



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:07 PM GMT

PDB ID : 1NF6
Title : X-ray structure of the Desulfovibrio desulfuricans bacterioferritin: the diiron site in different catalytic states ("cycled" structure: reduced in solution and allowed to reoxidise before crystallisation)
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 : 2.35 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (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

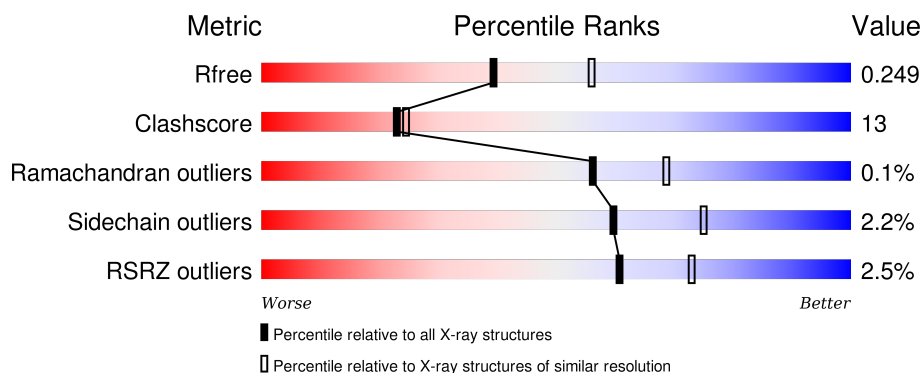
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1352 (2.38-2.34)
Clashscore	102246	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)
RSRZ outliers	91569	1358 (2.38-2.34)

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	179	<div> <div>3%</div> <div>74%</div> <div>21%</div> <div>• 5%</div> </div>
1	B	179	<div> <div>3%</div> <div>71%</div> <div>23%</div> <div>• 5%</div> </div>
1	C	179	<div> <div>3%</div> <div>72%</div> <div>22%</div> <div>• 5%</div> </div>
1	D	179	<div> <div>4%</div> <div>75%</div> <div>18%</div> <div>• 5%</div> </div>
1	E	179	<div> <div>2%</div> <div>66%</div> <div>27%</div> <div>• 5%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	179	
1	G	179	
1	H	179	
1	I	179	
1	J	179	
1	K	179	
1	L	179	
1	M	179	
1	N	179	
1	O	179	
1	P	179	

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	G	1701	-	-	-	X
3	SO4	I	1804	-	-	X	-
3	SO4	J	2001	-	-	-	X
3	SO4	J	2004	-	-	X	-
3	SO4	L	2204	-	-	X	-
3	SO4	N	1204	-	-	X	-
5	GOL	P	2615	-	X	X	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 23933 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	170	Total	C	N	O	S	0	0	0
			1324	824	228	266	6			
1	B	170	Total	C	N	O	S	0	0	0
			1321	824	228	263	6			
1	C	170	Total	C	N	O	S	0	0	0
			1324	824	228	266	6			
1	D	170	Total	C	N	O	S	0	0	0
			1320	822	227	265	6			
1	E	170	Total	C	N	O	S	0	0	0
			1315	820	225	264	6			
1	F	171	Total	C	N	O	S	0	0	0
			1319	821	225	267	6			
1	G	169	Total	C	N	O	S	0	1	0
			1324	825	226	267	6			
1	H	170	Total	C	N	O	S	0	0	0
			1328	828	229	265	6			
1	I	170	Total	C	N	O	S	0	0	0
			1318	820	224	268	6			
1	J	170	Total	C	N	O	S	0	1	0
			1333	833	230	264	6			
1	K	169	Total	C	N	O	S	0	0	0
			1321	823	226	266	6			
1	L	170	Total	C	N	O	S	0	1	0
			1325	825	229	265	6			
1	M	169	Total	C	N	O	S	0	0	0
			1316	820	226	264	6			
1	N	170	Total	C	N	O	S	0	0	0
			1317	820	227	264	6			
1	O	169	Total	C	N	O	S	0	0	0
			1313	817	224	266	6			
1	P	170	Total	C	N	O	S	0	0	0
			1328	827	228	267	6			

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	P	1	Total Fe 1 1	0	0
2	G	1	Total Fe 1 1	0	0
2	J	1	Total Fe 1 1	0	0
2	D	1	Total Fe 1 1	0	0
2	K	1	Total Fe 1 1	0	0
2	E	1	Total Fe 1 1	0	0
2	H	1	Total Fe 1 1	0	0
2	B	1	Total Fe 1 1	0	0
2	I	1	Total Fe 1 1	0	0
2	C	1	Total Fe 1 1	0	0
2	A	1	Total Fe 1 1	0	0
2	N	1	Total Fe 1 1	0	0
2	O	1	Total Fe 1 1	0	0
2	L	1	Total Fe 1 1	0	0
2	F	1	Total Fe 1 1	0	0
2	M	1	Total Fe 1 1	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



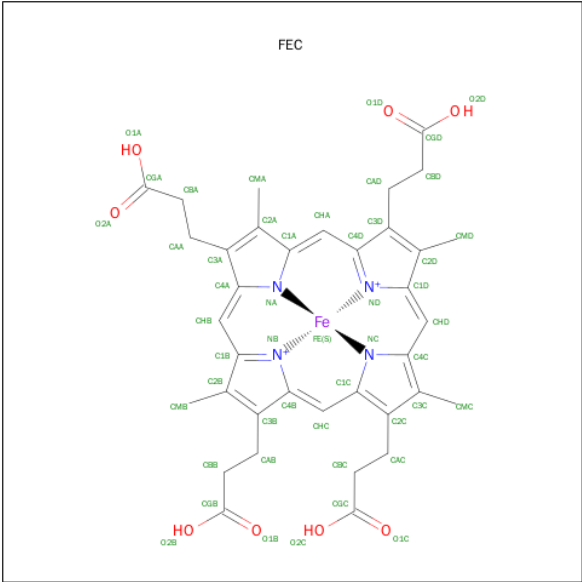
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	N	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	K	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 4 is 1,3,5,8-TETRAMETHYL-PORPHINE-2,4,6,7-TETRAPROPIONIC ACID FERROUS COMPLEX (three-letter code: FEC) (formula: C₃₆H₃₆FeN₄O₈).



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	F	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	K	1	Total	C	Fe	N	O	0	1
			98	72	2	8	16		
4	N	1	Total	C	Fe	N	O	0	1
			98	72	2	8	16		
4	O	1	Total	C	Fe	N	O	0	1
			98	72	2	8	16		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	P	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	121	Total	O	0	0
			121	121		
6	B	115	Total	O	0	0
			115	115		
6	C	92	Total	O	0	0
			92	92		
6	D	114	Total	O	0	0
			114	114		
6	E	92	Total	O	0	0
			92	92		
6	F	112	Total	O	0	0
			112	112		
6	G	130	Total	O	0	0
			130	130		
6	H	97	Total	O	0	0
			97	97		
6	I	132	Total	O	0	0
			132	132		
6	J	113	Total	O	0	0
			113	113		
6	K	133	Total	O	0	0
			133	133		

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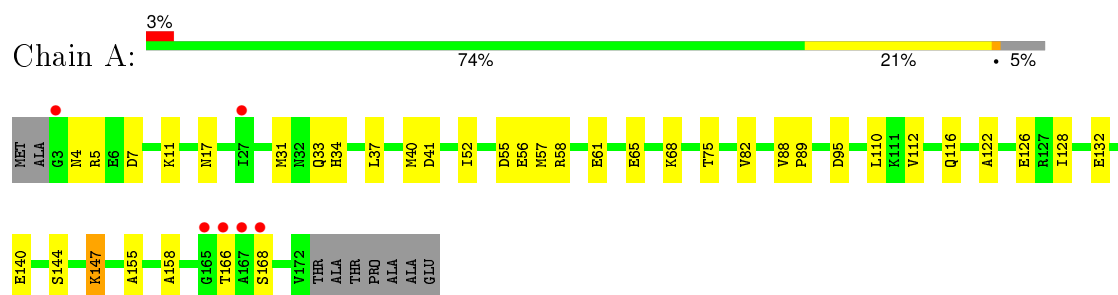
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	L	131	Total 131	O 131	0	0
6	M	128	Total 128	O 128	0	0
6	N	119	Total 119	O 119	0	0
6	O	77	Total 77	O 77	0	0
6	P	105	Total 105	O 105	0	0

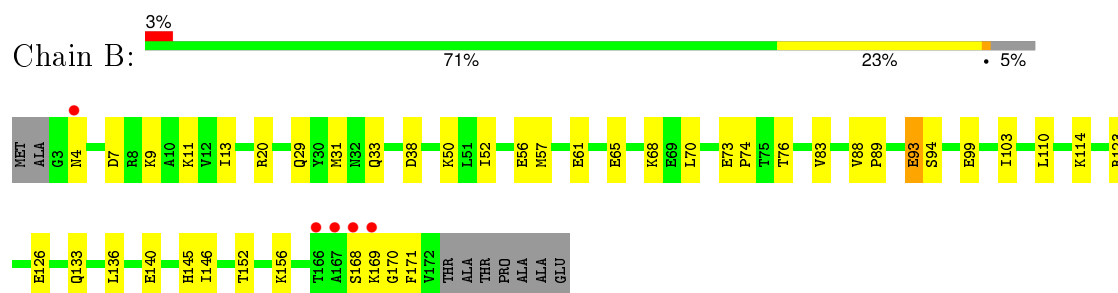
3 Residue-property plots [i](#)

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.

