Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:07 PM GMT

PDB ID	:	1NF4
Title	:	X-Ray Structure of the Desulfovibrio desulfuricans bacterioferritin: the diiron site in different states (reduced structure)
Authors	:	Macedo, S.; Romao, C.V.; Mitchell, E.; Matias, P.M.; Liu, M.Y.; Xavier, A.V.; LeGall, J.; Teixeira, M.; Lindley, P.; Carrondo, M.A.
Deposited on	:	2002-12-13
Resolution	:	2.05 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

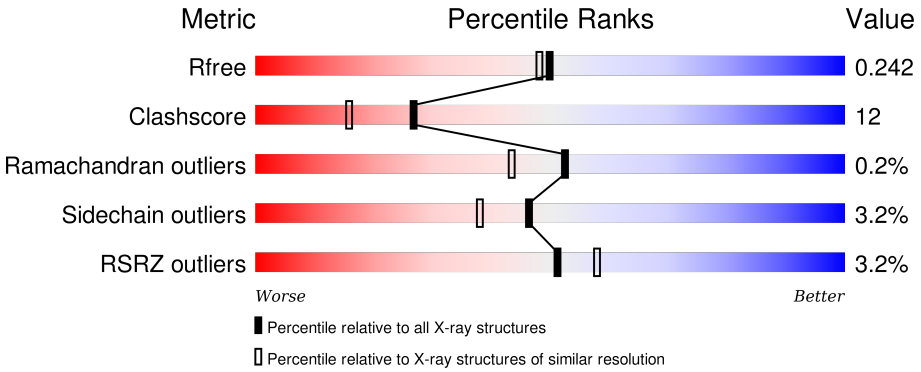
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	1192 (2.04-2.04)
Clashscore	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)
RSRZ outliers	91569	1194 (2.04-2.04)

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 <=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	179	3% 79% 13% • 6%
1	B	179	2% 77% 17% • 6%
1	C	179	4% 77% 17% • 6%
1	D	179	3% 77% 15% • 6%
1	E	179	3% 75% 18% •• 6%

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Mol	Chain	Length	Quality of chain
1	F	179	3% 77% 17% • 6%
1	G	179	3% 73% 20% • 6%
1	H	179	4% 77% 17% • 5%
1	I	179	3% 80% 13% • 5%
1	J	179	3% 78% 14% • 6%
1	K	179	2% 76% 17% • 6%
1	L	179	4% 78% 15% • 5%
1	M	179	3% 79% 16% • 5%
1	N	179	3% 79% 14% • 6%
1	O	179	2% 69% 25% • 6%
1	P	179	2% 77% 16% • 5%

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
3	SO4	A	1006	-	-	X	-
3	SO4	B	1005	-	-	X	X
3	SO4	B	1104	-	-	X	-
3	SO4	C	1206	-	-	X	-
3	SO4	D	1301	-	-	X	X
3	SO4	E	1403	-	-	X	-
3	SO4	F	1501	-	-	-	X
3	SO4	I	1704	-	-	X	-
3	SO4	I	1801	-	-	-	X
3	SO4	I	1802	-	-	X	-
3	SO4	J	1901	-	-	-	X
3	SO4	K	2001	-	-	-	X
3	SO4	L	2102	-	-	X	-
3	SO4	L	2104	-	-	X	-
3	SO4	M	2201	-	-	-	X
3	SO4	O	2406	-	-	X	-
3	SO4	P	1504	-	-	X	-
4	FEC	C	1207[B]	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	FEC	I	1805[B]	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 23945 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.

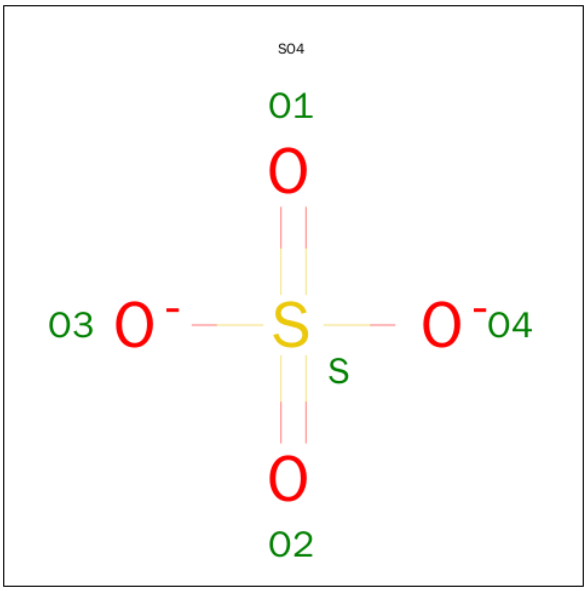
- Molecule 1 is a protein called bacterioferritin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	169	Total	C	N	O	S	0	0	0
			1328	828	229	265	6			
1	B	169	Total	C	N	O	S	0	0	0
			1321	823	227	265	6			
1	C	169	Total	C	N	O	S	0	0	0
			1318	821	227	264	6			
1	D	169	Total	C	N	O	S	0	1	0
			1328	828	228	266	6			
1	E	169	Total	C	N	O	S	0	0	0
			1322	824	228	264	6			
1	F	169	Total	C	N	O	S	0	0	0
			1324	825	227	266	6			
1	G	169	Total	C	N	O	S	0	0	0
			1321	823	226	266	6			
1	H	170	Total	C	N	O	S	0	0	0
			1324	824	228	266	6			
1	I	170	Total	C	N	O	S	0	0	0
			1328	827	229	266	6			
1	J	169	Total	C	N	O	S	0	1	0
			1311	818	224	263	6			
1	K	169	Total	C	N	O	S	0	0	0
			1322	824	228	264	6			
1	L	170	Total	C	N	O	S	0	1	0
			1336	832	231	267	6			
1	M	170	Total	C	N	O	S	0	2	0
			1338	832	232	268	6			
1	N	169	Total	C	N	O	S	0	0	0
			1326	826	228	266	6			
1	O	169	Total	C	N	O	S	0	0	0
			1315	819	225	265	6			
1	P	170	Total	C	N	O	S	0	0	0
			1328	827	229	266	6			

- Molecule 2 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	P	2	Total Fe 2 2	0	0
2	G	2	Total Fe 2 2	0	0
2	J	2	Total Fe 2 2	0	0
2	D	2	Total Fe 2 2	0	0
2	K	2	Total Fe 2 2	0	0
2	E	2	Total Fe 2 2	0	0
2	H	2	Total Fe 2 2	0	0
2	B	2	Total Fe 2 2	0	0
2	I	2	Total Fe 2 2	0	0
2	C	2	Total Fe 2 2	0	0
2	A	2	Total Fe 2 2	0	0
2	N	2	Total Fe 2 2	0	0
2	O	2	Total Fe 2 2	0	0
2	L	2	Total Fe 2 2	0	0
2	F	2	Total Fe 2 2	0	0
2	M	2	Total Fe 2 2	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0
3	P	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0
3	G	1	Total O S 5 4 1	0	0
3	G	1	Total O S 5 4 1	0	0
3	G	1	Total O S 5 4 1	0	0
3	H	1	Total O S 5 4 1	0	0
3	H	1	Total O S 5 4 1	0	0
3	H	1	Total O S 5 4 1	0	0
3	I	1	Total O S 5 4 1	0	0
3	H	1	Total O S 5 4 1	0	0
3	I	1	Total O S 5 4 1	0	0
3	I	1	Total O S 5 4 1	0	0
3	I	1	Total O S 5 4 1	0	0
3	I	1	Total O S 5 4 1	0	0
3	J	1	Total O S 5 4 1	0	0

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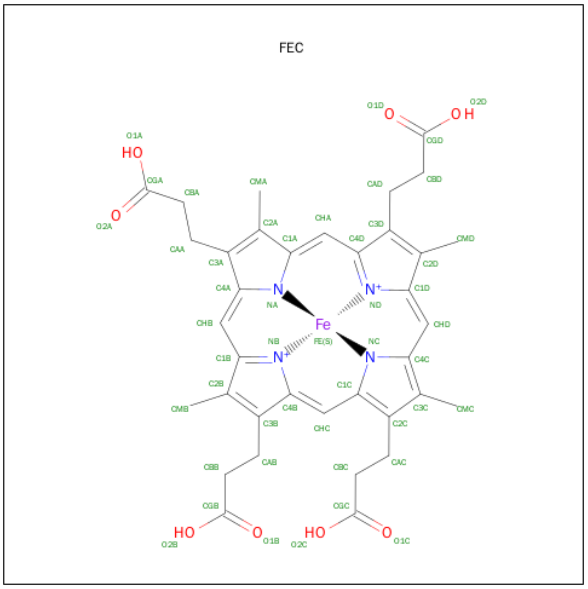
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	J	1	Total O S 5 4 1	0	0
3	J	1	Total O S 5 4 1	0	0
3	K	1	Total O S 5 4 1	0	0
3	K	1	Total O S 5 4 1	0	0
3	K	1	Total O S 5 4 1	0	0
3	L	1	Total O S 5 4 1	0	0
3	L	1	Total O S 5 4 1	0	0
3	L	1	Total O S 5 4 1	0	0
3	L	1	Total O S 5 4 1	0	0
3	M	1	Total O S 5 4 1	0	0
3	M	1	Total O S 5 4 1	0	0
3	M	1	Total O S 5 4 1	0	0
3	M	1	Total O S 5 4 1	0	0
3	N	1	Total O S 5 4 1	0	0
3	N	1	Total O S 5 4 1	0	0
3	N	1	Total O S 5 4 1	0	0
3	O	1	Total O S 5 4 1	0	0
3	O	1	Total O S 5 4 1	0	0
3	P	1	Total O S 5 4 1	0	0
3	P	1	Total O S 5 4 1	0	0
3	P	1	Total O S 5 4 1	0	0

- Molecule 4 is 1,3,5,8-TETRAMETHYL-PORPHINE-2,4,6,7-TETRAPROPIONIC ACID FERROUS COMPLEX (three-letter code: FEC) (formula: $C_{36}H_{36}FeN_4O_8$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Fe	N	O	0	1
			98	72	2	8	16		
4	C	1	Total	C	Fe	N	O	0	1
			98	72	2	8	16		
4	E	1	Total	C	Fe	N	O	0	1
			98	72	2	8	16		
4	G	1	Total	C	Fe	N	O	0	1
			98	72	2	8	16		
4	I	1	Total	C	Fe	N	O	0	1
			98	72	2	8	16		
4	L	1	Total	C	Fe	N	O	0	1
			98	72	2	8	16		
4	M	1	Total	C	Fe	N	O	0	1
			98	72	2	8	16		
4	P	1	Total	C	Fe	N	O	0	1
			98	72	2	8	16		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	123	Total	O	0	0
			123	123		
5	B	114	Total	O	0	0
			114	114		

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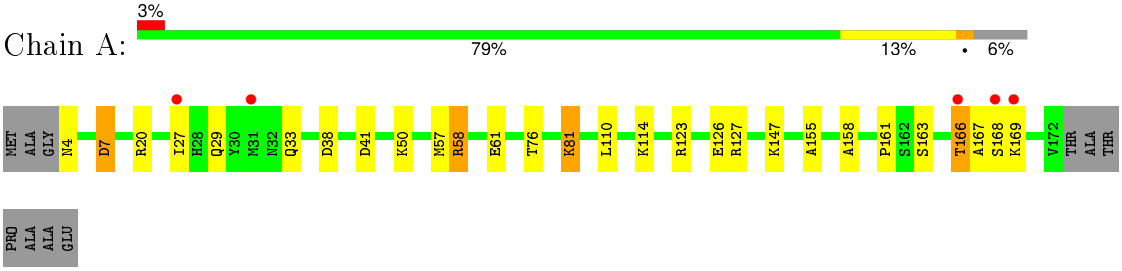
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	99	Total O 99 99	0	0
5	D	103	Total O 103 103	0	0
5	E	86	Total O 86 86	0	0
5	F	89	Total O 89 89	0	0
5	G	104	Total O 104 104	0	0
5	H	93	Total O 93 93	0	0
5	I	121	Total O 121 121	0	0
5	J	91	Total O 91 91	0	0
5	K	105	Total O 105 105	0	0
5	L	129	Total O 129 129	0	0
5	M	124	Total O 124 124	0	0
5	N	108	Total O 108 108	0	0
5	O	74	Total O 74 74	0	0
5	P	96	Total O 96 96	0	0

3 Residue-property plots (i)

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.

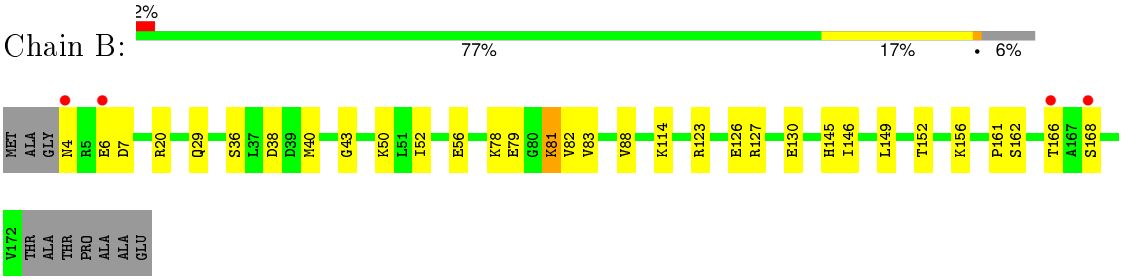
- Molecule 1: bacterioferritin

Chain A:



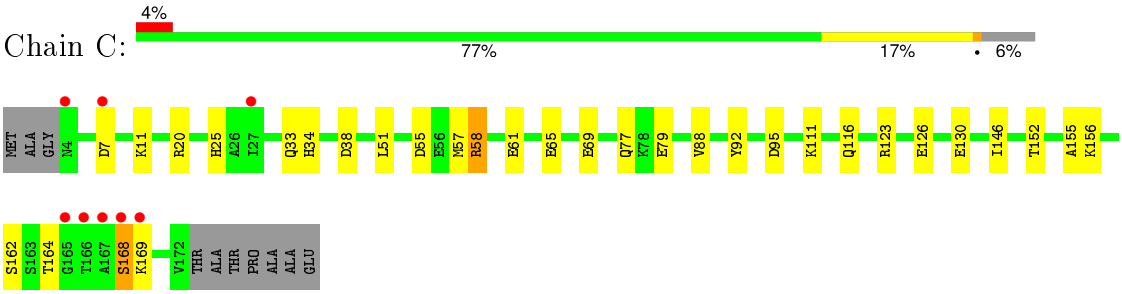
- Molecule 1: bacterioferritin

Chain B:



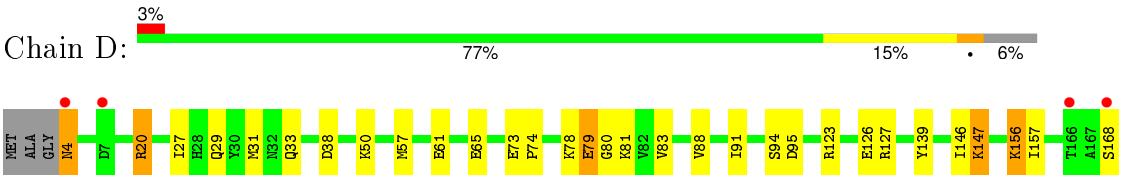
- Molecule 1: bacterioferritin

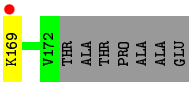
Chain C:



- Molecule 1: bacterioferritin

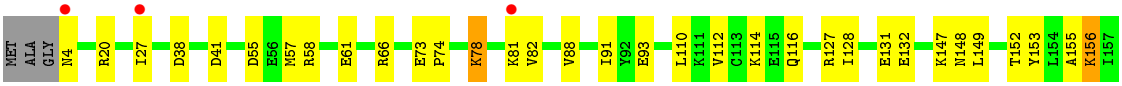
Chain D:

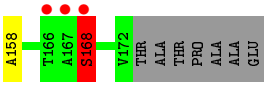




- Molecule 1: bacterioferritin

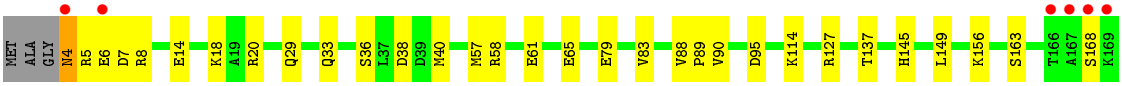
Chain E:





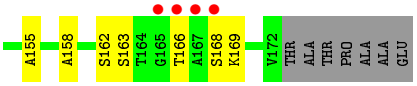
- Molecule 1: bacterioferritin

Chain F:



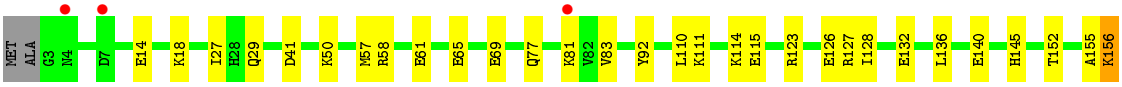
- Molecule 1: bacterioferritin

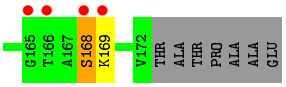
Chain G:



- Molecule 1: bacterioferritin

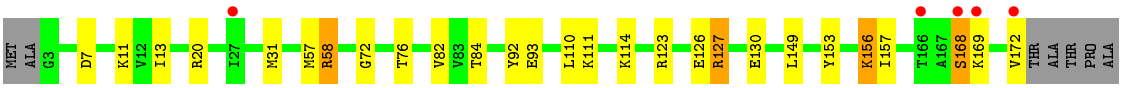
Chain H:





