



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 01:52 PM 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 wwPDB X-ray Structure Validation Summary 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

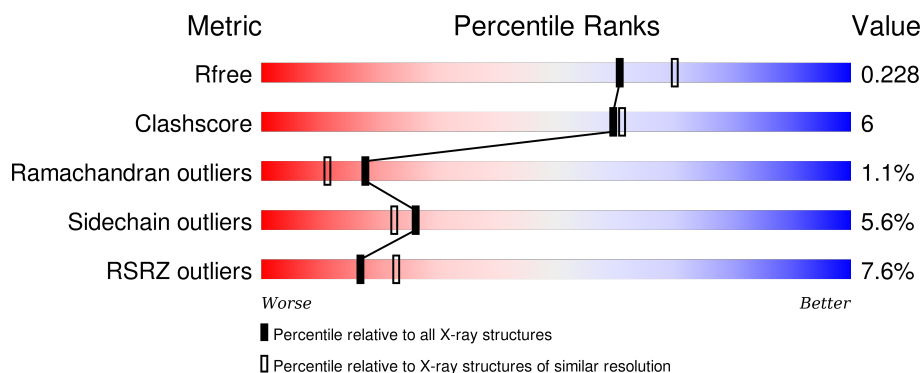
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (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>18%</div> <div> <div></div> <div>78%</div> <div>16%</div> <div>• •</div> </div> </div>
1	D	698	<div> <div>4%</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>

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Mol	Chain	Length	Quality of chain
1	F	698	

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.

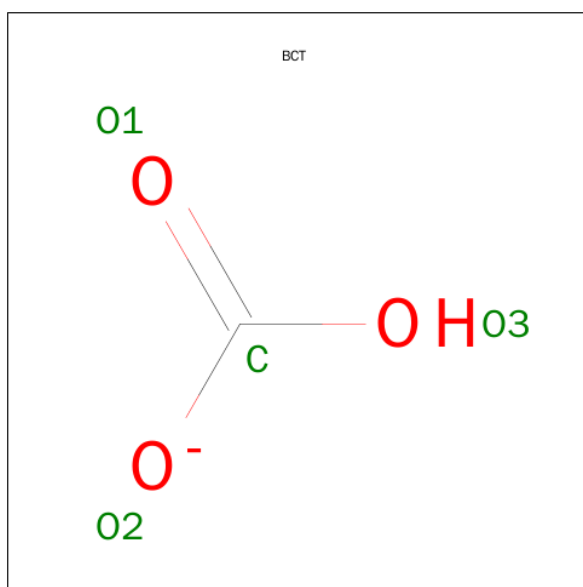
- Molecule 1 is a protein called Serotransferrin.

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).