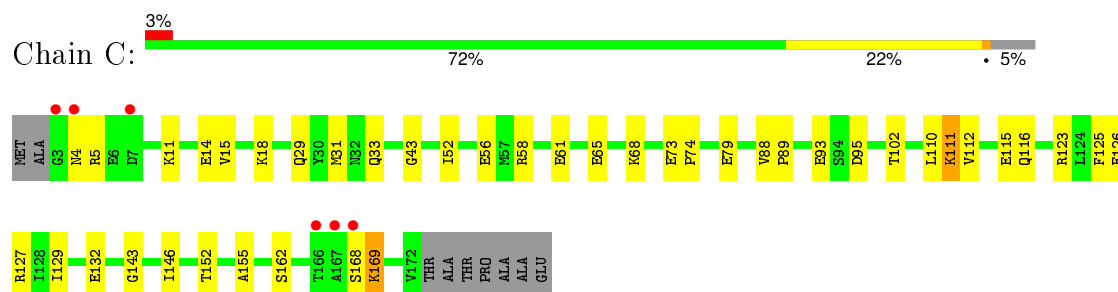
• Molecule 1: bacterioferritin



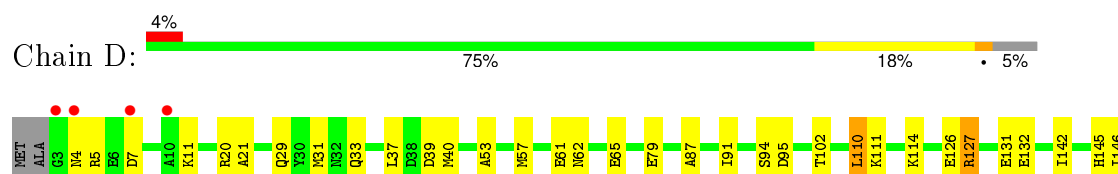
• Molecule 1: bacterioferritin



• Molecule 1: bacterioferritin

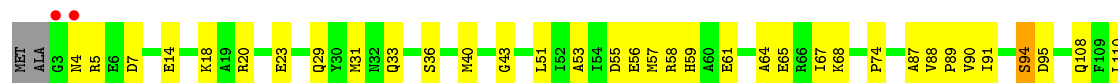


• Molecule 1: bacterioferritin

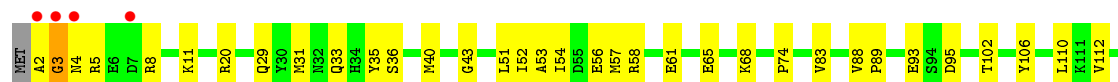




- Molecule 1: bacterioferritin



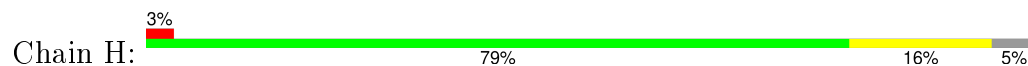
- Molecule 1: bacterioferritin



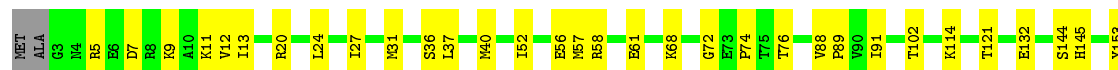
- Molecule 1: bacterioferritin

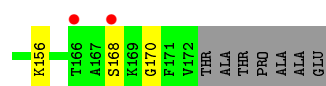


- Molecule 1: bacterioferritin



- Molecule 1: bacterioferritin

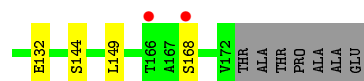
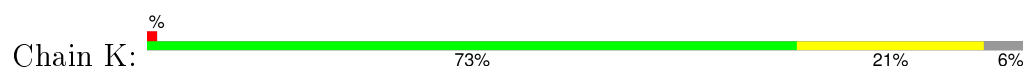




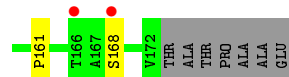
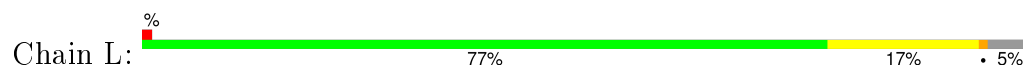
- Molecule 1: bacterioferritin



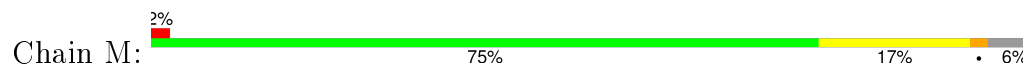
- Molecule 1: bacterioferritin



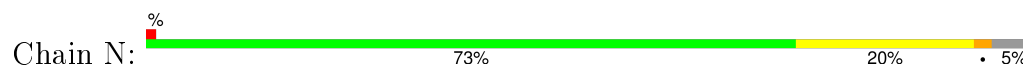
- Molecule 1: bacterioferritin



- Molecule 1: bacterioferritin



- Molecule 1: bacterioferritin





- Molecule 1: bacterioferritin



- Molecule 1: bacterioferritin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α , β , γ	225.79 Å 225.79 Å 225.79 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.35 29.91 – 2.35	Depositor EDS
% Data completeness (in resolution range)	96.5 (30.00-2.35) 96.1 (29.91-2.35)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.72 (at 2.36 Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.197 , 0.267 0.189 , 0.249	Depositor DCC
R_{free} test set	3041 reflections (2.04%)	DCC
Wilson B-factor (Å ²)	26.8	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 67.2	EDS
Estimated twinning fraction	0.048 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 152176 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	23933	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.84% 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: GOL, FE, SO4, FEC

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	0.27	0/1344	0.72	0/1813
1	B	0.27	0/1341	0.67	0/1808
1	C	0.27	0/1344	0.71	0/1813
1	D	0.27	0/1340	0.73	0/1808
1	E	0.27	0/1335	0.72	0/1802
1	F	0.27	0/1339	0.71	0/1809
1	G	0.28	0/1349	0.70	0/1818
1	H	0.27	0/1348	0.69	1/1816 (0.1%)
1	I	0.27	0/1338	0.72	0/1807
1	J	0.27	0/1357	0.71	0/1828
1	K	0.27	0/1341	0.70	0/1809
1	L	0.27	0/1350	0.72	0/1821
1	M	0.27	0/1336	0.66	0/1803
1	N	0.28	0/1337	0.72	0/1805
1	O	0.27	0/1333	0.70	0/1801
1	P	0.27	0/1348	0.74	1/1817 (0.1%)
All	All	0.27	0/21480	0.71	2/28978 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	92	TYR	CA-CB-CG	-5.36	103.22	113.40
1	P	92	TYR	CA-CB-CG	-5.04	103.82	113.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1324	0	1277	39	0
1	B	1321	0	1280	40	0
1	C	1324	0	1277	41	0
1	D	1320	0	1271	35	0
1	E	1315	0	1264	43	0
1	F	1319	0	1260	39	0
1	G	1324	0	1280	40	0
1	H	1328	0	1293	26	0
1	I	1318	0	1259	37	0
1	J	1333	0	1304	47	0
1	K	1321	0	1274	33	0
1	L	1325	0	1279	38	0
1	M	1316	0	1268	28	0
1	N	1317	0	1264	44	0
1	O	1313	0	1252	38	1
1	P	1328	0	1286	38	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
2	M	1	0	0	0	0
2	N	1	0	0	0	0
2	O	1	0	0	0	0
2	P	1	0	0	0	0
3	A	15	0	0	0	0
3	B	5	0	0	0	0
3	C	10	0	0	1	0
3	D	5	0	0	1	0
3	E	10	0	0	0	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	10	0	0	0	0
3	G	10	0	0	1	0
3	H	10	0	0	1	0
3	I	15	0	0	4	0
3	J	10	0	0	0	6
3	K	20	0	0	1	0
3	L	10	0	0	3	8
3	M	15	0	0	1	0
3	N	15	0	0	2	0
3	O	5	0	0	0	0
3	P	5	0	0	1	0
4	A	98	0	64	17	0
4	C	98	0	64	17	0
4	F	98	0	64	18	0
4	G	98	0	64	15	0
4	I	98	0	64	23	0
4	K	98	0	64	17	0
4	N	98	0	64	21	0
4	O	98	0	64	19	0
5	P	6	0	4	4	0
6	A	121	0	0	6	0
6	B	115	0	0	3	0
6	C	92	0	0	2	0
6	D	114	0	0	8	0
6	E	92	0	0	1	0
6	F	112	0	0	7	0
6	G	130	0	0	2	0
6	H	97	0	0	5	0
6	I	132	0	0	4	0
6	J	113	0	0	9	0
6	K	133	0	0	6	0
6	L	131	0	0	8	0
6	M	128	0	0	3	0
6	N	119	0	0	2	0
6	O	77	0	0	0	0
6	P	105	0	0	7	0
All	All	23933	0	20904	578	15

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 13.