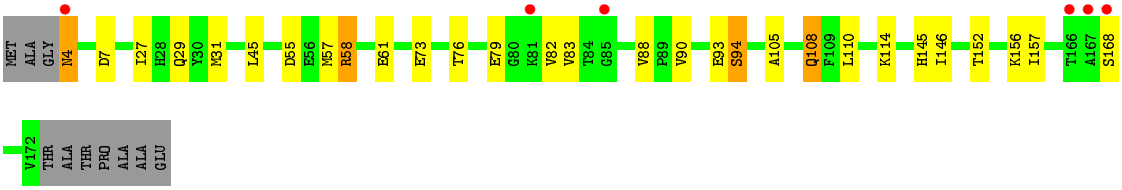
- Molecule 1: bacterioferritin

Chain I:



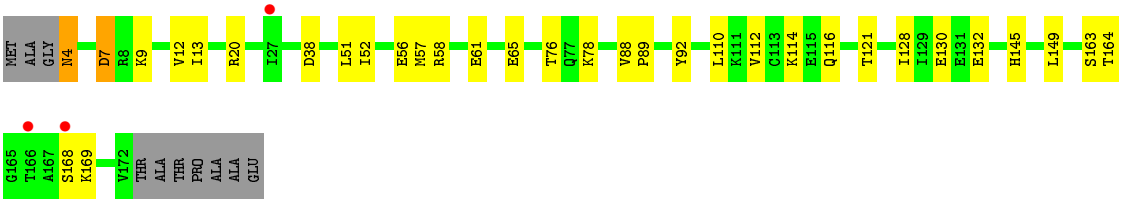
- Molecule 1: bacterioferritin

Chain J:



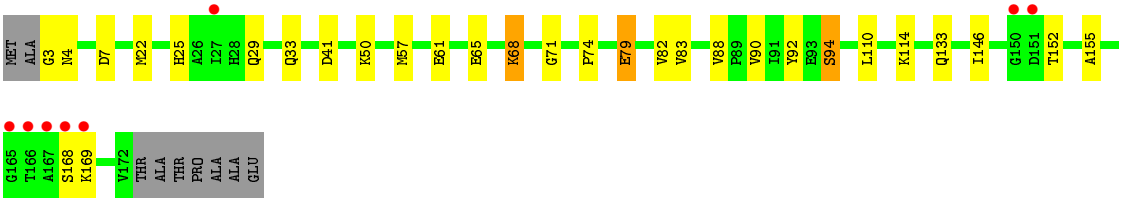
- Molecule 1: bacterioferritin

Chain K:



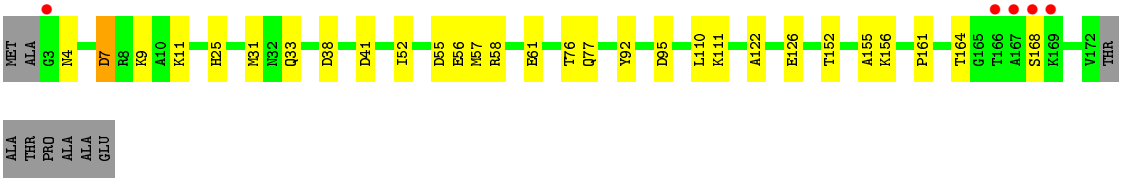
- Molecule 1: bacterioferritin

Chain L:



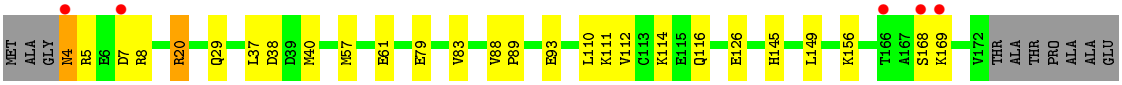
- Molecule 1: bacterioferritin

Chain M:



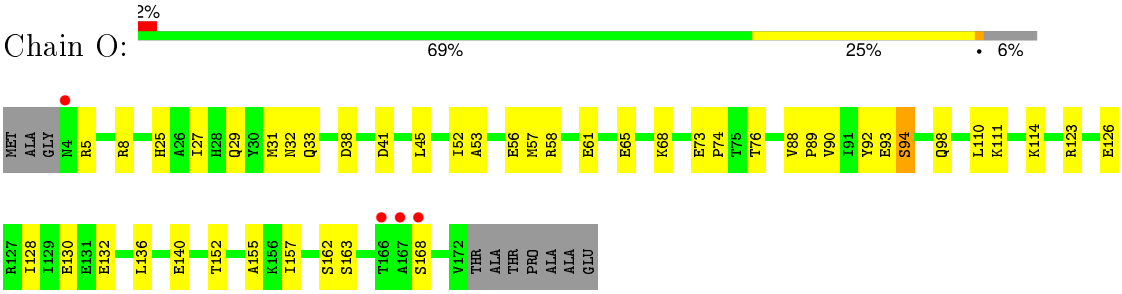
- Molecule 1: bacterioferritin

Chain N:



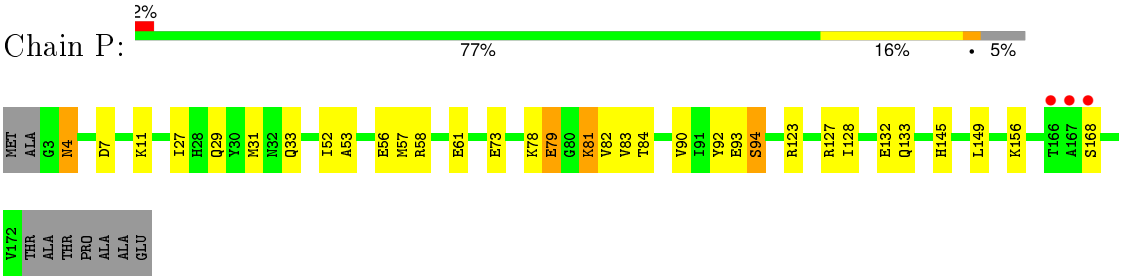
• Molecule 1: bacterioferritin

Chain O:



• Molecule 1: bacterioferritin

Chain P:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α, β, γ	225.68Å 225.68Å 225.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.05 29.63 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.0 (30.00-2.05) 98.8 (29.63-2.05)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.22 (at 2.04Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.231 , 0.270 0.196 , 0.242	Depositor DCC
R_{free} test set	4891 reflections (2.13%)	DCC
Wilson B-factor (Å^2)	28.1	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 60.6	EDS
Estimated twinning fraction	0.012 for l,-k,h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Outliers	1 of 234646 reflections (0.000%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	23945	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.46% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 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: FE2, FEC, 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	0.31	0/1348	0.85	5/1816 (0.3%)
1	B	0.35	0/1341	0.78	1/1809 (0.1%)
1	C	0.29	0/1338	0.83	3/1805 (0.2%)
1	D	0.31	0/1353	0.83	1/1823 (0.1%)
1	E	0.31	0/1342	0.84	2/1809 (0.1%)
1	F	0.37	1/1344 (0.1%)	0.79	0/1812
1	G	0.29	0/1341	0.85	5/1809 (0.3%)
1	H	0.30	0/1344	0.80	2/1813 (0.1%)
1	I	0.30	0/1348	0.80	3/1817 (0.2%)
1	J	0.37	2/1336 (0.1%)	0.76	0/1804
1	K	0.30	0/1342	0.82	1/1809 (0.1%)
1	L	0.32	0/1361	0.78	1/1833 (0.1%)
1	M	0.30	0/1368	0.79	1/1843 (0.1%)
1	N	0.31	0/1346	0.78	3/1814 (0.2%)
1	O	0.30	0/1335	0.83	2/1802 (0.1%)
1	P	0.31	0/1348	0.80	1/1817 (0.1%)
All	All	0.32	3/21535 (0.0%)	0.81	31/29035 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	6	GLU	CD-OE2	6.04	1.32	1.25
1	J	108[A]	GLN	CD-OE1	5.15	1.35	1.24
1	J	108[B]	GLN	CD-OE1	5.15	1.35	1.24

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	58	ARG	NE-CZ-NH1	8.53	124.57	120.30
1	E	127	ARG	NE-CZ-NH1	7.79	124.19	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	20	ARG	NE-CZ-NH1	7.66	124.13	120.30
1	A	20	ARG	NE-CZ-NH2	-7.02	116.79	120.30
1	G	127	ARG	NE-CZ-NH2	-6.57	117.02	120.30
1	C	58	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	E	66	ARG	NE-CZ-NH2	-6.27	117.17	120.30
1	G	92	TYR	CA-CB-CG	-6.12	101.77	113.40
1	A	127	ARG	CD-NE-CZ	5.93	131.90	123.60
1	A	20	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	L	92	TYR	CA-CB-CG	-5.81	102.37	113.40
1	A	58	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	H	58	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	D	20	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	G	127	ARG	NE-CZ-NH1	5.67	123.13	120.30
1	A	127	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	G	35	TYR	CB-CG-CD2	-5.60	117.64	121.00
1	O	58	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	K	92	TYR	CA-CB-CG	-5.43	103.09	113.40
1	H	92	TYR	CA-CB-CG	-5.34	103.26	113.40
1	N	20	ARG	NE-CZ-NH2	-5.29	117.65	120.30
1	C	92	TYR	CA-CB-CG	-5.29	103.36	113.40
1	N	20	ARG	CD-NE-CZ	5.28	130.99	123.60
1	I	92	TYR	CA-CB-CG	-5.27	103.39	113.40
1	I	58	ARG	NE-CZ-NH1	-5.22	117.69	120.30
1	M	92	TYR	CA-CB-CG	-5.13	103.64	113.40
1	O	92	TYR	CA-CB-CG	-5.11	103.69	113.40
1	P	92	TYR	CA-CB-CG	-5.08	103.74	113.40
1	I	127	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	G	58	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	B	127	ARG	NE-CZ-NH1	5.01	122.81	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	1328	0	1296	31	0
1	B	1321	0	1276	29	0
1	C	1318	0	1269	24	0
1	D	1328	0	1292	30	0
1	E	1322	0	1280	29	0
1	F	1324	0	1283	24	0
1	G	1321	0	1274	31	0
1	H	1324	0	1277	37	0
1	I	1328	0	1288	45	0
1	J	1311	0	1259	30	0
1	K	1322	0	1280	27	0
1	L	1336	0	1303	41	5
1	M	1338	0	1299	24	0
1	N	1326	0	1284	29	0
1	O	1315	0	1258	36	0
1	P	1328	0	1288	38	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	2	0	0	0	0
2	M	2	0	0	0	0
2	N	2	0	0	0	0
2	O	2	0	0	0	0
2	P	2	0	0	0	0
3	A	15	0	0	2	0
3	B	25	0	0	8	0
3	C	20	0	0	2	0
3	D	15	0	0	3	0
3	E	15	0	0	4	0
3	F	15	0	0	0	0
3	G	15	0	0	1	0
3	H	20	0	0	0	0
3	I	25	0	0	5	14
3	J	15	0	0	0	0
3	K	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	20	0	0	5	19
3	M	20	0	0	2	0
3	N	15	0	0	1	0
3	O	10	0	0	2	0
3	P	20	0	0	4	0
4	A	98	0	64	21	0
4	C	98	0	64	29	0
4	E	98	0	64	21	0
4	G	98	0	64	24	0
4	I	98	0	64	37	0
4	L	98	0	64	29	0
4	M	98	0	64	19	0
4	P	98	0	64	30	0
5	A	123	0	0	3	0
5	B	114	0	0	10	0
5	C	99	0	0	2	0
5	D	103	0	0	7	0
5	E	86	0	0	1	0
5	F	89	0	0	3	0
5	G	104	0	0	1	0
5	H	93	0	0	5	0
5	I	121	0	0	4	0
5	J	91	0	0	4	0
5	K	105	0	0	3	0
5	L	129	0	0	6	0
5	M	124	0	0	5	0
5	N	108	0	0	2	0
5	O	74	0	0	2	0
5	P	96	0	0	4	0
All	All	23945	0	21018	522	19

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 12.

