



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 10:32 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 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/ValidationPDFNotes.html>

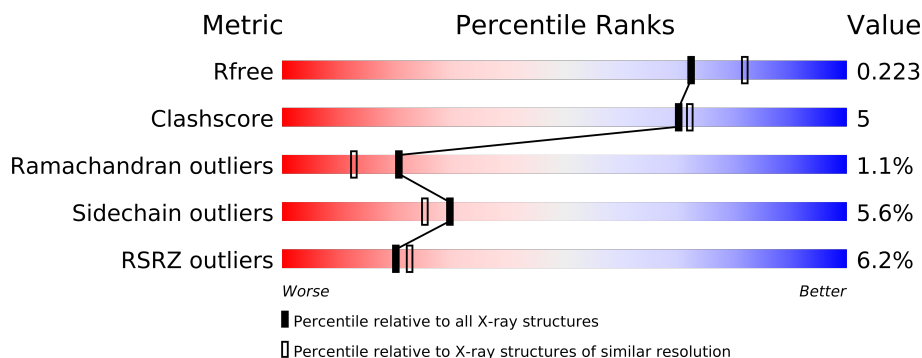
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	3012 (2.10-2.10)
Clashscore	79885	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (2.10-2.10)
RSRZ outliers	66119	3013 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	698	
1	B	698	
1	C	698	
1	D	698	
1	E	698	
1	F	698	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	BCT	D	702	-	X
2	BCT	E	702	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
2	BCT	F	702	-	X
3	FE	A	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	706	-	X
4	SO4	A	707	-	X
4	SO4	A	708	-	X
4	SO4	B	711	-	X
4	SO4	C	705	-	X
4	SO4	C	711	-	X
4	SO4	D	712	-	X
4	SO4	E	706	-	X
4	SO4	E	711	-	X
4	SO4	F	706	-	X
4	SO4	F	709	-	X
5	P6G	A	710	-	X
5	P6G	A	711	-	X
5	P6G	B	714	-	X
5	P6G	B	715	-	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 hydrogen and 0 are deuterium.

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.

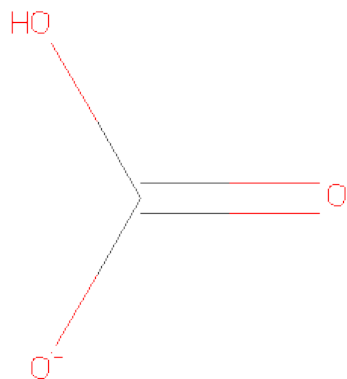
- Molecule 1 is a protein called Serotransferrin.

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).

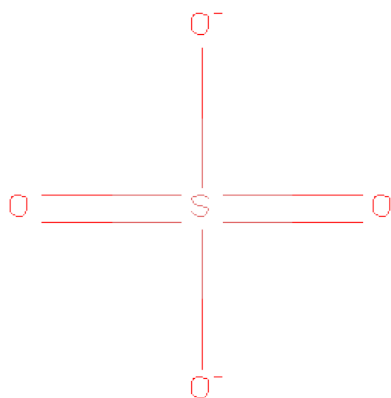


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	1	3		
2	A	1	Total	C	O	0	0
			4	1	3		
2	B	1	Total	C	O	0	0
			4	1	3		
2	B	1	Total	C	O	0	0
			4	1	3		
2	C	1	Total	C	O	0	0
			4	1	3		
2	C	1	Total	C	O	0	0
			4	1	3		
2	D	1	Total	C	O	0	0
			4	1	3		
2	D	1	Total	C	O	0	0
			4	1	3		
2	E	1	Total	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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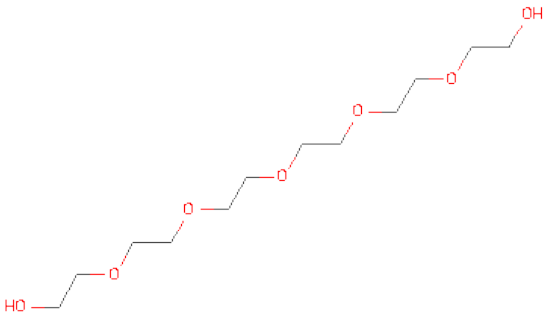
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	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	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.

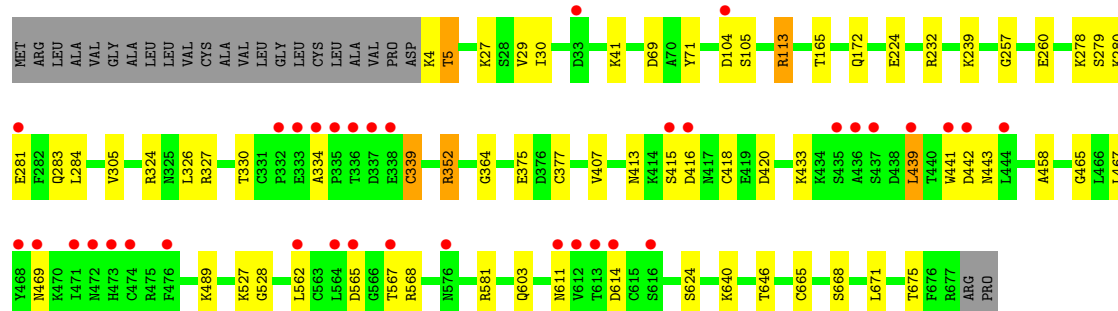
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	352	Total 352	O 352	0	0
6	B	454	Total 454	O 454	0	0
6	C	305	Total 305	O 305	0	0
6	D	398	Total 398	O 398	0	0
6	E	431	Total 431	O 431	0	0
6	F	393	Total 393	O 393	0	0

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 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.