All (578) 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:L:114:LYS:HD3	3:L:2204:SO4:O4	1.30	1.31
5:P:2615:GOL:C1	6:P:8947:HOH:O	1.82	1.25
1:L:114:LYS:CE	3:L:2204:SO4:O4	2.14	0.95
1:P:29:GLN:HE22	1:P:83:VAL:H	1.15	0.95
1:H:110:LEU:HD11	1:H:126:GLU:HG3	1.49	0.94
1:E:110:LEU:HD11	1:E:126:GLU:HG2	1.51	0.90
1:J:29:GLN:HE22	1:J:83:VAL:H	1.13	0.89
1:A:168:SER:HB3	4:A:1005[B]:FEC:HBB2	1.54	0.89
1:N:110:LEU:HD11	1:N:126:GLU:HG3	1.57	0.86
1:K:110:LEU:HD11	1:K:126:GLU:HG3	1.56	0.86
1:E:31:MET:HE2	4:F:1604[A]:FEC:HMD3	1.58	0.86
4:C:1305[B]:FEC:HBD1	1:D:31:MET:HG3	1.58	0.86
1:B:110:LEU:HD11	1:B:126:GLU:HG3	1.58	0.85
1:D:110:LEU:HD11	1:D:126:GLU:HG3	1.58	0.84
1:L:110:LEU:HD11	1:L:126:GLU:HG3	1.58	0.83
1:H:29:GLN:HE22	1:H:83:VAL:H	1.25	0.83
1:N:29:GLN:HE22	1:N:83:VAL:H	1.26	0.82
1:M:82:VAL:HG11	1:N:76:THR:HG21	1.61	0.82
1:C:31:MET:HG3	4:C:1305[A]:FEC:HBD1	1.62	0.81
1:L:114:LYS:HE2	3:L:2204:SO4:O4	1.81	0.79
4:K:2104[A]:FEC:HBB2	1:L:168:SER:HB3	1.65	0.79
1:O:61:GLU:O	1:O:65:GLU:HG3	1.82	0.79
6:M:9503:HOH:O	1:N:169:LYS:HE3	1.82	0.78
4:I:1903[A]:FEC:O2C	1:J:168:SER:HA	1.83	0.77
1:C:29:GLN:O	1:C:33:GLN:HG3	1.85	0.77
1:I:31:MET:HG3	4:I:1903[A]:FEC:HBD1	1.66	0.77
1:J:169:LYS:HB2	6:J:9637:HOH:O	1.85	0.77
1:M:111:LYS:O	1:M:115:GLU:HG3	1.85	0.77
1:I:114:LYS:NZ	3:I:1804:SO4:O4	2.14	0.77
1:C:111:LYS:HE2	1:C:115:GLU:OE2	1.84	0.76
1:L:29:GLN:HE22	1:L:83:VAL:H	1.33	0.76
3:D:1401:SO4:O2	6:D:9590:HOH:O	2.03	0.74
1:I:114:LYS:HD3	3:I:1804:SO4:O4	1.87	0.74
1:A:168:SER:HA	4:A:1005[B]:FEC:O2C	1.87	0.74
1:P:61:GLU:O	1:P:65:GLU:HG3	1.87	0.74
1:D:4:ASN:OD1	1:D:7:ASP:HB2	1.87	0.73
1:F:88:VAL:HG23	6:F:473:HOH:O	1.89	0.73
4:K:2104[A]:FEC:O1C	1:L:168:SER:HA	1.88	0.73
1:P:102:THR:HG21	1:P:132:GLU:OE2	1.89	0.72
1:M:127:ARG:HD2	6:M:682:HOH:O	1.89	0.72
1:B:88:VAL:HG23	6:B:1213:HOH:O	1.89	0.72
1:B:61:GLU:O	1:B:65:GLU:HG3	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:147:LYS:HG3	6:J:8944:HOH:O	1.90	0.72
1:L:152:THR:HG22	6:L:9827:HOH:O	1.88	0.72
1:E:87:ALA:O	1:E:91:ILE:HG13	1.89	0.72
1:O:9:LYS:HG2	1:O:70:LEU:HD22	1.70	0.72
1:E:29:GLN:O	1:E:33:GLN:HG3	1.90	0.72
1:I:7:ASP:OD2	1:I:11:LYS:HE3	1.89	0.71
4:I:1903[A]:FEC:HBB2	1:J:168:SER:HB3	1.73	0.70
1:K:149:LEU:HD13	1:O:155:ALA:HA	1.72	0.70
1:H:7:ASP:O	1:H:11:LYS:HG3	1.91	0.70
6:I:912:HOH:O	1:J:169:LYS:HB3	1.91	0.70
1:O:168:SER:HA	4:O:2502[A]:FEC:O1C	1.91	0.70
1:O:65:GLU:O	1:O:69:GLU:HG3	1.92	0.70
1:O:9:LYS:O	1:O:13:ILE:HG13	1.92	0.70
1:K:114:LYS:HE2	3:K:1604:SO4:O1	1.92	0.70
1:N:168:SER:HA	4:N:2403[A]:FEC:O2C	1.92	0.70
1:E:155:ALA:HA	1:P:149:LEU:HD13	1.71	0.70
1:J:29:GLN:HE22	1:J:83:VAL:N	1.89	0.69
1:P:108:GLN:HG2	6:P:9806:HOH:O	1.92	0.69
1:G:164:THR:HA	6:H:703:HOH:O	1.92	0.69
1:G:168:SER:HA	4:G:1704[A]:FEC:O1C	1.92	0.68
1:K:58:ARG:HD3	1:L:168:SER:OG	1.92	0.68
1:C:168:SER:HA	4:C:1305[A]:FEC:O1C	1.94	0.68
1:I:58:ARG:HD3	1:J:168:SER:OG	1.93	0.68
1:F:31:MET:HG3	4:F:1604[A]:FEC:HBA2	1.76	0.68
1:F:61:GLU:O	1:F:65:GLU:HG3	1.93	0.68
1:F:29:GLN:HE22	1:F:83:VAL:H	1.42	0.67
1:A:31:MET:HG3	4:A:1005[A]:FEC:HBD1	1.76	0.67
1:A:4:ASN:OD1	1:A:7:ASP:HB2	1.94	0.67
1:N:168:SER:HB3	4:N:2403[A]:FEC:HBB2	1.76	0.67
1:E:43:GLY:HA3	1:E:160:THR:O	1.95	0.67
4:A:1005[A]:FEC:HMD2	1:B:61:GLU:HB2	1.76	0.66
1:N:166:THR:HB	6:N:9734:HOH:O	1.96	0.66
1:O:53:ALA:O	1:O:57:MET:HG3	1.96	0.66
1:E:168:SER:OG	1:F:58:ARG:HD3	1.96	0.66
4:A:1005[B]:FEC:HBD1	1:B:31:MET:HG3	1.78	0.66
1:C:61:GLU:O	1:C:65:GLU:HG3	1.96	0.65
4:K:2104[A]:FEC:HHC	4:K:2104[A]:FEC:HBC2	1.78	0.65
1:L:61:GLU:O	1:L:65:GLU:HG3	1.96	0.65
3:H:1802:SO4:O1	6:H:721:HOH:O	2.12	0.65
1:J:104:GLU:HG2	6:J:9384:HOH:O	1.97	0.65
1:C:58:ARG:HD3	1:D:168:SER:OG	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:LEU:HA	1:A:40:MET:HE3	1.80	0.64
1:J:169:LYS:HG3	6:J:9558:HOH:O	1.97	0.64
1:H:29:GLN:HE22	1:H:83:VAL:N	1.93	0.64
1:A:112:VAL:O	1:A:116:GLN:HG2	1.98	0.64
4:A:1005[B]:FEC:HBC1	4:A:1005[B]:FEC:HHC	1.79	0.63
1:P:29:GLN:O	1:P:33:GLN:HG3	1.98	0.63
1:N:166:THR:HG23	6:N:9683:HOH:O	1.98	0.63
1:C:110:LEU:HD11	1:C:126:GLU:HG3	1.80	0.63
4:O:2502[A]:FEC:CGD	1:P:20:ARG:HH22	2.11	0.63
1:G:110:LEU:HD11	1:G:126:GLU:HG3	1.80	0.63
4:A:1005[A]:FEC:HHC	4:A:1005[A]:FEC:HBC2	1.79	0.63
1:H:110:LEU:HD23	1:H:114:LYS:HD2	1.80	0.63
1:O:58:ARG:HD3	1:P:168:SER:OG	1.98	0.63
1:J:29:GLN:NE2	1:J:83:VAL:H	1.93	0.62
5:P:2615:GOL:H11	6:P:8947:HOH:O	1.70	0.62
1:N:168:SER:HA	4:N:2403[B]:FEC:O1C	1.99	0.62
1:D:39:ASP:HA	6:D:386:HOH:O	1.98	0.62
1:E:88:VAL:HA	1:E:91:ILE:HD12	1.81	0.62
1:L:127:ARG:HD2	6:L:9796:HOH:O	1.99	0.62
1:G:164:THR:OG1	3:G:1701:SO4:O1	2.18	0.62
1:O:20:ARG:HH22	4:O:2502[B]:FEC:CGD	2.13	0.61
1:I:74:PRO:HB2	6:I:752:HOH:O	2.00	0.61
1:B:114:LYS:HD2	3:N:1204:SO4:O2	2.00	0.61
1:O:31:MET:HG3	4:O:2502[A]:FEC:HBD1	1.82	0.61
1:D:102:THR:HG21	1:D:132:GLU:OE2	2.00	0.61
1:K:8:ARG:O	1:K:12:VAL:HG23	2.00	0.61
1:K:12:VAL:HG11	1:K:118:ASP:OD2	2.02	0.60
1:K:31:MET:HG3	4:K:2104[B]:FEC:HBA2	1.83	0.60
1:O:168:SER:HA	4:O:2502[B]:FEC:O2C	2.02	0.60
4:O:2502[B]:FEC:HBD1	1:P:31:MET:HG3	1.84	0.59
1:E:20:ARG:HH22	4:F:1604[B]:FEC:CGD	2.15	0.59
1:I:20:ARG:HH22	4:I:1903[B]:FEC:CGD	2.15	0.59
1:L:79:GLU:HG2	6:L:8909:HOH:O	2.01	0.59
1:H:29:GLN:NE2	1:H:83:VAL:H	1.99	0.59
1:I:168:SER:HA	4:I:1903[B]:FEC:O2C	2.02	0.59
4:G:1704[A]:FEC:HBB2	1:H:168:SER:HB3	1.84	0.59
4:K:2104[B]:FEC:HBC2	4:K:2104[B]:FEC:HHC	1.83	0.59
4:O:2502[A]:FEC:CMD	1:P:61:GLU:HB2	2.33	0.59
1:E:53:ALA:O	1:E:57:MET:HG3	2.02	0.59
1:G:156:LYS:HA	1:I:156:LYS:HE3	1.84	0.59
1:E:61:GLU:O	1:E:65:GLU:HG3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:58:ARG:HD3	1:L:168:SER:HG	1.67	0.58
1:N:27:ILE:HD11	1:N:57:MET:HA	1.84	0.58
1:E:36:SER:O	1:E:40:MET:HG3	2.03	0.58
4:I:1903[A]:FEC:HHC	4:I:1903[A]:FEC:HBC2	1.84	0.58
1:C:93:GLU:OE1	1:G:6[A]:GLU:HB2	2.01	0.58
1:N:52:ILE:O	1:N:56:GLU:HG2	2.02	0.58
1:I:52:ILE:O	1:I:56:GLU:HG2	2.01	0.58
1:J:156:LYS:HD2	6:J:9663:HOH:O	2.03	0.58
4:C:1305[B]:FEC:HHC	4:C:1305[B]:FEC:HBC2	1.85	0.58
1:J:110:LEU:CD2	1:J:114:LYS:HE2	2.33	0.58
1:A:147:LYS:HE2	6:A:1120:HOH:O	2.03	0.58
1:A:55:ASP:OD2	1:B:171:PHE:HB3	2.04	0.58
1:K:125:PHE:O	1:K:129:ILE:HG13	2.04	0.58
1:I:61:GLU:HB2	4:I:1903[B]:FEC:HMD2	1.86	0.58
1:C:168:SER:CB	4:C:1305[A]:FEC:HBC1	2.34	0.58
1:H:65:GLU:O	1:H:69:GLU:HG3	2.04	0.58
1:K:168:SER:HB3	4:K:2104[B]:FEC:HBB2	1.86	0.58
4:O:2502[B]:FEC:HBC1	1:P:168:SER:HB2	1.86	0.57
1:F:145:HIS:HE1	1:L:41:ASP:OD2	1.86	0.57
1:A:122:ALA:O	1:A:126:GLU:HG3	2.04	0.57
1:I:114:LYS:CD	3:I:1804:SO4:O4	2.50	0.57
1:K:168:SER:HA	4:K:2104[B]:FEC:O2C	2.04	0.57
1:F:52:ILE:O	1:F:56:GLU:HG2	2.04	0.57
1:G:149:LEU:HD13	1:M:155:ALA:HA	1.86	0.57
1:J:77:GLN:HG2	6:J:9765:HOH:O	2.05	0.57
1:B:145:HIS:HE1	1:H:41:ASP:OD2	1.88	0.57
1:C:79:GLU:HG2	6:C:389:HOH:O	2.04	0.57
1:B:29:GLN:O	1:B:33:GLN:HG3	2.05	0.57
1:J:9:LYS:HG2	1:J:70:LEU:HD22	1.86	0.57
1:I:76:THR:HG21	1:J:82:VAL:HG11	1.86	0.57
4:A:1005[A]:FEC:CMD	1:B:61:GLU:HB2	2.34	0.57
1:J:61:GLU:O	1:J:65:GLU:HG3	2.05	0.57
1:F:68:LYS:HD3	1:F:74:PRO:HD3	1.87	0.57
1:O:27:ILE:HD11	1:O:57:MET:HA	1.87	0.56
1:K:31:MET:O	1:K:34:HIS:HB3	2.05	0.56
4:O:2502[A]:FEC:HMD2	1:P:61:GLU:HB2	1.88	0.56
1:I:58:ARG:HD3	1:J:168:SER:HG	1.68	0.56
1:M:4:ASN:ND2	3:M:2302:SO4:O1	2.39	0.56
1:O:61:GLU:HB2	4:O:2502[B]:FEC:HMD2	1.87	0.56
1:F:53:ALA:O	1:F:57:MET:HG3	2.04	0.56
1:B:9:LYS:HG2	1:B:70:LEU:HD22	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:44:GLU:OE1	1:O:157:ILE:HD12	2.06	0.56
1:G:52:ILE:O	1:G:56:GLU:HG2	2.04	0.56
1:M:31:MET:HG3	4:N:2403[A]:FEC:HBD1	1.87	0.56
1:A:166:THR:HG22	1:B:169:LYS:HE3	1.87	0.56
1:O:13:ILE:HD13	1:O:72:GLY:HA3	1.87	0.56
1:I:9:LYS:O	1:I:13:ILE:HG13	2.06	0.56
1:M:110:LEU:HD11	1:M:126:GLU:CG	2.35	0.56
1:A:58:ARG:HD3	1:B:168:SER:OG	2.04	0.55
6:K:977:HOH:O	1:L:65:GLU:HG2	2.06	0.55
1:N:29:GLN:NE2	1:N:83:VAL:H	2.01	0.55
1:D:7:ASP:O	1:D:11:LYS:HG3	2.05	0.55
1:E:4:ASN:HB3	1:E:7:ASP:CB	2.37	0.55
1:I:168:SER:HB3	4:I:1903[B]:FEC:HBB2	1.87	0.55
1:B:29:GLN:HE22	1:B:83:VAL:H	1.53	0.55
5:P:2615:GOL:O1	6:P:8947:HOH:O	1.73	0.55
1:F:149:LEU:HD13	1:L:155:ALA:HA	1.88	0.55
1:I:114:LYS:CE	3:I:1804:SO4:O4	2.54	0.55
1:P:110:LEU:HD11	1:P:126:GLU:HG3	1.89	0.55
6:A:1112:HOH:O	1:B:169:LYS:HE3	2.06	0.55
1:L:29:GLN:NE2	1:L:83:VAL:H	2.04	0.55
4:A:1005[A]:FEC:O2C	1:B:168:SER:HA	2.07	0.55
1:P:148:ASN:O	1:P:149:LEU:HD23	2.07	0.55
1:O:37:LEU:HA	1:O:40:MET:HE3	1.88	0.55
4:I:1903[A]:FEC:CMD	1:J:61:GLU:HB2	2.37	0.55
1:N:114:LYS:NZ	3:N:1204:SO4:O2	2.41	0.54
4:F:1604[B]:FEC:HBC2	4:F:1604[B]:FEC:HHC	1.88	0.54