All (522) 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)
4:L:2107[B]:FEC:NA	4:L:2107[B]:FEC:C4A	1.75	1.45
4:P:2507[B]:FEC:NA	4:P:2507[B]:FEC:C4A	1.80	1.44
4:C:1207[B]:FEC:NC	4:C:1207[B]:FEC:FE	0.70	1.43
4:E:1407[B]:FEC:NB	4:E:1407[B]:FEC:C4B	1.68	1.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1007[B]:FEC:NA	4:A:1007[B]:FEC:C1A	1.72	1.34
4:C:1207[B]:FEC:NB	4:C:1207[B]:FEC:C4B	1.84	1.34
4:I:1805[B]:FEC:C1D	4:I:1805[B]:FEC:ND	1.84	1.33
4:G:1607[B]:FEC:ND	4:G:1607[B]:FEC:C1D	1.76	1.32
4:A:1007[B]:FEC:C1D	4:A:1007[B]:FEC:ND	1.90	1.26
4:I:1805[B]:FEC:FE	4:I:1805[B]:FEC:NC	0.99	1.26
1:E:147:LYS:HE2	3:E:1403:SO4:O4	1.28	1.26
4:L:2107[B]:FEC:NA	4:L:2107[B]:FEC:C1A	1.97	1.25
1:P:168:SER:HA	4:P:2507[A]:FEC:O2C	1.21	1.24
4:G:1607[A]:FEC:O2C	1:H:168:SER:HA	1.28	1.24
1:A:168:SER:HA	4:A:1007[B]:FEC:O2C	1.38	1.23
4:P:2507[B]:FEC:NA	4:P:2507[B]:FEC:NB	1.87	1.22
1:C:168:SER:HA	4:C:1207[B]:FEC:O2C	1.12	1.21
1:I:168:SER:CA	4:I:1805[B]:FEC:O2C	1.88	1.20
4:C:1207[B]:FEC:NC	4:C:1207[B]:FEC:NB	1.89	1.19
1:I:168:SER:HA	4:I:1805[B]:FEC:O2C	0.98	1.13
4:C:1207[B]:FEC:NC	1:D:57:MET:SD	2.21	1.13
1:O:57:MET:SD	4:P:2507[B]:FEC:NA	2.23	1.12
1:P:168:SER:CA	4:P:2507[A]:FEC:O2C	1.98	1.11
1:L:114:LYS:CD	3:L:2104:SO4:O4	1.99	1.11
4:I:1805[B]:FEC:C1C	4:I:1805[B]:FEC:NC	2.13	1.10
1:A:168:SER:CA	4:A:1007[B]:FEC:O2C	2.00	1.09
1:L:114:LYS:NZ	3:L:2104:SO4:O4	1.87	1.07
1:C:168:SER:CA	4:C:1207[B]:FEC:O2C	2.02	1.07
4:I:1805[B]:FEC:C4C	4:I:1805[B]:FEC:NC	2.16	1.07
1:L:114:LYS:CE	3:L:2104:SO4:O4	2.04	1.04
1:L:168:SER:CB	4:L:2107[A]:FEC:O2C	2.06	1.04
4:P:2507[B]:FEC:NA	4:P:2507[B]:FEC:C1A	2.22	1.02
1:L:114:LYS:HD2	3:L:2104:SO4:O4	1.60	1.02
4:E:1407[B]:FEC:C4C	4:E:1407[B]:FEC:NC	2.25	0.99
4:I:1805[B]:FEC:NC	4:I:1805[B]:FEC:ND	2.11	0.97
1:L:168:SER:HA	4:L:2107[A]:FEC:O2C	1.63	0.96
1:L:168:SER:CA	4:L:2107[A]:FEC:O2C	2.14	0.95
1:N:29:GLN:HE22	1:N:83:VAL:H	1.08	0.94
4:G:1607[A]:FEC:O2C	1:H:168:SER:CA	2.15	0.93
3:B:1005:SO4:O2	5:B:1216:HOH:O	1.87	0.92
4:L:2107[B]:FEC:NA	4:L:2107[B]:FEC:FE	1.37	0.92
3:N:2301:SO4:O2	5:N:2413:HOH:O	1.86	0.92
1:L:29:GLN:HE22	1:L:83:VAL:H	1.12	0.91
1:D:29:GLN:HE22	1:D:83:VAL:H	1.20	0.90
1:I:168:SER:HB3	4:I:1805[B]:FEC:CGB	2.03	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:SER:CB	4:A:1007[B]:FEC:O2C	2.21	0.88
1:M:110:LEU:HD11	1:M:126[B]:GLU:HG2	1.54	0.88
4:C:1207[B]:FEC:C1C	4:C:1207[B]:FEC:NC	2.36	0.88
1:I:168:SER:HB3	4:I:1805[B]:FEC:HBB2	1.56	0.87
1:J:29:GLN:HE22	1:J:83:VAL:H	1.24	0.85
4:P:2507[B]:FEC:NA	4:P:2507[B]:FEC:CHB	2.39	0.85
1:E:147:LYS:CE	3:E:1403:SO4:O4	2.20	0.85
1:A:168:SER:HA	4:A:1007[B]:FEC:CGC	2.06	0.85
4:I:1805[B]:FEC:NC	1:J:57:MET:SD	2.51	0.84
1:L:168:SER:HA	4:L:2107[A]:FEC:CGC	2.07	0.84
3:C:1206:SO4:O3	5:C:9486:HOH:O	1.95	0.83
1:B:29:GLN:HE22	1:B:83:VAL:H	1.27	0.83
1:H:29:GLN:HE22	1:H:83:VAL:H	1.22	0.82
1:B:81:LYS:HE2	3:B:1005:SO4:O1	1.79	0.82
4:L:2107[B]:FEC:NB	4:L:2107[B]:FEC:NA	2.28	0.82
1:I:57:MET:SD	4:I:1805[B]:FEC:NC	2.52	0.81
1:A:168:SER:HB3	4:A:1007[B]:FEC:HBB2	1.63	0.80
1:F:114:LYS:NZ	3:P:1504:SO4:O3	2.15	0.80
4:P:2507[B]:FEC:NA	4:P:2507[B]:FEC:FE	1.48	0.80
1:P:93:GLU:HG3	5:P:9559:HOH:O	1.81	0.79
1:I:168:SER:HB3	4:I:1805[B]:FEC:CBB	2.11	0.79
4:L:2107[B]:FEC:NA	4:L:2107[B]:FEC:CHB	2.46	0.78
3:B:1005:SO4:S	5:B:1216:HOH:O	2.38	0.78
1:C:155:ALA:O	1:E:156:LYS:HE3	1.83	0.78
1:E:168:SER:HA	4:E:1407[B]:FEC:O2C	1.83	0.77
1:P:29:GLN:HE22	1:P:83:VAL:H	1.30	0.77
4:I:1805[B]:FEC:NB	4:I:1805[B]:FEC:NC	2.33	0.77
4:G:1607[A]:FEC:HBC2	4:G:1607[A]:FEC:HHC	1.66	0.77
1:H:156:LYS:HE2	5:H:9565:HOH:O	1.83	0.77
4:A:1007[B]:FEC:HHC	4:A:1007[B]:FEC:HBC2	1.65	0.77
1:M:122:ALA:O	1:M:126[B]:GLU:HG3	1.84	0.77
3:B:1104:SO4:O4	1:G:114:LYS:NZ	2.16	0.77
1:I:168:SER:HA	4:I:1805[B]:FEC:CGC	2.08	0.77
4:G:1607[A]:FEC:HBB2	1:H:168:SER:HB3	1.66	0.77
1:I:31:MET:HG3	4:I:1805[A]:FEC:HBD1	1.66	0.76
1:E:148:ASN:ND2	3:E:1403:SO4:O1	2.15	0.76
1:L:168:SER:HB2	4:L:2107[A]:FEC:O2C	1.84	0.75
1:B:123:ARG:HD3	1:N:126:GLU:OE1	1.87	0.75
1:P:4:ASN:ND2	1:P:7:ASP:H	1.84	0.74
1:P:168:SER:HB3	4:P:2507[A]:FEC:HBB2	1.67	0.74
1:K:114:LYS:HE2	3:P:1504:SO4:O1	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:169:LYS:HB3	5:D:9513:HOH:O	1.87	0.74
1:H:114:LYS:NZ	3:I:1704:SO4:O2	2.18	0.73
1:M:168:SER:HA	4:M:2207[B]:FEC:O2C	1.88	0.73
1:P:168:SER:HA	4:P:2507[A]:FEC:CGC	2.16	0.72
4:P:2507[B]:FEC:NA	4:P:2507[B]:FEC:C1B	2.53	0.72
1:F:29:GLN:HE22	1:F:83:VAL:H	1.36	0.72
1:C:57:MET:SD	4:C:1207[B]:FEC:NC	2.62	0.72
1:E:168:SER:OG	1:F:58:ARG:HD3	1.90	0.72
1:J:79:GLU:HG2	5:J:9508:HOH:O	1.88	0.72
1:P:78:LYS:HE2	1:P:81:LYS:NZ	2.05	0.72
1:O:57:MET:CE	4:P:2507[B]:FEC:NA	2.52	0.72
1:C:155:ALA:HA	1:E:149:LEU:HD13	1.71	0.72
1:F:4:ASN:ND2	1:F:7:ASP:H	1.87	0.71
1:C:7:ASP:O	1:C:11:LYS:HG3	1.91	0.71
1:A:168:SER:HB3	4:A:1007[B]:FEC:O2C	1.90	0.70
1:N:4:ASN:ND2	1:N:7:ASP:H	1.89	0.70
4:P:2507[A]:FEC:HBC2	4:P:2507[A]:FEC:HHC	1.73	0.70
1:I:114:LYS:NZ	3:I:1704:SO4:O4	2.22	0.70
1:I:168:SER:HB3	4:I:1805[B]:FEC:O2B	1.91	0.70
3:D:1301:SO4:O1	5:D:9670:HOH:O	0.72	0.70
4:M:2207[A]:FEC:HBB2	1:N:168:SER:HB3	1.73	0.70
4:C:1207[B]:FEC:NC	4:C:1207[B]:FEC:C4C	2.55	0.69
1:I:168:SER:CB	4:I:1805[B]:FEC:O2B	2.40	0.69
4:E:1407[A]:FEC:HBC2	1:F:168:SER:HB2	1.74	0.69
1:L:57:MET:SD	4:L:2107[B]:FEC:NA	2.66	0.69
1:O:31:MET:HG3	4:P:2507[A]:FEC:HBD1	1.74	0.69
1:E:147:LYS:HE2	3:E:1403:SO4:S	2.32	0.68
1:B:4:ASN:HD22	1:B:7:ASP:H	1.39	0.68
1:N:110:LEU:HD23	1:N:114:LYS:HE2	1.76	0.68
1:I:93:GLU:HG3	5:I:9455:HOH:O	1.92	0.68
1:B:4:ASN:ND2	1:B:7:ASP:H	1.89	0.68
1:P:78:LYS:HE2	1:P:81:LYS:HZ1	1.58	0.68
3:D:1306:SO4:O4	5:D:9704:HOH:O	2.11	0.68
4:L:2107[A]:FEC:HBC2	4:L:2107[A]:FEC:HHC	1.76	0.67
4:C:1207[B]:FEC:HHC	4:C:1207[B]:FEC:HBC2	1.76	0.67
3:B:1005:SO4:O4	5:B:1216:HOH:O	2.12	0.67
1:B:161:PRO:HA	5:B:1207:HOH:O	1.94	0.67
1:H:123:ARG:HG3	1:H:127:ARG:NH2	2.10	0.66
1:O:152:THR:HG22	5:O:9706:HOH:O	1.94	0.66
1:J:156:LYS:HE2	5:J:841:HOH:O	1.96	0.66
1:I:76:THR:HG21	1:J:82:VAL:HG11	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:4:ASN:ND2	1:J:7:ASP:H	1.93	0.66
1:G:155:ALA:HA	1:I:149:LEU:HD13	1.78	0.66
1:P:81:LYS:HD3	1:P:82:VAL:H	1.60	0.66
1:E:41:ASP:OD2	1:P:145:HIS:HE1	1.79	0.66
1:P:168:SER:CB	4:P:2507[A]:FEC:O2C	2.44	0.65
1:O:168:SER:OG	1:P:58:ARG:HD3	1.96	0.65
1:E:110:LEU:HD23	1:E:114:LYS:HD2	1.78	0.65
1:L:168:SER:HB3	4:L:2107[A]:FEC:HBB2	1.79	0.65
1:L:4:ASN:HD22	1:L:7:ASP:H	1.45	0.65
1:I:172:VAL:HG23	1:J:55:ASP:OD2	1.97	0.65
1:I:58:ARG:HD3	1:J:168:SER:OG	1.97	0.65
4:I:1805[B]:FEC:ND	1:J:57:MET:CE	2.60	0.64
1:F:61:GLU:O	1:F:65:GLU:HG3	1.97	0.64
1:E:155:ALA:HA	1:P:149:LEU:HD13	1.79	0.64
1:H:29:GLN:NE2	1:H:83:VAL:H	1.95	0.64
4:L:2107[B]:FEC:HBC2	4:L:2107[B]:FEC:HHC	1.78	0.64
1:H:65:GLU:O	1:H:69:GLU:HG3	1.98	0.64
1:G:149:LEU:HD13	1:M:155:ALA:HA	1.79	0.64
1:K:168:SER:HA	4:L:2107[B]:FEC:O2C	1.98	0.63
1:G:168:SER:HB3	4:G:1607[B]:FEC:HBB2	1.79	0.63
1:H:114:LYS:HD2	3:I:1704:SO4:O2	1.98	0.63
4:I:1805[A]:FEC:O2C	1:J:168:SER:HA	1.99	0.62
4:A:1007[A]:FEC:O2C	1:B:168:SER:HA	2.00	0.62
1:M:31:MET:HG3	4:M:2207[A]:FEC:HBD1	1.81	0.61
1:O:136:LEU:O	1:O:140:GLU:HG3	2.00	0.61
1:O:168:SER:HA	4:P:2507[B]:FEC:O2C	2.00	0.61
4:I:1805[A]:FEC:HHC	4:I:1805[A]:FEC:HBC2	1.81	0.61
1:N:29:GLN:NE2	1:N:83:VAL:H	1.90	0.61
1:D:80:GLY:O	1:D:81:LYS:HE2	2.00	0.61
1:A:155:ALA:HA	1:N:149:LEU:HD13	1.83	0.60
1:C:57:MET:HB3	4:C:1207[B]:FEC:C1D	2.32	0.60
4:I:1805[A]:FEC:C1D	1:J:57:MET:HB3	2.32	0.60
1:I:126:GLU:HG2	5:I:9732:HOH:O	2.00	0.60
1:A:169:LYS:HB3	5:B:1211:HOH:O	2.00	0.60
4:I:1805[A]:FEC:HMD2	1:J:61:GLU:HB2	1.83	0.60
1:P:128:ILE:O	1:P:132:GLU:HG2	2.02	0.60
1:M:76:THR:HG22	5:M:8936:HOH:O	2.01	0.60
1:I:168:SER:OG	1:J:58:ARG:HD3	2.01	0.60
1:K:58:ARG:HB2	5:L:9682:HOH:O	2.02	0.59
1:G:57:MET:HB3	4:G:1607[B]:FEC:C1D	2.32	0.59
1:B:82:VAL:HB	5:B:1216:HOH:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:4:ASN:HD22	1:P:7:ASP:H	1.50	0.59
1:B:152:THR:HG21	1:H:152:THR:HG23	1.84	0.59
1:B:156:LYS:HD3	5:H:9690:HOH:O	2.03	0.59
1:H:123:ARG:NH1	1:H:126:GLU:OE1	2.36	0.59
1:M:4:ASN:OD1	1:M:7:ASP:HB2	2.02	0.59
4:C:1207[A]:FEC:HBB2	1:D:168:SER:HB3	1.83	0.59
1:N:29:GLN:HE22	1:N:83:VAL:N	1.89	0.59
1:C:152:THR:HA	1:E:152:THR:HG21	1.85	0.59
1:L:22:MET:HA	1:L:79:GLU:OE1	2.02	0.59
4:E:1407[B]:FEC:CHD	4:E:1407[B]:FEC:NC	2.65	0.59
1:D:4:ASN:HD22	1:D:4:ASN:N	2.00	0.59
1:B:126:GLU:O	1:B:130:GLU:HG3	2.03	0.58
1:O:5:ARG:HD2	1:O:8:ARG:NH1	2.18	0.58
1:J:110:LEU:CD2	1:J:114:LYS:HE2	2.33	0.58
1:E:20:ARG:HH22	4:E:1407[A]:FEC:CGA	2.17	0.58
1:E:61:GLU:HB2	4:E:1407[B]:FEC:CMD	2.33	0.58
1:I:168:SER:CB	4:I:1805[B]:FEC:HBB2	2.32	0.58
1:L:68:LYS:HD3	1:L:74:PRO:HD3	1.86	0.58
4:L:2107[B]:FEC:C1B	4:L:2107[B]:FEC:NA	2.66	0.58
4:M:2207[A]:FEC:CMD	1:N:61:GLU:HB2	2.34	0.58
4:I:1805[B]:FEC:HBC1	4:I:1805[B]:FEC:HHC	1.86	0.58
4:M:2207[A]:FEC:C1D	1:N:57:MET:HB3	2.33	0.58
1:M:25:HIS:HD2	5:M:9724:HOH:O	1.86	0.58
4:C:1207[B]:FEC:NC	4:C:1207[B]:FEC:C4B	2.66	0.57
1:J:29:GLN:NE2	1:J:83:VAL:H	1.98	0.57
1:O:61:GLU:HB2	4:P:2507[B]:FEC:HMD2	1.84	0.57
1:P:57:MET:HB3	4:P:2507[A]:FEC:C1D	2.34	0.57
1:H:169:LYS:HB2	5:H:9507:HOH:O	2.05	0.57
1:C:20:ARG:HH22	4:C:1207[B]:FEC:CGD	2.17	0.57
1:G:128:ILE:O	1:G:132:GLU:HG2	2.04	0.57
1:L:57:MET:HB3	4:L:2107[A]:FEC:C1D	2.35	0.57
1:K:110:LEU:HD23	1:K:114:LYS:HD2	1.87	0.56
1:K:114:LYS:CE	3:P:1504:SO4:O1	2.53	0.56
1:L:168:SER:HB3	4:L:2107[A]:FEC:O2C	2.03	0.56
1:B:81:LYS:HE2	5:B:1202:HOH:O	2.05	0.56
1:K:149:LEU:HD13	1:O:155:ALA:HA	1.86	0.56
1:P:31:MET:HG3	4:P:2507[B]:FEC:HBD1	1.88	0.56
4:E:1407[A]:FEC:O2C	1:F:168:SER:HA	2.06	0.56
4:A:1007[A]:FEC:HHC	4:A:1007[A]:FEC:HBC2	1.87	0.56
1:L:114:LYS:NZ	3:L:2104:SO4:S	2.65	0.56
1:C:126:GLU:O	1:C:130:GLU:HG3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:110:LEU:HD23	1:I:114:LYS:HD2	1.86	0.56
1:G:152:THR:HG21	1:M:152:THR:HG23	1.86	0.56
4:E:1407[B]:FEC:NC	4:E:1407[B]:FEC:C1C	2.69	0.55
4:M:2207[B]:FEC:HHC	4:M:2207[B]:FEC:HBC2	1.87	0.55
1:L:61:GLU:O	1:L:65:GLU:HG3	2.06	0.55
1:M:9:LYS:HE2	5:M:9323:HOH:O	2.06	0.55
1:A:169:LYS:HB2	5:A:1118:HOH:O	2.05	0.55
1:K:114:LYS:HE2	3:P:1504:SO4:S	2.47	0.55
1:E:78:LYS:HE2	5:E:490:HOH:O	2.05	0.55
1:B:50:LYS:HD3	5:B:1219:HOH:O	2.05	0.55
1:K:145:HIS:CE1	1:O:41:ASP:HB3	2.42	0.55
1:C:168:SER:HB3	4:C:1207[B]:FEC:HBB2	1.88	0.54
1:J:27:ILE:HD11	1:J:57:MET:HA	1.90	0.54
1:O:57:MET:HE2	4:P:2507[B]:FEC:NA	2.22	0.54
1:P:53:ALA:O	1:P:57:MET:HG3	2.07	0.54
1:N:4:ASN:HD21	1:N:7:ASP:H	1.56	0.54
1:I:57:MET:HB3	4:I:1805[A]:FEC:C1B	2.37	0.54
1:O:57:MET:HB3	4:P:2507[B]:FEC:C1D	2.38	0.54
4:E:1407[B]:FEC:C1D	4:E:1407[B]:FEC:NC	2.49	0.54
1:H:145:HIS:HD2	5:H:9052:HOH:O	1.90	0.54
1:F:145:HIS:HE1	1:L:41:ASP:OD2	1.90	0.54
1:P:27:ILE:HD11	1:P:57:MET:HA	1.90	0.54
1:I:57:MET:HB3	4:I:1805[B]:FEC:C1D	2.37	0.54
1:A:81:LYS:HE2	5:A:1076:HOH:O	2.08	0.54
1:F:5:ARG:HD2	1:F:8:ARG:NH1	2.24	0.53
1:H:123:ARG:HE	1:H:127:ARG:HE	1.55	0.53
1:O:88:VAL:HB	1:O:89:PRO:HD3	1.90	0.53
1:L:168:SER:HB3	4:L:2107[A]:FEC:CGB	2.38	0.53
4:E:1407[B]:FEC:HAC2	1:F:168:SER:HB2	1.89	0.53
1:A:58:ARG:HB2	5:B:1220:HOH:O	2.09	0.53
1:A:166:THR:HG22	1:A:167:ALA:O	2.09	0.53
4:M:2207[A]:FEC:CGC	1:N:168:SER:HA	2.39	0.52
1:J:145:HIS:HD2	5:J:786:HOH:O	1.91	0.52
1:K:12:VAL:CG1	1:K:121:THR:HG21	2.40	0.52
1:G:61:GLU:HB2	4:G:1607[B]:FEC:HMD2	1.92	0.52
1:H:110:LEU:CD2	1:H:114:LYS:HE2	2.40	0.52
1:K:57:MET:HB3	4:L:2107[A]:FEC:C1B	2.39	0.52
1:D:27:ILE:HD11	1:D:57:MET:HA	1.92	0.52
1:L:88:VAL:HG12	1:L:146:ILE:HD13	1.92	0.52
4:E:1407[A]:FEC:HBC2	1:F:168:SER:CB	2.39	0.52
1:L:110:LEU:CD2	1:L:114:LYS:HE3	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:156:LYS:HD3	5:J:9480:HOH:O	2.10	0.51
1:B:145:HIS:HE1	1:H:41:ASP:OD2	1.93	0.51
1:K:164:THR:O	1:L:169:LYS:HD3	2.10	0.51
1:C:55:ASP:OD1	1:C:58:ARG:NH2	2.43	0.51
1:C:61:GLU:HB2	4:C:1207[B]:FEC:HMD2	1.93	0.51
1:C:162:SER:N	3:C:1206:SO4:O3	2.32	0.51
1:G:61:GLU:HB2	4:G:1607[B]:FEC:CMD	2.41	0.51
4:G:1607[A]:FEC:CBB	1:H:168:SER:HB3	2.40	0.51
1:H:156:LYS:HD3	5:H:9520:HOH:O	2.11	0.51
1:H:136:LEU:HD11	1:H:140:GLU:OE2	2.10	0.51
1:I:84:THR:HB	1:J:73:GLU:OE2	2.11	0.51
1:O:53:ALA:O	1:O:57:MET:HG3	2.11	0.51
1:O:61:GLU:HB2	4:P:2507[B]:FEC:CMD	2.40	0.51
1:M:57:MET:HB3	4:M:2207[A]:FEC:C1B	2.41	0.51
1:A:161:PRO:HB3	3:A:1006:SO4:O2	2.11	0.51
1:D:81:LYS:HD3	5:D:296:HOH:O	2.10	0.50
1:I:114:LYS:CE	3:I:1704:SO4:O4	2.58	0.50
1:P:90:VAL:O	1:P:94:SER:OG	2.28	0.50
1:B:88:VAL:HG12	1:B:146:ILE:HD13	1.93	0.50
4:I:1805[A]:FEC:HBB2	1:J:168:SER:HB3	1.94	0.50
1:N:111:LYS:HA	1:N:114:LYS:CE	2.41	0.50
1:N:37:LEU:HA	1:N:40:MET:HE3	1.94	0.50
1:P:52:ILE:O	1:P:56:GLU:HG2	2.12	0.50
1:I:168:SER:OG	4:I:1805[B]:FEC:O2B	2.28	0.50
1:A:168:SER:HB3	4:A:1007[B]:FEC:CBB	2.40	0.49
1:J:88:VAL:HG12	1:J:146:ILE:HD13	1.94	0.49
1:N:88:VAL:HB	1:N:89:PRO:HD3	1.94	0.49
1:O:29:GLN:O	1:O:33:GLN:HG3	2.12	0.49
1:I:82:VAL:HG11	1:J:76:THR:HG21	1.93	0.49
1:H:110:LEU:HD22	1:H:114:LYS:HE2	1.94	0.49
1:K:130:GLU:OE1	1:P:123:ARG:HG2	2.12	0.49
1:L:168:SER:HB3	4:L:2107[A]:FEC:O2B	2.13	0.49
1:E:128:ILE:O	1:E:132:GLU:HG2	2.12	0.49
1:H:114:LYS:CD	3:I:1704:SO4:O2	2.60	0.49
1:E:158:ALA:HB1	1:P:145:HIS:CD2	2.48	0.49
1:L:168:SER:HA	4:L:2107[A]:FEC:O1C	2.13	0.49
1:O:32:ASN:OD1	1:P:73:GLU:OE2	2.29	0.49
1:L:61:GLU:HB2	4:L:2107[A]:FEC:HMD2	1.95	0.48
4:E:1407[A]:FEC:CGD	1:F:20:ARG:HH22	2.26	0.48
1:B:78:LYS:HE2	3:B:1005:SO4:O2	2.13	0.48
1:B:114:LYS:NZ	3:B:1104:SO4:O3	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:1607[A]:FEC:C1D	1:H:57:MET:HB3	2.43	0.48
1:K:88:VAL:HB	1:K:89:PRO:HD3	1.95	0.48
1:A:158:ALA:O	1:N:156:LYS:NZ	2.46	0.48
1:K:20:ARG:HH22	4:L:2107[B]:FEC:CGD	2.26	0.48
4:G:1607[B]:FEC:ND	1:H:57:MET:CE	2.76	0.48
1:A:169:LYS:NZ	1:B:166:THR:HG22	2.29	0.48
1:K:52:ILE:O	1:K:56:GLU:HG2	2.13	0.48
1:L:29:GLN:O	1:L:33:GLN:HG3	2.13	0.48
1:A:50:LYS:HE3	4:A:1007[B]:FEC:HAB2	1.94	0.48
1:K:61:GLU:O	1:K:65:GLU:HG3	2.13	0.48
1:O:128:ILE:O	1:O:132:GLU:HG2	2.12	0.48
1:I:57:MET:HB3	4:I:1805[A]:FEC:CHB	2.43	0.48
1:A:29:GLN:O	1:A:33:GLN:HG3	2.13	0.48
1:G:145:HIS:CE1	1:M:41:ASP:HB3	2.49	0.48
4:C:1207[A]:FEC:O2C	1:D:168:SER:HB3	2.14	0.48
4:E:1407[B]:FEC:HBC1	4:E:1407[B]:FEC:HHC	1.96	0.48
4:M:2207[A]:FEC:HMD2	1:N:61:GLU:HB2	1.95	0.48
1:P:133:GLN:NE2	5:P:517:HOH:O	2.46	0.48
1:D:156:LYS:HG2	1:D:157:ILE:HD13	1.95	0.48
1:G:88:VAL:HB	1:G:89:PRO:HD3	1.94	0.48
4:C:1207[A]:FEC:CGD	1:D:20:ARG:HH22	2.26	0.48
1:I:58:ARG:HG2	5:I:9611:HOH:O	2.13	0.48
1:A:41:ASP:OD2	1:N:145:HIS:HE1	1.97	0.48
1:L:61:GLU:HB2	4:L:2107[A]:FEC:CMD	2.44	0.48
1:A:163:SER:HB2	3:A:1006:SO4:O4	2.14	0.48
1:E:20:ARG:HH22	4:E:1407[B]:FEC:CGD	2.25	0.48
1:G:5:ARG:HG2	5:G:9341:HOH:O	2.14	0.48
1:B:130:GLU:OE2	1:G:127:ARG:NH2	2.47	0.47
3:D:1301:SO4:S	5:D:9670:HOH:O	1.98	0.47
1:B:36:SER:C	1:B:40:MET:HE3	2.34	0.47
1:I:169:LYS:N	4:I:1805[B]:FEC:O2C	2.47	0.47
1:E:78:LYS:HE3	1:E:82:VAL:HG23	1.96	0.47
1:H:14:GLU:O	1:H:18:LYS:HG3	2.14	0.47
1:B:149:LEU:HD13	1:H:155:ALA:HA	1.95	0.47
1:D:123:ARG:NH1	1:D:126:GLU:OE1	2.47	0.47
1:O:57:MET:CE	4:P:2507[B]:FEC:NB	2.77	0.47
1:L:168:SER:HB3	4:L:2107[A]:FEC:CBB	2.43	0.47
1:N:111:LYS:HA	1:N:114:LYS:HE3	1.96	0.47
1:P:168:SER:HB3	4:P:2507[A]:FEC:CBB	2.40	0.47
1:I:58:ARG:HD3	1:J:168:SER:HG	1.79	0.47
1:B:123:ARG:NH1	1:B:126:GLU:OE1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:3:GLY:HA3	5:L:9493:HOH:O	2.14	0.47
4:I:1805[B]:FEC:NC	4:I:1805[B]:FEC:C4B	2.77	0.47
1:C:65:GLU:O	1:C:69:GLU:HG3	2.14	0.47
1:O:123:ARG:NH1	1:O:126:GLU:OE1	2.47	0.47
1:G:14:GLU:O	1:G:18:LYS:HG3	2.13	0.47
1:C:51:LEU:HD21	1:C:164:THR:HB	1.96	0.47
1:F:5:ARG:HD2	1:F:8:ARG:HH11	1.80	0.47
1:O:25:HIS:HE1	1:O:98:GLN:OE1	1.98	0.47
1:A:76:THR:OG1	5:B:1216:HOH:O	2.20	0.47
1:O:8:ARG:NH1	5:O:9358:HOH:O	2.48	0.47
1:J:90:VAL:O	1:J:94:SER:OG	2.33	0.47
4:E:1407[A]:FEC:C1D	1:F:57:MET:HB3	2.45	0.46
4:I:1805[B]:FEC:HBD1	1:J:31:MET:HG3	1.97	0.46
4:G:1607[A]:FEC:O2B	1:H:168:SER:HB3	2.15	0.46
1:O:110:LEU:CD2	1:O:114:LYS:HE3	2.45	0.46
1:I:123:ARG:NH1	5:I:9732:HOH:O	2.47	0.46
1:A:110:LEU:HD23	1:A:114:LYS:HD2	1.97	0.46
1:I:123:ARG:NH1	1:I:127:ARG:HG3	2.30	0.46
1:A:123:ARG:NH1	1:A:126:GLU:OE1	2.48	0.46
1:P:57:MET:CE	4:P:2507[B]:FEC:ND	2.78	0.46
1:C:123:ARG:NH1	1:C:126:GLU:OE1	2.49	0.46
1:M:55:ASP:OD1	1:M:58:ARG:NH2	2.48	0.46
1:P:168:SER:HB3	4:P:2507[A]:FEC:O2B	2.15	0.46
1:O:76:THR:O	1:P:78:LYS:HE3	2.15	0.46
1:F:127:ARG:NH2	5:F:9540:HOH:O	2.49	0.46
1:P:79:GLU:HB2	5:P:9131:HOH:O	2.15	0.46
1:P:29:GLN:O	1:P:33:GLN:HG3	2.15	0.46
1:K:112:VAL:O	1:K:116:GLN:HG2	2.14	0.46
1:K:128:ILE:O	1:K:132:GLU:HG2	2.16	0.46
1:D:147:LYS:HE3	1:D:147:LYS:HB2	1.74	0.46
1:K:57:MET:HB3	4:L:2107[A]:FEC:CHB	2.46	0.46
4:C:1207[B]:FEC:HHB	4:C:1207[B]:FEC:HBA2	1.97	0.46
1:G:158:ALA:O	1:I:156:LYS:NZ	2.48	0.46
4:G:1607[A]:FEC:HMD2	1:H:61:GLU:HB2	1.96	0.46
1:D:61:GLU:O	1:D:65:GLU:HG3	2.16	0.46
4:E:1407[A]:FEC:HMD2	1:F:61:GLU:HB2	1.97	0.46
4:I:1805[B]:FEC:CHC	4:I:1805[B]:FEC:NC	2.74	0.46
1:G:53:ALA:O	1:G:57:MET:HG3	2.16	0.46
1:A:169:LYS:HZ2	1:B:166:THR:HG22	1.81	0.46
1:M:57:MET:HB3	4:M:2207[B]:FEC:C1D	2.45	0.46
4:M:2207[A]:FEC:O1C	1:N:168:SER:HA	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:2207[B]:FEC:C1B	1:N:57:MET:HB3	2.45	0.45
1:J:157:ILE:N	1:J:157:ILE:HD13	2.30	0.45
1:G:31:MET:HG3	4:G:1607[A]:FEC:HBD1	1.99	0.45
1:G:123:ARG:NH1	1:G:126:GLU:OE1	2.49	0.45
5:K:9231:HOH:O	1:P:127:ARG:NH2	2.49	0.45
1:G:27:ILE:HD11	1:G:57:MET:HA	1.99	0.45
4:M:2207[A]:FEC:NB	1:N:57:MET:CE	2.79	0.45
1:H:111:LYS:O	1:H:115:GLU:HG3	2.17	0.45
4:G:1607[B]:FEC:C1B	1:H:57:MET:HB3	2.46	0.45
1:G:68:LYS:HA	1:G:68:LYS:HD2	1.81	0.45
1:L:50:LYS:HE3	4:L:2107[B]:FEC:HMC2	1.99	0.45
1:M:7:ASP:OD2	1:M:11:LYS:NZ	2.49	0.45
1:L:133:GLN:NE2	5:L:9208:HOH:O	2.48	0.45
1:M:164:THR:N	5:M:9457:HOH:O	2.47	0.45
1:F:149:LEU:HD13	1:L:155:ALA:HA	1.99	0.45
1:E:55:ASP:OD1	1:E:58:ARG:NH2	2.49	0.45
1:P:61:GLU:HB2	4:P:2507[A]:FEC:HMD2	1.99	0.45
4:C:1207[B]:FEC:C1B	1:D:57:MET:HB3	2.47	0.45
4:G:1607[A]:FEC:CMD	1:H:61:GLU:HB2	2.47	0.45
1:G:43:GLY:HA2	1:G:162:SER:HB3	1.98	0.45
1:L:25:HIS:HD2	5:L:9609:HOH:O	1.99	0.45
1:D:127:ARG:NH2	5:D:410:HOH:O	2.49	0.45
1:L:90:VAL:O	1:L:94:SER:OG	2.28	0.45
1:C:33:GLN:NE2	1:C:95:ASP:OD2	2.48	0.45
1:A:61:GLU:HB2	4:A:1007[B]:FEC:CMD	2.47	0.44
1:E:27:ILE:HD11	1:E:57:MET:HA	1.98	0.44
4:A:1007[B]:FEC:CGA	1:B:20:ARG:HH22	2.30	0.44
1:C:11:LYS:HD2	1:C:116:GLN:NE2	2.32	0.44
1:E:88:VAL:HA	1:E:91:ILE:HD12	1.99	0.44
4:C:1207[A]:FEC:HBA2	1:D:31:MET:HG3	2.00	0.44
1:M:4:ASN:HB2	3:M:2202:SO4:O1	2.17	0.44
1:D:79:GLU:O	1:D:79:GLU:OE1	2.35	0.44
1:H:128:ILE:O	1:H:132:GLU:HG2	2.18	0.44
1:G:20:ARG:HH22	4:G:1607[B]:FEC:CGD	2.29	0.44
1:D:88:VAL:HG12	1:D:146:ILE:HD13	1.99	0.44
1:O:61:GLU:O	1:O:65:GLU:HG3	2.17	0.44
4:A:1007[A]:FEC:CGD	1:B:20:ARG:HH22	2.30	0.44
1:K:58:ARG:HG3	5:K:9548:HOH:O	2.18	0.44
4:M:2207[B]:FEC:CGA	1:N:20:ARG:HH22	2.31	0.44
1:I:123:ARG:NH1	1:I:126:GLU:OE1	2.51	0.44
1:K:78:LYS:NZ	5:K:924:HOH:O	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:163:SER:N	3:O:2406:SO4:O3	2.46	0.44
1:G:163:SER:HA	3:G:1601:SO4:O4	2.18	0.44
1:A:57:MET:HB3	4:A:1007[A]:FEC:C1B	2.47	0.44
4:C:1207[A]:FEC:CGC	1:D:168:SER:HA	2.47	0.44
1:M:61:GLU:HB2	4:M:2207[B]:FEC:HMD2	2.00	0.44
1:K:51:LEU:HD21	1:K:164:THR:HB	1.99	0.44
1:I:20:ARG:HH22	4:I:1805[B]:FEC:CGD	2.30	0.43
1:D:95:ASP:HB3	1:D:139:TYR:CE1	2.53	0.43
1:O:45:LEU:HG	1:O:157:ILE:HG21	2.00	0.43
1:M:161:PRO:HB3	3:M:2206:SO4:O2	2.18	0.43
1:A:57:MET:HB3	4:A:1007[B]:FEC:C1D	2.48	0.43
4:A:1007[A]:FEC:CGB	1:B:168:SER:HB3	2.47	0.43
1:C:57:MET:CE	4:C:1207[B]:FEC:NB	2.81	0.43
1:K:110:LEU:CD2	1:K:114:LYS:HD2	2.48	0.43
4:C:1207[B]:FEC:HMC2	1:D:50:LYS:CE	2.48	0.43
4:G:1607[B]:FEC:HMC2	1:H:50:LYS:HE3	2.01	0.43
1:L:68:LYS:HA	1:L:68:LYS:HD2	1.74	0.43
1:E:58:ARG:NH1	1:E:131:GLU:OE1	2.51	0.43
1:O:73:GLU:OE2	1:P:84:THR:HB	2.18	0.43
1:D:33:GLN:OE1	1:D:95:ASP:OD2	2.36	0.43
1:G:168:SER:HB3	4:G:1607[B]:FEC:O2C	2.18	0.43
1:N:5:ARG:HD2	1:N:8:ARG:NH1	2.33	0.43
1:O:90:VAL:O	1:O:94:SER:OG	2.37	0.43
1:K:57:MET:HB3	4:L:2107[B]:FEC:C1D	2.49	0.43
1:B:78:LYS:CE	3:B:1005:SO4:O2	2.66	0.43
1:L:29:GLN:NE2	1:L:83:VAL:H	1.96	0.43
4:C:1207[B]:FEC:NC	4:C:1207[B]:FEC:CHC	2.82	0.43
1:F:137:THR:HG23	5:F:999:HOH:O	2.19	0.43
1:I:7:ASP:OD2	1:I:11:LYS:NZ	2.38	0.43
4:P:2507[A]:FEC:CHC	4:P:2507[A]:FEC:HBC2	2.47	0.43
5:A:1068:HOH:O	1:N:145:HIS:HD2	2.02	0.43
4:C:1207[A]:FEC:HMD2	1:D:61:GLU:HB2	2.01	0.43
1:I:168:SER:C	4:I:1805[B]:FEC:O2C	2.52	0.43
1:I:153:TYR:O	1:I:156:LYS:HB3	2.19	0.43
1:B:52:ILE:O	1:B:56:GLU:HG2	2.19	0.43
4:E:1407[B]:FEC:CGA	1:F:20:ARG:HH22	2.30	0.42
1:I:156:LYS:HD3	1:I:157:ILE:HD13	2.00	0.42
1:D:95:ASP:HB3	1:D:139:TYR:CD1	2.53	0.42
4:M:2207[A]:FEC:O2C	1:N:168:SER:HA	2.19	0.42
1:D:127:ARG:NE	5:D:9572:HOH:O	2.49	0.42
1:O:52:ILE:O	1:O:56:GLU:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:25:HIS:HB2	1:C:79:GLU:O	2.19	0.42
1:G:168:SER:HA	4:G:1607[B]:FEC:O2C	2.20	0.42
1:M:168:SER:HB3	4:M:2207[B]:FEC:HBB2	2.00	0.42
1:E:112:VAL:O	1:E:116:GLN:HG2	2.19	0.42
1:G:168:SER:HA	4:G:1607[B]:FEC:CGC	2.49	0.42
1:H:27:ILE:HD11	1:H:57:MET:HA	2.02	0.42
1:E:61:GLU:HB2	4:E:1407[B]:FEC:HMD2	2.00	0.42
1:J:45:LEU:HG	1:J:157:ILE:HG21	2.01	0.42
1:P:11:LYS:NZ	5:P:9174:HOH:O	2.48	0.42
1:G:8:ARG:HG2	1:G:116:GLN:OE1	2.20	0.42
1:O:27:ILE:HD11	1:O:57:MET:HA	2.02	0.42
4:I:1805[A]:FEC:CMD	1:J:61:GLU:HB2	2.50	0.42
1:H:123:ARG:HE	1:H:127:ARG:NE	2.16	0.42
1:D:88:VAL:HA	1:D:91:ILE:HD12	2.01	0.42
4:I:1805[A]:FEC:O2B	1:J:168:SER:HB3	2.20	0.42
1:B:43:GLY:HA2	1:B:162:SER:HB3	2.00	0.42
1:D:73:GLU:HA	1:D:74:PRO:HD3	1.88	0.42
1:O:162:SER:N	3:O:2406:SO4:O3	2.53	0.42
1:C:88:VAL:HG12	1:C:146:ILE:HD13	2.02	0.42
1:K:76:THR:HG21	1:L:82:VAL:HG11	2.02	0.42
1:F:33:GLN:OE1	1:F:95:ASP:OD2	2.37	0.42
4:G:1607[B]:FEC:HBC2	4:G:1607[B]:FEC:HHC	2.01	0.41
1:K:9:LYS:O	1:K:13:ILE:HG13	2.20	0.41
1:F:36:SER:HB3	1:F:40:MET:HE2	2.02	0.41
1:A:27:ILE:HD11	1:A:57:MET:HA	2.03	0.41
1:M:61:GLU:HB2	4:M:2207[B]:FEC:CMD	2.50	0.41
1:G:155:ALA:CA	1:I:149:LEU:HD13	2.48	0.41
1:E:158:ALA:O	1:P:156:LYS:NZ	2.48	0.41
1:F:88:VAL:HB	1:F:89:PRO:HD3	2.02	0.41
1:F:14:GLU:O	1:F:18:LYS:HG3	2.20	0.41
1:F:90:VAL:HG21	5:F:9309:HOH:O	2.19	0.41
1:C:77:GLN:NE2	1:D:78:LYS:NZ	2.68	0.41
1:K:4:ASN:OD1	1:K:7:ASP:HB2	2.20	0.41
1:E:153:TYR:O	1:E:156:LYS:HB3	2.21	0.41
1:L:4:ASN:HB3	5:L:9356:HOH:O	2.21	0.41
1:J:105:ALA:HA	1:J:108[A]:GLN:NE2	2.35	0.41
1:G:57:MET:HB3	4:G:1607[A]:FEC:C1B	2.50	0.41
4:M:2207[B]:FEC:CHB	1:N:57:MET:HB3	2.51	0.41
1:N:169:LYS:HB3	5:N:2404:HOH:O	2.20	0.41
1:M:52:ILE:O	1:M:56:GLU:HG2	2.19	0.41
1:E:57:MET:HB3	4:E:1407[A]:FEC:C1B	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:LYS:CE	4:A:1007[B]:FEC:HAB2	2.51	0.41
1:H:123:ARG:HG3	1:H:127:ARG:HH21	1.85	0.41
4:C:1207[B]:FEC:NC	4:C:1207[B]:FEC:ND	2.68	0.41
1:I:110:LEU:CD2	1:I:114:LYS:HD2	2.51	0.41
1:G:155:ALA:O	1:I:156:LYS:NZ	2.44	0.41
1:N:112:VAL:O	1:N:116:GLN:HG2	2.21	0.41
1:C:34:HIS:HE1	5:C:371:HOH:O	2.03	0.41
4:P:2507[B]:FEC:HHC	4:P:2507[B]:FEC:HBC2	2.02	0.41
1:H:110:LEU:O	1:H:114:LYS:HG3	2.21	0.41
1:O:5:ARG:HA	1:O:8:ARG:HH11	1.86	0.41
1:L:71:GLY:HA2	5:L:956:HOH:O	2.21	0.41
1:O:73:GLU:HA	1:O:74:PRO:HD3	1.90	0.40
1:I:13:ILE:HD13	1:I:72:GLY:HA3	2.02	0.40
4:C:1207[A]:FEC:HHC	4:C:1207[A]:FEC:HBC2	2.03	0.40
1:M:77:GLN:NE2	5:M:8918:HOH:O	2.54	0.40
1:O:68:LYS:HA	1:O:68:LYS:HD2	1.95	0.40
4:C:1207[A]:FEC:C1D	1:D:57:MET:HB3	2.51	0.40
4:E:1407[B]:FEC:HHB	4:E:1407[B]:FEC:HBA2	2.04	0.40
1:I:58:ARG:HH11	1:I:58:ARG:HD2	1.67	0.40
1:M:33:GLN:NE2	1:M:95:ASP:OD2	2.49	0.40
1:I:126:GLU:O	1:I:130:GLU:HG3	2.21	0.40
1:E:73:GLU:HA	1:E:74:PRO:HD3	1.83	0.40
1:A:4:ASN:HB3	1:A:7:ASP:HB2	2.04	0.40
1:P:57:MET:CE	4:P:2507[A]:FEC:NB	2.84	0.40
1:A:57:MET:HB3	4:A:1007[A]:FEC:CHB	2.51	0.40
1:G:33:GLN:NE2	1:G:95:ASP:OD2	2.53	0.40

