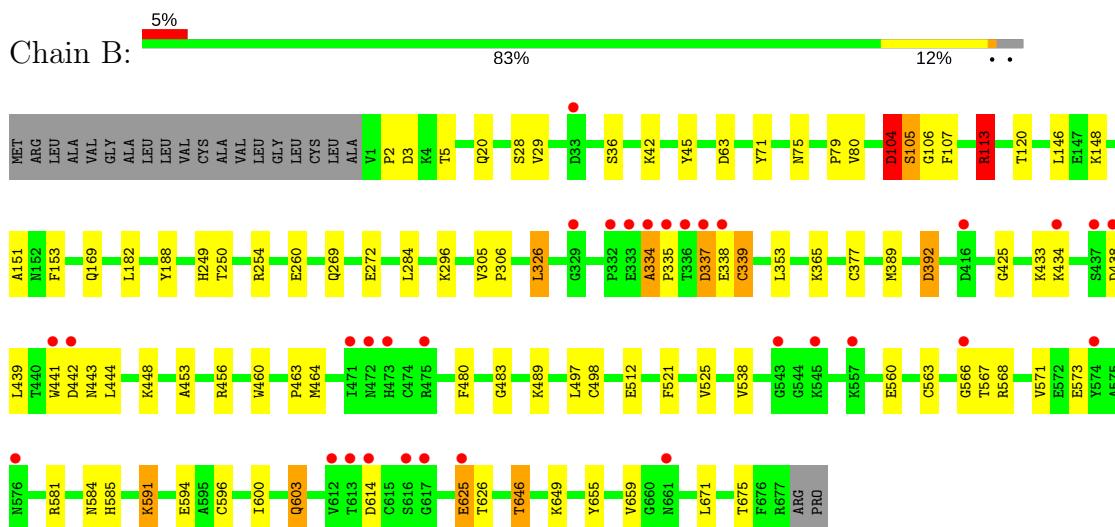
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

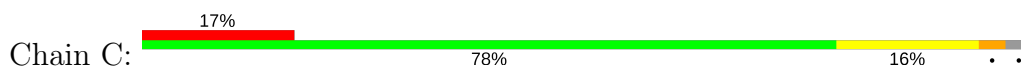
• Molecule 1: Serotransferrin



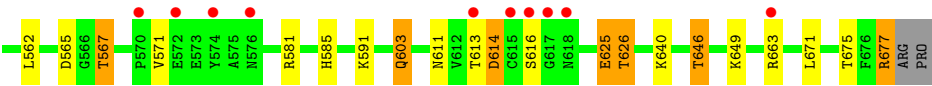
• Molecule 1: Serotransferrin



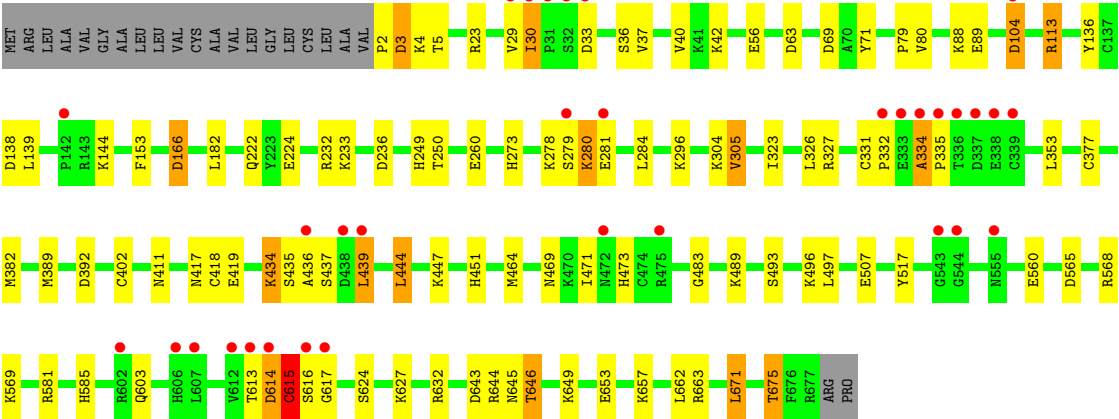
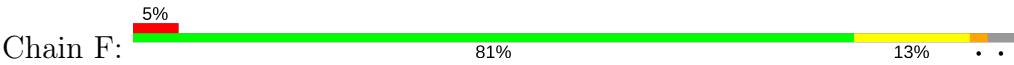
• Molecule 1: Serotransferrin







● Molecule 1: Serotransferrin



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	254.53Å 173.00Å 150.15Å 90.00° 123.26° 90.00°	Depositor
Resolution (Å)	29.95 – 2.10 49.25 – 2.10	Depositor EDS
% Data completeness (in resolution range)	94.4 (29.95-2.10) 94.4 (49.25-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 2.10Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.180 , 0.230 0.180 , 0.224	Depositor DCC
R_{free} test set	15035 reflections (5.06%)	DCC
Wilson B-factor (Å ²)	27.0	Xtriage
Anisotropy	0.250	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 60.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.014 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	33928	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.33% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: BCT, FE, P6G, 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	0.38	0/5278	0.54	1/7144 (0.0%)
1	B	0.42	0/5298	0.57	2/7169 (0.0%)
1	C	0.39	0/5240	0.54	0/7097
1	D	0.41	0/5311	0.57	2/7184 (0.0%)
1	E	0.42	0/5320	0.57	2/7196 (0.0%)
1	F	0.40	0/5309	0.58	2/7183 (0.0%)
All	All	0.40	0/31756	0.56	9/42973 (0.0%)

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
1	D	0	2
1	E	0	2
All	All	0	4

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	113	ARG	NE-CZ-NH1	6.35	123.47	120.30
1	E	113	ARG	NE-CZ-NH1	6.23	123.41	120.30
1	D	113	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	B	113	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	F	113	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	B	113	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	A	113	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	E	113	ARG	NE-CZ-NH2	-5.04	117.78	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	113	ARG	NE-CZ-NH2	-5.01	117.79	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	278	LYS	Peptide
1	D	279	SER	Peptide
1	E	613	THR	Peptide
1	E	614	ASP	Peptide