1:A:61:GLU:OE1	4:A:1005[A]:FEC:HMB2	2.07	0.54
1:M:110:LEU:HD11	1:M:126:GLU:HG3	1.89	0.54
1:D:145:HIS:HD2	6:D:9670:HOH:O	1.90	0.54
1:P:145:HIS:O	1:P:149:LEU:HB2	2.08	0.54
1:N:61:GLU:O	1:N:65:GLU:HG3	2.08	0.54
1:G:88:VAL:HB	1:G:89:PRO:HD3	1.88	0.54
1:O:18:LYS:O	1:O:22:MET:HG3	2.08	0.54
1:F:51:LEU:HD21	1:F:164:THR:HB	1.88	0.54
1:A:11:LYS:HE2	6:A:1124:HOH:O	2.08	0.54
1:I:88:VAL:HA	1:I:91:ILE:HD12	1.90	0.54
1:A:34:HIS:HE1	6:A:1051:HOH:O	1.91	0.54
1:O:111:LYS:O	1:O:114:LYS:HB2	2.08	0.54
1:E:58:ARG:HD3	1:F:168:SER:OG	2.07	0.54
4:C:1305[B]:FEC:HBC1	1:D:168:SER:HB2	1.90	0.54
1:K:79:GLU:HG2	6:K:8937:HOH:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:102:THR:HG21	1:I:132:GLU:OE2	2.08	0.54
1:F:168:SER:HB3	4:F:1604[A]:FEC:HBB2	1.90	0.54
1:N:25:HIS:HA	1:N:78:LYS:HD3	1.90	0.54
1:A:140:GLU:O	1:A:144:SER:HB2	2.08	0.53
1:P:8:ARG:O	1:P:12:VAL:HG23	2.09	0.53
4:I:1903[B]:FEC:HBC2	4:I:1903[B]:FEC:HHC	1.90	0.53
1:E:55:ASP:OD2	1:F:172:VAL:HG22	2.09	0.53
1:F:110:LEU:HD11	1:F:126:GLU:HG3	1.90	0.53
1:J:88:VAL:HG12	1:J:146:ILE:HD13	1.91	0.53
1:H:16:LEU:HD21	1:H:121:THR:HG23	1.89	0.53
1:G:110:LEU:HD11	1:G:126:GLU:CG	2.37	0.53
1:E:122:ALA:O	1:E:126:GLU:HG3	2.09	0.53
1:C:168:SER:HB3	4:C:1305[B]:FEC:HBB2	1.89	0.53
1:M:50:LYS:HE3	4:N:2403[A]:FEC:HMC2	1.91	0.53
1:E:108:GLN:O	1:E:111:LYS:HB3	2.08	0.53
1:B:88:VAL:HB	1:B:89:PRO:HD3	1.91	0.53
1:A:41:ASP:OD2	1:N:145:HIS:HE1	1.92	0.53
4:O:2502[B]:FEC:HBC2	4:O:2502[B]:FEC:HHC	1.90	0.53
1:G:112:VAL:O	1:G:116:GLN:HG2	2.09	0.53
1:P:43:GLY:HA3	1:P:160:THR:O	2.08	0.53
1:A:7:ASP:O	1:A:11:LYS:HG3	2.08	0.52
1:F:145:HIS:HD2	6:L:8990:HOH:O	1.91	0.52
1:M:57:MET:HB3	4:N:2403[A]:FEC:C1B	2.39	0.52
1:H:145:HIS:HD2	6:H:9179:HOH:O	1.92	0.52
1:A:155:ALA:HA	1:N:149:LEU:HD13	1.91	0.52
1:G:7:ASP:OD2	1:G:11:LYS:HE3	2.09	0.52
1:G:142:ILE:HG22	1:G:146:ILE:HD12	1.90	0.52
1:C:58:ARG:HD3	1:D:168:SER:HG	1.73	0.52
1:B:136:LEU:HD11	1:B:140:GLU:OE2	2.10	0.52
1:C:152:THR:HA	1:E:152:THR:HG21	1.91	0.52
1:C:155:ALA:HA	1:E:149:LEU:HD13	1.92	0.52
4:K:2104[B]:FEC:C1B	1:L:57:MET:HB3	2.40	0.52
1:N:57:MET:HB3	4:N:2403[B]:FEC:C1B	2.40	0.52
1:P:120:VAL:HG23	6:P:9227:HOH:O	2.09	0.52
1:J:7:ASP:O	1:J:11:LYS:HG3	2.09	0.52
1:C:112:VAL:O	1:C:116:GLN:HG2	2.10	0.52
1:L:88:VAL:HB	1:L:89:PRO:HD3	1.92	0.52
1:F:93:GLU:HG3	6:F:9406:HOH:O	2.10	0.52
1:A:57:MET:HB3	4:A:1005[A]:FEC:CHB	2.40	0.52
4:I:1903[A]:FEC:HMD2	1:J:61:GLU:HB2	1.92	0.52
1:D:33:GLN:OE1	1:D:95:ASP:OD2	2.27	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:43:GLY:HA2	1:O:162:SER:HB3	1.93	0.51
1:P:29:GLN:NE2	1:P:83:VAL:H	1.97	0.51
1:A:57:MET:HB3	4:A:1005[B]:FEC:C1D	2.41	0.51
1:B:152:THR:HG21	1:H:152:THR:HA	1.92	0.51
1:I:61:GLU:HB2	4:I:1903[B]:FEC:CMD	2.41	0.51
1:D:37:LEU:HA	1:D:40:MET:HE3	1.92	0.51
1:A:58:ARG:HG2	6:A:1119:HOH:O	2.10	0.51
1:K:110:LEU:HD11	1:K:126:GLU:CG	2.34	0.51
1:J:50:LYS:HD3	1:J:164:THR:HG21	1.92	0.51
4:G:1704[A]:FEC:HMD2	1:H:61:GLU:HB2	1.91	0.51
1:K:31:MET:HG3	4:K:2104[A]:FEC:HBD1	1.93	0.51
1:I:31:MET:HG3	4:I:1903[B]:FEC:HBA2	1.92	0.51
1:M:143:GLY:O	1:M:147:LYS:HE3	2.11	0.51
1:K:61:GLU:HB2	4:K:2104[B]:FEC:HMD2	1.93	0.50
4:I:1903[A]:FEC:HAB2	1:J:50:LYS:CE	2.41	0.50
1:E:88:VAL:HB	1:E:89:PRO:HD3	1.92	0.50
1:G:110:LEU:HD21	1:G:114:LYS:HE3	1.93	0.50
1:A:110:LEU:HD11	1:A:126:GLU:HG2	1.93	0.50
1:F:2:ALA:O	1:F:3:GLY:O	2.29	0.50
1:E:14:GLU:O	1:E:18:LYS:HG3	2.11	0.50
1:D:142:ILE:HG22	1:D:146:ILE:HD12	1.93	0.50
1:D:21:ALA:HB1	1:D:79:GLU:HB2	1.93	0.50
1:N:88:VAL:HB	1:N:89:PRO:HD3	1.94	0.50
1:O:125:PHE:O	1:O:129:ILE:HG13	2.11	0.50
4:F:1604[B]:FEC:HBC1	6:F:9471:HOH:O	2.11	0.50
1:K:120:VAL:HG23	6:K:946:HOH:O	2.10	0.50
1:A:52:ILE:O	1:A:56:GLU:HG2	2.11	0.50
1:A:166:THR:HG22	1:B:169:LYS:CE	2.42	0.50
1:O:47:ALA:HB2	1:O:162:SER:O	2.11	0.50
1:O:33:GLN:HE22	1:O:95:ASP:CG	2.15	0.50
6:A:1105:HOH:O	1:B:68:LYS:HE2	2.12	0.50
1:N:61:GLU:HB2	4:N:2403[A]:FEC:HMD2	1.93	0.50
1:L:12:VAL:HG21	6:L:1000:HOH:O	2.12	0.50
4:C:1305[A]:FEC:HMD2	1:D:61:GLU:HB2	1.94	0.49
1:D:4:ASN:ND2	1:D:7:ASP:H	2.10	0.49
1:E:31:MET:HE2	4:F:1604[A]:FEC:CMD	2.38	0.49
1:H:88:VAL:HG12	1:H:146:ILE:HD13	1.93	0.49
1:J:29:GLN:O	1:J:33:GLN:HG3	2.12	0.49
1:N:14:GLU:O	1:N:18:LYS:HG3	2.12	0.49
1:F:88:VAL:HB	1:F:89:PRO:HD3	1.95	0.49
1:K:88:VAL:HB	1:K:89:PRO:HD3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:88:VAL:HG12	1:M:146:ILE:HD13	1.94	0.49
1:K:61:GLU:HB2	4:K:2104[B]:FEC:CMD	2.42	0.49
1:G:50:LYS:HE3	4:G:1704[A]:FEC:HMC2	1.95	0.49
1:M:50:LYS:HZ1	4:N:2403[B]:FEC:CGB	2.25	0.49
1:N:57:MET:HB3	4:N:2403[A]:FEC:C1D	2.43	0.49
1:A:37:LEU:HD23	1:A:40:MET:HE3	1.93	0.49
1:B:9:LYS:O	1:B:13:ILE:HG13	2.12	0.49
1:N:123:ARG:HH12	1:N:127:ARG:HG3	1.78	0.49
1:D:61:GLU:O	1:D:65:GLU:HG3	2.13	0.49
1:G:18:LYS:O	1:G:22:MET:HG3	2.12	0.49
1:L:110:LEU:HD11	1:L:126:GLU:CG	2.38	0.48
1:G:61:GLU:HB2	4:G:1704[B]:FEC:CMD	2.43	0.48
1:F:33:GLN:OE1	1:F:95:ASP:OD2	2.31	0.48
1:A:61:GLU:HB2	4:A:1005[B]:FEC:HMD2	1.95	0.48
1:A:82:VAL:HG11	1:B:76:THR:HG21	1.95	0.48
1:O:61:GLU:HB2	4:O:2502[B]:FEC:CMD	2.43	0.48
1:M:61:GLU:HB2	4:N:2403[B]:FEC:CMD	2.42	0.48
1:N:88:VAL:HG12	1:N:146:ILE:HD13	1.95	0.48
1:P:12:VAL:HG21	5:P:2615:GOL:O3	2.14	0.48
1:F:61:GLU:HB2	4:F:1604[A]:FEC:HMD2	1.95	0.48
1:D:110:LEU:HD23	1:D:114:LYS:HE3	1.96	0.48
1:O:57:MET:HB3	4:O:2502[B]:FEC:C1D	2.44	0.48
1:G:168:SER:HA	4:G:1704[B]:FEC:O2C	2.13	0.48
1:F:8:ARG:HG3	6:F:9666:HOH:O	2.14	0.48
1:C:11:LYS:O	1:C:14:GLU:HB3	2.13	0.48
1:E:90:VAL:O	1:E:94:SER:OG	2.27	0.48
1:B:88:VAL:HG12	1:B:146:ILE:HD13	1.96	0.48
1:F:152:THR:HG21	1:L:152:THR:HA	1.96	0.48
1:F:36:SER:O	1:F:40:MET:HG3	2.14	0.48
1:F:31:MET:CE	4:F:1604[B]:FEC:HMD3	2.43	0.47
4:K:2104[A]:FEC:HMD2	1:L:61:GLU:HB2	1.96	0.47
1:D:7:ASP:OD1	1:D:11:LYS:HE3	2.14	0.47
1:C:5:ARG:HD2	1:C:5:ARG:HA	1.68	0.47
4:G:1704[B]:FEC:HBC1	1:H:168:SER:HB2	1.95	0.47
1:I:9:LYS:HA	6:I:801:HOH:O	2.12	0.47
1:D:53:ALA:O	1:D:57:MET:HG3	2.14	0.47
1:J:81:LYS:HE2	1:J:83:VAL:HA	1.97	0.47
1:N:31:MET:CE	4:N:2403[B]:FEC:HMD3	2.45	0.47
4:F:1604[A]:FEC:HHC	4:F:1604[A]:FEC:CGC	2.45	0.47
4:C:1305[A]:FEC:HBB2	1:D:168:SER:HB3	1.96	0.47
1:N:57:MET:HB3	4:N:2403[B]:FEC:CHB	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:1903[A]:FEC:CGD	1:J:20:ARG:HH22	2.27	0.47
1:K:5:ARG:HD2	1:K:8:ARG:NH1	2.30	0.47
1:G:12:VAL:HG21	6:G:1739:HOH:O	2.15	0.47
1:M:4:ASN:OD1	1:M:7:ASP:HB2	2.15	0.47
1:M:171:PHE:HB3	1:N:55:ASP:OD2	2.15	0.47
1:E:68:LYS:HD3	1:E:74:PRO:HD3	1.97	0.47
1:M:43:GLY:HA3	1:M:160:THR:O	2.15	0.47
1:P:5:ARG:HA	1:P:5:ARG:HD2	1.65	0.47
1:I:88:VAL:HB	1:I:89:PRO:HD3	1.97	0.47
1:C:88:VAL:HB	1:C:89:PRO:HD3	1.96	0.47
1:G:33:GLN:NE2	1:G:95:ASP:OD2	2.47	0.47
1:E:61:GLU:HB2	4:F:1604[B]:FEC:HMD2	1.96	0.47
1:G:27:ILE:HD11	1:G:57:MET:HA	1.97	0.47
1:B:145:HIS:CD2	1:H:158:ALA:HB1	2.49	0.47
1:J:161[B]:PRO:HG2	6:J:893:HOH:O	2.13	0.47
1:D:127:ARG:NH2	1:D:131:GLU:OE2	2.48	0.47
1:G:8:ARG:O	1:G:12:VAL:HG23	2.14	0.47
1:J:150:GLY:O	1:J:153:TYR:N	2.47	0.47
1:D:169:LYS:HD2	1:D:169:LYS:HA	1.52	0.47
1:F:29:GLN:O	1:F:33:GLN:HG3	2.14	0.46
1:C:123:ARG:NH1	1:C:126:GLU:HB2	2.30	0.46
1:N:23:GLU:HA	1:N:23:GLU:OE1	2.14	0.46
1:I:12:VAL:CG1	1:I:121:THR:HG21	2.45	0.46
1:M:61:GLU:HB2	4:N:2403[B]:FEC:HMD2	1.97	0.46
1:O:52:ILE:O	1:O:56:GLU:HG2	2.15	0.46
1:P:12:VAL:HG11	1:P:118:ASP:OD2	2.14	0.46
1:J:88:VAL:HB	1:J:89:PRO:HD3	1.96	0.46
4:K:2104[A]:FEC:HBB2	1:L:168:SER:CB	2.40	0.46
1:D:127:ARG:NH2	6:D:9562:HOH:O	2.46	0.46
1:I:36:SER:O	1:I:40:MET:HG3	2.16	0.46
1:B:133:GLN:NE2	6:B:1264:HOH:O	2.49	0.46
1:I:168:SER:CB	4:I:1903[B]:FEC:HBB2	2.46	0.46
1:J:53:ALA:O	1:J:57:MET:HG3	2.16	0.46
4:G:1704[B]:FEC:HBC1	1:H:168:SER:CB	2.45	0.46
1:H:61:GLU:O	1:H:65:GLU:HG3	2.16	0.46
1:E:51:LEU:HD21	1:E:164:THR:HB	1.97	0.46
1:A:17:ASN:OD1	1:A:75:THR:HG22	2.16	0.46
1:E:168:SER:HA	4:F:1604[B]:FEC:O1C	2.15	0.46
1:G:8:ARG:NE	1:G:116:GLN:O	2.49	0.46
1:J:55:ASP:OD1	1:J:58:ARG:NH2	2.47	0.46
1:P:55:ASP:OD1	1:P:58:ARG:NH2	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:LYS:NZ	6:B:1255:HOH:O	2.49	0.46
4:F:1604[B]:FEC:HHB	4:F:1604[B]:FEC:HBA2	1.96	0.46
1:P:20:ARG:NH2	6:P:9233:HOH:O	2.49	0.46
1:P:27:ILE:HD11	1:P:57:MET:HA	1.98	0.46
1:N:169:LYS:N	4:N:2403[B]:FEC:O1C	2.49	0.46
4:I:1903[A]:FEC:O1A	1:J:35:TYR:OH	2.30	0.46
1:E:88:VAL:HG12	1:E:146:ILE:HD13	1.98	0.46
1:G:158:ALA:O	1:I:156:LYS:NZ	2.48	0.46
1:P:58:ARG:O	1:P:62:ASN:ND2	2.49	0.46
1:J:104:GLU:HA	1:J:104:GLU:OE1	2.16	0.45
1:P:164:THR:OG1	3:P:2601:SO4:O1	2.30	0.45
1:L:52:ILE:O	1:L:56:GLU:HG2	2.16	0.45
1:M:55:ASP:OD1	1:M:58:ARG:NH2	2.49	0.45