All (19) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:1802:SO4:O3	3:L:2102:SO4:O1[9_465]	0.18	2.02
3:I:1802:SO4:O2	3:L:2102:SO4:O4[9_465]	0.28	1.92
3:I:1802:SO4:O1	3:L:2102:SO4:O3[9_465]	0.31	1.89
3:I:1802:SO4:O4	3:L:2102:SO4:O2[9_465]	0.50	1.70
3:I:1802:SO4:S	3:L:2102:SO4:S[9_465]	0.56	1.64
3:I:1802:SO4:O1	3:L:2102:SO4:S[9_465]	1.22	0.98
3:I:1802:SO4:S	3:L:2102:SO4:O1[9_465]	1.23	0.97
3:I:1802:SO4:O2	3:L:2102:SO4:S[9_465]	1.38	0.82
3:I:1802:SO4:S	3:L:2102:SO4:O2[9_465]	1.44	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:1802:SO4:S	3:L:2102:SO4:O4[9_465]	1.63	0.57
3:I:1802:SO4:O4	3:L:2102:SO4:S[9_465]	1.65	0.55
3:I:1802:SO4:O3	3:L:2102:SO4:S[9_465]	1.76	0.44
1:L:114:LYS:NZ	3:L:2104:SO4:O2[12_554]	1.80	0.40
3:I:1802:SO4:S	3:L:2102:SO4:O3[9_465]	1.81	0.39
1:L:114:LYS:CE	3:L:2104:SO4:O2[12_554]	2.09	0.11
1:L:114:LYS:NZ	3:L:2104:SO4:O1[6_555]	2.15	0.05
3:I:1802:SO4:O1	3:L:2102:SO4:O2[9_465]	2.16	0.04
1:L:114:LYS:CD	3:L:2104:SO4:O1[6_555]	2.16	0.04
1:L:114:LYS:CE	3:L:2104:SO4:O1[6_555]	2.19	0.01