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	5160	0	4928	50	0
1	B	5179	0	4949	54	0
1	C	5124	0	4868	84	0
1	D	5193	0	4970	57	0
1	E	5202	0	4992	51	0
1	F	5191	0	4969	62	0
2	A	8	0	1	0	0
2	B	8	0	0	0	0
2	C	8	0	1	3	0
2	D	8	0	1	0	0
2	E	8	0	1	0	0
2	F	8	0	1	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
4	A	25	0	0	1	0
4	B	45	0	0	1	0
4	C	35	0	0	0	0
4	D	45	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	45	0	0	0	0
4	F	25	0	0	0	0
5	A	57	0	78	4	0
5	B	38	0	52	6	0
5	C	57	0	78	4	0
5	D	38	0	52	7	0
5	E	38	0	52	4	0
5	F	38	0	52	6	0
6	A	352	0	0	6	0
6	B	454	0	0	9	0
6	C	305	0	0	10	0
6	D	398	0	0	10	0
6	E	431	0	0	9	0
6	F	393	0	0	5	0
All	All	33928	0	30045	353	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (353) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:436:ALA:H	1:C:437:SER:HA	1.23	1.00
1:B:566:GLY:H	1:B:567:THR:HA	1.39	0.85
1:A:113:ARG:HD2	1:E:254:ARG:HD2	1.59	0.82
1:A:646:THR:HG22	1:A:649:LYS:H	1.48	0.79
1:E:646:THR:HG22	1:E:649:LYS:H	1.48	0.78
1:D:169:GLN:NE2	6:D:936:HOH:O	2.16	0.78
1:C:436:ALA:N	1:C:437:SER:HA	2.00	0.76
1:C:524:LEU:HB2	1:C:531:ALA:HB2	1.67	0.76
1:C:657:LYS:O	1:C:661:ASN:N	2.19	0.76
1:A:327:ARG:NH2	6:A:825:HOH:O	2.19	0.75
1:F:435:SER:H	1:F:436:ALA:HA	1.50	0.75
1:C:664:LYS:O	6:C:942:HOH:O	2.04	0.74
1:D:507:GLU:OE2	6:D:979:HOH:O	2.06	0.74
1:F:42:LYS:HZ2	5:F:711:P6G:H91	1.52	0.74
1:C:327:ARG:NH2	6:C:858:HOH:O	2.22	0.72
1:A:439:LEU:O	1:A:568:ARG:NH1	2.23	0.72
1:C:665:CYS:SG	6:C:1067:HOH:O	2.49	0.71
1:C:662:LEU:O	6:C:942:HOH:O	2.09	0.70
1:E:565:ASP:OD1	1:E:567:THR:OG1	2.10	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:483:GLY:HA2	1:F:497:LEU:HD22	1.74	0.69
1:E:208:SER:HB2	5:E:714:P6G:H112	1.74	0.69
1:B:20:GLN:NE2	6:B:1222:HOH:O	2.26	0.69
1:E:493:SER:HA	1:E:496:LYS:HD3	1.74	0.69
1:C:646:THR:HG22	1:C:649:LYS:H	1.57	0.68
1:C:603:GLN:OE1	1:C:604:GLN:NE2	2.24	0.68
1:C:69:ASP:OD1	1:C:327:ARG:NH1	2.26	0.67
1:C:483:GLY:HA2	1:C:497:LEU:HD22	1.76	0.66
1:A:439:LEU:HD21	1:A:447:LYS:HG2	1.76	0.66
1:A:465:GLY:O	1:A:469:ASN:ND2	2.28	0.66
1:B:339:CYS:SG	6:B:1202:HOH:O	2.53	0.65
1:F:4:LYS:NZ	1:F:33:ASP:O	2.26	0.65
1:F:616:SER:HB2	1:F:617:GLY:HA2	1.77	0.65
1:F:671:LEU:O	1:F:675:THR:HB	1.95	0.65
1:B:254:ARG:HD2	1:F:113:ARG:HD2	1.78	0.65
1:D:350:HIS:ND1	6:D:991:HOH:O	2.29	0.65
1:F:493:SER:HA	1:F:496:LYS:HD2	1.79	0.64
1:B:646:THR:HG22	1:B:649:LYS:H	1.63	0.64
1:A:324:ARG:NH2	6:A:1126:HOH:O	2.30	0.63
1:F:646:THR:HG22	1:F:649:LYS:H	1.63	0.63
1:B:104:ASP:O	1:B:106:GLY:N	2.31	0.63
1:F:323:ILE:O	1:F:327:ARG:HG2	1.98	0.63
1:B:591:LYS:NZ	6:B:949:HOH:O	2.32	0.63
1:C:115:LYS:NZ	6:C:954:HOH:O	2.28	0.63
1:B:2:PRO:HD2	1:B:5:THR:OG1	1.99	0.63
1:F:434:LYS:HD2	1:F:560:GLU:HG3	1.79	0.63
1:E:56:GLU:OE1	5:E:715:P6G:O19	2.14	0.62
1:A:254:ARG:HD2	1:C:113:ARG:HD2	1.82	0.62
1:C:452:THR:OG1	2:C:702:BCT:O3	2.08	0.61
1:D:239:LYS:NZ	6:D:1053:HOH:O	2.27	0.61
1:C:5:THR:HG22	1:C:36:SER:HB2	1.83	0.61
1:C:79:PRO:HB3	1:C:250:THR:HG21	1.82	0.61
1:E:113:ARG:HD3	6:E:1031:HOH:O	1.99	0.61
1:F:42:LYS:NZ	5:F:711:P6G:H91	2.16	0.60
1:D:600:ILE:HD11	5:D:715:P6G:H122	1.83	0.60
1:F:5:THR:HG22	1:F:36:SER:HB2	1.82	0.60
1:C:63:ASP:HA	1:C:249:HIS:CD2	2.37	0.60
1:C:413:ASN:ND2	6:C:1006:HOH:O	2.34	0.60
1:A:323:ILE:O	1:A:327:ARG:HG2	2.02	0.60
1:C:664:LYS:O	1:C:666:SER:N	2.34	0.60
1:F:304:LYS:NZ	6:F:1103:HOH:O	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:249:HIS:CE1	1:D:296:LYS:HD2	2.37	0.59
1:F:643:ASP:O	1:F:645:ASN:ND2	2.36	0.59
1:E:105:SER:O	6:E:827:HOH:O	2.16	0.59
1:A:352:ARG:NH2	6:A:1076:HOH:O	2.34	0.59
1:B:566:GLY:N	1:B:567:THR:HA	2.06	0.58
1:C:646:THR:HB	1:C:649:LYS:HD2	1.84	0.58
1:A:524:LEU:HB2	1:A:531:ALA:HB2	1.85	0.58
1:D:654:GLU:CD	1:D:654:GLU:H	2.07	0.58
1:F:40:VAL:HG13	5:F:711:P6G:H141	1.85	0.58
1:C:517:TYR:OH	1:C:632:ARG:NH1	2.36	0.58
1:F:278:LYS:O	1:F:280:LYS:HG2	2.03	0.58
1:F:507:GLU:OE2	6:F:865:HOH:O	2.17	0.57
1:A:483:GLY:HA2	1:A:497:LEU:HD22	1.85	0.57
1:B:42:LYS:HZ3	5:B:715:P6G:C14	2.17	0.57
1:E:42:LYS:HD2	5:E:715:P6G:H61	1.87	0.57
1:A:432:VAL:HG11	1:A:439:LEU:HD12	1.87	0.57
1:D:441:TRP:HZ2	1:D:579:LEU:HD21	1.70	0.57
1:C:514:TYR:CD2	1:C:523:CYS:HB2	2.40	0.56
1:B:596:CYS:HB2	6:B:1202:HOH:O	2.05	0.56
1:C:456:ARG:NE	2:C:702:BCT:O1	2.37	0.56
1:F:417:ASN:O	1:F:419:GLU:N	2.37	0.56
1:A:441:TRP:HE3	1:A:562:LEU:HD13	1.69	0.56
1:D:654:GLU:HG2	6:D:849:HOH:O	2.05	0.56
1:C:671:LEU:O	1:C:675:THR:HG22	2.06	0.56
5:D:714:P6G:O19	6:D:897:HOH:O	2.18	0.55
5:A:712:P6G:O1	6:A:1097:HOH:O	2.16	0.54
1:F:79:PRO:HB3	1:F:250:THR:HG21	1.88	0.54
1:C:50:ARG:HD3	5:C:713:P6G:H182	1.90	0.54
1:F:392:ASP:HA	1:F:585:HIS:CD2	2.43	0.54
1:C:464:MET:HG3	1:C:476:PHE:CG	2.43	0.54
1:E:677:ARG:NH2	6:E:1197:HOH:O	2.40	0.54
1:B:453:ALA:HB3	1:B:456:ARG:HD3	1.91	0.53
1:C:107:PHE:CD1	1:C:115:LYS:HE2	2.43	0.53
1:B:483:GLY:HA2	1:B:497:LEU:HD22	1.90	0.53
1:C:323:ILE:O	1:C:327:ARG:HG2	2.09	0.53
1:D:453:ALA:HB3	1:D:456:ARG:HD3	1.90	0.53
1:F:436:ALA:HB3	1:F:437:SER:HA	1.90	0.53
1:A:41:LYS:O	5:A:710:P6G:H32	2.08	0.53
1:A:570:PRO:HG2	1:A:573:GLU:HG3	1.90	0.53
1:D:646:THR:HG23	1:D:649:LYS:H	1.73	0.53
1:F:23:ARG:HA	1:F:37:VAL:HG13	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:LYS:NZ	5:B:715:P6G:H172	2.23	0.52
1:D:93:THR:H	1:D:677:ARG:HH21	1.55	0.52
1:B:42:LYS:HZ3	5:B:715:P6G:H142	1.74	0.52
1:B:392:ASP:HA	1:B:585:HIS:CD2	2.44	0.52
1:D:80:VAL:C	1:D:305:VAL:HG13	2.29	0.52
1:E:280:LYS:NZ	6:E:1037:HOH:O	2.42	0.52
1:C:565:ASP:HB3	1:F:273:HIS:CD2	2.44	0.52
1:F:138:ASP:OD1	6:F:897:HOH:O	2.19	0.52
1:C:467:LEU:HD11	1:C:479:PHE:CE1	2.44	0.52
1:A:136:TYR:HA	1:A:139:LEU:HG	1.91	0.51
1:C:142:PRO:O	1:C:143:ARG:HB2	2.10	0.51
1:C:451:HIS:ND1	1:C:459:GLY:O	2.33	0.51
1:D:136:TYR:HA	1:D:139:LEU:HG	1.90	0.51
1:D:42:LYS:HD2	5:D:714:P6G:H92	1.91	0.51
1:F:113:ARG:HG3	1:F:153:PHE:CD1	2.45	0.51
1:D:535:HIS:CD2	1:D:536:GLN:HG2	2.46	0.51
1:D:483:GLY:HA2	1:D:497:LEU:HD22	1.92	0.51
1:A:407:VAL:HG22	1:A:408:LEU:HG	1.91	0.51
1:C:608:PHE:HA	1:C:612:VAL:HG21	1.93	0.51
1:D:42:LYS:HZ3	5:D:714:P6G:H122	1.74	0.51
1:E:433:LYS:HG2	6:E:1039:HOH:O	2.11	0.51
1:F:613:THR:O	1:F:614:ASP:HB2	2.10	0.51
1:C:279:SER:HB2	1:F:565:ASP:HB3	1.92	0.50
1:C:623:ARG:NH2	1:C:633:ASP:O	2.43	0.50
1:F:42:LYS:HD2	5:F:711:P6G:H52	1.93	0.50
1:E:136:TYR:HA	1:E:139:LEU:HG	1.93	0.50
1:F:63:ASP:HA	1:F:249:HIS:CD2	2.46	0.50
1:E:30:ILE:HD13	1:E:35:PRO:HD2	1.94	0.50
1:B:655:TYR:O	1:B:659:VAL:HG23	2.12	0.50
1:C:417:ASN:O	1:C:419:GLU:N	2.43	0.50
1:D:337:ASP:OD1	6:D:1068:HOH:O	2.19	0.50
1:C:565:ASP:HB2	1:F:29:VAL:HG22	1.93	0.50
1:E:453:ALA:HB3	1:E:456:ARG:HD3	1.94	0.49
1:F:517:TYR:HE2	1:F:632:ARG:HD2	1.77	0.49
1:E:442:ASP:OD1	1:E:442:ASP:N	2.44	0.49
1:C:498:CYS:HA	1:C:514:TYR:HD2	1.77	0.49
1:F:653:GLU:N	1:F:653:GLU:OE1	2.44	0.49
1:C:467:LEU:HD21	1:C:479:PHE:CG	2.47	0.49
1:A:365:LYS:HZ3	5:A:712:P6G:H182	1.76	0.49
1:E:80:VAL:C	1:E:305:VAL:HG13	2.33	0.49
1:C:660:GLY:C	1:C:662:LEU:H	2.15	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:436:ALA:H	1:C:437:SER:CA	2.10	0.49
1:A:464:MET:HE3	1:A:476:PHE:HB3	1.95	0.49
1:A:93:THR:OG1	1:A:677:ARG:HG2	2.13	0.49
1:B:249:HIS:CE1	1:B:296:LYS:HD2	2.47	0.49
1:A:63:ASP:HA	1:A:249:HIS:CD2	2.48	0.49
1:D:103:LYS:HE2	1:D:221:ASP:O	2.13	0.49
1:D:113:ARG:HG3	1:D:153:PHE:CD1	2.48	0.49
1:A:69:ASP:OD1	1:A:327:ARG:NH1	2.46	0.48
1:A:364:GLY:N	6:A:887:HOH:O	2.44	0.48
1:B:80:VAL:C	1:B:305:VAL:HG13	2.33	0.48
1:B:377:CYS:HB3	1:B:389:MET:SD	2.53	0.48
1:C:42:LYS:HZ2	5:C:713:P6G:H91	1.79	0.48
1:C:29:VAL:HG21	1:F:565:ASP:O	2.13	0.48
1:A:362:SER:HB2	1:A:365:LYS:HB2	1.95	0.48
5:C:712:P6G:O1	5:C:712:P6G:O19	2.23	0.48
1:D:667:THR:HG22	6:D:1044:HOH:O	2.14	0.48
1:E:113:ARG:HG3	1:E:153:PHE:CD1	2.48	0.48
1:F:435:SER:N	1:F:436:ALA:HA	2.23	0.48
1:A:441:TRP:O	1:A:443:ASN:N	2.47	0.48
1:B:151:ALA:HB1	1:B:169:GLN:HB2	1.96	0.48
1:B:594:GLU:OE2	6:B:1174:HOH:O	2.20	0.47
1:D:432:VAL:HG11	1:D:439:LEU:HD12	1.96	0.47
1:D:382:MET:SD	1:D:402:CYS:HB3	2.54	0.47
1:D:562:LEU:HD23	1:D:568:ARG:HG2	1.96	0.47
1:D:627:LYS:HB3	1:D:629:LEU:HG	1.96	0.47
1:F:166:ASP:OD1	1:F:166:ASP:N	2.47	0.47
1:E:392:ASP:HA	1:E:585:HIS:CD2	2.49	0.47
1:C:474:CYS:HA	6:C:1067:HOH:O	2.14	0.47
1:C:652:GLY:O	1:C:656:VAL:HG23	2.13	0.47
1:F:411:ASN:ND2	1:F:418:CYS:O	2.48	0.47
1:B:563:CYS:HB2	1:B:566:GLY:HA3	1.95	0.47