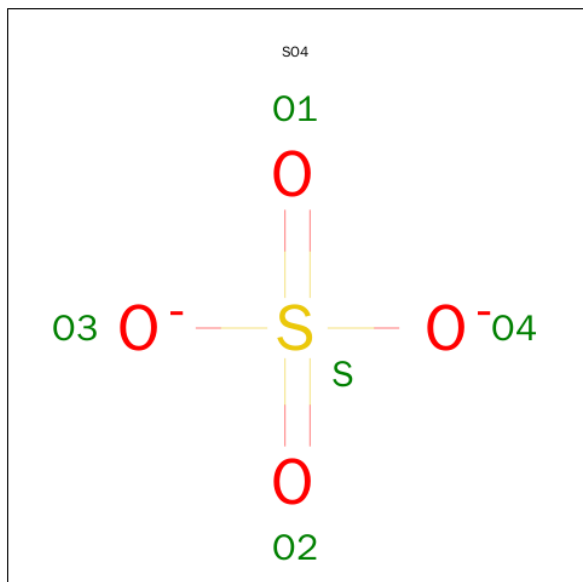


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	1	3		
2	A	1	Total	C	O	0	0
			4	1	3		
2	B	1	Total	C	O	0	0
			4	1	3		
2	B	1	Total	C	O	0	0
			4	1	3		
2	C	1	Total	C	O	0	0
			4	1	3		
2	C	1	Total	C	O	0	0
			4	1	3		
2	D	1	Total	C	O	0	0
			4	1	3		
2	D	1	Total	C	O	0	0
			4	1	3		
2	E	1	Total	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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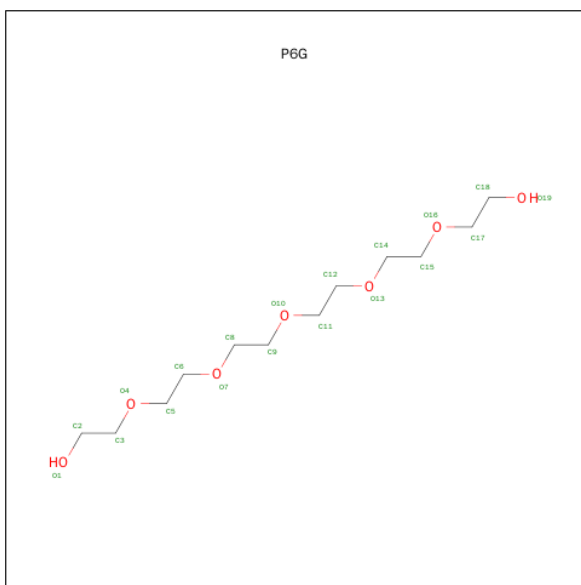
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	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 19	C 12	O 7	0	0
5	A	1	Total 19	C 12	O 7	0	0
5	A	1	Total 19	C 12	O 7	0	0
5	B	1	Total 19	C 12	O 7	0	0
5	B	1	Total 19	C 12	O 7	0	0
5	C	1	Total 19	C 12	O 7	0	0
5	C	1	Total 19	C 12	O 7	0	0
5	C	1	Total 19	C 12	O 7	0	0
5	D	1	Total 19	C 12	O 7	0	0
5	D	1	Total 19	C 12	O 7	0	0
5	E	1	Total 19	C 12	O 7	0	0
5	E	1	Total 19	C 12	O 7	0	0
5	F	1	Total 19	C 12	O 7	0	0
5	F	1	Total 19	C 12	O 7	0	0

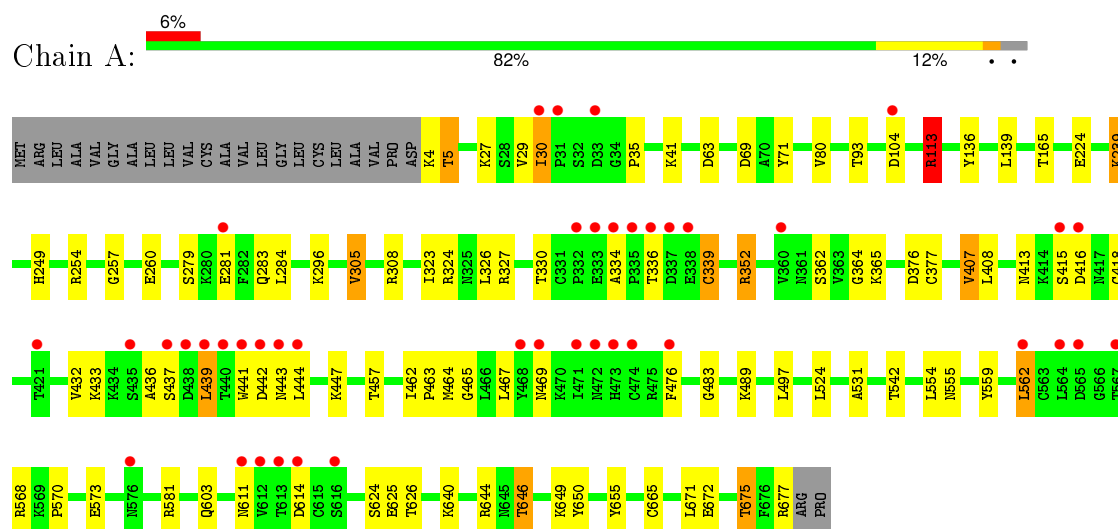
- Molecule 6 is water.