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	167/179 (93%)	163 (98%)	4 (2%)	0	100	100
1	B	167/179 (93%)	164 (98%)	3 (2%)	0	100	100
1	C	167/179 (93%)	165 (99%)	1 (1%)	1 (1%)	30	18
1	D	168/179 (94%)	166 (99%)	2 (1%)	0	100	100
1	E	167/179 (93%)	163 (98%)	3 (2%)	1 (1%)	30	18
1	F	167/179 (93%)	165 (99%)	2 (1%)	0	100	100
1	G	167/179 (93%)	163 (98%)	3 (2%)	1 (1%)	30	18
1	H	168/179 (94%)	165 (98%)	2 (1%)	1 (1%)	30	18
1	I	168/179 (94%)	164 (98%)	3 (2%)	1 (1%)	30	18
1	J	168/179 (94%)	165 (98%)	3 (2%)	0	100	100
1	K	167/179 (93%)	165 (99%)	2 (1%)	0	100	100
1	L	169/179 (94%)	166 (98%)	3 (2%)	0	100	100
1	M	170/179 (95%)	166 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	N	167/179 (93%)	164 (98%)	3 (2%)	0	100	100
1	O	167/179 (93%)	165 (99%)	2 (1%)	0	100	100
1	P	168/179 (94%)	163 (97%)	5 (3%)	0	100	100
All	All	2682/2864 (94%)	2632 (98%)	45 (2%)	5 (0%)	52	43

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	168	SER
1	I	168	SER
1	C	168	SER
1	E	168	SER
1	G	151	ASP

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	139/145 (96%)	134 (96%)	5 (4%)	42	34
1	B	137/145 (94%)	133 (97%)	4 (3%)	50	42
1	C	136/145 (94%)	132 (97%)	4 (3%)	50	42
1	D	139/145 (96%)	133 (96%)	6 (4%)	35	27
1	E	137/145 (94%)	130 (95%)	7 (5%)	29	19
1	F	138/145 (95%)	133 (96%)	5 (4%)	42	34
1	G	137/145 (94%)	133 (97%)	4 (3%)	50	42
1	H	137/145 (94%)	134 (98%)	3 (2%)	60	53
1	I	138/145 (95%)	136 (99%)	2 (1%)	74	72
1	J	135/145 (93%)	130 (96%)	5 (4%)	41	32
1	K	137/145 (94%)	132 (96%)	5 (4%)	42	34
1	L	140/145 (97%)	136 (97%)	4 (3%)	50	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	140/145 (97%)	136 (97%)	4 (3%)	50	42
1	N	138/145 (95%)	134 (97%)	4 (3%)	50	42
1	O	135/145 (93%)	130 (96%)	5 (4%)	41	32
1	P	138/145 (95%)	134 (97%)	4 (3%)	50	42
All	All	2201/2320 (95%)	2130 (97%)	71 (3%)	46	38

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASP
1	A	38	ASP
1	A	81	LYS
1	A	147	LYS
1	A	166	THR
1	B	6	GLU
1	B	38	ASP
1	B	79	GLU
1	B	81	LYS
1	C	38	ASP
1	C	111	LYS
1	C	156	LYS
1	C	169	LYS
1	D	4	ASN
1	D	38	ASP
1	D	79	GLU
1	D	94	SER
1	D	147	LYS
1	D	156	LYS
1	E	4	ASN
1	E	38	ASP
1	E	78	LYS
1	E	81	LYS
1	E	93	GLU
1	E	156	LYS
1	E	168	SER
1	F	4	ASN
1	F	38	ASP
1	F	79	GLU
1	F	156	LYS
1	F	163	SER
1	G	38	ASP

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Mol	Chain	Res	Type
1	G	152	THR
1	G	166	THR
1	G	169	LYS
1	H	77	GLN
1	H	81	LYS
1	H	156	LYS
1	I	111	LYS
1	I	156	LYS
1	J	4	ASN
1	J	58	ARG
1	J	93	GLU
1	J	94	SER
1	J	152	THR
1	K	4	ASN
1	K	7	ASP
1	K	38	ASP
1	K	163	SER
1	K	169	LYS
1	L	68	LYS
1	L	79	GLU
1	L	94	SER
1	L	152	THR
1	M	7	ASP
1	M	38	ASP
1	M	111	LYS
1	M	156	LYS
1	N	4	ASN
1	N	38	ASP
1	N	79	GLU
1	N	93	GLU
1	O	38	ASP
1	O	93	GLU
1	O	94	SER
1	O	111	LYS
1	O	130	GLU
1	P	4	ASN
1	P	79	GLU
1	P	81	LYS
1	P	94	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	33	GLN
1	B	4	ASN
1	B	29	GLN
1	B	62	ASN
1	B	133	GLN
1	B	145	HIS
1	C	25	HIS
1	C	32	ASN
1	C	33	GLN
1	C	77	GLN
1	C	108	GLN
1	D	29	GLN
1	D	98	GLN
1	D	133	GLN
1	E	4	ASN
1	E	32	ASN
1	F	4	ASN
1	F	29	GLN
1	F	133	GLN
1	F	145	HIS
1	G	32	ASN
1	G	33	GLN
1	H	25	HIS
1	H	29	GLN
1	H	133	GLN
1	H	145	HIS
1	I	32	ASN
1	I	33	GLN
1	J	4	ASN
1	J	25	HIS
1	J	29	GLN
1	J	98	GLN
1	J	145	HIS
1	J	148	ASN
1	K	32	ASN
1	K	33	GLN
1	K	108	GLN
1	L	4	ASN
1	L	25	HIS
1	L	29	GLN
1	L	133	GLN
1	M	32	ASN

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Mol	Chain	Res	Type
1	M	33	GLN
1	M	77	GLN
1	M	108	GLN
1	N	4	ASN
1	N	29	GLN
1	N	133	GLN
1	N	145	HIS
1	O	25	HIS
1	O	32	ASN
1	O	33	GLN
1	O	77	GLN
1	P	4	ASN
1	P	25	HIS
1	P	29	GLN
1	P	98	GLN
1	P	133	GLN
1	P	145	HIS

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 104 ligands modelled in this entry, 32 are monoatomic - leaving 72 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	$\#\|Z\|>2$
3	SO4	A	1001	-	4,4,4	3.05	2 (50%)	6,6,6	1.02	0
3	SO4	A	1003	-	4,4,4	3.25	2 (50%)	6,6,6	0.92	0
3	SO4	A	1006	-	4,4,4	0.54	0	6,6,6	0.86	0
4	FEC	A	1007[A]	1	34,56,56	3.05	5 (14%)	43,90,90	2.40	7 (16%)
4	FEC	A	1007[B]	1	34,56,56	6.91	7 (20%)	43,90,90	6.42	20 (46%)
3	SO4	B	1005	-	4,4,4	1.02	0	6,6,6	1.83	2 (33%)
3	SO4	B	1101	-	4,4,4	3.09	2 (50%)	6,6,6	0.93	0
3	SO4	B	1103	-	4,4,4	0.46	0	6,6,6	0.47	0
3	SO4	B	1104	-	4,4,4	3.31	2 (50%)	6,6,6	1.02	0
3	SO4	B	1106	-	4,4,4	0.45	0	6,6,6	1.42	1 (16%)
3	SO4	C	1201	-	4,4,4	3.13	2 (50%)	6,6,6	0.95	0
3	SO4	C	1203	-	4,4,4	0.46	0	6,6,6	1.61	1 (16%)
3	SO4	C	1204	-	4,4,4	3.28	2 (50%)	6,6,6	0.94	0
3	SO4	C	1206	-	4,4,4	0.73	0	6,6,6	0.37	0
4	FEC	C	1207[A]	1	34,56,56	2.69	4 (11%)	43,90,90	2.19	9 (20%)
4	FEC	C	1207[B]	1	34,56,56	5.79	9 (26%)	43,90,90	6.64	17 (39%)
3	SO4	D	1301	-	4,4,4	3.29	2 (50%)	6,6,6	0.94	0
3	SO4	D	1303	-	4,4,4	0.43	0	6,6,6	0.52	0
3	SO4	D	1306	-	4,4,4	0.77	0	6,6,6	1.12	1 (16%)
3	SO4	E	1304	-	4,4,4	3.13	2 (50%)	6,6,6	0.96	0
3	SO4	E	1403	-	4,4,4	0.80	0	6,6,6	0.82	0
3	SO4	E	1406	-	4,4,4	0.44	0	6,6,6	0.93	0
4	FEC	E	1407[A]	1	34,56,56	2.88	4 (11%)	43,90,90	2.44	10 (23%)
4	FEC	E	1407[B]	1	34,56,56	3.95	6 (17%)	43,90,90	4.00	15 (34%)
3	SO4	F	1501	-	4,4,4	3.33	2 (50%)	6,6,6	0.90	0
3	SO4	F	1502	-	4,4,4	3.18	2 (50%)	6,6,6	1.04	0
3	SO4	F	1506	-	4,4,4	0.47	0	6,6,6	1.64	1 (16%)
3	SO4	G	1601	-	4,4,4	3.55	2 (50%)	6,6,6	1.00	0
3	SO4	G	1603	-	4,4,4	3.31	2 (50%)	6,6,6	1.02	0
3	SO4	G	1606	-	4,4,4	0.40	0	6,6,6	0.67	0
4	FEC	G	1607[A]	1	34,56,56	2.90	5 (14%)	43,90,90	2.72	13 (30%)
4	FEC	G	1607[B]	1	34,56,56	4.43	6 (17%)	43,90,90	5.22	15 (34%)
3	SO4	H	1701	-	4,4,4	3.05	2 (50%)	6,6,6	0.95	0
3	SO4	H	1702	-	4,4,4	3.18	2 (50%)	6,6,6	0.98	0
3	SO4	H	1703	-	4,4,4	0.62	0	6,6,6	0.54	0
3	SO4	H	1706	-	4,4,4	0.71	0	6,6,6	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	SO4	I	1704	-	4,4,4	3.36	2 (50%)	6,6,6	0.97	0
3	SO4	I	1801	-	4,4,4	3.24	2 (50%)	6,6,6	1.00	0
3	SO4	I	1802	-	4,4,4	3.37	2 (50%)	6,6,6	0.97	0
3	SO4	I	1803	-	4,4,4	0.30	0	6,6,6	0.50	0
3	SO4	I	1804	-	4,4,4	0.63	0	6,6,6	0.52	0
4	FEC	I	1805[A]	1	34,56,56	2.73	4 (11%)	43,90,90	2.06	10 (23%)
4	FEC	I	1805[B]	1	34,56,56	5.72	8 (23%)	43,90,90	5.75	14 (32%)
3	SO4	J	1901	-	4,4,4	3.08	2 (50%)	6,6,6	0.94	0
3	SO4	J	1904	-	4,4,4	3.23	2 (50%)	6,6,6	1.00	0
3	SO4	J	1906	-	4,4,4	0.34	0	6,6,6	0.60	0
3	SO4	K	2001	-	4,4,4	3.21	2 (50%)	6,6,6	1.05	0
3	SO4	K	2003	-	4,4,4	3.16	2 (50%)	6,6,6	1.04	0
3	SO4	K	2006	-	4,4,4	0.51	0	6,6,6	1.05	1 (16%)
3	SO4	L	2101	-	4,4,4	3.16	2 (50%)	6,6,6	0.92	0
3	SO4	L	2102	-	4,4,4	3.19	2 (50%)	6,6,6	0.95	0
3	SO4	L	2104	-	4,4,4	3.20	2 (50%)	6,6,6	0.95	0
3	SO4	L	2106	-	4,4,4	0.41	0	6,6,6	1.16	0
4	FEC	L	2107[A]	1	34,56,56	1.92	5 (14%)	43,90,90	1.98	12 (27%)
4	FEC	L	2107[B]	1	34,56,56	10.02	9 (26%)	43,90,90	8.31	15 (34%)
3	SO4	M	2201	-	4,4,4	3.16	2 (50%)	6,6,6	0.96	0
3	SO4	M	2202	-	4,4,4	3.25	2 (50%)	6,6,6	0.93	0
3	SO4	M	2203	-	4,4,4	3.20	2 (50%)	6,6,6	0.92	0
3	SO4	M	2206	-	4,4,4	0.59	0	6,6,6	0.32	0
4	FEC	M	2207[A]	1	34,56,56	3.45	4 (11%)	43,90,90	3.25	12 (27%)
4	FEC	M	2207[B]	1	34,56,56	3.32	7 (20%)	43,90,90	3.32	10 (23%)
3	SO4	N	2301	-	4,4,4	3.20	2 (50%)	6,6,6	0.92	0
3	SO4	N	2303	-	4,4,4	0.21	0	6,6,6	0.77	0
3	SO4	N	2306	-	4,4,4	0.51	0	6,6,6	0.67	0
3	SO4	O	2403	-	4,4,4	0.49	0	6,6,6	0.27	0
3	SO4	O	2406	-	4,4,4	0.60	0	6,6,6	1.54	1 (16%)
3	SO4	P	1504	-	4,4,4	3.18	2 (50%)	6,6,6	0.94	0
3	SO4	P	2501	-	4,4,4	3.15	2 (50%)	6,6,6	0.98	0
3	SO4	P	2503	-	4,4,4	0.51	0	6,6,6	0.72	0
3	SO4	P	2506	-	4,4,4	0.80	0	6,6,6	0.34	0
4	FEC	P	2507[A]	1	34,56,56	3.02	5 (14%)	43,90,90	3.23	9 (20%)
4	FEC	P	2507[B]	1	34,56,56	12.64	6 (17%)	43,90,90	4.23	16 (37%)