1:B:538:VAL:HG11	1:B:571:VAL:HG21	1.95	0.47
1:E:444:LEU:HA	1:E:444:LEU:HD12	1.78	0.47
1:E:517:TYR:CZ	1:E:534:LYS:HD3	2.49	0.47
1:A:672:GLU:HA	1:A:675:THR:HG22	1.97	0.47
1:A:436:ALA:N	1:A:437:SER:HA	2.30	0.47
1:A:27:LYS:NZ	6:A:942:HOH:O	2.47	0.47
1:B:42:LYS:NZ	5:B:715:P6G:H112	2.30	0.47
1:D:107:PHE:CD1	1:D:115:LYS:HE3	2.49	0.47
1:D:444:LEU:O	1:D:447:LYS:HB2	2.15	0.47
1:D:599:LYS:HE3	5:D:715:P6G:H181	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:334:ALA:HA	1:B:335:PRO:HD3	1.81	0.47
1:C:645:ASN:ND2	6:C:1052:HOH:O	2.44	0.46
1:D:18:LYS:HD3	1:D:293:LEU:HB2	1.97	0.46
1:D:646:THR:HG22	1:D:649:LYS:HD3	1.97	0.46
1:F:435:SER:H	1:F:436:ALA:CA	2.23	0.46
1:F:56:GLU:OE1	5:F:711:P6G:O19	2.22	0.46
1:A:80:VAL:C	1:A:305:VAL:HG13	2.36	0.46
1:B:433:LYS:NZ	6:B:1150:HOH:O	2.47	0.46
1:C:613:THR:HA	1:C:614:ASP:HA	1.58	0.46
1:E:377:CYS:HB3	1:E:389:MET:SD	2.55	0.46
1:C:450:CYS:HB2	1:C:531:ALA:HA	1.97	0.46
1:C:603:GLN:NE2	6:C:1100:HOH:O	2.49	0.46
1:E:249:HIS:CE1	1:E:296:LYS:HD2	2.51	0.46
1:B:120:THR:HG22	1:B:188:TYR:HA	1.98	0.46
1:D:392:ASP:HA	1:D:585:HIS:CD2	2.51	0.46
1:A:365:LYS:HZ1	5:A:712:P6G:H92	1.81	0.46
1:B:3:ASP:N	1:B:3:ASP:OD1	2.49	0.46
1:D:419:GLU:OE1	1:D:602:ARG:NH2	2.48	0.46
1:D:42:LYS:NZ	5:D:714:P6G:H122	2.30	0.46
1:E:498:CYS:HB3	1:E:512:GLU:OE1	2.15	0.46
1:E:524:LEU:HB2	1:E:531:ALA:HB2	1.98	0.46
5:E:715:P6G:H91	5:E:715:P6G:H121	1.40	0.46
1:A:542:THR:HB	1:A:555:ASN:HA	1.98	0.46
1:C:377:CYS:HB3	1:C:389:MET:SD	2.55	0.46
1:D:524:LEU:HB2	1:D:531:ALA:HB2	1.96	0.46
1:A:644:ARG:HB3	1:A:650:TYR:HA	1.98	0.46
1:B:105:SER:HB2	1:B:107:PHE:CE1	2.50	0.46
1:D:63:ASP:HA	1:D:249:HIS:CD2	2.51	0.46
1:F:80:VAL:C	1:F:305:VAL:HG13	2.36	0.46
1:A:433:LYS:HE3	1:A:524:LEU:O	2.16	0.46
1:C:600:ILE:O	1:C:603:GLN:HG3	2.16	0.46
1:B:63:ASP:HA	1:B:249:HIS:CD2	2.51	0.45
1:C:664:LYS:C	1:C:666:SER:H	2.20	0.45
1:F:382:MET:SD	1:F:402:CYS:HB3	2.55	0.45
1:B:448:LYS:HD2	1:B:497:LEU:HD21	1.98	0.45
1:F:224:GLU:OE2	1:F:232:ARG:HD3	2.17	0.45
1:F:2:PRO:O	1:F:3:ASP:HB2	2.16	0.45
1:A:308:ARG:HH11	1:A:376:ASP:HA	1.80	0.45
1:B:600:ILE:O	1:B:603:GLN:HG3	2.17	0.45
1:C:453:ALA:HB3	1:C:456:ARG:HD3	1.98	0.45
1:C:483:GLY:C	1:C:497:LEU:HB2	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:623:ARG:NH1	1:C:633:ASP:HB3	2.32	0.45
1:C:458:ALA:N	2:C:702:BCT:O2	2.50	0.45
1:F:249:HIS:CE1	1:F:296:LYS:HD2	2.52	0.45
1:D:671:LEU:O	1:D:675:THR:HG22	2.17	0.45
1:A:462:ILE:HB	1:A:463:PRO:HD3	1.99	0.45
1:F:280:LYS:HB3	1:F:281:GLU:H	1.56	0.45
1:B:438:ASP:O	1:B:443:ASN:ND2	2.48	0.45
1:F:136:TYR:HA	1:F:139:LEU:HG	1.99	0.45
1:B:42:LYS:HZ3	5:B:715:P6G:H141	1.82	0.44
1:A:437:SER:HB3	1:F:104:ASP:OD1	2.18	0.44
1:B:464:MET:HE1	1:B:480:PHE:HE2	1.82	0.44
1:C:113:ARG:HG3	1:C:153:PHE:CD1	2.52	0.44
1:E:603:GLN:HE21	1:E:603:GLN:HB2	1.59	0.44
1:E:677:ARG:N	1:E:677:ARG:HD2	2.31	0.44
1:B:269:GLN:NE2	6:B:983:HOH:O	2.20	0.44
1:F:353:LEU:HA	1:F:353:LEU:HD23	1.74	0.44
1:E:107:PHE:CD1	1:E:115:LYS:HE2	2.52	0.44
1:F:69:ASP:OD1	1:F:327:ARG:NH1	2.47	0.44
1:D:224:GLU:HB2	1:D:233:LYS:O	2.18	0.44
1:D:84:PHE:HZ	1:D:88:LYS:HE3	1.82	0.44
1:A:640:LYS:HB3	4:A:705:SO4:O3	2.18	0.44
1:B:521:PHE:O	1:B:525:VAL:HG23	2.18	0.44
1:B:337:ASP:HA	1:B:338:GLU:HA	1.65	0.44
1:B:42:LYS:HZ1	5:B:715:P6G:H172	1.83	0.44
1:C:457:THR:HG23	1:C:655:TYR:CE1	2.52	0.44
1:F:334:ALA:HA	1:F:335:PRO:HD2	1.87	0.44
1:A:336:THR:HB	1:E:349:HIS:HB2	2.00	0.44
1:C:305:VAL:HA	1:C:306:PRO:HD3	1.90	0.44
1:A:4:LYS:HG3	1:A:5:THR:H	1.83	0.43
1:C:80:VAL:C	1:C:305:VAL:HG13	2.38	0.43
1:C:382:MET:SD	1:C:402:CYS:HB3	2.58	0.43
1:E:468:TYR:HB2	1:E:476:PHE:HZ	1.83	0.43
1:C:105:SER:HG	1:C:232:ARG:HH22	1.66	0.43
1:C:644:ARG:HA	1:C:649:LYS:HB3	2.00	0.43
1:F:233:LYS:NZ	6:F:957:HOH:O	2.34	0.43
1:A:441:TRP:H	1:A:562:LEU:HD11	1.83	0.43
1:B:434:LYS:HG3	1:B:560:GLU:HG3	2.00	0.43
1:E:334:ALA:HB3	1:E:337:ASP:OD1	2.18	0.43
1:E:353:LEU:HA	1:E:353:LEU:HD23	1.81	0.43
1:D:471:ILE:HD12	1:D:473:HIS:CE1	2.53	0.43
1:E:143:ARG:HB3	6:E:1200:HOH:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:460:TRP:O	1:C:464:MET:HB2	2.19	0.43
1:E:448:LYS:HD2	1:E:497:LEU:HD21	2.00	0.43
1:E:280:LYS:H	1:E:280:LYS:CD	2.31	0.43
1:C:249:HIS:CE1	1:C:296:LYS:HD2	2.54	0.43
1:E:527:LYS:HE2	6:E:1170:HOH:O	2.19	0.43
1:A:444:LEU:O	1:A:447:LYS:HB2	2.19	0.42
1:C:498:CYS:HA	1:C:514:TYR:CD2	2.54	0.42
1:F:278:LYS:O	1:F:280:LYS:N	2.52	0.42
1:F:444:LEU:HA	1:F:444:LEU:HD12	1.86	0.42
1:A:439:LEU:HD22	1:A:439:LEU:HA	1.82	0.42
1:B:105:SER:HB2	1:B:107:PHE:HE1	1.84	0.42
1:C:430:ALA:HB3	1:C:562:LEU:HB2	2.00	0.42
1:D:601:LEU:HD23	1:D:601:LEU:HA	1.90	0.42
1:C:471:ILE:HD12	1:C:473:HIS:CE1	2.54	0.42
1:E:467:LEU:HD21	1:E:479:PHE:CE1	2.55	0.42
1:A:249:HIS:CE1	1:A:296:LYS:HD2	2.55	0.42
1:D:419:GLU:OE2	1:D:606:HIS:NE2	2.53	0.42
1:A:554:LEU:HD22	1:A:559:TYR:OH	2.19	0.42
1:D:224:GLU:OE2	1:D:232:ARG:HD3	2.20	0.42
1:D:434:LYS:HD3	1:D:557:LYS:O	2.20	0.42
1:E:382:MET:SD	1:E:402:CYS:HB3	2.60	0.42
1:A:625:GLU:HB2	1:A:626:THR:H	1.65	0.42
1:C:643:ASP:O	1:C:649:LYS:HD3	2.20	0.42
1:E:63:ASP:HA	1:E:249:HIS:CD2	2.54	0.42
1:E:538:VAL:HB	1:E:571:VAL:HG11	2.02	0.42
1:A:457:THR:HG23	1:A:655:TYR:CE1	2.54	0.42
1:E:349:HIS:HA	1:E:352:ARG:HB3	2.02	0.42
1:F:377:CYS:HB3	1:F:389:MET:SD	2.59	0.42
1:B:460:TRP:O	1:B:463:PRO:HD2	2.20	0.41
1:B:75:ASN:ND2	6:B:1047:HOH:O	2.43	0.41
1:D:279:SER:CB	1:D:283:GLN:HG3	2.50	0.41
1:B:625:GLU:HA	1:B:626:THR:HA	1.67	0.41
1:D:141:GLU:HA	6:D:1079:HOH:O	2.19	0.41
1:E:625:GLU:HA	1:E:626:THR:HA	1.70	0.41
1:D:279:SER:CB	1:D:280:LYS:HA	2.50	0.41
1:D:18:LYS:HD2	1:D:287:SER:HB2	2.01	0.41
1:D:421:THR:HA	1:D:422:PRO:HD2	1.89	0.41
1:D:465:GLY:HA2	1:D:662:LEU:HD13	2.02	0.41
1:E:471:ILE:HD12	1:E:473:HIS:CE1	2.55	0.41
1:E:520:ALA:O	1:E:523:CYS:HB3	2.21	0.41
1:C:662:LEU:HG	6:C:942:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:365:LYS:HZ3	5:D:715:P6G:H151	1.85	0.41
1:B:260:GLU:HB2	4:B:707:SO4:O3	2.21	0.41
1:D:300:HIS:ND1	4:D:710:SO4:O2	2.42	0.41
1:E:517:TYR:CE2	1:E:534:LYS:HD3	2.56	0.41
1:B:305:VAL:HA	1:B:306:PRO:HD3	1.92	0.41
1:C:622:PHE:HZ	1:C:638:LEU:HG	1.84	0.41
1:E:29:VAL:HG12	1:E:30:ILE:HG23	2.03	0.41
1:E:358:TRP:CE2	1:E:366:ILE:HG13	2.55	0.41
1:F:331:CYS:HA	1:F:332:PRO:HD2	1.85	0.41
1:F:614:ASP:HB3	1:F:615:CYS:H	1.67	0.41
1:B:425:GLY:HA2	1:B:584:ASN:OD1	2.21	0.41
1:E:555:ASN:HB2	1:E:558:ASP:OD2	2.21	0.41
1:F:113:ARG:HG2	1:F:153:PHE:O	2.21	0.41
1:F:439:LEU:HD21	1:F:447:LYS:HG2	2.03	0.41
1:B:79:PRO:HB3	1:B:250:THR:HG21	2.02	0.41
1:D:273:HIS:HD2	6:D:1160:HOH:O	2.04	0.41
1:C:402:CYS:HA	1:C:674:CYS:HB3	2.03	0.41
1:F:444:LEU:O	1:F:447:LYS:HB2	2.21	0.41
1:C:654:GLU:OE1	1:F:88:LYS:NZ	2.54	0.41
1:A:30:ILE:HD13	1:A:35:PRO:HD2	2.02	0.41
1:B:45:TYR:OH	6:B:910:HOH:O	2.22	0.41
1:B:460:TRP:C	1:B:463:PRO:HD2	2.41	0.41
1:C:4:LYS:HD2	1:C:4:LYS:HA	1.85	0.41
1:E:675:THR:HG21	6:E:1132:HOH:O	2.21	0.41
1:A:239:LYS:HB2	1:A:239:LYS:HE2	1.92	0.41
1:B:113:ARG:HG3	1:B:153:PHE:CE1	2.56	0.41
1:C:192:PHE:CE1	1:C:210:ILE:HG13	2.55	0.41
1:C:326:LEU:HA	1:C:326:LEU:HD23	1.88	0.41
1:C:42:LYS:NZ	5:C:713:P6G:H91	2.35	0.41
1:E:12:SER:HA	6:E:938:HOH:O	2.21	0.41
1:B:146:LEU:HD22	1:B:326:LEU:HD22	2.02	0.40
1:D:471:ILE:HD12	1:D:473:HIS:NE2	2.36	0.40
1:E:30:ILE:HD12	1:E:31:PRO:O	2.20	0.40
1:A:441:TRP:N	1:A:562:LEU:HD21	2.37	0.40
1:D:676:PHE:O	1:D:677:ARG:HB2	2.21	0.40
1:C:174:CYS:O	1:C:174:CYS:SG	2.79	0.40
1:C:448:LYS:O	1:C:530:VAL:HG12	2.21	0.40
1:D:68:TYR:CE2	1:D:72:LEU:HD11	2.56	0.40
1:B:498:CYS:HB3	1:B:512:GLU:OE1	2.21	0.40
1:C:146:LEU:HD22	1:C:326:LEU:HD22	2.03	0.40
1:C:466:LEU:HA	1:C:466:LEU:HD23	1.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:470:LYS:HE2	1:D:470:LYS:HB3	1.88	0.40
1:F:451:HIS:CE1	1:F:464:MET:HE2	2.57	0.40
5:F:711:P6G:H81	6:F:890:HOH:O	2.22	0.40
1:C:335:PRO:C	1:C:337:ASP:H	2.25	0.40
1:C:589:THR:HG21	1:C:594:GLU:HA	2.03	0.40
1:F:29:VAL:HG12	1:F:30:ILE:HG22	2.03	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	672/698 (96%)	621 (92%)	42 (6%)	9 (1%)	14	8
1	B	675/698 (97%)	630 (93%)	39 (6%)	6 (1%)	20	14
1	C	672/698 (96%)	617 (92%)	46 (7%)	9 (1%)	14	8
1	D	673/698 (96%)	630 (94%)	37 (6%)	6 (1%)	20	14
1	E	672/698 (96%)	632 (94%)	35 (5%)	5 (1%)	25	20
1	F	674/698 (97%)	623 (92%)	43 (6%)	8 (1%)	15	9
All	All	4038/4188 (96%)	3753 (93%)	242 (6%)	43 (1%)	17	11