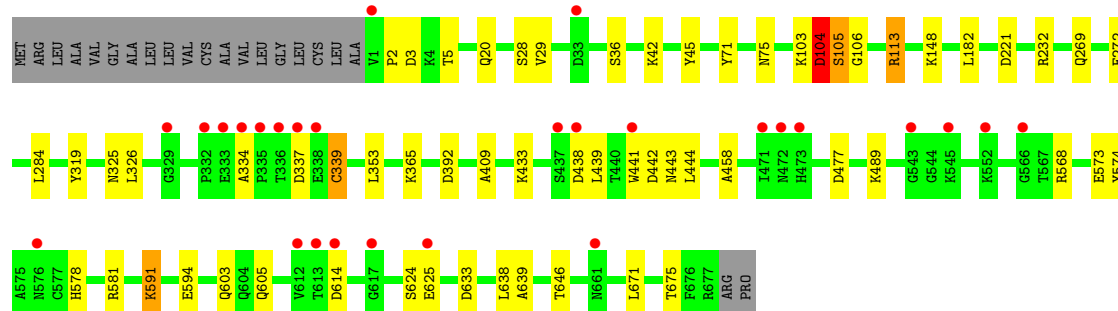
• Molecule 1: Serotransferrin

Chain A: 



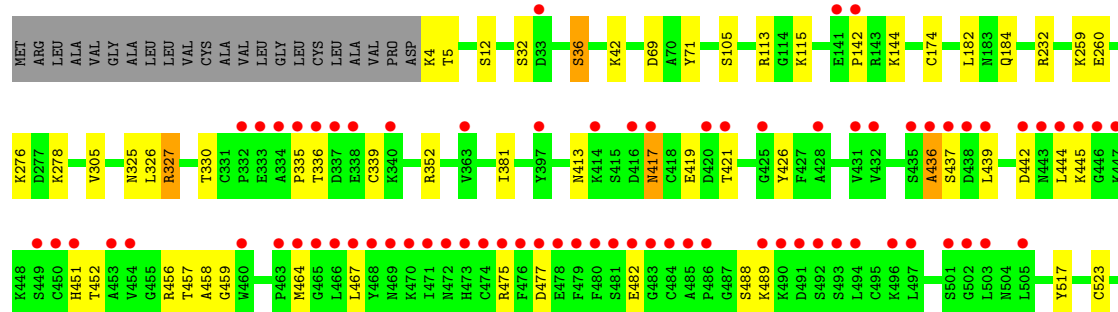
• Molecule 1: Serotransferrin

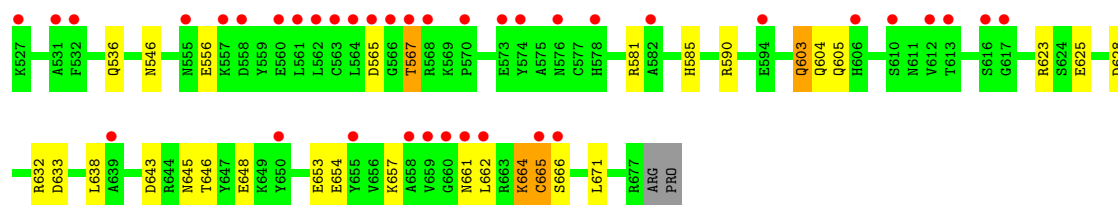
Chain B: 



• Molecule 1: Serotransferrin

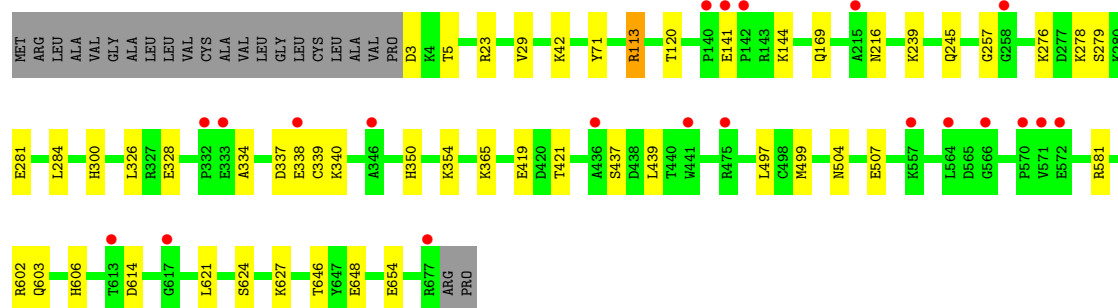
Chain C: 





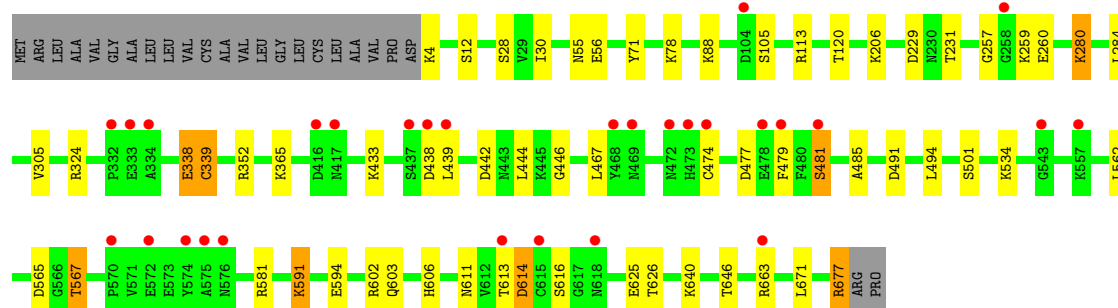
• Molecule 1: Serotransferrin

Chain D:



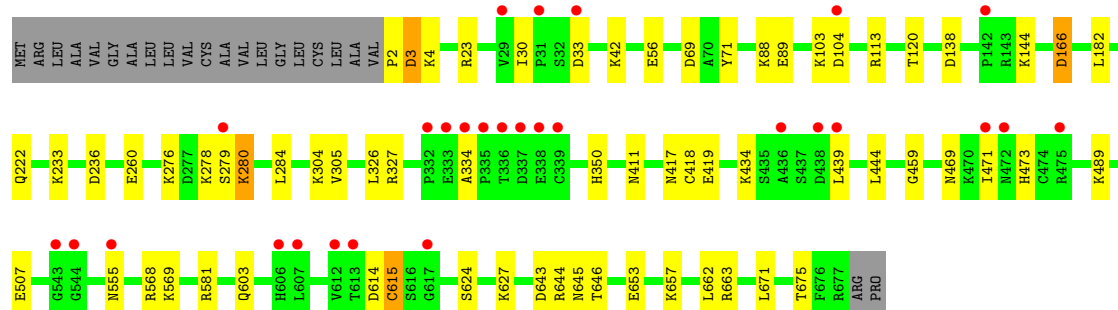
• Molecule 1: Serotransferrin

Chain E:



• Molecule 1: Serotransferrin

Chain F:



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 0.181 , 0.223	Depositor DCC
R_{free} test set	15028 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)	0.37 , 46.2	EDS
Estimated twinning fraction	0.014 for -h-2*1,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 297219 reflections (0.000%)	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.