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

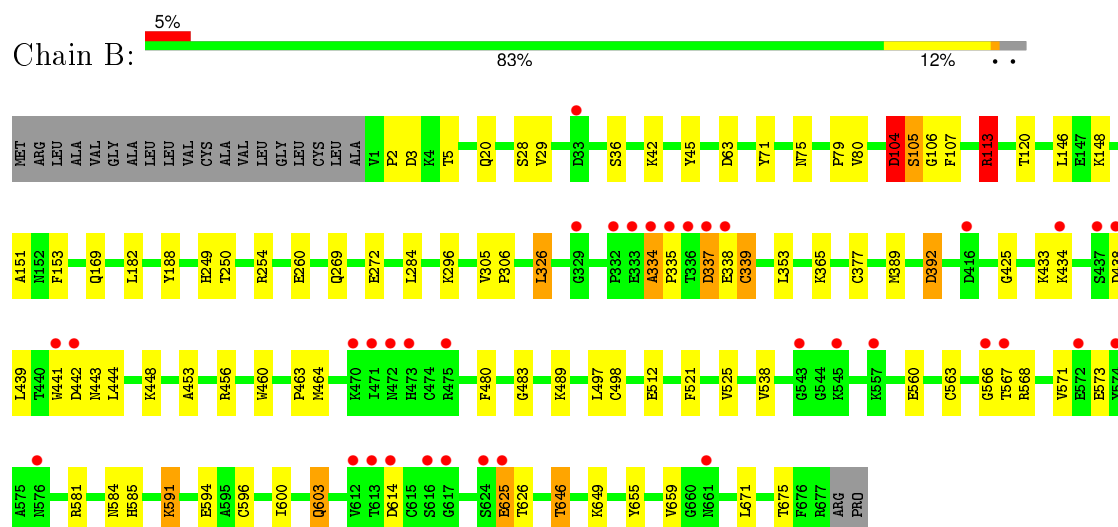
3 Residue-property plots

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.

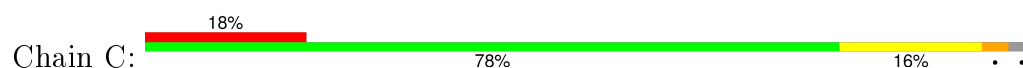
• Molecule 1: Serotransferrin

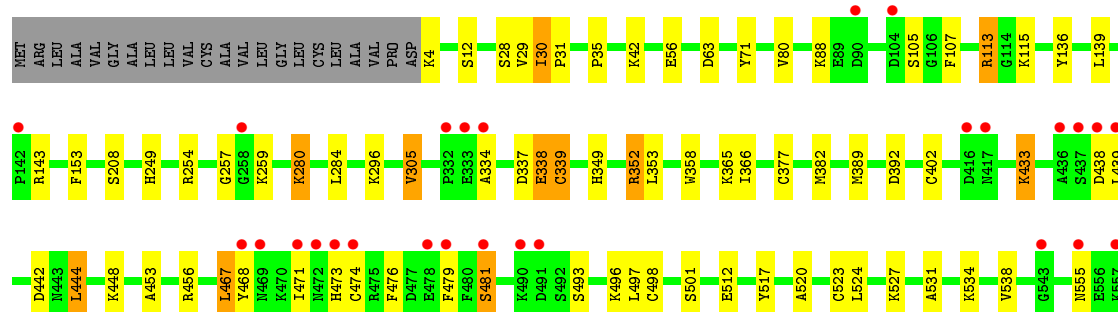
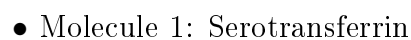


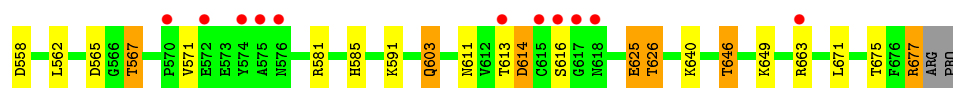
• Molecule 1: Serotransferrin



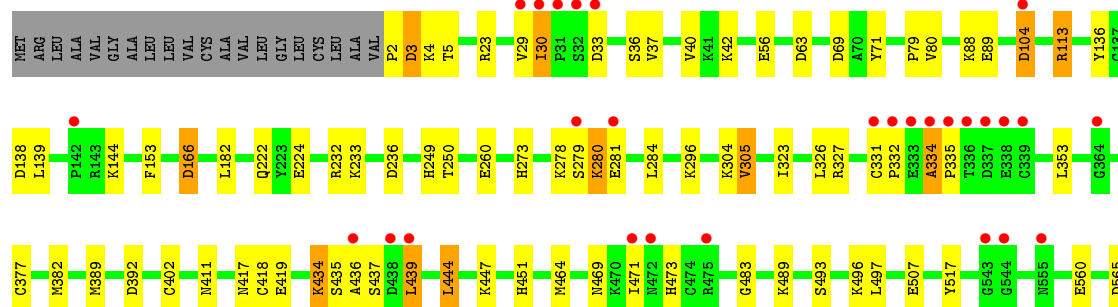
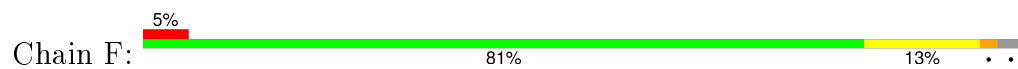
• Molecule 1: Serotransferrin