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	416	ASP
1	A	442	ASP
1	A	614	ASP
1	B	104	ASP
1	B	105	SER
1	E	614	ASP

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Mol	Chain	Res	Type
1	F	279	SER
1	F	614	ASP
1	B	442	ASP
1	C	439	LEU
1	C	445	LYS
1	C	625	GLU
1	D	339	CYS
1	D	437	SER
1	E	338	GLU
1	E	481	SER
1	F	3	ASP
1	A	334	ALA
1	A	415	SER
1	A	665	CYS
1	C	457	THR
1	C	665	CYS
1	F	439	LEU
1	F	615	CYS
1	F	624	SER
1	A	624	SER
1	B	334	ALA
1	C	436	ALA
1	D	334	ALA
1	D	624	SER
1	F	280	LYS
1	A	257	GLY
1	A	339	CYS
1	B	625	GLU
1	C	417	ASN
1	D	614	ASP
1	E	339	CYS
1	B	614	ASP
1	C	664	LYS
1	D	257	GLY
1	F	334	ALA
1	E	257	GLY
1	C	142	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	547/585 (94%)	514 (94%)	33 (6%)	22	19
1	B	547/585 (94%)	519 (95%)	28 (5%)	28	25
1	C	539/585 (92%)	503 (93%)	36 (7%)	19	15
1	D	555/585 (95%)	535 (96%)	20 (4%)	40	41
1	E	560/585 (96%)	525 (94%)	35 (6%)	21	17
1	F	553/585 (94%)	521 (94%)	32 (6%)	23	20
All	All	3301/3510 (94%)	3117 (94%)	184 (6%)	25	21