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5160	0	144	21	0
1	B	5179	0	138	24	0
1	C	5124	0	144	38	0
1	D	5193	0	139	19	0
1	E	5202	0	144	21	0
1	F	5191	0	136	23	0
2	A	8	0	1	1	0
2	B	8	0	0	1	0
2	C	8	0	1	3	0
2	D	8	0	1	1	0
2	E	8	0	1	1	0
2	F	8	0	1	2	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	0	0
4	B	45	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	35	0	0	0	0
4	D	45	0	0	2	0
4	E	45	0	0	0	0
4	F	25	0	0	1	0
5	A	57	0	78	2	0
5	B	38	0	52	2	0
5	C	57	0	78	2	0
5	D	38	0	52	2	0
5	E	38	0	52	2	0
5	F	38	0	52	3	0
6	A	352	0	0	9	0
6	B	454	0	0	10	0
6	C	305	0	0	13	0
6	D	398	0	0	12	0
6	E	431	0	0	10	0
6	F	393	0	0	9	0
All	All	33928	0	1214	150	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

All (150) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:169:GLN:NE2	6:D:936:HOH:O	2.16	0.78
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:C:664:LYS:O	6:C:942:HOH:O	2.04	0.74
1:B:269:GLN:NE2	6:B:983:HOH:O	2.20	0.74
1:D:507:GLU:OE2	6:D:979:HOH:O	2.06	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:603:GLN:OE1	1:C:604:GLN:NE2	2.24	0.70
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
1:B:20:GLN:NE2	6:B:1222:HOH:O	2.26	0.69
1:F:459:GLY:N	2:F:702:BCT:HO3	1.91	0.68
1:C:69:ASP:OD1	1:C:327:ARG:NH1	2.26	0.68
1:C:452:THR:OG1	2:C:702:BCT:O3	2.08	0.68
1:D:239:LYS:NZ	6:D:1053:HOH:O	2.27	0.67
1:F:350:HIS:ND1	6:F:911:HOH:O	2.28	0.66
1:C:327:ARG:NH2	6:C:965:HOH:O	2.28	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:465:GLY:O	1:A:469:ASN:ND2	2.28	0.66
1:F:4:LYS:NZ	1:F:33:ASP:O	2.26	0.65
1:B:339:CYS:SG	6:B:1202:HOH:O	2.53	0.65
1:C:115:LYS:NZ	6:C:954:HOH:O	2.28	0.65
1:D:350:HIS:ND1	6:D:991:HOH:O	2.29	0.65
1:A:324:ARG:NH2	6:A:1126:HOH:O	2.30	0.63
1:B:104:ASP:O	1:B:106:GLY:N	2.31	0.63
1:B:591:LYS:NZ	6:B:949:HOH:O	2.32	0.63
1:B:2:PRO:HD2	1:B:5:THR:OG1	1.99	0.63
1:E:56:GLU:OE1	5:E:715:P6G:O19	2.14	0.62
1:C:451:HIS:ND1	1:C:459:GLY:O	2.33	0.61
1:F:42:LYS:NZ	5:F:711:P6G:H91	2.16	0.60
1:C:413:ASN:ND2	6:C:1006:HOH:O	2.34	0.60
1:C:664:LYS:O	1:C:666:SER:N	2.34	0.60
1:B:103:LYS:NZ	1:B:221:ASP:O	2.34	0.60
1:F:304:LYS:NZ	6:F:1103:HOH:O	2.34	0.60
1:F:276:LYS:NZ	6:F:1064:HOH:O	2.33	0.60
1:F:233:LYS:NZ	6:F:957:HOH:O	2.34	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:325:ASN:ND2	6:B:1185:HOH:O	2.36	0.58
1:C:517:TYR:OH	1:C:632:ARG:NH1	2.36	0.58
1:F:507:GLU:OE2	6:F:865:HOH:O	2.17	0.57
1:B:105:SER:OG	1:B:232:ARG:NH2	2.37	0.57
1:F:417:ASN:O	1:F:419:GLU:N	2.37	0.57
1:C:456:ARG:NE	2:C:702:BCT:O1	2.37	0.56
1:E:78:LYS:NZ	1:E:260:GLU:OE1	2.38	0.56
1:E:591:LYS:NZ	1:E:594:GLU:OE1	2.38	0.56
1:D:216:ASN:N	6:D:1151:HOH:O	2.39	0.56
1:A:172:GLN:NE2	6:A:1042:HOH:O	2.39	0.56
5:D:714:P6G:O19	6:D:897:HOH:O	2.18	0.55
1:A:105:SER:OG	1:A:232:ARG:NH2	2.40	0.55
5:A:712:P6G:O1	6:A:1097:HOH:O	2.16	0.54
1:C:536:GLN:N	6:C:832:HOH:O	2.41	0.54
1:E:491:ASP:N	6:E:912:HOH:O	2.40	0.54
1:E:677:ARG:NH2	6:E:1197:HOH:O	2.40	0.54
1:A:41:LYS:O	5:A:710:P6G:H32	2.08	0.53
1:B:42:LYS:NZ	5:B:715:P6G:H172	2.23	0.52
1:D:300:HIS:ND1	4:D:710:SO4:O2	2.42	0.52
1:E:280:LYS:NZ	6:E:1037:HOH:O	2.42	0.52
1:A:433:LYS:NZ	1:A:528:GLY:O	2.43	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:41:LYS:NZ	6:A:1091:HOH:O	2.43	0.52
1:F:138:ASP:OD1	6:F:897:HOH:O	2.19	0.52
1:C:623:ARG:NH2	1:C:633:ASP:O	2.43	0.52
1:B:75:ASN:ND2	6:B:1047:HOH:O	2.43	0.52
1:F:653:GLU:OE1	1:F:653:GLU:N	2.44	0.51
1:A:364:GLY:N	6:A:887:HOH:O	2.44	0.51
1:E:206:LYS:NZ	6:E:1071:HOH:O	2.42	0.51
1:C:417:ASN:O	1:C:419:GLU:N	2.43	0.50
1:C:645:ASN:ND2	6:C:1052:HOH:O	2.44	0.50
1:C:605:GLN:OE1	1:C:638:LEU:N	2.44	0.50
1:B:574:TYR:O	1:B:578:HIS:ND1	2.44	0.50