1:G:23:GLU:OE1	1:G:23:GLU:HA	2.16	0.45
1:I:5:ARG:NH1	6:I:924:HOH:O	2.46	0.45
1:N:110:LEU:CD2	1:N:114:LYS:HE3	2.45	0.45
1:F:35:TYR:OH	4:F:1604[A]:FEC:O1A	2.28	0.45
1:B:88:VAL:HG12	1:B:146:ILE:CD1	2.47	0.45
1:O:88:VAL:HB	1:O:89:PRO:HD3	1.98	0.45
1:A:128:ILE:O	1:A:132:GLU:HG2	2.16	0.45
1:K:9:LYS:HG2	1:K:70:LEU:HD22	1.98	0.45
1:O:33:GLN:NE2	1:O:95:ASP:OD2	2.46	0.45
4:G:1704[A]:FEC:CMD	1:H:61:GLU:HB2	2.47	0.45
1:P:88:VAL:HB	1:P:89:PRO:HD3	1.99	0.45
1:E:144:SER:O	1:E:148:ASN:ND2	2.49	0.45
1:C:168:SER:HB2	4:C:1305[A]:FEC:HBC1	1.99	0.45
1:K:11:LYS:HD3	1:K:116:GLN:NE2	2.31	0.45
1:J:62:ASN:ND2	6:J:9845:HOH:O	2.50	0.45
1:E:33:GLN:NE2	1:E:95:ASP:OD2	2.46	0.45
1:M:68:LYS:HD2	1:M:68:LYS:HA	1.78	0.45
1:O:57:MET:HB3	4:O:2502[A]:FEC:CHB	2.47	0.45
1:B:7:ASP:O	1:B:11:LYS:HG3	2.17	0.45
1:J:111:LYS:O	1:J:115:GLU:HG3	2.17	0.45
1:E:5:ARG:HA	1:E:5:ARG:HD2	1.78	0.45
4:A:1005[B]:FEC:C1B	1:B:57:MET:HB3	2.46	0.45
1:D:110:LEU:CD2	1:D:114:LYS:HE3	2.47	0.45
1:A:61:GLU:O	1:A:65:GLU:HG3	2.17	0.44
1:C:168:SER:HB3	4:C:1305[B]:FEC:CBB	2.48	0.44
1:C:33:GLN:HE22	1:C:95:ASP:CG	2.21	0.44
1:G:110:LEU:HD13	1:N:119:ILE:HG13	1.99	0.44
1:N:110:LEU:HD11	1:N:126:GLU:CG	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:29:GLN:O	1:N:33:GLN:HG3	2.18	0.44
1:H:168:SER:N	6:H:9612:HOH:O	2.49	0.44
1:E:23:GLU:OE1	1:E:23:GLU:HA	2.18	0.44
1:O:168:SER:HB3	4:O:2502[B]:FEC:O2B	2.17	0.44
6:M:9691:HOH:O	4:N:2403[B]:FEC:HBB2	2.17	0.44
1:K:111:LYS:HE2	1:K:115:GLU:OE2	2.18	0.44
1:K:68:LYS:HA	1:K:68:LYS:HD2	1.73	0.44
1:N:61:GLU:OE1	4:N:2403[B]:FEC:HMB2	2.17	0.44
1:L:59:HIS:CE1	1:L:128:ILE:HG23	2.52	0.44
1:C:68:LYS:HD2	1:C:68:LYS:HA	1.81	0.44
1:J:33:GLN:OE1	1:J:95:ASP:OD2	2.35	0.44
4:C:1305[B]:FEC:HBC1	1:D:168:SER:CB	2.47	0.44
1:N:31:MET:HE2	4:N:2403[B]:FEC:HMD3	1.99	0.44
1:A:55:ASP:OD1	1:B:170:GLY:HA3	2.18	0.44
1:F:3:GLY:N	6:F:9666:HOH:O	2.49	0.44
1:K:56:GLU:HA	1:K:56:GLU:OE1	2.18	0.44
1:D:29:GLN:NE2	6:D:338:HOH:O	2.49	0.44
1:C:61:GLU:HB2	4:C:1305[B]:FEC:HMD2	1.98	0.44
1:M:123:ARG:NH1	1:M:126:GLU:OE1	2.49	0.44
1:P:153:TYR:O	1:P:156:LYS:HB3	2.17	0.44
1:B:52:ILE:O	1:B:56:GLU:HG2	2.17	0.44
1:N:123:ARG:HA	1:N:123:ARG:HD2	1.72	0.44
1:K:33:GLN:NE2	1:K:95:ASP:OD2	2.47	0.44
1:C:43:GLY:HA2	1:C:162:SER:HB3	2.00	0.44
1:M:110:LEU:HD11	1:M:126:GLU:HG2	2.00	0.44
1:J:150:GLY:O	1:J:153:TYR:HB3	2.18	0.44
1:I:37:LEU:HD23	1:I:40:MET:HE3	2.00	0.44
1:C:102:THR:HG21	1:C:132:GLU:OE2	2.17	0.44
1:N:20:ARG:HH22	4:N:2403[A]:FEC:CGD	2.30	0.44
1:O:12:VAL:O	1:O:15:VAL:HG22	2.18	0.44
4:C:1305[B]:FEC:HBD1	1:D:31:MET:CG	2.39	0.43
1:D:169:LYS:N	6:D:9425:HOH:O	2.49	0.43
1:B:93:GLU:HG2	1:B:94:SER:N	2.33	0.43
1:J:27:ILE:HD11	1:J:57:MET:HA	2.00	0.43
1:L:127:ARG:HB3	6:L:9796:HOH:O	2.18	0.43
1:K:12:VAL:HG21	6:K:996:HOH:O	2.17	0.43
1:J:88:VAL:CG1	1:J:146:ILE:HD13	2.47	0.43
1:F:2:ALA:N	6:F:9654:HOH:O	2.49	0.43
1:B:99:GLU:O	1:B:103:ILE:HG13	2.18	0.43
4:I:1903[B]:FEC:HBD1	1:J:31:MET:HG3	1.99	0.43
1:E:64:ALA:HA	1:E:67:ILE:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:K:9009:HOH:O	1:L:68:LYS:HE2	2.19	0.43
1:F:112:VAL:O	1:F:116:GLN:HG2	2.18	0.43
4:A:1005[A]:FEC:CGD	1:B:20:ARG:HH22	2.32	0.43
4:O:2502[B]:FEC:CBD	1:P:31:MET:HG3	2.48	0.43
1:I:57:MET:HB3	4:I:1903[B]:FEC:C1D	2.48	0.43
1:G:57:MET:HB3	4:G:1704[A]:FEC:C1B	2.49	0.43
1:G:58:ARG:HD3	1:H:168:SER:HG	1.83	0.43
1:G:110:LEU:CD2	1:G:114:LYS:HE3	2.49	0.43
1:F:54:ILE:O	1:F:57:MET:HB2	2.18	0.43
1:C:155:ALA:O	1:E:156:LYS:NZ	2.50	0.43
1:O:17:ASN:OD1	1:O:75:THR:HG22	2.19	0.43
1:M:52:ILE:O	1:M:56:GLU:HG2	2.17	0.43
1:A:5:ARG:HA	1:A:5:ARG:HD2	1.74	0.43
1:E:168:SER:HB3	4:F:1604[B]:FEC:HBB2	2.01	0.43
1:G:50:LYS:O	1:G:54:ILE:HG13	2.19	0.43
1:O:128:ILE:O	1:O:132:GLU:HG2	2.19	0.43
1:G:57:MET:HB3	4:G:1704[B]:FEC:C1D	2.48	0.43
4:G:1704[B]:FEC:HHC	4:G:1704[B]:FEC:HBC2	2.01	0.43
1:H:8:ARG:O	1:H:12:VAL:HG23	2.18	0.43
1:M:132:GLU:HA	1:M:132:GLU:OE1	2.18	0.43
1:F:157:ILE:O	1:F:157:ILE:HG22	2.18	0.43
1:C:125:PHE:O	1:C:129:ILE:HG13	2.18	0.43
1:C:88:VAL:HG12	1:C:146:ILE:HD13	2.00	0.43
1:G:30:TYR:OH	1:G:99:GLU:OE2	2.27	0.43
1:A:33:GLN:NE2	1:A:95:ASP:OD2	2.51	0.43
1:L:161:PRO:HA	6:L:9420:HOH:O	2.17	0.43
1:O:83:VAL:HG12	1:O:86:GLN:HG3	2.01	0.43
1:H:27:ILE:HD11	1:H:57:MET:HA	2.01	0.43
1:C:123:ARG:HH11	1:C:126:GLU:HB2	1.84	0.43
1:C:15:VAL:HA	1:C:18:LYS:HD2	2.01	0.43
1:M:112:VAL:O	1:M:116:GLN:HG2	2.19	0.43
1:E:20:ARG:NH1	4:F:1604[B]:FEC:O2D	2.49	0.42
1:F:20:ARG:HH22	4:F:1604[A]:FEC:CGD	2.32	0.42
1:F:31:MET:HE1	4:F:1604[B]:FEC:HMD3	2.01	0.42
1:N:168:SER:HB3	4:N:2403[A]:FEC:CBB	2.48	0.42
4:I:1903[A]:FEC:HAB2	1:J:50:LYS:HE2	2.01	0.42
1:E:33:GLN:HE22	1:E:95:ASP:CG	2.21	0.42
1:F:5:ARG:HD2	1:F:8:ARG:NH1	2.34	0.42
1:P:15:VAL:O	1:P:18:LYS:HB2	2.19	0.42
1:I:68:LYS:HD2	1:I:68:LYS:HA	1.76	0.42
1:C:123:ARG:O	1:C:127:ARG:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:56:GLU:HA	1:E:56:GLU:OE1	2.20	0.42
1:B:4:ASN:N	1:B:4:ASN:OD1	2.51	0.42
1:B:73:GLU:HA	1:B:74:PRO:HD3	1.81	0.42
1:O:123:ARG:NH1	1:O:126:GLU:OE1	2.49	0.42
1:J:9:LYS:O	1:J:13:ILE:HG13	2.18	0.42
1:P:88:VAL:CG1	1:P:146:ILE:HD13	2.49	0.42
1:C:143:GLY:HA3	6:C:328:HOH:O	2.19	0.42
1:N:128:ILE:O	1:N:132:GLU:HG2	2.20	0.42
1:K:102:THR:HG21	1:K:132:GLU:OE2	2.19	0.42
1:M:20:ARG:HH22	4:N:2403[B]:FEC:CGD	2.32	0.42
1:I:153:TYR:O	1:I:156:LYS:HB3	2.19	0.42
1:D:127:ARG:NH1	6:D:9562:HOH:O	2.52	0.42
1:F:11:LYS:HE3	6:F:9526:HOH:O	2.19	0.42
1:A:168:SER:HB3	4:A:1005[B]:FEC:CBB	2.38	0.42
1:D:87:ALA:O	1:D:91:ILE:HG13	2.20	0.42
4:O:2502[B]:FEC:HBC1	1:P:168:SER:CB	2.48	0.42
1:C:14:GLU:O	1:C:18:LYS:HG3	2.18	0.42
1:L:104:GLU:O	1:L:108:GLN:NE2	2.53	0.42
1:P:9:LYS:HG2	1:P:70:LEU:HD22	2.01	0.42
4:I:1903[A]:FEC:O2B	1:J:168:SER:OG	2.33	0.42
1:K:68:LYS:HD3	1:K:74:PRO:HD3	2.02	0.42
1:L:33:GLN:OE1	1:L:95:ASP:OD2	2.37	0.42
1:E:118:ASP:OD2	1:E:121:THR:OG1	2.31	0.42
1:O:8:ARG:HA	1:O:116:GLN:OE1	2.20	0.42
1:A:88:VAL:HB	1:A:89:PRO:HD3	2.01	0.42
1:C:169:LYS:N	4:C:1305[A]:FEC:O1C	2.50	0.42
1:C:33:GLN:NE2	1:C:95:ASP:OD2	2.43	0.42
1:A:55:ASP:CG	1:B:171:PHE:H	2.23	0.42
1:B:123:ARG:HD2	1:B:123:ARG:HA	1.92	0.42
4:K:2104[A]:FEC:C1D	1:L:57:MET:HB3	2.50	0.41
4:K:2104[A]:FEC:CMD	1:L:61:GLU:HB2	2.50	0.41
1:P:74:PRO:HB2	6:P:9225:HOH:O	2.20	0.41
1:H:58:ARG:HD2	6:H:740:HOH:O	2.19	0.41
4:I:1903[A]:FEC:C1D	1:J:57:MET:HB3	2.50	0.41
1:G:88:VAL:HG23	6:G:1748:HOH:O	2.20	0.41
1:K:86:GLN:HB3	1:K:90:VAL:HG12	2.03	0.41
1:I:20:ARG:NH2	4:I:1903[B]:FEC:O2D	2.50	0.41
4:G:1704[A]:FEC:C1D	1:H:57:MET:HB3	2.50	0.41
1:I:170:GLY:HA3	1:J:55:ASP:OD1	2.19	0.41
1:E:112:VAL:O	1:E:116:GLN:HG2	2.20	0.41
1:C:4:ASN:HB2	3:C:1302:SO4:O1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:68:LYS:HA	1:E:68:LYS:HD2	1.89	0.41
4:A:1005[A]:FEC:HAB2	1:B:50:LYS:CE	2.50	0.41
1:G:41:ASP:HB3	1:I:145:HIS:CE1	2.55	0.41
1:L:5:ARG:HD2	6:L:8969:HOH:O	2.20	0.41
1:G:90:VAL:O	1:G:94:SER:HB2	2.20	0.41
1:A:158:ALA:O	1:N:156:LYS:NZ	2.49	0.41
1:G:31:MET:HG3	4:G:1704[A]:FEC:HBD1	2.03	0.41
1:C:93:GLU:CD	1:G:6[A]:GLU:HB2	2.41	0.41
1:O:102:THR:HG21	1:O:132:GLU:OE2	2.20	0.41
1:L:5:ARG:HD2	1:L:5:ARG:HA	1.89	0.41
1:D:5:ARG:HD2	1:D:5:ARG:HA	1.71	0.41
4:C:1305[A]:FEC:HBB2	1:D:168:SER:CB	2.51	0.41
1:N:29:GLN:HE22	1:N:83:VAL:N	2.06	0.41
1:P:145:HIS:O	1:P:149:LEU:N	2.54	0.41
1:K:89:PRO:HD3	6:K:9527:HOH:O	2.21	0.41
1:M:29:GLN:O	1:M:33:GLN:HG3	2.21	0.41
1:I:24:LEU:HA	1:I:27:ILE:HD12	2.03	0.41
1:F:128:ILE:O	1:F:132:GLU:HG2	2.21	0.41
1:P:4:ASN:OD1	1:P:7:ASP:OD1	2.37	0.41
1:E:59:HIS:HD2	6:E:9698:HOH:O	2.04	0.41
1:F:102:THR:HG23	1:F:106:TYR:CE1	2.56	0.41
1:J:127:ARG:HB3	6:J:9732:HOH:O	2.21	0.41
1:A:68:LYS:HD2	1:A:68:LYS:HA	1.83	0.41
4:K:2104[A]:FEC:CGD	1:L:20:ARG:HH22	2.34	0.40
1:D:62:ASN:ND2	6:D:9562:HOH:O	2.54	0.40
1:G:55:ASP:OD2	1:H:172:VAL:HG22	2.21	0.40
1:K:82:VAL:HG11	1:L:76:THR:HG21	2.03	0.40
1:C:73:GLU:HA	1:C:74:PRO:HD3	1.93	0.40
1:L:73:GLU:HA	1:L:74:PRO:HD3	1.93	0.40
4:C:1305[B]:FEC:CGA	1:D:20:ARG:HH22	2.35	0.40
4:O:2502[B]:FEC:CGA	1:P:20:ARG:HH22	2.33	0.40
1:K:31:MET:HE2	4:K:2104[A]:FEC:HMD3	2.03	0.40
1:O:169:LYS:N	4:O:2502[A]:FEC:O1C	2.50	0.40
1:A:41:ASP:HB3	1:N:145:HIS:CE1	2.57	0.40
1:G:168:SER:HB3	4:G:1704[B]:FEC:CBB	2.52	0.40
1:O:157:ILE:HG22	1:O:157:ILE:O	2.20	0.40
1:I:13:ILE:HD13	1:I:72:GLY:HA3	2.04	0.40
1:C:155:ALA:CB	1:E:152:THR:HG22	2.51	0.40
1:M:23:GLU:OE1	1:M:56:GLU:HB3	2.21	0.40
1:N:8:ARG:HA	1:N:116:GLN:OE1	2.22	0.40
1:F:43:GLY:HA3	1:F:160:THR:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:104:GLU:O	1:N:108:GLN:HG3	2.22	0.40
1:C:52:ILE:O	1:C:56:GLU:HG2	2.21	0.40