All (184) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	29	VAL
1	A	30	ILE
1	A	71	TYR
1	A	104	ASP
1	A	113	ARG
1	A	165	THR
1	A	224	GLU
1	A	239	LYS
1	A	260	GLU
1	A	279	SER
1	A	281	GLU
1	A	283	GLN
1	A	284	LEU
1	A	305	VAL
1	A	326	LEU
1	A	330	THR
1	A	339	CYS
1	A	352	ARG
1	A	377	CYS
1	A	407	VAL
1	A	413	ASN
1	A	418	CYS
1	A	439	LEU
1	A	467	LEU
1	A	489	LYS

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Mol	Chain	Res	Type
1	A	562	LEU
1	A	581	ARG
1	A	603	GLN
1	A	611	ASN
1	A	646	THR
1	A	671	LEU
1	A	675	THR
1	B	28	SER
1	B	29	VAL
1	B	36	SER
1	B	71	TYR
1	B	104	ASP
1	B	113	ARG
1	B	148	LYS
1	B	182	LEU
1	B	272	GLU
1	B	284	LEU
1	B	326	LEU
1	B	337	ASP
1	B	339	CYS
1	B	353	LEU
1	B	365	LYS
1	B	392	ASP
1	B	439	LEU
1	B	441	TRP
1	B	444	LEU
1	B	489	LYS
1	B	568	ARG
1	B	573	GLU
1	B	581	ARG
1	B	591	LYS
1	B	603	GLN
1	B	646	THR
1	B	671	LEU
1	B	675	THR
1	C	12	SER
1	C	32	SER
1	C	36	SER
1	C	71	TYR
1	C	113	ARG
1	C	144	LYS
1	C	182	LEU

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Mol	Chain	Res	Type
1	C	184	GLN
1	C	259	LYS
1	C	260	GLU
1	C	276	LYS
1	C	305	VAL
1	C	326	LEU
1	C	327	ARG
1	C	330	THR
1	C	339	CYS
1	C	352	ARG
1	C	421	THR
1	C	442	ASP
1	C	444	LEU
1	C	464	MET
1	C	467	LEU
1	C	475	ARG
1	C	482	GLU
1	C	488	SER
1	C	489	LYS
1	C	523	CYS
1	C	556	GLU
1	C	567	THR
1	C	581	ARG
1	C	603	GLN
1	C	643	ASP
1	C	646	THR
1	C	648	GLU
1	C	653	GLU
1	C	671	LEU
1	D	3	ASP
1	D	5	THR
1	D	29	VAL
1	D	71	TYR
1	D	113	ARG
1	D	141	GLU
1	D	144	LYS
1	D	281	GLU
1	D	284	LEU
1	D	326	LEU
1	D	328	GLU
1	D	338	GLU
1	D	365	LYS

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Mol	Chain	Res	Type
1	D	421	THR
1	D	439	LEU
1	D	497	LEU
1	D	499	MET
1	D	581	ARG
1	D	603	GLN
1	D	654	GLU
1	E	4	LYS
1	E	28	SER
1	E	30	ILE
1	E	71	TYR
1	E	88	LYS
1	E	259	LYS
1	E	280	LYS
1	E	284	LEU
1	E	305	VAL
1	E	338	GLU
1	E	339	CYS
1	E	352	ARG
1	E	365	LYS
1	E	433	LYS
1	E	438	ASP
1	E	439	LEU
1	E	444	LEU
1	E	467	LEU
1	E	474	CYS
1	E	481	SER
1	E	501	SER
1	E	562	LEU
1	E	567	THR
1	E	581	ARG
1	E	591	LYS
1	E	603	GLN
1	E	611	ASN
1	E	616	SER
1	E	625	GLU
1	E	626	THR
1	E	640	LYS
1	E	646	THR
1	E	663	ARG
1	E	671	LEU
1	E	677	ARG

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Mol	Chain	Res	Type
1	F	30	ILE
1	F	71	TYR
1	F	89	GLU
1	F	104	ASP
1	F	144	LYS
1	F	166	ASP
1	F	182	LEU
1	F	222	GLN
1	F	236	ASP
1	F	260	GLU
1	F	284	LEU
1	F	305	VAL
1	F	326	LEU
1	F	434	LYS
1	F	444	LEU
1	F	469	ASN
1	F	471	ILE
1	F	473	HIS
1	F	489	LYS
1	F	568	ARG
1	F	569	LYS
1	F	581	ARG
1	F	603	GLN
1	F	615	CYS
1	F	627	LYS
1	F	644	ARG
1	F	646	THR
1	F	657	LYS
1	F	662	LEU
1	F	663	ARG
1	F	671	LEU
1	F	675	THR