1:E:446:GLY:N	1:E:479:PHE:O	2.45	0.50
1:A:420:ASP:OD1	1:A:640:LYS:NZ	2.45	0.50
1:D:337:ASP:OD1	6:D:1068:HOH:O	2.19	0.50
1:F:103:LYS:NZ	6:F:896:HOH:O	2.45	0.50
1:E:442:ASP:OD1	1:E:442:ASP:N	2.44	0.49
1:A:69:ASP:OD1	1:A:327:ARG:NH1	2.46	0.48
1:E:602:ARG:O	1:E:606:HIS:ND1	2.46	0.48
1:E:485:ALA:N	1:E:494:LEU:O	2.46	0.48
1:F:69:ASP:OD1	1:F:327:ARG:NH1	2.47	0.48
5:C:712:P6G:O19	5:C:712:P6G:O1	2.23	0.48
1:A:441:TRP:O	1:A:443:ASN:N	2.47	0.48
1:C:278:LYS:NZ	6:C:1088:HOH:O	2.46	0.47
1:B:594:GLU:OE2	6:B:1174:HOH:O	2.20	0.47
1:F:166:ASP:OD1	1:F:166:ASP:N	2.47	0.47
1:A:527:LYS:NZ	6:A:947:HOH:O	2.46	0.47
1:C:546:ASN:N	6:C:1003:HOH:O	2.47	0.47
1:F:411:ASN:ND2	1:F:418:CYS:O	2.48	0.47
1:C:426:TYR:OH	1:C:585:HIS:NE2	2.48	0.47
1:B:624:SER:OG	1:B:633:ASP:OD1	2.33	0.47
1:B:42:LYS:NZ	5:B:715:P6G:H112	2.30	0.47
1:F:555:ASN:N	6:F:1094:HOH:O	2.47	0.47
1:A:27:LYS:NZ	6:A:942:HOH:O	2.47	0.47
1:C:325:ASN:ND2	6:C:878:HOH:O	2.47	0.47
1:F:56:GLU:OE1	5:F:711:P6G:O19	2.22	0.46
1:D:504:ASN:ND2	6:D:932:HOH:O	2.47	0.46
1:B:433:LYS:NZ	6:B:1150:HOH:O	2.47	0.46
1:C:603:GLN:NE2	6:C:1100:HOH:O	2.49	0.46
1:E:534:LYS:NZ	6:E:917:HOH:O	2.48	0.46
1:B:438:ASP:O	1:B:443:ASN:ND2	2.48	0.46
5:E:715:P6G:H121	5:E:715:P6G:H91	1.40	0.46
1:D:42:LYS:NZ	5:D:714:P6G:H122	2.30	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:3:ASP:N	1:B:3:ASP:OD1	2.49	0.46
1:C:565:ASP:OD1	1:C:567:THR:OG1	2.34	0.46
1:D:419:GLU:OE1	1:D:602:ARG:NH2	2.48	0.46
1:A:375:GLU:OE2	1:A:668:SER:OG	2.32	0.46
1:B:458:ALA:N	2:B:702:BCT:O2	2.50	0.45
1:E:280:LYS:NZ	6:E:1174:HOH:O	2.49	0.45
1:F:2:PRO:O	1:F:3:ASP:HB2	2.16	0.45
1:D:23:ARG:NE	4:D:709:SO4:O3	2.48	0.45
1:C:458:ALA:N	2:C:702:BCT:O2	2.50	0.45
1:C:381:ILE:O	1:C:590:ARG:NH1	2.50	0.45
1:E:324:ARG:NH2	6:E:887:HOH:O	2.50	0.45
1:B:605:GLN:OE1	1:B:638:LEU:N	2.50	0.44
1:D:646:THR:OG1	1:D:648:GLU:OE1	2.36	0.44
1:E:55:ASN:ND2	6:E:926:HOH:O	2.50	0.44
1:B:409:ALA:O	1:B:639:ALA:N	2.50	0.44
1:A:565:ASP:OD1	1:A:567:THR:OG1	2.36	0.44
1:A:4:LYS:HG3	1:A:5:THR:H	1.83	0.43
1:D:120:THR:OG1	2:D:701:BCT:O3	2.36	0.43
1:C:628:ASP:OD1	1:C:633:ASP:N	2.51	0.43
1:D:245:GLN:NE2	6:D:1104:HOH:O	2.52	0.43
1:A:278:LYS:O	1:A:280:LYS:N	2.51	0.43
1:C:5:THR:HG22	1:C:36:SER:CB	2.49	0.42
1:F:278:LYS:O	1:F:280:LYS:N	2.52	0.42
1:A:458:ALA:N	2:A:702:BCT:O2	2.51	0.42
1:C:436:ALA:N	1:C:437:SER:CA	2.82	0.42
1:D:419:GLU:OE2	1:D:606:HIS:NE2	2.53	0.42
1:E:120:THR:OG1	2:E:701:BCT:O3	2.38	0.42
1:D:340:LYS:NZ	6:D:1143:HOH:O	2.52	0.42
1:F:120:THR:OG1	2:F:701:BCT:O3	2.37	0.41
1:D:627:LYS:NZ	6:D:1119:HOH:O	2.53	0.41
1:E:477:ASP:OD1	1:E:477:ASP:N	2.53	0.41
1:C:105:SER:OG	1:C:232:ARG:NH2	2.53	0.41
1:C:335:PRO:O	1:C:336:THR:OG1	2.38	0.41
1:E:229:ASP:OD1	1:E:231:THR:OG1	2.39	0.41
1:B:477:ASP:N	1:B:477:ASP:OD1	2.54	0.41
1:D:276:LYS:NZ	6:D:987:HOH:O	2.53	0.41
1:C:654:GLU:OE1	1:F:88:LYS:NZ	2.54	0.41
1:B:45:TYR:OH	6:B:910:HOH:O	2.22	0.41
1:C:4:LYS:HA	1:C:4:LYS:HD2	1.85	0.41
1:D:354:LYS:NZ	1:D:621:LEU:O	2.53	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:23:ARG:NE	4:F:709:SO4:O4	2.53	0.40
1:C:477:ASP:N	1:C:477:ASP:OD1	2.53	0.40
1:C:174:CYS:SG	1:C:174:CYS:O	2.79	0.40
5:F:711:P6G:H81	6:F:890:HOH:O	2.22	0.40
1:B:319:TYR:N	6:B:1098:HOH:O	2.55	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	672/698 (96%)	621 (92%)	42 (6%)	9 (1%)	18	10
1	B	675/698 (97%)	630 (93%)	39 (6%)	6 (1%)	25	17
1	C	672/698 (96%)	617 (92%)	46 (7%)	9 (1%)	18	10
1	D	673/698 (96%)	630 (94%)	37 (6%)	6 (1%)	25	17
1	E	672/698 (96%)	632 (94%)	35 (5%)	5 (1%)	30	23
1	F	674/698 (97%)	623 (92%)	43 (6%)	8 (1%)	19	11
All	All	4038/4188 (96%)	3753 (93%)	242 (6%)	43 (1%)	21	13