All (15) 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:J:2004:SO4:O3	3:J:2004:SO4:O4[8_555]	0.24	1.96
3:J:2004:SO4:O1	3:J:2004:SO4:O3[8_555]	0.29	1.91
3:J:2004:SO4:O1	3:J:2004:SO4:O4[11_455]	0.30	1.90
3:L:2204:SO4:O2	3:L:2204:SO4:O4[6_555]	0.32	1.88
3:L:2204:SO4:O1	3:L:2204:SO4:O2[6_555]	0.45	1.75
3:L:2204:SO4:O1	3:L:2204:SO4:O4[12_554]	0.48	1.72
3:L:2204:SO4:S	3:L:2204:SO4:O2[12_554]	1.25	0.95
3:J:2004:SO4:S	3:J:2004:SO4:O1[11_455]	1.31	0.89
3:L:2204:SO4:S	3:L:2204:SO4:O3[6_555]	1.32	0.88
3:L:2204:SO4:S	3:L:2204:SO4:O1[6_555]	1.47	0.73
3:J:2004:SO4:S	3:J:2004:SO4:O2[11_455]	1.48	0.72
3:J:2004:SO4:S	3:J:2004:SO4:O3[11_455]	1.48	0.72
3:L:2204:SO4:S	3:L:2204:SO4:O4[12_554]	1.70	0.50
1:O:114:LYS:NZ	3:E:1404:SO4:O2[6_555]	2.12	0.08
3:L:2204:SO4:O2	3:L:2204:SO4:O3[12_554]	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	168/179 (94%)	165 (98%)	3 (2%)	0	100	100
1	B	168/179 (94%)	163 (97%)	5 (3%)	0	100	100
1	C	168/179 (94%)	166 (99%)	2 (1%)	0	100	100
1	D	168/179 (94%)	163 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	168/179 (94%)	163 (97%)	5 (3%)	0	100	100
1	F	169/179 (94%)	166 (98%)	2 (1%)	1 (1%)	30	34
1	G	168/179 (94%)	161 (96%)	5 (3%)	2 (1%)	16	15
1	H	168/179 (94%)	162 (96%)	6 (4%)	0	100	100
1	I	168/179 (94%)	165 (98%)	3 (2%)	0	100	100
1	J	169/179 (94%)	166 (98%)	3 (2%)	0	100	100
1	K	167/179 (93%)	164 (98%)	3 (2%)	0	100	100
1	L	169/179 (94%)	166 (98%)	3 (2%)	0	100	100
1	M	167/179 (93%)	165 (99%)	2 (1%)	0	100	100
1	N	168/179 (94%)	165 (98%)	3 (2%)	0	100	100
1	O	167/179 (93%)	165 (99%)	2 (1%)	0	100	100
1	P	168/179 (94%)	162 (96%)	6 (4%)	0	100	100
All	All	2688/2864 (94%)	2627 (98%)	58 (2%)	3 (0%)	56	69