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

Mol	Chain	Res	Type
1	A	469	ASN
1	A	603	GLN
1	F	222	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 82 ligands modelled in this entry, 12 are monoatomic - leaving 70 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	$\# Z > 2$
2	BCT	A	701	3	0,3,3	0.00	-	0,3,3	0.00	-
2	BCT	A	702	3	0,3,3	0.00	-	0,3,3	0.00	-
4	SO4	A	705	-	4,4,4	0.19	0	6,6,6	0.15	0
4	SO4	A	706	-	4,4,4	0.20	0	6,6,6	0.21	0
4	SO4	A	707	-	4,4,4	0.13	0	6,6,6	0.16	0
4	SO4	A	708	-	4,4,4	0.19	0	6,6,6	0.11	0
4	SO4	A	709	-	4,4,4	0.16	0	6,6,6	0.08	0
5	P6G	A	710	-	18,18,18	0.71	0	17,17,17	1.49	0
5	P6G	A	711	-	18,18,18	0.66	0	17,17,17	1.54	0
5	P6G	A	712	-	18,18,18	0.71	0	17,17,17	1.47	0
2	BCT	B	701	3	0,3,3	0.00	-	0,3,3	0.00	-
2	BCT	B	702	3	0,3,3	0.00	-	0,3,3	0.00	-
4	SO4	B	705	-	4,4,4	0.15	0	6,6,6	0.30	0
4	SO4	B	706	-	4,4,4	0.21	0	6,6,6	0.12	0
4	SO4	B	707	-	4,4,4	0.18	0	6,6,6	0.12	0
4	SO4	B	708	-	4,4,4	0.18	0	6,6,6	0.22	0
4	SO4	B	709	-	4,4,4	0.14	0	6,6,6	0.15	0
4	SO4	B	710	-	4,4,4	0.17	0	6,6,6	0.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	B	711	-	4,4,4	0.19	0	6,6,6	0.13	0
4	SO4	B	712	-	4,4,4	0.17	0	6,6,6	0.06	0
4	SO4	B	713	-	4,4,4	0.17	0	6,6,6	0.11	0
5	P6G	B	714	-	18,18,18	0.74	0	17,17,17	1.29	1 (5%)
5	P6G	B	715	-	18,18,18	0.72	0	17,17,17	1.48	0
2	BCT	C	701	3	0,3,3	0.00	-	0,3,3	0.00	-
2	BCT	C	702	3	0,3,3	0.00	-	0,3,3	0.00	-
4	SO4	C	705	-	4,4,4	0.13	0	6,6,6	0.10	0
4	SO4	C	706	-	4,4,4	0.18	0	6,6,6	0.10	0
4	SO4	C	707	-	4,4,4	0.16	0	6,6,6	0.22	0
4	SO4	C	708	-	4,4,4	0.14	0	6,6,6	0.15	0
4	SO4	C	709	-	4,4,4	0.19	0	6,6,6	0.12	0
4	SO4	C	710	-	4,4,4	0.18	0	6,6,6	0.09	0
4	SO4	C	711	-	4,4,4	0.15	0	6,6,6	0.06	0
5	P6G	C	712	-	18,18,18	0.73	0	17,17,17	1.44	0
5	P6G	C	713	-	18,18,18	0.68	0	17,17,17	1.54	1 (5%)
5	P6G	C	714	-	18,18,18	0.66	0	17,17,17	1.54	0
2	BCT	D	701	3	0,3,3	0.00	-	0,3,3	0.00	-
2	BCT	D	702	3	0,3,3	0.00	-	0,3,3	0.00	-
4	SO4	D	705	-	4,4,4	0.17	0	6,6,6	0.08	0
4	SO4	D	706	-	4,4,4	0.16	0	6,6,6	0.11	0
4	SO4	D	707	-	4,4,4	0.15	0	6,6,6	0.16	0
4	SO4	D	708	-	4,4,4	0.13	0	6,6,6	0.14	0
4	SO4	D	709	-	4,4,4	0.19	0	6,6,6	0.14	0
4	SO4	D	710	-	4,4,4	0.14	0	6,6,6	0.19	0
4	SO4	D	711	-	4,4,4	0.17	0	6,6,6	0.12	0
4	SO4	D	712	-	4,4,4	0.14	0	6,6,6	0.12	0
4	SO4	D	713	-	4,4,4	0.17	0	6,6,6	0.08	0
5	P6G	D	714	-	18,18,18	0.69	0	17,17,17	1.56	0
5	P6G	D	715	-	18,18,18	0.62	0	17,17,17	1.75	3 (17%)
2	BCT	E	701	3	0,3,3	0.00	-	0,3,3	0.00	-
2	BCT	E	702	3	0,3,3	0.00	-	0,3,3	0.00	-
4	SO4	E	705	-	4,4,4	0.16	0	6,6,6	0.06	0
4	SO4	E	706	-	4,4,4	0.68	0	6,6,6	1.07	1 (16%)
4	SO4	E	707	-	4,4,4	0.17	0	6,6,6	0.16	0
4	SO4	E	708	-	4,4,4	0.17	0	6,6,6	0.08	0
4	SO4	E	709	-	4,4,4	0.15	0	6,6,6	0.16	0
4	SO4	E	710	-	4,4,4	0.16	0	6,6,6	0.12	0
4	SO4	E	711	-	4,4,4	0.15	0	6,6,6	0.16	0
4	SO4	E	712	-	4,4,4	0.17	0	6,6,6	0.17	0
4	SO4	E	713	-	4,4,4	0.16	0	6,6,6	0.09	0
5	P6G	E	714	-	18,18,18	0.69	0	17,17,17	1.57	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	P6G	E	715	-	18,18,18	0.73	0	17,17,17	1.40	0
2	BCT	F	701	3	0,3,3	0.00	-	0,3,3	0.00	-
2	BCT	F	702	3	0,3,3	0.00	-	0,3,3	0.00	-
4	SO4	F	705	-	4,4,4	0.15	0	6,6,6	0.11	0
4	SO4	F	706	-	4,4,4	0.21	0	6,6,6	0.14	0
4	SO4	F	707	-	4,4,4	0.16	0	6,6,6	0.15	0
4	SO4	F	708	-	4,4,4	0.18	0	6,6,6	0.13	0
4	SO4	F	709	-	4,4,4	0.17	0	6,6,6	0.12	0
5	P6G	F	710	-	18,18,18	0.72	0	17,17,17	1.52	0
5	P6G	F	711	-	18,18,18	0.70	0	17,17,17	1.64	2 (11%)

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
2	BCT	A	701	3	-	0/0/0/0	0/0/0/0
2	BCT	A	702	3	-	0/0/0/0	0/0/0/0
4	SO4	A	705	-	-	0/0/0/0	0/0/0/0
4	SO4	A	706	-	-	0/0/0/0	0/0/0/0
4	SO4	A	707	-	-	0/0/0/0	0/0/0/0
4	SO4	A	708	-	-	0/0/0/0	0/0/0/0
4	SO4	A	709	-	-	0/0/0/0	0/0/0/0
5	P6G	A	710	-	-	0/16/16/16	0/0/0/0
5	P6G	A	711	-	-	0/16/16/16	0/0/0/0
5	P6G	A	712	-	-	0/16/16/16	0/0/0/0
2	BCT	B	701	3	-	0/0/0/0	0/0/0/0
2	BCT	B	702	3	-	0/0/0/0	0/0/0/0
4	SO4	B	705	-	-	0/0/0/0	0/0/0/0
4	SO4	B	706	-	-	0/0/0/0	0/0/0/0
4	SO4	B	707	-	-	0/0/0/0	0/0/0/0
4	SO4	B	708	-	-	0/0/0/0	0/0/0/0
4	SO4	B	709	-	-	0/0/0/0	0/0/0/0
4	SO4	B	710	-	-	0/0/0/0	0/0/0/0
4	SO4	B	711	-	-	0/0/0/0	0/0/0/0
4	SO4	B	712	-	-	0/0/0/0	0/0/0/0
4	SO4	B	713	-	-	0/0/0/0	0/0/0/0
5	P6G	B	714	-	-	0/16/16/16	0/0/0/0
5	P6G	B	715	-	-	0/16/16/16	0/0/0/0
2	BCT	C	701	3	-	0/0/0/0	0/0/0/0
2	BCT	C	702	3	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SO4	C	705	-	-	0/0/0/0	0/0/0/0
4	SO4	C	706	-	-	0/0/0/0	0/0/0/0
4	SO4	C	707	-	-	0/0/0/0	0/0/0/0
4	SO4	C	708	-	-	0/0/0/0	0/0/0/0
4	SO4	C	709	-	-	0/0/0/0	0/0/0/0
4	SO4	C	710	-	-	0/0/0/0	0/0/0/0
4	SO4	C	711	-	-	0/0/0/0	0/0/0/0
5	P6G	C	712	-	-	0/16/16/16	0/0/0/0
5	P6G	C	713	-	-	0/16/16/16	0/0/0/0
5	P6G	C	714	-	-	0/16/16/16	0/0/0/0
2	BCT	D	701	3	-	0/0/0/0	0/0/0/0
2	BCT	D	702	3	-	0/0/0/0	0/0/0/0
4	SO4	D	705	-	-	0/0/0/0	0/0/0/0
4	SO4	D	706	-	-	0/0/0/0	0/0/0/0
4	SO4	D	707	-	-	0/0/0/0	0/0/0/0
4	SO4	D	708	-	-	0/0/0/0	0/0/0/0
4	SO4	D	709	-	-	0/0/0/0	0/0/0/0
4	SO4	D	710	-	-	0/0/0/0	0/0/0/0
4	SO4	D	711	-	-	0/0/0/0	0/0/0/0
4	SO4	D	712	-	-	0/0/0/0	0/0/0/0
4	SO4	D	713	-	-	0/0/0/0	0/0/0/0
5	P6G	D	714	-	-	0/16/16/16	0/0/0/0
5	P6G	D	715	-	-	0/16/16/16	0/0/0/0
2	BCT	E	701	3	-	0/0/0/0	0/0/0/0
2	BCT	E	702	3	-	0/0/0/0	0/0/0/0
4	SO4	E	705	-	-	0/0/0/0	0/0/0/0
4	SO4	E	706	-	-	0/0/0/0	0/0/0/0
4	SO4	E	707	-	-	0/0/0/0	0/0/0/0
4	SO4	E	708	-	-	0/0/0/0	0/0/0/0
4	SO4	E	709	-	-	0/0/0/0	0/0/0/0
4	SO4	E	710	-	-	0/0/0/0	0/0/0/0
4	SO4	E	711	-	-	0/0/0/0	0/0/0/0
4	SO4	E	712	-	-	0/0/0/0	0/0/0/0
4	SO4	E	713	-	-	0/0/0/0	0/0/0/0
5	P6G	E	714	-	-	0/16/16/16	0/0/0/0
5	P6G	E	715	-	-	0/16/16/16	0/0/0/0
2	BCT	F	701	3	-	0/0/0/0	0/0/0/0
2	BCT	F	702	3	-	0/0/0/0	0/0/0/0
4	SO4	F	705	-	-	0/0/0/0	0/0/0/0
4	SO4	F	706	-	-	0/0/0/0	0/0/0/0
4	SO4	F	707	-	-	0/0/0/0	0/0/0/0
4	SO4	F	708	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SO4	F	709	-	-	0/0/0/0	0/0/0/0
5	P6G	F	710	-	-	0/16/16/16	0/0/0/0
5	P6G	F	711	-	-	0/16/16/16	0/0/0/0