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
3	SO4	A	1001	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1003	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1006	-	-	0/0/0/0	0/0/0/0
4	FEC	A	1007[A]	1	-	0/12/100/100	0/0/8/8
4	FEC	A	1007[B]	1	-	0/12/100/100	0/0/8/8
3	SO4	B	1005	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1101	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1103	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1104	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1106	-	-	0/0/0/0	0/0/0/0
3	SO4	C	1201	-	-	0/0/0/0	0/0/0/0
3	SO4	C	1203	-	-	0/0/0/0	0/0/0/0
3	SO4	C	1204	-	-	0/0/0/0	0/0/0/0
3	SO4	C	1206	-	-	0/0/0/0	0/0/0/0
4	FEC	C	1207[A]	1	-	0/12/100/100	0/0/8/8
4	FEC	C	1207[B]	1	-	0/12/100/100	0/0/8/8
3	SO4	D	1301	-	-	0/0/0/0	0/0/0/0
3	SO4	D	1303	-	-	0/0/0/0	0/0/0/0
3	SO4	D	1306	-	-	0/0/0/0	0/0/0/0
3	SO4	E	1304	-	-	0/0/0/0	0/0/0/0
3	SO4	E	1403	-	-	0/0/0/0	0/0/0/0
3	SO4	E	1406	-	-	0/0/0/0	0/0/0/0
4	FEC	E	1407[A]	1	-	0/12/100/100	0/0/8/8
4	FEC	E	1407[B]	1	-	0/12/100/100	0/0/8/8
3	SO4	F	1501	-	-	0/0/0/0	0/0/0/0
3	SO4	F	1502	-	-	0/0/0/0	0/0/0/0
3	SO4	F	1506	-	-	0/0/0/0	0/0/0/0
3	SO4	G	1601	-	-	0/0/0/0	0/0/0/0
3	SO4	G	1603	-	-	0/0/0/0	0/0/0/0
3	SO4	G	1606	-	-	0/0/0/0	0/0/0/0
4	FEC	G	1607[A]	1	-	0/12/100/100	0/0/8/8
4	FEC	G	1607[B]	1	-	0/12/100/100	0/0/8/8
3	SO4	H	1701	-	-	0/0/0/0	0/0/0/0
3	SO4	H	1702	-	-	0/0/0/0	0/0/0/0
3	SO4	H	1703	-	-	0/0/0/0	0/0/0/0
3	SO4	H	1706	-	-	0/0/0/0	0/0/0/0
3	SO4	I	1704	-	-	0/0/0/0	0/0/0/0
3	SO4	I	1801	-	-	0/0/0/0	0/0/0/0
3	SO4	I	1802	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	I	1803	-	-	0/0/0/0	0/0/0/0
3	SO4	I	1804	-	-	0/0/0/0	0/0/0/0
4	FEC	I	1805[A]	1	-	0/12/100/100	0/0/8/8
4	FEC	I	1805[B]	1	-	0/12/100/100	0/0/8/8
3	SO4	J	1901	-	-	0/0/0/0	0/0/0/0
3	SO4	J	1904	-	-	0/0/0/0	0/0/0/0
3	SO4	J	1906	-	-	0/0/0/0	0/0/0/0
3	SO4	K	2001	-	-	0/0/0/0	0/0/0/0
3	SO4	K	2003	-	-	0/0/0/0	0/0/0/0
3	SO4	K	2006	-	-	0/0/0/0	0/0/0/0
3	SO4	L	2101	-	-	0/0/0/0	0/0/0/0
3	SO4	L	2102	-	-	0/0/0/0	0/0/0/0
3	SO4	L	2104	-	-	0/0/0/0	0/0/0/0
3	SO4	L	2106	-	-	0/0/0/0	0/0/0/0
4	FEC	L	2107[A]	1	-	0/12/100/100	0/0/8/8
4	FEC	L	2107[B]	1	-	0/12/100/100	0/0/8/8
3	SO4	M	2201	-	-	0/0/0/0	0/0/0/0
3	SO4	M	2202	-	-	0/0/0/0	0/0/0/0
3	SO4	M	2203	-	-	0/0/0/0	0/0/0/0
3	SO4	M	2206	-	-	0/0/0/0	0/0/0/0
4	FEC	M	2207[A]	1	-	0/12/100/100	0/0/8/8
4	FEC	M	2207[B]	1	-	0/12/100/100	0/0/8/8
3	SO4	N	2301	-	-	0/0/0/0	0/0/0/0
3	SO4	N	2303	-	-	0/0/0/0	0/0/0/0
3	SO4	N	2306	-	-	0/0/0/0	0/0/0/0
3	SO4	O	2403	-	-	0/0/0/0	0/0/0/0
3	SO4	O	2406	-	-	0/0/0/0	0/0/0/0
3	SO4	P	1504	-	-	0/0/0/0	0/0/0/0
3	SO4	P	2501	-	-	0/0/0/0	0/0/0/0
3	SO4	P	2503	-	-	0/0/0/0	0/0/0/0
3	SO4	P	2506	-	-	0/0/0/0	0/0/0/0
4	FEC	P	2507[A]	1	-	0/12/100/100	0/0/8/8
4	FEC	P	2507[B]	1	-	0/12/100/100	0/0/8/8

All (154) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1207[B]	FEC	C4A-NA	-18.81	1.11	1.36
4	L	2107[B]	FEC	C4D-ND	-18.76	1.00	1.38
4	I	1805[B]	FEC	C4A-NA	-17.42	1.13	1.36
4	E	1407[B]	FEC	C1A-NA	-13.23	1.18	1.36
4	M	2207[A]	FEC	C1A-NA	-12.87	1.19	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1207[B]	FEC	C1D-ND	-12.32	1.14	1.39
4	E	1407[A]	FEC	C1A-NA	-12.32	1.20	1.36
4	I	1805[A]	FEC	C1A-NA	-12.14	1.20	1.36
4	C	1207[A]	FEC	C1A-NA	-10.94	1.21	1.36
4	A	1007[A]	FEC	C1A-NA	-10.36	1.22	1.36
4	G	1607[A]	FEC	C4A-NA	-9.82	1.23	1.36
4	P	2507[A]	FEC	C4A-NA	-8.84	1.24	1.36
4	A	1007[A]	FEC	C4A-NA	-8.54	1.25	1.36
4	G	1607[A]	FEC	C1A-NA	-8.46	1.25	1.36
4	I	1805[B]	FEC	C1B-NB	-8.26	1.22	1.38
4	A	1007[B]	FEC	FE-ND	-7.89	1.58	1.97
4	M	2207[B]	FEC	C4B-NB	-7.70	1.23	1.39
4	A	1007[B]	FEC	C1B-NB	-7.39	1.23	1.38
4	M	2207[B]	FEC	C1A-NA	-7.37	1.26	1.36
4	P	2507[A]	FEC	C1A-NA	-6.48	1.27	1.36
4	L	2107[A]	FEC	C1A-NA	-5.69	1.29	1.36
4	I	1805[B]	FEC	FE-ND	-5.69	1.69	1.97
4	M	2207[A]	FEC	C4A-NA	-5.22	1.29	1.36
4	G	1607[B]	FEC	FE-ND	-5.20	1.71	1.97
4	E	1407[A]	FEC	C4A-NA	-5.12	1.29	1.36
4	M	2207[B]	FEC	C4A-NA	-5.04	1.29	1.36
4	L	2107[A]	FEC	C4A-NA	-4.62	1.30	1.36
4	C	1207[A]	FEC	C4A-NA	-4.53	1.30	1.36
3	I	1802	SO4	O3-S	-4.49	1.31	1.47
3	I	1704	SO4	O3-S	-4.49	1.31	1.47
3	A	1001	SO4	O3-S	-4.07	1.32	1.47
3	J	1904	SO4	O3-S	-4.07	1.32	1.47
3	I	1801	SO4	O3-S	-4.07	1.32	1.47
4	L	2107[B]	FEC	C1D-ND	-4.02	1.31	1.39
3	M	2201	SO4	O3-S	-4.00	1.33	1.47
3	K	2001	SO4	O3-S	-3.99	1.33	1.47
3	F	1501	SO4	O3-S	-3.95	1.33	1.47
3	D	1301	SO4	O3-S	-3.91	1.33	1.47
3	C	1204	SO4	O3-S	-3.89	1.33	1.47
3	F	1502	SO4	O3-S	-3.87	1.33	1.47
3	L	2101	SO4	O3-S	-3.85	1.33	1.47
4	E	1407[B]	FEC	C1B-NB	-3.85	1.31	1.38
3	K	2003	SO4	O3-S	-3.84	1.33	1.47
3	H	1701	SO4	O3-S	-3.83	1.33	1.47
3	P	2501	SO4	O3-S	-3.82	1.33	1.47
3	M	2203	SO4	O3-S	-3.81	1.33	1.47
3	N	2301	SO4	O3-S	-3.81	1.33	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	1601	SO4	O3-S	-3.81	1.33	1.47
3	B	1104	SO4	O3-S	-3.80	1.33	1.47
3	G	1603	SO4	O3-S	-3.78	1.33	1.47
3	L	2104	SO4	O3-S	-3.71	1.34	1.47
3	L	2102	SO4	O3-S	-3.71	1.34	1.47
3	P	1504	SO4	O3-S	-3.67	1.34	1.47
3	H	1702	SO4	O3-S	-3.66	1.34	1.47
3	B	1101	SO4	O3-S	-3.65	1.34	1.47
3	M	2202	SO4	O3-S	-3.57	1.34	1.47
3	C	1201	SO4	O3-S	-3.56	1.34	1.47
3	A	1003	SO4	O3-S	-3.56	1.34	1.47
3	E	1304	SO4	O3-S	-3.56	1.34	1.47
3	J	1901	SO4	O3-S	-3.53	1.34	1.47
4	E	1407[B]	FEC	FE-ND	-3.52	1.80	1.97
4	C	1207[B]	FEC	C1A-NA	-3.36	1.32	1.36
4	C	1207[B]	FEC	FE-NB	-3.10	1.82	1.97
4	M	2207[B]	FEC	FE-ND	-2.86	1.83	1.97
4	I	1805[A]	FEC	C4D-ND	-2.82	1.33	1.38
4	G	1607[B]	FEC	FE-NB	-2.73	1.83	1.97
4	P	2507[B]	FEC	FE-NB	-2.72	1.83	1.97
4	L	2107[B]	FEC	C4B-NB	-2.65	1.34	1.39
4	P	2507[A]	FEC	C4D-ND	-2.16	1.34	1.38
4	A	1007[A]	FEC	FE-NB	-2.11	1.86	1.97
4	G	1607[A]	FEC	C4D-ND	-2.05	1.34	1.38
4	A	1007[B]	FEC	CMB-C2B	2.00	1.55	1.50
4	C	1207[B]	FEC	CMD-C2D	2.01	1.55	1.50
4	L	2107[B]	FEC	CMD-C2D	2.05	1.55	1.50
4	L	2107[A]	FEC	CMB-C2B	2.07	1.55	1.50
4	G	1607[A]	FEC	FE-ND	2.07	2.07	1.97
4	A	1007[A]	FEC	CMD-C2D	2.09	1.55	1.50
4	M	2207[B]	FEC	FE-NB	2.09	2.07	1.97
4	I	1805[A]	FEC	C1D-ND	2.11	1.44	1.39
4	C	1207[B]	FEC	CMB-C2B	2.16	1.55	1.50
4	L	2107[B]	FEC	CMB-C2B	2.19	1.55	1.50
4	L	2107[A]	FEC	C1D-ND	2.23	1.44	1.39
4	I	1805[B]	FEC	FE-NB	2.58	2.09	1.97
4	C	1207[B]	FEC	C1B-NB	3.56	1.46	1.38
4	E	1407[B]	FEC	C4D-ND	3.86	1.46	1.38
4	E	1407[A]	FEC	C1D-ND	4.18	1.48	1.39
4	M	2207[B]	FEC	C1B-NB	4.36	1.47	1.38
3	A	1001	SO4	O1-S	4.54	1.62	1.47
3	H	1701	SO4	O1-S	4.74	1.63	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	1704	SO4	O1-S	4.87	1.63	1.47
3	I	1802	SO4	O1-S	4.89	1.63	1.47
3	M	2201	SO4	O1-S	4.89	1.63	1.47
3	B	1101	SO4	O1-S	4.98	1.64	1.47
3	L	2101	SO4	O1-S	4.99	1.64	1.47
3	J	1904	SO4	O1-S	5.00	1.64	1.47
3	P	2501	SO4	O1-S	5.00	1.64	1.47
3	K	2001	SO4	O1-S	5.00	1.64	1.47
3	J	1901	SO4	O1-S	5.01	1.64	1.47
3	I	1801	SO4	O1-S	5.01	1.64	1.47
4	I	1805[B]	FEC	C4B-NB	5.02	1.50	1.39
3	K	2003	SO4	O1-S	5.02	1.64	1.47
3	F	1502	SO4	O1-S	5.04	1.64	1.47
3	C	1201	SO4	O1-S	5.12	1.64	1.47
3	M	2203	SO4	O1-S	5.13	1.64	1.47
3	N	2301	SO4	O1-S	5.13	1.64	1.47
3	E	1304	SO4	O1-S	5.14	1.64	1.47
3	P	1504	SO4	O1-S	5.17	1.64	1.47
3	L	2102	SO4	O1-S	5.18	1.64	1.47
3	L	2104	SO4	O1-S	5.19	1.64	1.47
3	H	1702	SO4	O1-S	5.21	1.65	1.47
3	C	1204	SO4	O1-S	5.23	1.65	1.47
3	D	1301	SO4	O1-S	5.25	1.65	1.47
4	P	2507[A]	FEC	C4B-NB	5.26	1.50	1.39
3	F	1501	SO4	O1-S	5.30	1.65	1.47
4	L	2107[A]	FEC	C1B-NB	5.37	1.49	1.38
3	B	1104	SO4	O1-S	5.43	1.65	1.47
3	M	2202	SO4	O1-S	5.43	1.65	1.47
3	G	1603	SO4	O1-S	5.43	1.65	1.47
3	A	1003	SO4	O1-S	5.44	1.65	1.47
4	C	1207[A]	FEC	C1D-ND	5.50	1.51	1.39
4	G	1607[B]	FEC	C4D-ND	5.63	1.50	1.38
3	G	1601	SO4	O1-S	5.98	1.67	1.47
4	L	2107[B]	FEC	C1B-NB	5.99	1.51	1.38
4	M	2207[A]	FEC	C4B-NB	6.12	1.52	1.39
4	C	1207[A]	FEC	C1B-NB	6.18	1.51	1.38
4	E	1407[A]	FEC	C1B-NB	7.19	1.53	1.38
4	A	1007[B]	FEC	C4D-ND	7.43	1.53	1.38
4	I	1805[A]	FEC	C1B-NB	7.65	1.54	1.38
4	P	2507[B]	FEC	C1D-ND	7.71	1.55	1.39
4	G	1607[A]	FEC	C1B-NB	8.39	1.55	1.38
4	P	2507[B]	FEC	C1B-NB	9.30	1.57	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	1805[B]	FEC	C1A-NA	9.63	1.49	1.36
4	E	1407[B]	FEC	C1D-ND	9.66	1.59	1.39
4	A	1007[A]	FEC	C1B-NB	9.70	1.58	1.38
4	C	1207[B]	FEC	FE-ND	9.77	2.44	1.97
4	I	1805[B]	FEC	C4D-ND	9.94	1.59	1.38
4	L	2107[B]	FEC	FE-ND	10.68	2.48	1.97
4	P	2507[B]	FEC	C4B-NB	10.74	1.62	1.39
4	P	2507[A]	FEC	C1B-NB	11.13	1.61	1.38
4	G	1607[B]	FEC	C4B-NB	11.41	1.63	1.39
4	G	1607[B]	FEC	C1A-NA	11.43	1.52	1.36
4	A	1007[B]	FEC	C4B-NB	11.52	1.63	1.39
4	M	2207[A]	FEC	C1B-NB	11.66	1.62	1.38
4	M	2207[B]	FEC	C4D-ND	13.11	1.65	1.38
4	E	1407[B]	FEC	C4B-NB	13.60	1.68	1.39
4	G	1607[B]	FEC	C1D-ND	17.48	1.76	1.39
4	I	1805[B]	FEC	C1D-ND	21.37	1.84	1.39
4	C	1207[B]	FEC	C4B-NB	21.69	1.84	1.39
4	A	1007[B]	FEC	C1D-ND	24.18	1.90	1.39
4	A	1007[B]	FEC	C1A-NA	26.41	1.72	1.36
4	L	2107[B]	FEC	C4A-NA	28.98	1.75	1.36
4	P	2507[B]	FEC	C4A-NA	32.41	1.80	1.36
4	L	2107[B]	FEC	C1A-NA	44.89	1.97	1.36
4	P	2507[B]	FEC	C1A-NA	63.83	2.22	1.36