• 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 0.186 , 0.228	Depositor DCC
R_{free} test set	15028 reflections (5.33%)	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
Estimated twinning fraction	0.014 for -h-2*k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

The worst 5 of 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

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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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.

The worst 5 of 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

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%)	15 9
1	B	675/698 (97%)	630 (93%)	39 (6%)	6 (1%)	21 15
1	C	672/698 (96%)	617 (92%)	46 (7%)	9 (1%)	15 9
1	D	673/698 (96%)	630 (94%)	37 (6%)	6 (1%)	21 15
1	E	672/698 (96%)	632 (94%)	35 (5%)	5 (1%)	26 21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	674/698 (97%)	623 (92%)	43 (6%)	8 (1%)	16	10
All	All	4038/4188 (96%)	3753 (93%)	242 (6%)	43 (1%)	17	11

5 of 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

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%)	24	20
1	B	547/585 (94%)	519 (95%)	28 (5%)	29	26
1	C	539/585 (92%)	503 (93%)	36 (7%)	20	16
1	D	555/585 (95%)	535 (96%)	20 (4%)	42	43
1	E	560/585 (96%)	525 (94%)	35 (6%)	22	18
1	F	553/585 (94%)	521 (94%)	32 (6%)	25	21
All	All	3301/3510 (94%)	3117 (94%)	184 (6%)	26	22