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	706	SO4	O4-S-O3	-2.39	98.17	108.96
5	D	715	P6G	O4-C5-C6	2.02	119.69	110.41
5	E	714	P6G	C17-O16-C15	2.04	122.16	113.30
5	B	714	P6G	O13-C14-C15	2.09	120.01	110.41
5	D	715	P6G	O13-C12-C11	2.12	120.13	110.41
5	C	713	P6G	O10-C9-C8	2.16	120.33	110.41
5	D	715	P6G	O7-C6-C5	2.19	120.46	110.41
5	F	711	P6G	C8-O7-C6	2.24	123.00	113.30
5	F	711	P6G	O4-C5-C6	2.31	121.00	110.41
5	E	714	P6G	C14-O13-C12	2.48	124.04	113.30

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	705	SO4	1	0
5	A	710	P6G	1	0
5	A	712	P6G	3	0
4	B	707	SO4	1	0
5	B	715	P6G	6	0
2	C	702	BCT	3	0
5	C	712	P6G	1	0
5	C	713	P6G	3	0
4	D	710	SO4	1	0
5	D	714	P6G	4	0
5	D	715	P6G	3	0
5	E	714	P6G	1	0
5	E	715	P6G	3	0
5	F	711	P6G	6	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	674/698 (96%)	0.03	39 (5%) 24 30	15, 39, 77, 97	0
1	B	677/698 (96%)	-0.09	32 (4%) 32 38	13, 33, 72, 97	0
1	C	674/698 (96%)	0.81	122 (18%) 1 2	13, 46, 117, 151	0
1	D	675/698 (96%)	-0.03	23 (3%) 46 53	16, 34, 66, 94	0
1	E	674/698 (96%)	0.02	35 (5%) 28 34	13, 35, 73, 93	0
1	F	676/698 (96%)	-0.04	33 (4%) 30 37	13, 36, 70, 98	0
All	All	4050/4188 (96%)	0.12	284 (7%) 17 22	13, 36, 83, 151	0

All (284) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	479	PHE	14.5
1	C	474	CYS	13.6
1	C	478	GLU	13.0
1	C	564	LEU	11.7
1	C	445	LYS	11.1
1	C	468	TYR	10.5
1	C	472	ASN	10.4
1	C	447	LYS	10.1
1	C	493	SER	8.9
1	C	567	THR	8.5
1	C	612	VAL	8.1
1	C	471	ILE	8.1
1	F	334	ALA	8.0
1	C	480	PHE	7.7
1	A	333	GLU	7.2
1	C	613	THR	7.1
1	C	483	GLY	7.1
1	C	335	PRO	7.1
1	C	476	PHE	6.6