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	3	GLY
1	G	151	ASP
1	G	150	GLY

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	137/145 (94%)	136 (99%)	1 (1%)	88	95
1	B	136/145 (94%)	133 (98%)	3 (2%)	60	75
1	C	137/145 (94%)	135 (98%)	2 (2%)	72	85
1	D	136/145 (94%)	131 (96%)	5 (4%)	41	53
1	E	135/145 (93%)	132 (98%)	3 (2%)	60	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	135/145 (93%)	134 (99%)	1 (1%)	88	95
1	G	138/145 (95%)	132 (96%)	6 (4%)	35	45
1	H	138/145 (95%)	136 (99%)	2 (1%)	74	86
1	I	136/145 (94%)	135 (99%)	1 (1%)	88	95
1	J	139/145 (96%)	134 (96%)	5 (4%)	42	55
1	K	137/145 (94%)	134 (98%)	3 (2%)	60	75
1	L	137/145 (94%)	134 (98%)	3 (2%)	60	75
1	M	136/145 (94%)	132 (97%)	4 (3%)	50	64
1	N	135/145 (93%)	132 (98%)	3 (2%)	60	75
1	O	135/145 (93%)	133 (98%)	2 (2%)	72	85
1	P	138/145 (95%)	134 (97%)	4 (3%)	50	64
All	All	2185/2320 (94%)	2137 (98%)	48 (2%)	60	75