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
1	F	279	SER
1	F	614	ASP
1	B	442	ASP
1	C	439	LEU

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Mol	Chain	Res	Type
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%)	27	22
1	B	547/585 (94%)	519 (95%)	28 (5%)	33	29
1	C	539/585 (92%)	503 (93%)	36 (7%)	23	18
1	D	555/585 (95%)	535 (96%)	20 (4%)	47	46
1	E	560/585 (96%)	525 (94%)	35 (6%)	25	21
1	F	553/585 (94%)	521 (94%)	32 (6%)	28	23
All	All	3301/3510 (94%)	3117 (94%)	184 (6%)	30	25

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
1	A	562	LEU
1	A	581	ARG
1	A	603	GLN
1	A	611	ASN

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Mol	Chain	Res	Type
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
1	C	184	GLN
1	C	259	LYS
1	C	260	GLU
1	C	276	LYS

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Mol	Chain	Res	Type
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
1	D	421	THR
1	D	439	LEU
1	D	497	LEU
1	D	499	MET

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Mol	Chain	Res	Type
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
1	F	30	ILE
1	F	71	TYR
1	F	89	GLU
1	F	104	ASP

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Mol	Chain	Res	Type
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. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains 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	0.17	0	6,6,6	0.10	0
4	SO4	A	706	-	4,4,4	0.07	0	6,6,6	0.22	0
4	SO4	A	707	-	4,4,4	0.17	0	6,6,6	0.18	0
4	SO4	A	708	-	4,4,4	0.25	0	6,6,6	0.10	0
4	SO4	A	709	-	4,4,4	0.20	0	6,6,6	0.10	0
5	P6G	A	710	-	18,18,18	0.70	0	17,17,17	1.45	0
5	P6G	A	711	-	18,18,18	0.65	0	17,17,17	1.50	0
5	P6G	A	712	-	18,18,18	0.70	0	17,17,17	1.43	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	0.26	0	6,6,6	0.28	0
4	SO4	B	706	-	4,4,4	0.18	0	6,6,6	0.16	0
4	SO4	B	707	-	4,4,4	0.20	0	6,6,6	0.09	0
4	SO4	B	708	-	4,4,4	0.09	0	6,6,6	0.24	0
4	SO4	B	709	-	4,4,4	0.21	0	6,6,6	0.21	0
4	SO4	B	710	-	4,4,4	0.16	0	6,6,6	0.16	0
4	SO4	B	711	-	4,4,4	0.23	0	6,6,6	0.10	0
4	SO4	B	712	-	4,4,4	0.14	0	6,6,6	0.06	0
4	SO4	B	713	-	4,4,4	0.18	0	6,6,6	0.14	0
5	P6G	B	714	-	18,18,18	0.73	0	17,17,17	1.25	1 (5%)
5	P6G	B	715	-	18,18,18	0.70	0	17,17,17	1.44	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	0.24	0	6,6,6	0.09	0
4	SO4	C	706	-	4,4,4	0.11	0	6,6,6	0.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	C	707	-	4,4,4	0.21	0	6,6,6	0.23	0
4	SO4	C	708	-	4,4,4	0.17	0	6,6,6	0.14	0
4	SO4	C	709	-	4,4,4	0.16	0	6,6,6	0.16	0
4	SO4	C	710	-	4,4,4	0.16	0	6,6,6	0.10	0
4	SO4	C	711	-	4,4,4	0.15	0	6,6,6	0.08	0
5	P6G	C	712	-	18,18,18	0.72	0	17,17,17	1.40	0
5	P6G	C	713	-	18,18,18	0.67	0	17,17,17	1.50	1 (5%)
5	P6G	C	714	-	18,18,18	0.65	0	17,17,17	1.50	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	0.13	0	6,6,6	0.11	0
4	SO4	D	706	-	4,4,4	0.21	0	6,6,6	0.10	0
4	SO4	D	707	-	4,4,4	0.16	0	6,6,6	0.22	0
4	SO4	D	708	-	4,4,4	0.19	0	6,6,6	0.12	0
4	SO4	D	709	-	4,4,4	0.22	0	6,6,6	0.15	0
4	SO4	D	710	-	4,4,4	0.16	0	6,6,6	0.17	0
4	SO4	D	711	-	4,4,4	0.20	0	6,6,6	0.09	0
4	SO4	D	712	-	4,4,4	0.17	0	6,6,6	0.14	0
4	SO4	D	713	-	4,4,4	0.22	0	6,6,6	0.07	0
5	P6G	D	714	-	18,18,18	0.68	0	17,17,17	1.52	0
5	P6G	D	715	-	18,18,18	0.61	0	17,17,17	1.72	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	0.19	0	6,6,6	0.07	0
4	SO4	E	706	-	4,4,4	1.73	1 (25%)	6,6,6	1.21	1 (16%)
4	SO4	E	707	-	4,4,4	0.11	0	6,6,6	0.17	0
4	SO4	E	708	-	4,4,4	0.16	0	6,6,6	0.07	0
4	SO4	E	709	-	4,4,4	0.18	0	6,6,6	0.15	0
4	SO4	E	710	-	4,4,4	0.17	0	6,6,6	0.14	0
4	SO4	E	711	-	4,4,4	0.16	0	6,6,6	0.12	0
4	SO4	E	712	-	4,4,4	0.14	0	6,6,6	0.14	0
4	SO4	E	713	-	4,4,4	0.15	0	6,6,6	0.08	0
5	P6G	E	714	-	18,18,18	0.67	0	17,17,17	1.52	1 (5%)
5	P6G	E	715	-	18,18,18	0.72	0	17,17,17	1.36	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	0.18	0	6,6,6	0.09	0
4	SO4	F	706	-	4,4,4	0.15	0	6,6,6	0.12	0
4	SO4	F	707	-	4,4,4	0.18	0	6,6,6	0.11	0
4	SO4	F	708	-	4,4,4	0.16	0	6,6,6	0.10	0
4	SO4	F	709	-	4,4,4	0.16	0	6,6,6	0.08	0
5	P6G	F	710	-	18,18,18	0.71	0	17,17,17	1.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	P6G	F	711	-	18,18,18	0.69	0	17,17,17	1.61	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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	706	SO4	O4-S	-2.31	1.39	1.47