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Mol	Chain	Res	Type	RSRZ
1	C	436	ALA	6.5
1	C	491	ASP	6.5
1	C	665	CYS	6.4
1	C	467	LEU	6.4
1	C	466	LEU	6.4
1	C	497	LEU	6.4
1	B	332	PRO	6.2
1	C	562	LEU	6.2
1	C	570	PRO	6.2
1	F	335	PRO	6.1
1	C	417	ASN	6.0
1	C	481	SER	5.9
1	C	496	LYS	5.9
1	C	473	HIS	5.9
1	C	438	ASP	5.8
1	F	333	GLU	5.8
1	C	449	SER	5.7
1	C	469	ASN	5.7
1	C	332	PRO	5.7
1	C	482	GLU	5.6
1	C	444	LEU	5.5
1	C	475	ARG	5.5
1	F	337	ASP	5.3
1	A	332	PRO	5.3
1	C	485	ALA	5.1
1	F	613	THR	5.1
1	C	494	LEU	4.9
1	C	435	SER	4.9
1	F	279	SER	4.9
1	C	659	VAL	4.9
1	C	477	ASP	4.9
1	C	639	ALA	4.8
1	B	441	TRP	4.7
1	A	334	ALA	4.7
1	C	463	PRO	4.6
1	E	333	GLU	4.6
1	C	561	LEU	4.6
1	C	333	GLU	4.5
1	A	335	PRO	4.5
1	D	613	THR	4.5
1	D	333	GLU	4.4
1	C	336	THR	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	613	THR	4.4
1	C	142	PRO	4.4
1	B	613	THR	4.4
1	F	336	THR	4.4
1	A	336	THR	4.2
1	E	615	CYS	4.2
1	C	610	SER	4.2
1	C	446	GLY	4.2
1	D	332	PRO	4.1
1	C	470	LYS	4.1
1	C	582	ALA	4.1
1	C	437	SER	4.1
1	C	662	LEU	4.1
1	D	441	TRP	4.0
1	B	334	ALA	4.0
1	E	618	ASN	4.0
1	C	141	GLU	3.9
1	C	660	GLY	3.9
1	C	484	CYS	3.9
1	C	431	VAL	3.9
1	D	140	PRO	3.8
1	C	490	LYS	3.8
1	E	478	GLU	3.8
1	C	443	ASN	3.8
1	D	141	GLU	3.8
1	C	606	HIS	3.7
1	A	612	VAL	3.7
1	A	474	CYS	3.7
1	C	489	LYS	3.6
1	C	334	ALA	3.6
1	A	562	LEU	3.6
1	C	337	ASP	3.6
1	C	532	PHE	3.6
1	C	425	GLY	3.6
1	E	576	ASN	3.6
1	A	472	ASN	3.6
1	D	436	ALA	3.6
1	F	439	LEU	3.6
1	A	416	ASP	3.6
1	F	617	GLY	3.6
1	F	436	ALA	3.5
1	F	104	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	442	ASP	3.5
1	A	441	TRP	3.5
1	E	617	GLY	3.5
1	C	439	LEU	3.5
1	F	332	PRO	3.5
1	C	565	ASP	3.4
1	D	564	LEU	3.4
1	B	617	GLY	3.4
1	F	29	VAL	3.4
1	A	468	TYR	3.3
1	F	544	GLY	3.3
1	E	416	ASP	3.3
1	E	613	THR	3.3
1	C	566	GLY	3.2
1	B	473	HIS	3.2
1	E	472	ASN	3.2
1	C	655	TYR	3.2
1	C	464	MET	3.2
1	C	573	GLU	3.2
1	D	617	GLY	3.2
1	A	338	GLU	3.1
1	A	564	LEU	3.1
1	E	557	LYS	3.1
1	A	33	ASP	3.1
1	C	527	LYS	3.1
1	C	563	CYS	3.1
1	C	617	GLY	3.1
1	C	574	TYR	3.1
1	A	614	ASP	3.1
1	C	460	TRP	3.0
1	A	281	GLU	3.0
1	E	468	TYR	3.0
1	B	614	ASP	3.0
1	B	336	THR	3.0
1	F	606	HIS	3.0
1	C	450	CYS	3.0
1	C	560	GLU	2.9
1	C	33	ASP	2.9
1	E	574	TYR	2.9
1	A	565	ASP	2.9
1	D	142	PRO	2.9
1	B	612	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	558	ASP	2.9
1	C	465	GLY	2.9
1	B	33	ASP	2.9
1	C	503	LEU	2.9
1	B	335	PRO	2.9
1	F	543	GLY	2.8
1	A	616	SER	2.8
1	F	612	VAL	2.8
1	A	435	SER	2.8
1	C	421	THR	2.8
1	F	142	PRO	2.8
1	A	576	ASN	2.8
1	D	572	GLU	2.8
1	E	481	SER	2.8
1	B	661	ASN	2.8
1	A	611	ASN	2.7
1	C	661	ASN	2.7
1	B	625	GLU	2.7
1	C	416	ASP	2.7
1	C	338	GLU	2.7
1	F	475	ARG	2.7
1	C	523	CYS	2.7
1	D	570	PRO	2.7
1	B	333	GLU	2.7
1	B	337	ASP	2.7
1	E	334	ALA	2.7
1	E	572	GLU	2.7
1	D	475	ARG	2.7
1	A	476	PHE	2.7
1	A	439	LEU	2.7
1	E	104	ASP	2.7
1	C	501	SER	2.7
1	C	531	ALA	2.7
1	F	33	ASP	2.6
1	B	566	GLY	2.6
1	D	338	GLU	2.6
1	C	492	SER	2.6
1	F	616	SER	2.6
1	C	571	VAL	2.6
1	C	611	ASN	2.6
1	E	616	SER	2.6
1	A	473	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	614	ASP	2.6
1	E	663	ARG	2.6
1	C	432	VAL	2.6
1	B	438	ASP	2.6
1	E	479	PHE	2.5
1	A	444	LEU	2.5
1	B	437	SER	2.5
1	C	616	SER	2.5
1	E	258	GLY	2.5
1	C	578	HIS	2.5
1	C	666	SER	2.5
1	F	607	LEU	2.5
1	D	571	VAL	2.5
1	A	442	ASP	2.5
1	F	602	ARG	2.5
1	A	337	ASP	2.5
1	C	363	VAL	2.5
1	C	495	CYS	2.5
1	E	474	CYS	2.5
1	C	397	TYR	2.5
1	D	677	ARG	2.5
1	F	438	ASP	2.5
1	D	557	LYS	2.5
1	A	437	SER	2.5
1	B	616	SER	2.5
1	B	543	GLY	2.5
1	C	502	GLY	2.5
1	D	566	GLY	2.5
1	F	31	PRO	2.4
1	C	486	PRO	2.4
1	E	437	SER	2.4
1	C	572	GLU	2.4
1	E	142	PRO	2.4
1	F	339	CYS	2.4
1	A	104	ASP	2.4
1	C	414	LYS	2.4
1	C	658	ALA	2.4
1	A	415	SER	2.4
1	F	30	ILE	2.4
1	C	576	ASN	2.3
1	E	438	ASP	2.3
1	C	448	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	90	ASP	2.3
1	F	614	ASP	2.3
1	B	545	LYS	2.3
1	F	338	GLU	2.3
1	F	32	SER	2.3
1	B	338	GLU	2.3
1	A	469	ASN	2.3
1	B	576	ASN	2.3
1	C	454	VAL	2.3
1	C	568	ARG	2.3
1	A	438	ASP	2.3
1	B	471	ILE	2.3
1	E	471	ILE	2.3
1	B	574	TYR	2.3
1	D	335	PRO	2.3
1	C	426	TYR	2.2
1	E	473	HIS	2.2
1	B	475	ARG	2.2
1	C	594	GLU	2.2
1	C	555	ASN	2.2
1	F	555	ASN	2.2
1	A	31	PRO	2.2
1	E	570	PRO	2.2
1	F	281	GLU	2.2
1	C	505	LEU	2.2
1	F	472	ASN	2.2
1	C	524	LEU	2.2
1	C	528	GLY	2.2
1	B	472	ASN	2.2
1	B	416	ASP	2.2
1	E	543	GLY	2.2
1	E	555	ASN	2.1
1	B	557	LYS	2.1
1	C	451	HIS	2.1
1	E	490	LYS	2.1
1	D	344	TRP	2.1
1	C	418	CYS	2.1
1	E	332	PRO	2.1
1	D	477	ASP	2.1
1	D	258	GLY	2.1
1	E	417	ASN	2.1
1	B	442	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	650	TYR	2.1
1	B	329	GLY	2.1
1	A	443	ASN	2.1
1	D	346	ALA	2.1
1	C	557	LYS	2.1
1	B	434	LYS	2.0
1	A	421	THR	2.0
1	C	461	ASN	2.0
1	A	471	ILE	2.0
1	A	567	THR	2.0
1	C	462	ILE	2.0
1	E	436	ALA	2.0
1	E	491	ASP	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	FE	E	703	1/1	1.00	0.14	9.00	19,19,19,19	0
5	P6G	E	714	19/19	0.90	0.21	8.66	28,45,83,84	0
5	P6G	F	710	19/19	0.92	0.16	8.16	37,48,68,71	0
5	P6G	B	714	19/19	0.93	0.14	8.13	22,32,87,87	0
3	FE	D	703	1/1	0.99	0.15	7.99	26,26,26,26	0
3	FE	F	703	1/1	1.00	0.14	6.05	16,16,16,16	0
3	FE	A	703	1/1	1.00	0.15	5.79	19,19,19,19	0
5	P6G	A	711	19/19	0.85	0.16	5.60	46,66,84,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	P6G	C	712	19/19	0.94	0.14	5.28	28,48,79,81	0
3	FE	B	704	1/1	1.00	0.14	4.77	15,15,15,15	0
4	SO4	C	705	5/5	0.97	0.21	4.31	77,78,83,83	0
5	P6G	F	711	19/19	0.90	0.19	4.08	28,48,98,100	0
3	FE	C	704	1/1	1.00	0.14	3.93	16,16,16,16	0
5	P6G	D	714	19/19	0.89	0.18	3.84	41,54,79,79	0
2	BCT	D	702	4/4	0.98	0.12	3.70	23,26,29,32	0
3	FE	D	704	1/1	1.00	0.15	3.53	20,20,20,20	0
4	SO4	A	705	5/5	0.84	0.19	3.47	93,94,95,97	0
5	P6G	A	710	19/19	0.93	0.17	3.42	37,48,77,77	0
4	SO4	A	708	5/5	0.89	0.19	3.12	95,98,99,100	0
5	P6G	E	715	19/19	0.93	0.17	2.95	44,56,71,71	0
4	SO4	F	706	5/5	0.83	0.16	2.93	89,92,95,98	0
2	BCT	F	702	4/4	0.99	0.13	2.81	19,20,21,24	0
3	FE	F	704	1/1	0.99	0.14	2.77	31,31,31,31	0
5	P6G	D	715	19/19	0.79	0.20	2.62	56,74,84,86	0
3	FE	B	703	1/1	1.00	0.12	2.46	29,29,29,29	0
2	BCT	E	701	4/4	0.99	0.10	2.14	14,17,17,18	0
4	SO4	B	708	5/5	0.81	0.21	1.81	86,88,92,96	0
5	P6G	C	714	19/19	0.85	0.20	1.79	56,79,99,100	0
3	FE	E	704	1/1	0.98	0.14	1.76	32,32,32,32	0
4	SO4	A	706	5/5	0.95	0.15	1.69	51,66,69,77	0
5	P6G	B	715	19/19	0.95	0.15	1.68	32,46,94,95	0
2	BCT	E	702	4/4	0.95	0.13	1.53	26,28,29,30	0
4	SO4	C	706	5/5	0.91	0.12	1.50	94,95,97,98	0
5	P6G	C	713	19/19	0.90	0.16	1.45	43,57,83,83	0
4	SO4	D	708	5/5	0.98	0.12	1.39	46,49,58,58	0
2	BCT	B	701	4/4	0.99	0.11	1.24	13,14,15,16	0
4	SO4	D	705	5/5	0.97	0.19	1.23	68,71,72,78	0
4	SO4	F	705	5/5	0.87	0.14	1.21	97,97,98,100	0
3	FE	A	704	1/1	0.99	0.12	1.17	34,34,34,34	0
4	SO4	B	706	5/5	0.94	0.15	1.13	72,79,81,82	0
5	P6G	A	712	19/19	0.83	0.20	0.59	74,81,91,92	0
4	SO4	F	707	5/5	0.94	0.15	0.57	85,87,87,90	0
4	SO4	C	710	5/5	0.96	0.15	0.56	73,77,79,83	0
4	SO4	D	710	5/5	0.98	0.16	0.54	55,55,65,66	0
4	SO4	E	713	5/5	0.89	0.16	0.50	93,95,95,96	0
4	SO4	E	708	5/5	0.94	0.12	0.36	94,95,96,96	0
2	BCT	C	701	4/4	0.99	0.09	0.24	14,15,15,17	0
2	BCT	B	702	4/4	0.98	0.10	0.06	27,27,28,31	0
2	BCT	D	701	4/4	0.98	0.11	0.00	15,17,21,24	0
2	BCT	A	701	4/4	0.99	0.10	-0.07	14,14,16,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	SO4	B	707	5/5	0.91	0.12	-0.09	85,87,90,92	0
4	SO4	E	712	5/5	0.98	0.11	-0.11	44,48,49,50	0
4	SO4	C	707	5/5	0.97	0.10	-0.21	38,55,63,63	0
4	SO4	B	710	5/5	0.97	0.11	-0.40	44,61,65,72	0
2	BCT	A	702	4/4	0.98	0.10	-0.64	28,31,34,38	0
4	SO4	D	713	5/5	0.96	0.12	-0.67	72,73,74,78	0
4	SO4	D	707	5/5	0.98	0.09	-0.80	57,58,59,65	0
2	BCT	F	701	4/4	0.99	0.09	-0.82	8,9,10,11	0
4	SO4	E	707	5/5	0.98	0.09	-0.98	41,55,61,63	0
2	BCT	C	702	4/4	0.95	0.13	-1.69	32,36,38,44	0
3	FE	C	703	1/1	0.96	0.12	-2.52	38,38,38,38	0
4	SO4	D	706	5/5	0.90	0.15	-	101,103,106,109	0
4	SO4	B	713	5/5	0.88	0.20	-	105,107,108,109	0
4	SO4	A	707	5/5	0.90	0.18	-	77,87,88,92	0
4	SO4	A	709	5/5	0.89	0.13	-	97,97,99,99	0
4	SO4	B	709	5/5	0.97	0.10	-	66,67,68,73	0
4	SO4	F	708	5/5	0.95	0.14	-	80,85,87,90	0
4	SO4	C	708	5/5	0.97	0.10	-	70,75,76,79	0
4	SO4	C	709	5/5	0.92	0.13	-	76,77,80,80	0
4	SO4	E	705	5/5	0.91	0.16	-	107,108,109,110	0
4	SO4	C	711	5/5	0.84	0.20	-	106,109,109,110	0
4	SO4	E	711	5/5	0.94	0.17	-	73,77,84,87	0
4	SO4	B	705	5/5	0.98	0.10	-	44,45,49,50	0
4	SO4	B	711	5/5	0.96	0.19	-	63,68,74,77	0
4	SO4	F	709	5/5	0.91	0.13	-	89,89,92,93	0
4	SO4	B	712	5/5	0.95	0.11	-	77,80,83,84	0
4	SO4	E	710	5/5	0.97	0.12	-	73,73,75,79	0
4	SO4	D	709	5/5	0.95	0.11	-	70,72,75,76	0
4	SO4	D	711	5/5	0.97	0.21	-	62,67,73,74	0
4	SO4	D	712	5/5	0.88	0.16	-	95,95,99,100	0
4	SO4	E	709	5/5	0.95	0.11	-	76,77,79,81	0
4	SO4	E	706	5/5	0.84	0.42	-	111,112,113,113	5

6.5 Other polymers [i](#)

There are no such residues in this entry.