All (212) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1007[B]	FEC	C1D-ND-C4D	-28.77	78.80	105.00
4	I	1805[B]	FEC	C1D-ND-C4D	-27.98	79.52	105.00
4	C	1207[B]	FEC	C4B-NB-C1B	-24.24	82.93	105.00
4	G	1607[B]	FEC	C1D-ND-C4D	-22.38	84.62	105.00
4	P	2507[B]	FEC	C4B-NB-C1B	-19.45	87.29	105.00
4	C	1207[B]	FEC	C3D-C4D-ND	-19.42	90.10	110.35
4	M	2207[A]	FEC	C4B-NB-C1B	-17.67	88.91	105.00
4	L	2107[B]	FEC	C2D-C1D-ND	-17.13	88.09	109.78
4	P	2507[A]	FEC	C4B-NB-C1B	-16.92	89.59	105.00
4	L	2107[B]	FEC	C3D-C4D-ND	-16.57	93.07	110.35
4	A	1007[B]	FEC	CHA-C4D-ND	-16.17	105.54	124.47
4	I	1805[B]	FEC	CHA-C4D-ND	-14.69	107.28	124.47
4	C	1207[B]	FEC	CHB-C1B-NB	-14.02	108.06	124.47
4	E	1407[B]	FEC	C1D-ND-C4D	-13.54	92.67	105.00
4	M	2207[B]	FEC	C1D-ND-C4D	-12.62	93.51	105.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	1607[B]	FEC	C4B-NB-C1B	-12.34	93.76	105.00
4	G	1607[B]	FEC	CHA-C4D-ND	-11.78	110.68	124.47
4	E	1407[B]	FEC	C4B-NB-C1B	-11.61	94.43	105.00
4	P	2507[B]	FEC	C1D-ND-C4D	-11.52	94.51	105.00
4	C	1207[B]	FEC	C2D-C1D-ND	-11.17	95.63	109.78
4	A	1007[A]	FEC	C4B-NB-C1B	-10.12	95.78	105.00
4	E	1407[B]	FEC	CHB-C1B-NB	-9.86	112.92	124.47
4	G	1607[A]	FEC	C4B-NB-C1B	-9.61	96.24	105.00
4	A	1007[B]	FEC	CHB-C1B-NB	-9.05	113.88	124.47
4	G	1607[B]	FEC	CHB-C1B-NB	-9.03	113.89	124.47
4	M	2207[B]	FEC	CHD-C1D-ND	-7.64	114.11	124.35
4	P	2507[B]	FEC	CHB-C1B-NB	-7.53	115.66	124.47
4	G	1607[A]	FEC	CHC-C4B-NB	-7.35	114.50	124.35
4	E	1407[A]	FEC	C4B-NB-C1B	-7.26	98.39	105.00
4	A	1007[B]	FEC	C4B-NB-C1B	-7.17	98.46	105.00
4	I	1805[A]	FEC	C4B-NB-C1B	-6.76	98.84	105.00
4	C	1207[A]	FEC	C4B-NB-C1B	-6.75	98.85	105.00
4	E	1407[B]	FEC	CHA-C4D-ND	-5.93	117.52	124.47
4	M	2207[A]	FEC	CHC-C4B-NB	-5.92	116.41	124.35
4	A	1007[A]	FEC	CHC-C4B-NB	-5.71	116.69	124.35
4	L	2107[A]	FEC	C4B-NB-C1B	-5.64	99.86	105.00
4	I	1805[B]	FEC	C3B-C4B-NB	-5.60	103.45	110.12
4	P	2507[B]	FEC	CHC-C4B-NB	-5.58	116.86	124.35
4	E	1407[A]	FEC	CHC-C4B-NB	-5.51	116.97	124.35
4	P	2507[A]	FEC	CHC-C4B-NB	-5.43	117.06	124.35
4	P	2507[B]	FEC	CHA-C4D-ND	-5.36	118.20	124.47
4	I	1805[B]	FEC	CHD-C1D-ND	-5.00	117.65	124.35
4	E	1407[A]	FEC	C1D-ND-C4D	-4.88	100.56	105.00
4	I	1805[B]	FEC	CAA-C3A-C4A	-4.73	121.87	127.01
4	I	1805[A]	FEC	CHC-C4B-NB	-4.72	118.02	124.35
4	C	1207[A]	FEC	CHC-C4B-NB	-4.49	118.33	124.35
4	C	1207[A]	FEC	C1D-ND-C4D	-4.41	100.98	105.00
4	M	2207[B]	FEC	C2B-C1B-NB	-4.28	104.95	110.04
4	I	1805[B]	FEC	CMC-C3C-C4C	-4.27	121.29	128.36
4	P	2507[B]	FEC	CAA-C3A-C4A	-4.21	122.43	127.01
4	M	2207[B]	FEC	CAA-C3A-C4A	-4.20	122.44	127.01
4	I	1805[A]	FEC	CAA-C3A-C4A	-4.05	122.61	127.01
4	C	1207[A]	FEC	CAA-C3A-C4A	-4.05	122.61	127.01
4	E	1407[B]	FEC	CAA-C3A-C4A	-3.98	122.69	127.01
4	A	1007[B]	FEC	CHD-C1D-ND	-3.79	119.28	124.35
4	M	2207[A]	FEC	CAA-C3A-C4A	-3.76	122.93	127.01
4	L	2107[B]	FEC	CHC-C4B-NB	-3.72	119.36	124.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	1506	SO4	O2-S-O1	-3.72	97.70	109.50
4	P	2507[A]	FEC	CMC-C3C-C4C	-3.66	122.31	128.36
4	A	1007[B]	FEC	CMC-C3C-C4C	-3.64	122.34	128.36
4	L	2107[B]	FEC	C4B-NB-C1B	-3.58	101.74	105.00
3	B	1005	SO4	O4-S-O3	-3.51	94.70	108.98
4	L	2107[A]	FEC	CHC-C4B-NB	-3.45	119.73	124.35
4	G	1607[A]	FEC	CMC-C3C-C4C	-3.42	122.70	128.36
4	E	1407[A]	FEC	CAA-C3A-C4A	-3.42	123.30	127.01
4	L	2107[A]	FEC	CAA-C3A-C4A	-3.29	123.44	127.01
4	L	2107[A]	FEC	CMC-C3C-C4C	-3.14	123.16	128.36
4	M	2207[A]	FEC	CMC-C3C-C4C	-3.14	123.17	128.36
4	A	1007[A]	FEC	CAA-C3A-C4A	-3.14	123.60	127.01
4	L	2107[B]	FEC	CAA-C3A-C4A	-3.13	123.61	127.01
4	P	2507[A]	FEC	CHB-C1B-NB	-3.13	120.81	124.47
4	A	1007[B]	FEC	CAA-C3A-C4A	-3.10	123.64	127.01
4	A	1007[B]	FEC	C3B-C4B-NB	-3.08	106.46	110.12
4	E	1407[A]	FEC	CMC-C3C-C4C	-3.06	123.29	128.36
4	M	2207[B]	FEC	CMC-C3C-C4C	-3.02	123.37	128.36
4	G	1607[B]	FEC	CAA-C3A-C4A	-3.01	123.74	127.01
4	M	2207[A]	FEC	CHB-C1B-NB	-2.99	120.97	124.47
4	C	1207[B]	FEC	CMC-C3C-C4C	-2.93	123.52	128.36
4	G	1607[A]	FEC	CAA-C3A-C4A	-2.84	123.92	127.01
4	I	1805[A]	FEC	C2D-C1D-ND	-2.81	106.21	109.78
4	L	2107[B]	FEC	C4C-CHD-C1D	-2.80	123.24	129.26
4	A	1007[A]	FEC	CMC-C3C-C4C	-2.79	123.74	128.36
4	P	2507[B]	FEC	CMC-C3C-C4C	-2.75	123.82	128.36
4	G	1607[B]	FEC	CHD-C1D-ND	-2.74	120.68	124.35
4	E	1407[A]	FEC	C2D-C1D-ND	-2.69	106.37	109.78
3	D	1306	SO4	O2-S-O1	-2.68	101.01	109.50
4	P	2507[A]	FEC	CAA-C3A-C4A	-2.64	124.14	127.01
4	C	1207[A]	FEC	CHA-C4D-ND	-2.62	121.40	124.47
4	E	1407[B]	FEC	CMC-C3C-C4C	-2.62	124.04	128.36
4	A	1007[B]	FEC	C4C-CHD-C1D	-2.56	123.76	129.26
4	E	1407[B]	FEC	C4C-CHD-C1D	-2.52	123.85	129.26
4	G	1607[B]	FEC	CMC-C3C-C4C	-2.49	124.24	128.36
4	P	2507[B]	FEC	C4C-CHD-C1D	-2.49	123.92	129.26
4	M	2207[A]	FEC	C4C-CHD-C1D	-2.47	123.95	129.26
4	C	1207[B]	FEC	CMB-C2B-C1B	-2.44	121.24	125.02
4	C	1207[A]	FEC	C2D-C1D-ND	-2.42	106.71	109.78
3	K	2006	SO4	O2-S-O1	-2.42	101.84	109.50
4	I	1805[A]	FEC	CMC-C3C-C4C	-2.37	124.44	128.36
4	I	1805[A]	FEC	C4C-CHD-C1D	-2.24	124.44	129.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	1407[B]	FEC	CHD-C1D-ND	-2.23	121.36	124.35
4	C	1207[B]	FEC	CAA-C3A-C4A	-2.23	124.59	127.01
4	M	2207[A]	FEC	CAC-C2C-C1C	-2.21	124.61	127.01
4	G	1607[A]	FEC	C4C-CHD-C1D	-2.20	124.54	129.26
4	G	1607[B]	FEC	C4C-CHD-C1D	-2.20	124.54	129.26
4	L	2107[B]	FEC	CMC-C3C-C4C	-2.20	124.73	128.36
4	L	2107[A]	FEC	C2D-C1D-ND	-2.19	107.00	109.78
4	E	1407[B]	FEC	CAC-C2C-C1C	-2.12	124.71	127.01
4	C	1207[B]	FEC	C4C-CHD-C1D	-2.11	124.73	129.26
4	G	1607[B]	FEC	CAC-C2C-C1C	-2.08	124.75	127.01
4	I	1805[B]	FEC	CHB-C1B-NB	-2.05	122.07	124.47
4	C	1207[A]	FEC	CMD-C2D-C1D	-2.01	121.91	125.02
4	M	2207[A]	FEC	CMC-C3C-C2C	2.00	129.42	125.24
4	C	1207[B]	FEC	CMC-C3C-C2C	2.03	129.47	125.24
4	A	1007[A]	FEC	CMA-C2A-C3A	2.04	129.50	125.24
4	C	1207[B]	FEC	C4A-CHB-C1B	2.06	125.71	122.60
4	L	2107[A]	FEC	CMC-C3C-C2C	2.06	129.54	125.24
4	P	2507[A]	FEC	CMC-C3C-C2C	2.06	129.54	125.24
4	L	2107[A]	FEC	CAA-CBA-CGA	2.07	116.54	112.75
4	L	2107[B]	FEC	CAB-CBB-CGB	2.07	116.55	112.75
4	A	1007[B]	FEC	CMC-C3C-C2C	2.08	129.59	125.24
4	M	2207[A]	FEC	CAA-CBA-CGA	2.09	116.58	112.75
4	G	1607[A]	FEC	CMC-C3C-C2C	2.15	129.73	125.24
4	E	1407[B]	FEC	C2D-C1D-ND	2.16	112.51	109.78
4	P	2507[A]	FEC	CMA-C2A-C3A	2.16	129.76	125.24
4	G	1607[A]	FEC	CAD-CBD-CGD	2.16	116.71	112.75
4	A	1007[B]	FEC	CMA-C2A-C3A	2.21	129.85	125.24
4	P	2507[B]	FEC	CMC-C3C-C2C	2.22	129.88	125.24
4	L	2107[A]	FEC	CMA-C2A-C3A	2.23	129.90	125.24
4	I	1805[A]	FEC	CMA-C2A-C3A	2.25	129.95	125.24
4	L	2107[A]	FEC	C4A-CHB-C1B	2.27	126.03	122.60
3	B	1005	SO4	O4-S-O1	2.29	131.49	110.19
3	B	1106	SO4	O2-S-O1	2.29	116.76	109.50
4	M	2207[A]	FEC	C3B-C4B-NB	2.30	112.86	110.12
4	P	2507[B]	FEC	CBA-CAA-C3A	2.32	116.70	112.53
4	L	2107[B]	FEC	C4A-CHB-C1B	2.34	126.14	122.60
4	I	1805[A]	FEC	CHD-C1D-ND	2.36	127.52	124.35
4	I	1805[B]	FEC	C4B-NB-C1B	2.41	107.19	105.00
4	G	1607[A]	FEC	CBA-CAA-C3A	2.41	116.86	112.53
4	E	1407[A]	FEC	C1A-CHA-C4D	2.43	126.28	122.60
4	E	1407[B]	FEC	CAB-CBB-CGB	2.45	117.24	112.75
4	I	1805[B]	FEC	CBA-CAA-C3A	2.46	116.93	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	L	2107[A]	FEC	CBA-CAA-C3A	2.49	116.99	112.53
4	M	2207[A]	FEC	CAB-CBB-CGB	2.49	117.31	112.75
4	G	1607[B]	FEC	C4A-CHB-C1B	2.53	126.42	122.60
4	G	1607[A]	FEC	CHD-C1D-ND	2.57	127.79	124.35
4	P	2507[B]	FEC	CAB-CBB-CGB	2.59	117.49	112.75
4	P	2507[B]	FEC	CMA-C2A-C3A	2.59	130.66	125.24
4	A	1007[B]	FEC	CAC-CBC-CGC	2.64	117.58	112.75
4	A	1007[B]	FEC	CHC-C4B-NB	2.73	128.01	124.35
4	G	1607[B]	FEC	C2D-C1D-ND	2.82	113.34	109.78
4	I	1805[B]	FEC	CMC-C3C-C2C	2.83	131.15	125.24
4	G	1607[B]	FEC	CAA-CBA-CGA	2.88	118.02	112.75
4	A	1007[B]	FEC	CBA-CAA-C3A	2.95	117.81	112.53
4	L	2107[B]	FEC	C3B-C4B-NB	3.03	113.72	110.12
4	E	1407[B]	FEC	CBA-CAA-C3A	3.13	118.13	112.53
4	P	2507[A]	FEC	CAC-CBC-CGC	3.13	118.48	112.75
4	M	2207[B]	FEC	CAB-CBB-CGB	3.18	118.58	112.75
4	A	1007[B]	FEC	C4A-CHB-C1B	3.22	127.47	122.60
4	G	1607[A]	FEC	CAB-CBB-CGB	3.28	118.75	112.75
4	C	1207[B]	FEC	CBA-CAA-C3A	3.31	118.46	112.53
4	L	2107[B]	FEC	CBA-CAA-C3A	3.37	118.58	112.53
4	C	1207[B]	FEC	CAB-CBB-CGB	3.43	119.03	112.75
4	P	2507[B]	FEC	C3D-C4D-ND	3.45	113.95	110.35
3	O	2406	SO4	O2-S-O1	3.46	120.46	109.50
4	L	2107[A]	FEC	C3B-C4B-NB	3.51	114.29	110.12
4	M	2207[A]	FEC	CBC-CAC-C2C	3.56	118.91	112.53
4	M	2207[B]	FEC	C4B-NB-C1B	3.60	108.27	105.00
4	E	1407[A]	FEC	CAB-CBB-CGB	3.68	119.49	112.75
4	A	1007[B]	FEC	CAB-CBB-CGB	3.69	119.52	112.75
4	A	1007[B]	FEC	C2D-C1D-ND	3.74	114.51	109.78
3	C	1203	SO4	O2-S-O1	3.77	121.45	109.50
4	P	2507[B]	FEC	CBC-CAC-C2C	3.81	119.36	112.53
4	P	2507[B]	FEC	C3B-C4B-NB	3.84	114.68	110.12
4	G	1607[A]	FEC	C1D-ND-C4D	3.95	108.59	105.00
4	G	1607[B]	FEC	CBC-CAC-C2C	4.18	120.02	112.53
4	I	1805[A]	FEC	CBC-CAC-C2C	4.22	120.10	112.53
4	I	1805[B]	FEC	C2D-C1D-ND	4.47	115.43	109.78
4	C	1207[A]	FEC	CBC-CAC-C2C	4.67	120.89	112.53
4	C	1207[A]	FEC	C3B-C4B-NB	4.72	115.73	110.12
4	E	1407[B]	FEC	CBC-CAC-C2C	4.72	120.99	112.53
4	P	2507[B]	FEC	C2B-C1B-NB	4.76	115.69	110.04
4	I	1805[B]	FEC	CHC-C4B-NB	4.77	130.75	124.35
4	I	1805[A]	FEC	C3B-C4B-NB	4.79	115.81	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	1607[A]	FEC	CBC-CAC-C2C	4.90	121.31	112.53
4	A	1007[A]	FEC	C3B-C4B-NB	4.94	115.99	110.12
4	L	2107[B]	FEC	CBC-CAC-C2C	5.00	121.49	112.53
4	A	1007[A]	FEC	CBC-CAC-C2C	5.01	121.50	112.53
4	L	2107[A]	FEC	CBC-CAC-C2C	5.07	121.61	112.53
4	M	2207[B]	FEC	CHB-C1B-NB	5.45	130.85	124.47
4	E	1407[A]	FEC	C3B-C4B-NB	5.47	116.62	110.12
4	C	1207[B]	FEC	CBC-CAC-C2C	5.52	122.43	112.53
4	G	1607[A]	FEC	C3B-C4B-NB	5.80	117.01	110.12
4	I	1805[B]	FEC	CBC-CAC-C2C	5.93	123.16	112.53
4	E	1407[B]	FEC	C3D-C4D-ND	6.10	116.71	110.35
4	M	2207[B]	FEC	CBC-CAC-C2C	6.11	123.49	112.53
4	E	1407[A]	FEC	CBC-CAC-C2C	6.37	123.95	112.53
4	C	1207[B]	FEC	CHD-C1D-ND	6.56	133.15	124.35
4	P	2507[A]	FEC	CBC-CAC-C2C	6.92	124.93	112.53
4	A	1007[B]	FEC	CBC-CAC-C2C	7.24	125.51	112.53
4	A	1007[B]	FEC	C2B-C1B-NB	7.50	118.95	110.04
4	G	1607[B]	FEC	C2B-C1B-NB	8.50	120.14	110.04
4	M	2207[B]	FEC	C2D-C1D-ND	8.87	121.00	109.78
4	C	1207[B]	FEC	C2B-C1B-NB	9.49	121.31	110.04
4	E	1407[B]	FEC	C2B-C1B-NB	9.63	121.48	110.04
4	G	1607[B]	FEC	C3D-C4D-ND	11.04	121.86	110.35
4	C	1207[B]	FEC	CHA-C4D-ND	12.91	139.58	124.47
4	I	1805[B]	FEC	C3D-C4D-ND	13.83	124.77	110.35
4	C	1207[B]	FEC	C1D-ND-C4D	13.92	117.67	105.00
4	L	2107[B]	FEC	CHA-C4D-ND	15.03	142.06	124.47
4	A	1007[B]	FEC	C3D-C4D-ND	17.08	128.15	110.35
4	L	2107[B]	FEC	CHD-C1D-ND	17.60	147.96	124.35
4	L	2107[B]	FEC	C1D-ND-C4D	41.58	142.85	105.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