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	706	SO4	O4-S-O3	-2.58	98.17	109.08
5	E	714	P6G	C14-O13-C12	2.42	124.04	113.38
5	F	711	P6G	O4-C5-C6	2.32	121.00	110.47
5	D	715	P6G	O7-C6-C5	2.20	120.46	110.47
5	F	711	P6G	C8-O7-C6	2.19	123.00	113.38
5	C	713	P6G	O10-C9-C8	2.17	120.33	110.47
5	D	715	P6G	O13-C12-C11	2.13	120.13	110.47
5	B	714	P6G	O13-C14-C15	2.10	120.01	110.47
5	D	715	P6G	O4-C5-C6	2.03	119.69	110.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.01	36 (5%)	25	28	15, 39, 77, 97	0
1	B	677/698 (96%)	-0.10	27 (3%)	36	41	13, 33, 72, 97	0
1	C	674/698 (96%)	0.74	113 (16%)	2	2	13, 46, 117, 151	0
1	D	675/698 (96%)	-0.06	21 (3%)	47	52	16, 34, 66, 94	0
1	E	674/698 (96%)	-0.02	29 (4%)	34	38	13, 35, 73, 93	0
1	F	676/698 (96%)	-0.07	28 (4%)	35	40	13, 36, 70, 98	0
All	All	4050/4188 (96%)	0.08	254 (6%)	20	22	13, 36, 83, 151	0

All (254) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	479	PHE	13.6
1	C	474	CYS	12.8
1	C	478	GLU	12.1
1	C	564	LEU	11.1
1	C	445	LYS	10.8
1	C	468	TYR	9.8
1	C	472	ASN	9.3
1	C	567	THR	8.9
1	C	447	LYS	8.2
1	F	334	ALA	7.7
1	C	612	VAL	7.5
1	A	333	GLU	7.3
1	C	613	THR	7.3
1	C	471	ILE	7.2
1	C	493	SER	7.1
1	C	480	PHE	6.7
1	C	436	ALA	6.5
1	C	335	PRO	6.4
1	C	467	LEU	6.3

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Mol	Chain	Res	Type	RSRZ
1	C	570	PRO	6.2
1	C	483	GLY	6.2
1	C	497	LEU	6.2
1	C	476	PHE	6.1
1	C	491	ASP	6.1
1	C	438	ASP	6.1
1	C	469	ASN	6.1
1	C	466	LEU	5.9
1	B	332	PRO	5.6
1	C	475	ARG	5.6
1	C	562	LEU	5.6
1	C	417	ASN	5.5
1	C	665	CYS	5.4
1	F	333	GLU	5.4
1	C	496	LYS	5.3
1	F	335	PRO	5.3
1	C	481	SER	5.3
1	C	332	PRO	5.3
1	F	337	ASP	5.3
1	C	473	HIS	5.2
1	C	449	SER	5.2
1	C	659	VAL	5.2
1	C	444	LEU	5.1
1	C	435	SER	5.0
1	C	485	ALA	4.9
1	A	332	PRO	4.8
1	C	482	GLU	4.6
1	F	279	SER	4.6
1	C	439	LEU	4.5
1	B	441	TRP	4.5
1	A	336	THR	4.4
1	F	336	THR	4.4
1	A	613	THR	4.4
1	C	561	LEU	4.3
1	B	613	THR	4.2
1	C	336	THR	4.2
1	D	333	GLU	4.2
1	C	437	SER	4.1
1	A	334	ALA	4.1
1	C	639	ALA	4.1
1	C	494	LEU	4.1
1	E	333	GLU	4.1