5 of 184 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	475	ARG
1	D	141	GLU
1	F	489	LYS
1	C	488	SER
1	C	646	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 [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	0.11	0
4	SO4	A	706	-	4,4,4	0.08	0	6,6,6	0.24	0
4	SO4	A	707	-	4,4,4	0.19	0	6,6,6	0.19	0
4	SO4	A	708	-	4,4,4	0.26	0	6,6,6	0.10	0
4	SO4	A	709	-	4,4,4	0.21	0	6,6,6	0.11	0
5	P6G	A	710	-	18,18,18	0.71	0	17,17,17	1.51	0
5	P6G	A	711	-	18,18,18	0.66	0	17,17,17	1.56	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	P6G	A	712	-	18,18,18	0.71	0	17,17,17	1.49	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	0.27	0	6,6,6	0.28	0
4	SO4	B	706	-	4,4,4	0.19	0	6,6,6	0.17	0
4	SO4	B	707	-	4,4,4	0.21	0	6,6,6	0.09	0
4	SO4	B	708	-	4,4,4	0.11	0	6,6,6	0.26	0
4	SO4	B	709	-	4,4,4	0.23	0	6,6,6	0.22	0
4	SO4	B	710	-	4,4,4	0.18	0	6,6,6	0.17	0
4	SO4	B	711	-	4,4,4	0.24	0	6,6,6	0.10	0
4	SO4	B	712	-	4,4,4	0.16	0	6,6,6	0.07	0
4	SO4	B	713	-	4,4,4	0.20	0	6,6,6	0.15	0
5	P6G	B	714	-	18,18,18	0.75	0	17,17,17	1.30	1 (5%)
5	P6G	B	715	-	18,18,18	0.72	0	17,17,17	1.50	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	0.26	0	6,6,6	0.10	0
4	SO4	C	706	-	4,4,4	0.13	0	6,6,6	0.11	0
4	SO4	C	707	-	4,4,4	0.22	0	6,6,6	0.24	0
4	SO4	C	708	-	4,4,4	0.19	0	6,6,6	0.15	0
4	SO4	C	709	-	4,4,4	0.17	0	6,6,6	0.18	0
4	SO4	C	710	-	4,4,4	0.18	0	6,6,6	0.11	0
4	SO4	C	711	-	4,4,4	0.18	0	6,6,6	0.09	0
5	P6G	C	712	-	18,18,18	0.73	0	17,17,17	1.45	0
5	P6G	C	713	-	18,18,18	0.68	0	17,17,17	1.56	1 (5%)
5	P6G	C	714	-	18,18,18	0.67	0	17,17,17	1.56	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	0.15	0	6,6,6	0.12	0
4	SO4	D	706	-	4,4,4	0.23	0	6,6,6	0.11	0
4	SO4	D	707	-	4,4,4	0.18	0	6,6,6	0.22	0
4	SO4	D	708	-	4,4,4	0.21	0	6,6,6	0.13	0
4	SO4	D	709	-	4,4,4	0.23	0	6,6,6	0.16	0
4	SO4	D	710	-	4,4,4	0.18	0	6,6,6	0.18	0
4	SO4	D	711	-	4,4,4	0.22	0	6,6,6	0.09	0
4	SO4	D	712	-	4,4,4	0.19	0	6,6,6	0.15	0
4	SO4	D	713	-	4,4,4	0.23	0	6,6,6	0.07	0
5	P6G	D	714	-	18,18,18	0.70	0	17,17,17	1.58	0
5	P6G	D	715	-	18,18,18	0.62	0	17,17,17	1.78	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	0.21	0	6,6,6	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	E	706	-	4,4,4	1.67	1 (25%)	6,6,6	1.25	1 (16%)
4	SO4	E	707	-	4,4,4	0.13	0	6,6,6	0.18	0
4	SO4	E	708	-	4,4,4	0.17	0	6,6,6	0.07	0
4	SO4	E	709	-	4,4,4	0.20	0	6,6,6	0.16	0
4	SO4	E	710	-	4,4,4	0.19	0	6,6,6	0.15	0
4	SO4	E	711	-	4,4,4	0.18	0	6,6,6	0.12	0
4	SO4	E	712	-	4,4,4	0.16	0	6,6,6	0.13	0
4	SO4	E	713	-	4,4,4	0.17	0	6,6,6	0.08	0
5	P6G	E	714	-	18,18,18	0.69	0	17,17,17	1.58	2 (11%)
5	P6G	E	715	-	18,18,18	0.74	0	17,17,17	1.42	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	0.20	0	6,6,6	0.09	0
4	SO4	F	706	-	4,4,4	0.16	0	6,6,6	0.12	0
4	SO4	F	707	-	4,4,4	0.20	0	6,6,6	0.11	0
4	SO4	F	708	-	4,4,4	0.18	0	6,6,6	0.09	0
4	SO4	F	709	-	4,4,4	0.18	0	6,6,6	0.08	0
5	P6G	F	710	-	18,18,18	0.72	0	17,17,17	1.54	0
5	P6G	F	711	-	18,18,18	0.71	0	17,17,17	1.67	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-2.21	1.39	1.47

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	706	SO4	O4-S-O3	-2.66	98.17	108.98
5	A	711	P6G	O13-C12-C11	2.05	119.48	110.36
5	E	714	P6G	C17-O16-C15	2.06	122.16	113.31
5	D	715	P6G	O4-C5-C6	2.10	119.69	110.36
5	B	714	P6G	O13-C14-C15	2.17	120.01	110.36

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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	0.09	42 (6%) 24 32	15, 39, 77, 97	0
1	B	677/698 (96%)	-0.04	36 (5%) 30 39	13, 33, 72, 97	0
1	C	674/698 (96%)	0.89	128 (18%) 2 2	13, 46, 117, 151	0
1	D	675/698 (96%)	0.02	26 (3%) 43 52	16, 34, 66, 94	0
1	E	674/698 (96%)	0.08	38 (5%) 28 36	13, 35, 73, 93	0
1	F	676/698 (96%)	0.01	36 (5%) 30 39	13, 36, 70, 98	0
All	All	4050/4188 (96%)	0.17	306 (7%) 17 23	13, 36, 83, 151	0

The worst 5 of 306 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	479	PHE	15.2
1	C	474	CYS	14.0
1	C	478	GLU	13.3
1	C	564	LEU	12.2
1	C	445	LYS	11.4

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 ⓘ

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	7.92	26,26,26,26	0
3	FE	F	703	1/1	1.00	0.14	6.09	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
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	3.71	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	2.61	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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
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
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	-0.65	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	-0.81	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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
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.