33 monomers are involved in 268 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1006	SO4	2	0
4	A	1007[A]	FEC	6	0
4	A	1007[B]	FEC	15	0
3	B	1005	SO4	6	0
3	B	1104	SO4	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1206	SO4	2	0
4	C	1207[A]	FEC	8	0
4	C	1207[B]	FEC	21	0
3	D	1301	SO4	2	0
3	D	1306	SO4	1	0
3	E	1403	SO4	4	0
4	E	1407[A]	FEC	8	0
4	E	1407[B]	FEC	13	0
3	G	1601	SO4	1	0
4	G	1607[A]	FEC	11	0
4	G	1607[B]	FEC	13	0
3	I	1704	SO4	5	0
3	I	1802	SO4	0	14
4	I	1805[A]	FEC	10	0
4	I	1805[B]	FEC	27	0
3	L	2102	SO4	0	14
3	L	2104	SO4	5	5
4	L	2107[A]	FEC	17	0
4	L	2107[B]	FEC	12	0
3	M	2202	SO4	1	0
3	M	2206	SO4	1	0
4	M	2207[A]	FEC	10	0
4	M	2207[B]	FEC	9	0
3	N	2301	SO4	1	0
3	O	2406	SO4	2	0
3	P	1504	SO4	4	0
4	P	2507[A]	FEC	13	0
4	P	2507[B]	FEC	17	0

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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	169/179 (94%)	-0.17	5 (2%)	54	61	17, 26, 42, 66	0
1	B	169/179 (94%)	-0.15	4 (2%)	62	68	17, 25, 47, 66	0
1	C	169/179 (94%)	-0.27	8 (4%)	35	41	18, 26, 42, 64	0
1	D	169/179 (94%)	-0.18	5 (2%)	54	61	17, 26, 43, 66	0
1	E	169/179 (94%)	-0.24	6 (3%)	46	53	18, 26, 45, 64	0
1	F	169/179 (94%)	-0.28	6 (3%)	46	53	18, 26, 44, 66	0
1	G	169/179 (94%)	-0.20	6 (3%)	46	53	17, 26, 42, 66	0
1	H	170/179 (94%)	-0.24	7 (4%)	41	47	17, 26, 48, 68	0
1	I	170/179 (94%)	-0.25	5 (2%)	55	62	17, 26, 43, 66	0
1	J	169/179 (94%)	-0.26	6 (3%)	46	53	18, 26, 42, 66	0
1	K	169/179 (94%)	-0.25	3 (1%)	71	76	17, 26, 42, 64	0
1	L	170/179 (94%)	-0.18	8 (4%)	35	41	17, 26, 44, 66	0
1	M	170/179 (94%)	-0.25	5 (2%)	55	62	16, 25, 44, 66	0
1	N	169/179 (94%)	-0.23	5 (2%)	54	61	17, 25, 44, 64	0
1	O	169/179 (94%)	-0.19	4 (2%)	62	68	18, 26, 42, 64	0
1	P	170/179 (94%)	-0.34	3 (1%)	71	76	17, 26, 48, 66	0
All	All	2709/2864 (94%)	-0.23	86 (3%)	51	58	16, 26, 46, 68	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	168	SER	7.2
1	B	166	THR	6.8
1	I	166	THR	6.8
1	A	166	THR	6.5
1	N	168	SER	6.3

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Mol	Chain	Res	Type	RSRZ
1	G	166	THR	6.3
1	J	168	SER	6.0
1	H	166	THR	5.9
1	G	168	SER	5.9
1	F	168	SER	5.7
1	M	168	SER	5.6
1	C	168	SER	5.3
1	A	168	SER	5.3
1	P	168	SER	5.2
1	K	166	THR	5.0
1	O	168	SER	5.0
1	H	168	SER	4.8
1	F	166	THR	4.7
1	J	166	THR	4.7
1	E	166	THR	4.5
1	L	166	THR	4.5
1	K	168	SER	4.4
1	C	166	THR	4.4
1	L	168	SER	4.3
1	D	166	THR	4.3
1	O	166	THR	4.3
1	D	168	SER	4.3
1	E	167	ALA	4.1
1	C	165	GLY	3.9
1	I	169	LYS	3.9
1	C	7	ASP	3.8
1	B	168	SER	3.7
1	F	167	ALA	3.6
1	D	4	ASN	3.4
1	M	166	THR	3.3
1	I	168	SER	3.3
1	H	81	LYS	3.3
1	P	167	ALA	3.3
1	P	166	THR	3.2
1	H	169	LYS	3.1
1	G	165	GLY	3.1
1	M	3	GLY	3.1
1	K	27	ILE	3.1
1	H	165	GLY	3.0
1	G	167	ALA	2.9
1	H	7	ASP	2.9
1	G	150	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	N	169	LYS	2.7
1	N	166	THR	2.7
1	M	169	LYS	2.6
1	J	4	ASN	2.6
1	J	85	GLY	2.6
1	L	150	GLY	2.6
1	A	27	ILE	2.6
1	C	169	LYS	2.5
1	M	167	ALA	2.5
1	B	4	ASN	2.5
1	L	27	ILE	2.5
1	A	169	LYS	2.5
1	F	169	LYS	2.5
1	L	165	GLY	2.4
1	G	27	ILE	2.4
1	L	167	ALA	2.4
1	B	6	GLU	2.4
1	D	169	LYS	2.4
1	O	4	ASN	2.4
1	H	4	ASN	2.4
1	E	4	ASN	2.3
1	C	167	ALA	2.3
1	O	167	ALA	2.3
1	F	4	ASN	2.3
1	C	27	ILE	2.3
1	E	27	ILE	2.3
1	E	81	LYS	2.3
1	J	81	LYS	2.3
1	A	31	MET	2.3
1	I	172	VAL	2.2
1	L	151	ASP	2.2
1	F	6	GLU	2.2
1	I	27	ILE	2.1
1	N	4	ASN	2.1
1	L	169	LYS	2.1
1	C	4	ASN	2.1
1	D	7	ASP	2.0
1	N	7	ASP	2.0
1	J	167	ALA	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	SO4	I	1801	5/5	0.89	0.29	10.08	61,61,62,63	0
3	SO4	F	1501	5/5	0.91	0.26	4.33	66,66,67,67	0
3	SO4	J	1901	5/5	0.70	0.25	4.24	66,67,67,69	0
3	SO4	B	1005	5/5	0.95	0.27	3.24	51,53,55,61	0
3	SO4	D	1301	5/5	0.84	0.24	3.21	58,59,60,60	0
3	SO4	M	2201	5/5	0.95	0.19	2.36	51,51,52,53	0
3	SO4	K	2001	5/5	0.86	0.22	2.27	51,53,53,54	0
3	SO4	N	2301	5/5	0.91	0.19	1.90	62,63,63,63	0
3	SO4	A	1001	5/5	0.91	0.16	1.19	53,54,54,55	0
3	SO4	G	1601	5/5	0.82	0.22	1.10	74,74,74,75	0
3	SO4	P	2501	5/5	0.89	0.15	0.79	62,62,63,63	0
3	SO4	H	1701	5/5	0.89	0.19	0.79	54,54,55,56	0
3	SO4	I	1802	5/5	0.93	0.17	0.74	36,37,38,38	0
4	FEC	L	2107[A]	49/49	0.96	0.22	0.59	15,20,31,36	49
4	FEC	L	2107[B]	49/49	0.96	0.22	0.58	13,20,28,30	49
4	FEC	P	2507[B]	49/49	0.97	0.19	0.54	14,20,29,36	49
4	FEC	P	2507[A]	49/49	0.97	0.19	0.48	15,20,31,35	49
4	FEC	A	1007[A]	49/49	0.97	0.22	0.39	15,20,31,36	49
4	FEC	C	1207[A]	49/49	0.96	0.20	0.31	15,20,30,37	49
4	FEC	A	1007[B]	49/49	0.97	0.22	0.30	9,19,28,34	49
3	SO4	L	2101	5/5	0.87	0.15	0.30	64,64,65,65	0
3	SO4	B	1101	5/5	0.90	0.14	0.27	66,66,67,67	0
3	SO4	L	2102	5/5	0.94	0.15	0.24	78,78,78,79	5
4	FEC	M	2207[B]	49/49	0.96	0.19	0.23	12,20,29,32	49
4	FEC	M	2207[A]	49/49	0.96	0.19	0.22	15,20,31,37	49

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	FEC	C	1207[B]	49/49	0.96	0.20	0.22	12,20,32,35	49
4	FEC	G	1607[B]	49/49	0.97	0.20	0.21	9,20,32,38	49
4	FEC	G	1607[A]	49/49	0.97	0.20	0.16	15,20,31,36	49
4	FEC	I	1805[B]	49/49	0.96	0.17	0.12	13,21,30,33	49
3	SO4	C	1201	5/5	0.88	0.16	0.11	65,65,67,67	0
4	FEC	E	1407[A]	49/49	0.96	0.18	0.08	16,20,31,36	49
4	FEC	E	1407[B]	49/49	0.96	0.18	0.06	15,20,29,36	49
4	FEC	I	1805[A]	49/49	0.96	0.17	0.01	15,20,31,36	49
2	FE2	B	200	1/1	0.99	0.07	-1.18	29,29,29,29	0
2	FE2	O	200	1/1	0.99	0.07	-1.32	34,34,34,34	0
2	FE2	L	201	1/1	0.98	0.05	-1.38	32,32,32,32	0
2	FE2	D	200	1/1	0.99	0.06	-1.77	32,32,32,32	0
2	FE2	J	200	1/1	0.99	0.05	-1.83	33,33,33,33	0
2	FE2	B	201	1/1	0.99	0.05	-2.10	31,31,31,31	0
2	FE2	K	201	1/1	0.99	0.03	-2.19	36,36,36,36	0
2	FE2	N	200	1/1	0.98	0.06	-2.22	29,29,29,29	0
2	FE2	G	200	1/1	0.98	0.07	-2.22	32,32,32,32	0
2	FE2	A	201	1/1	0.96	0.04	-2.24	34,34,34,34	0
2	FE2	N	201	1/1	0.99	0.05	-2.24	34,34,34,34	0
2	FE2	L	200	1/1	1.00	0.06	-2.40	30,30,30,30	0
2	FE2	I	200	1/1	0.99	0.05	-2.46	30,30,30,30	0
2	FE2	P	200	1/1	0.99	0.05	-2.47	32,32,32,32	0
2	FE2	E	200	1/1	0.97	0.05	-2.48	34,34,34,34	0
2	FE2	C	201	1/1	0.98	0.04	-2.50	36,36,36,36	0
2	FE2	J	201	1/1	0.98	0.04	-2.54	36,36,36,36	0
2	FE2	I	201	1/1	0.99	0.03	-2.61	33,33,33,33	0
2	FE2	M	200	1/1	0.99	0.06	-2.63	29,29,29,29	0
2	FE2	M	201	1/1	0.98	0.04	-2.64	33,33,33,33	0
2	FE2	D	201	1/1	0.99	0.04	-2.83	34,34,34,34	0
2	FE2	G	201	1/1	0.99	0.03	-2.83	33,33,33,33	0
2	FE2	A	200	1/1	0.99	0.06	-2.99	31,31,31,31	0
2	FE2	K	200	1/1	0.99	0.05	-3.06	30,30,30,30	0
2	FE2	H	201	1/1	0.99	0.03	-3.10	34,34,34,34	0
2	FE2	H	200	1/1	0.99	0.04	-3.17	31,31,31,31	0
2	FE2	O	201	1/1	0.99	0.02	-3.35	37,37,37,37	0
2	FE2	F	200	1/1	0.99	0.05	-3.71	33,33,33,33	0
2	FE2	E	201	1/1	0.99	0.02	-3.97	35,35,35,35	0
2	FE2	F	201	1/1	0.97	0.04	-4.73	35,35,35,35	0
2	FE2	P	201	1/1	0.99	0.03	-5.20	34,34,34,34	0
2	FE2	C	200	1/1	1.00	0.03	-7.15	31,31,31,31	0
3	SO4	L	2104	5/5	0.77	0.34	-	78,78,78,79	5
3	SO4	A	1006	5/5	0.91	0.40	-	56,67,69,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	SO4	E	1403	5/5	0.91	0.35	-	44,47,49,52	0
3	SO4	B	1103	5/5	0.92	0.19	-	70,71,72,74	0
3	SO4	B	1106	5/5	0.94	0.34	-	64,66,74,75	0
3	SO4	P	1504	5/5	0.91	0.13	-	78,78,78,79	0
3	SO4	H	1703	5/5	0.96	0.17	-	40,43,48,48	5
3	SO4	H	1706	5/5	0.92	0.23	-	47,55,58,60	0
3	SO4	L	2106	5/5	0.92	0.33	-	60,65,69,72	0
3	SO4	C	1204	5/5	0.93	0.19	-	58,59,60,60	5
3	SO4	N	2303	5/5	0.94	0.24	-	64,68,70,72	0
3	SO4	G	1603	5/5	0.92	0.16	-	73,73,74,75	0
3	SO4	M	2206	5/5	0.89	0.32	-	58,60,67,70	0
3	SO4	I	1804	5/5	0.94	0.26	-	62,65,67,69	0
3	SO4	G	1606	5/5	0.95	0.33	-	58,65,67,73	0
3	SO4	F	1506	5/5	0.95	0.23	-	65,67,68,69	0
3	SO4	J	1906	5/5	0.95	0.28	-	50,51,59,59	0
3	SO4	P	2503	5/5	0.93	0.24	-	42,43,47,49	5
3	SO4	O	2406	5/5	0.85	0.18	-	41,44,46,47	5
3	SO4	E	1406	5/5	0.88	0.26	-	62,67,67,70	0
3	SO4	E	1304	5/5	0.88	0.21	-	65,65,67,67	0
3	SO4	D	1303	5/5	0.85	0.43	-	39,44,45,50	0
3	SO4	N	2306	5/5	0.91	0.31	-	60,65,69,71	0
3	SO4	P	2506	5/5	0.93	0.31	-	57,63,66,67	0
3	SO4	A	1003	5/5	0.91	0.27	-	73,73,73,74	0
3	SO4	B	1104	5/5	0.89	0.13	-	73,73,74,75	0
3	SO4	I	1704	5/5	0.76	0.35	-	36,37,38,38	0
3	SO4	O	2403	5/5	0.95	0.26	-	63,66,67,68	0
3	SO4	C	1206	5/5	0.92	0.14	-	46,46,47,49	5
3	SO4	I	1803	5/5	0.95	0.24	-	67,67,70,70	0
3	SO4	M	2203	5/5	0.91	0.41	-	62,63,63,63	0
3	SO4	F	1502	5/5	0.90	0.35	-	69,69,69,71	0
3	SO4	K	2003	5/5	0.94	0.22	-	69,69,69,71	0
3	SO4	M	2202	5/5	0.78	0.42	-	73,73,73,74	0
3	SO4	J	1904	5/5	0.93	0.18	-	61,61,62,63	5
3	SO4	H	1702	5/5	0.76	0.47	-	72,72,73,73	0
3	SO4	K	2006	5/5	0.90	0.23	-	52,55,60,61	0
3	SO4	C	1203	5/5	0.96	0.18	-	56,58,62,64	0
3	SO4	D	1306	5/5	0.94	0.45	-	45,45,48,48	0

6.5 Other polymers (i)

There are no such residues in this entry.