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Mol	Chain	Res	Type	RSRZ
1	C	470	LYS	4.1
1	C	606	HIS	4.1
1	D	441	TRP	4.0
1	A	562	LEU	3.9
1	C	333	GLU	3.9
1	C	662	LEU	3.9
1	F	439	LEU	3.9
1	C	582	ALA	3.9
1	E	576	ASN	3.8
1	E	478	GLU	3.8
1	C	446	GLY	3.8
1	C	463	PRO	3.8
1	C	142	PRO	3.8
1	C	141	GLU	3.7
1	F	436	ALA	3.7
1	F	613	THR	3.7
1	C	565	ASP	3.6
1	D	332	PRO	3.6
1	A	335	PRO	3.6
1	C	532	PHE	3.5
1	C	431	VAL	3.5
1	D	613	THR	3.5
1	C	465	GLY	3.5
1	D	141	GLU	3.5
1	C	442	ASP	3.5
1	C	425	GLY	3.5
1	C	477	ASP	3.5
1	D	436	ALA	3.4
1	A	612	VAL	3.4
1	B	473	HIS	3.4
1	C	489	LYS	3.4
1	F	29	VAL	3.4
1	C	337	ASP	3.4
1	D	564	LEU	3.3
1	F	332	PRO	3.3
1	F	104	ASP	3.3
1	A	441	TRP	3.3
1	A	439	LEU	3.3
1	C	610	SER	3.3
1	C	655	TYR	3.3
1	A	472	ASN	3.3
1	B	334	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	443	ASN	3.2
1	A	435	SER	3.2
1	A	565	ASP	3.2
1	E	615	CYS	3.2
1	C	566	GLY	3.1
1	C	490	LYS	3.1
1	C	484	CYS	3.1
1	B	333	GLU	3.1
1	C	464	MET	3.1
1	E	468	TYR	3.1
1	E	472	ASN	3.1
1	A	576	ASN	3.0
1	E	572	GLU	3.0
1	B	617	GLY	2.9
1	A	338	GLU	2.9
1	C	573	GLU	2.9
1	E	557	LYS	2.9
1	D	140	PRO	2.9
1	C	560	GLU	2.9
1	C	660	GLY	2.9
1	A	416	ASP	2.9
1	E	481	SER	2.9
1	A	468	TYR	2.9
1	C	576	ASN	2.8
1	E	618	ASN	2.8
1	E	613	THR	2.8
1	C	334	ALA	2.8
1	D	142	PRO	2.8
1	C	527	LYS	2.7
1	C	531	ALA	2.7
1	C	574	TYR	2.7
1	B	33	ASP	2.7
1	B	612	VAL	2.7
1	D	566	GLY	2.7
1	B	336	THR	2.7
1	A	564	LEU	2.7
1	E	543	GLY	2.7
1	A	474	CYS	2.7
1	B	576	ASN	2.7
1	C	421	THR	2.7
1	B	438	ASP	2.7
1	C	450	CYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	574	TYR	2.7
1	A	614	ASP	2.6
1	D	570	PRO	2.6
1	A	415	SER	2.6
1	A	616	SER	2.6
1	C	338	GLU	2.6
1	E	104	ASP	2.6
1	C	563	CYS	2.6
1	C	503	LEU	2.6
1	F	617	GLY	2.6
1	B	614	ASP	2.6
1	A	476	PHE	2.6
1	C	617	GLY	2.6
1	D	338	GLU	2.6
1	E	575	ALA	2.6
1	B	335	PRO	2.6
1	F	339	CYS	2.6
1	C	558	ASP	2.6
1	D	475	ARG	2.6
1	D	215	ALA	2.6
1	A	436	ALA	2.5
1	F	142	PRO	2.5
1	C	33	ASP	2.5
1	F	544	GLY	2.5
1	F	438	ASP	2.5
1	A	444	LEU	2.5
1	E	332	PRO	2.5
1	F	543	GLY	2.5
1	A	104	ASP	2.5
1	F	475	ARG	2.5
1	E	439	LEU	2.5
1	A	469	ASN	2.4
1	C	414	LYS	2.4
1	D	572	GLU	2.4
1	E	416	ASP	2.4
1	D	571	VAL	2.4
1	F	338	GLU	2.4
1	B	1	VAL	2.4
1	C	460	TRP	2.4
1	C	578	HIS	2.4
1	A	437	SER	2.4
1	A	611	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	661	ASN	2.4
1	C	616	SER	2.4
1	B	472	ASN	2.4
1	C	363	VAL	2.4
1	C	650	TYR	2.4
1	E	479	PHE	2.4
1	B	543	GLY	2.4
1	C	502	GLY	2.3
1	D	258	GLY	2.3
1	D	617	GLY	2.3
1	B	471	ILE	2.3
1	B	545	LYS	2.3
1	C	416	ASP	2.3
1	B	566	GLY	2.3
1	F	607	LEU	2.3
1	C	432	VAL	2.3
1	C	555	ASN	2.3
1	A	281	GLU	2.3
1	B	338	GLU	2.3
1	E	258	GLY	2.3
1	E	334	ALA	2.3
1	B	437	SER	2.2
1	C	568	ARG	2.2
1	E	663	ARG	2.2
1	B	661	ASN	2.2
1	A	337	ASP	2.2
1	F	471	ILE	2.2
1	D	677	ARG	2.2
1	F	472	ASN	2.2
1	B	337	ASP	2.2
1	A	567	THR	2.2
1	A	473	HIS	2.2
1	C	397	TYR	2.2
1	A	471	ILE	2.2
1	C	340	LYS	2.2
1	C	454	VAL	2.2
1	E	438	ASP	2.2
1	C	492	SER	2.2
1	B	329	GLY	2.1
1	A	442	ASP	2.1
1	E	469	ASN	2.1
1	E	570	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	612	VAL	2.1
1	E	474	CYS	2.1
1	C	453	ALA	2.1
1	C	451	HIS	2.1
1	E	473	HIS	2.1
1	F	606	HIS	2.1
1	C	666	SER	2.1
1	C	420	ASP	2.1
1	C	557	LYS	2.1
1	F	33	ASP	2.1
1	C	594	GLU	2.1
1	F	31	PRO	2.1
1	E	437	SER	2.1
1	C	505	LEU	2.1
1	D	346	ALA	2.1
1	C	486	PRO	2.1
1	B	552	LYS	2.1
1	C	658	ALA	2.0
1	A	33	ASP	2.0
1	C	501	SER	2.0
1	B	625	GLU	2.0
1	E	417	ASN	2.0
1	F	555	ASN	2.0
1	C	428	ALA	2.0
1	D	557	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	SO4	E	706	5/5	0.44	14.87	111,112,113,113	5
4	SO4	B	711	5/5	0.19	12.69	63,68,74,77	0
5	P6G	F	710	19/19	0.16	9.18	37,48,68,71	0
3	FE	E	703	1/1	0.13	8.25	19,19,19,19	0
5	P6G	B	714	19/19	0.14	7.85	22,32,87,87	0
4	SO4	A	707	5/5	0.18	7.71	77,87,88,92	0
3	FE	A	703	1/1	0.15	7.53	19,19,19,19	0
5	P6G	E	714	19/19	0.20	7.06	28,45,83,84	0
4	SO4	E	711	5/5	0.17	6.82	73,77,84,87	0
5	P6G	A	711	19/19	0.17	6.08	46,66,84,85	0
4	SO4	C	711	5/5	0.19	5.78	106,109,109,110	0
3	FE	B	704	1/1	0.14	5.75	15,15,15,15	0
3	FE	F	703	1/1	0.13	5.71	16,16,16,16	0
3	FE	D	703	1/1	0.14	5.47	26,26,26,26	0
5	P6G	D	714	19/19	0.18	4.23	41,54,79,79	0
5	P6G	C	712	19/19	0.15	4.13	28,48,79,81	0
5	P6G	F	711	19/19	0.18	4.02	28,48,98,100	0
4	SO4	F	709	5/5	0.13	4.01	89,89,92,93	0
4	SO4	A	705	5/5	0.21	3.95	93,94,95,97	0
4	SO4	C	705	5/5	0.20	3.90	77,78,83,83	0
4	SO4	A	708	5/5	0.19	3.82	95,98,99,100	0
3	FE	D	704	1/1	0.14	3.62	20,20,20,20	0
3	FE	F	704	1/1	0.14	3.48	31,31,31,31	0
5	P6G	D	715	19/19	0.23	3.39	56,74,84,86	0
3	FE	C	704	1/1	0.13	3.32	16,16,16,16	0
2	BCT	F	702	4/4	0.13	3.04	19,20,21,24	0
2	BCT	D	702	4/4	0.12	2.98	23,26,29,32	0
4	SO4	D	712	5/5	0.18	2.86	95,95,99,100	0
4	SO4	F	706	5/5	0.15	2.84	89,92,95,98	0
5	P6G	E	715	19/19	0.16	2.78	44,56,71,71	0
5	P6G	A	710	19/19	0.15	2.50	37,48,77,77	0
5	P6G	B	715	19/19	0.16	2.32	32,46,94,95	0
2	BCT	E	702	4/4	0.13	2.15	26,28,29,30	0
4	SO4	A	706	5/5	0.15	2.04	51,66,69,77	0
2	BCT	E	701	4/4	0.10	1.95	14,17,17,18	0
3	FE	E	704	1/1	0.14	1.95	32,32,32,32	0
3	FE	B	703	1/1	0.11	1.90	29,29,29,29	0
5	P6G	C	713	19/19	0.16	1.74	43,57,83,83	0
3	FE	A	704	1/1	0.12	1.74	34,34,34,34	0
4	SO4	E	705	5/5	0.15	1.72	107,108,109,110	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	P6G	C	714	19/19	0.20	1.69	56,79,99,100	0
4	SO4	B	713	5/5	0.20	1.68	105,107,108,109	0
2	BCT	B	701	4/4	0.11	1.48	13,14,15,16	0
4	SO4	C	706	5/5	0.12	1.34	94,95,97,98	0
4	SO4	D	705	5/5	0.18	1.17	68,71,72,78	0
4	SO4	D	708	5/5	0.12	1.15	46,49,58,58	0
4	SO4	B	708	5/5	0.20	1.08	86,88,92,96	0
2	BCT	C	701	4/4	0.09	1.06	14,15,15,17	0
4	SO4	E	713	5/5	0.16	1.00	93,95,95,96	0
4	SO4	F	705	5/5	0.13	0.89	97,97,98,100	0
5	P6G	A	712	19/19	0.22	0.88	74,81,91,92	0
4	SO4	D	710	5/5	0.16	0.86	55,55,65,66	0
4	SO4	A	709	5/5	0.14	0.85	97,97,99,99	0
4	SO4	D	711	5/5	0.19	0.82	62,67,73,74	0
4	SO4	B	705	5/5	0.10	0.74	44,45,49,50	0
4	SO4	E	709	5/5	0.10	0.70	76,77,79,81	0
4	SO4	C	709	5/5	0.11	0.63	76,77,80,80	0
4	SO4	F	707	5/5	0.15	0.56	85,87,87,90	0
4	SO4	E	708	5/5	0.12	0.45	94,95,96,96	0
4	SO4	C	710	5/5	0.14	0.40	73,77,79,83	0
4	SO4	D	706	5/5	0.12	0.31	101,103,106,109	0
2	BCT	B	702	4/4	0.10	0.23	27,27,28,31	0
4	SO4	B	706	5/5	0.14	0.22	72,79,81,82	0
2	BCT	A	701	4/4	0.09	0.13	14,14,16,19	0
4	SO4	B	707	5/5	0.12	-0.01	85,87,90,92	0
2	BCT	D	701	4/4	0.10	-0.06	15,17,21,24	0
4	SO4	F	708	5/5	0.13	-0.18	80,85,87,90	0
4	SO4	C	707	5/5	0.10	-0.18	38,55,63,63	0
4	SO4	B	709	5/5	0.09	-0.31	66,67,68,73	0
4	SO4	D	709	5/5	0.10	-0.35	70,72,75,76	0
4	SO4	E	710	5/5	0.10	-0.44	73,73,75,79	0
2	BCT	A	702	4/4	0.10	-0.50	28,31,34,38	0
4	SO4	E	712	5/5	0.10	-0.53	44,48,49,50	0
4	SO4	C	708	5/5	0.09	-0.60	70,75,76,79	0
4	SO4	D	707	5/5	0.08	-0.81	57,58,59,65	0
4	SO4	D	713	5/5	0.11	-0.81	72,73,74,78	0
4	SO4	E	707	5/5	0.09	-0.83	41,55,61,63	0
4	SO4	B	710	5/5	0.09	-1.03	44,61,65,72	0
2	BCT	F	701	4/4	0.08	-1.04	8,9,10,11	0
2	BCT	C	702	4/4	0.14	-1.33	32,36,38,44	0
4	SO4	B	712	5/5	0.11	-1.58	77,80,83,84	0
3	FE	C	703	1/1	0.11	-2.83	38,38,38,38	0

6.5 Other polymers ⓘ

There are no such residues in this entry.