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	147	LYS
1	B	38	ASP
1	B	93	GLU
1	B	156	LYS
1	C	111	LYS
1	C	169	LYS
1	D	94	SER
1	D	110	LEU
1	D	111	LYS
1	D	127	ARG
1	D	169	LYS
1	E	94	SER
1	E	111	LYS
1	E	144	SER
1	F	4	ASN
1	G	81	LYS
1	G	94	SER
1	G	123	ARG
1	G	144	SER
1	G	147	LYS
1	G	152	THR
1	H	77	GLN

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Mol	Chain	Res	Type
1	H	169	LYS
1	I	144	SER
1	J	81	LYS
1	J	104	GLU
1	J	111	LYS
1	J	144	SER
1	J	152	THR
1	K	7	ASP
1	K	81	LYS
1	K	144	SER
1	L	20	ARG
1	L	147	LYS
1	L	152	THR
1	M	4	ASN
1	M	7	ASP
1	M	111	LYS
1	M	169	LYS
1	N	78	LYS
1	N	123	ARG
1	N	169	LYS
1	O	36	SER
1	O	144	SER
1	P	78	LYS
1	P	81	LYS
1	P	144	SER
1	P	152	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	33	GLN
1	B	29	GLN
1	B	145	HIS
1	C	32	ASN
1	C	33	GLN
1	D	4	ASN
1	D	29	GLN
1	D	62	ASN
1	D	108	GLN
1	D	145	HIS
1	E	32	ASN

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Mol	Chain	Res	Type
1	E	33	GLN
1	E	148	ASN
1	F	29	GLN
1	F	133	GLN
1	F	145	HIS
1	G	32	ASN
1	G	33	GLN
1	H	29	GLN
1	H	62	ASN
1	H	145	HIS
1	I	32	ASN
1	I	33	GLN
1	I	62	ASN
1	I	148	ASN
1	J	29	GLN
1	J	148	ASN
1	K	33	GLN
1	L	29	GLN
1	L	108	GLN
1	L	133	GLN
1	M	32	ASN
1	M	33	GLN
1	N	29	GLN
1	N	62	ASN
1	N	133	GLN
1	N	145	HIS
1	O	32	ASN
1	O	33	GLN
1	O	62	ASN
1	P	29	GLN
1	P	62	ASN
1	P	145	HIS
1	P	148	ASN

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 67 ligands modelled in this entry, 16 are monoatomic - leaving 51 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	1004	-	4,4,4	3.09	2 (50%)	6,6,6	0.93	0
4	FEC	A	1005[A]	1	34,56,56	1.03	0	43,90,90	1.54	8 (18%)
4	FEC	A	1005[B]	1	34,56,56	1.04	0	43,90,90	1.70	8 (18%)
3	SO4	B	1201	-	4,4,4	3.09	2 (50%)	6,6,6	0.93	0
3	SO4	C	1302	-	4,4,4	3.11	2 (50%)	6,6,6	0.97	0
3	SO4	C	1304	-	4,4,4	3.28	2 (50%)	6,6,6	0.94	0
4	FEC	C	1305[A]	1	34,56,56	1.05	0	43,90,90	1.51	8 (18%)
4	FEC	C	1305[B]	1	34,56,56	1.05	0	43,90,90	1.61	9 (20%)
3	SO4	D	1401	-	4,4,4	3.28	2 (50%)	6,6,6	0.94	0
3	SO4	E	1404	-	4,4,4	3.13	2 (50%)	6,6,6	0.96	0
3	SO4	E	1501	-	4,4,4	3.15	2 (50%)	6,6,6	1.02	0
3	SO4	F	1601	-	4,4,4	3.33	2 (50%)	6,6,6	0.90	0
3	SO4	F	1603	-	4,4,4	3.18	2 (50%)	6,6,6	0.94	0
4	FEC	F	1604[A]	1	34,56,56	1.03	0	43,90,90	1.62	6 (13%)
4	FEC	F	1604[B]	1	34,56,56	1.03	0	43,90,90	1.65	6 (13%)
3	SO4	G	1701	-	4,4,4	3.55	2 (50%)	6,6,6	1.00	0
3	SO4	G	1703	-	4,4,4	3.32	2 (50%)	6,6,6	1.02	0
4	FEC	G	1704[A]	1	34,56,56	1.06	0	43,90,90	1.52	9 (20%)
4	FEC	G	1704[B]	1	34,56,56	1.07	0	43,90,90	1.68	9 (20%)
3	SO4	H	1801	-	4,4,4	3.05	2 (50%)	6,6,6	0.95	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	H	1802	-	4,4,4	3.18	2 (50%)	6,6,6	0.98	0
3	SO4	I	1804	-	4,4,4	3.36	2 (50%)	6,6,6	0.97	0
3	SO4	I	1901	-	4,4,4	3.24	2 (50%)	6,6,6	1.00	0
3	SO4	I	1902	-	4,4,4	3.37	2 (50%)	6,6,6	0.97	0
4	FEC	I	1903[A]	1	34,56,56	1.06	0	43,90,90	1.54	6 (13%)
4	FEC	I	1903[B]	1	34,56,56	1.05	0	43,90,90	1.51	6 (13%)
3	SO4	J	2001	-	4,4,4	3.08	2 (50%)	6,6,6	0.94	0
3	SO4	J	2004	-	4,4,4	3.23	2 (50%)	6,6,6	1.00	0
3	SO4	K	1604	-	4,4,4	3.18	2 (50%)	6,6,6	0.94	0
3	SO4	K	2101	-	4,4,4	3.21	2 (50%)	6,6,6	1.05	0
3	SO4	K	2102	-	4,4,4	3.19	2 (50%)	6,6,6	0.95	0
3	SO4	K	2103	-	4,4,4	3.17	2 (50%)	6,6,6	1.04	0
4	FEC	K	2104[A]	1	34,56,56	1.06	1 (2%)	43,90,90	1.64	8 (18%)
4	FEC	K	2104[B]	1	34,56,56	1.06	0	43,90,90	1.57	5 (11%)
3	SO4	L	2201	-	4,4,4	3.16	2 (50%)	6,6,6	0.92	0
3	SO4	L	2204	1	4,4,4	3.20	2 (50%)	6,6,6	0.95	0
3	SO4	M	2301	-	4,4,4	3.16	2 (50%)	6,6,6	0.96	0
3	SO4	M	2302	-	4,4,4	3.25	2 (50%)	6,6,6	0.93	0
3	SO4	M	2303	-	4,4,4	3.19	2 (50%)	6,6,6	0.92	0
3	SO4	N	1204	-	4,4,4	3.31	2 (50%)	6,6,6	1.02	0
3	SO4	N	2401	-	4,4,4	3.20	2 (50%)	6,6,6	0.92	0
3	SO4	N	2402	-	4,4,4	3.31	2 (50%)	6,6,6	1.02	0
4	FEC	N	2403[A]	1	34,56,56	1.04	0	43,90,90	1.48	7 (16%)
4	FEC	N	2403[B]	1	34,56,56	1.09	0	43,90,90	1.59	11 (25%)
3	SO4	O	2501	-	4,4,4	3.09	2 (50%)	6,6,6	0.99	0
4	FEC	O	2502[A]	1	34,56,56	1.02	0	43,90,90	1.56	9 (20%)
4	FEC	O	2502[B]	1	34,56,56	1.04	0	43,90,90	1.57	7 (16%)
3	SO4	P	2601	-	4,4,4	3.15	2 (50%)	6,6,6	0.98	0
5	GOL	P	2615	-	5,5,5	4.80	5 (100%)	5,5,5	4.76	3 (60%)

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	1004	-	-	0/0/0/0	0/0/0/0
4	FEC	A	1005[A]	1	-	0/12/100/100	0/0/8/8
4	FEC	A	1005[B]	1	-	0/12/100/100	0/0/8/8
3	SO4	B	1201	-	-	0/0/0/0	0/0/0/0
3	SO4	C	1302	-	-	0/0/0/0	0/0/0/0
3	SO4	C	1304	-	-	0/0/0/0	0/0/0/0
4	FEC	C	1305[A]	1	-	0/12/100/100	0/0/8/8
4	FEC	C	1305[B]	1	-	0/12/100/100	0/0/8/8
3	SO4	D	1401	-	-	0/0/0/0	0/0/0/0
3	SO4	E	1404	-	-	0/0/0/0	0/0/0/0
3	SO4	E	1501	-	-	0/0/0/0	0/0/0/0
3	SO4	F	1601	-	-	0/0/0/0	0/0/0/0
3	SO4	F	1603	-	-	0/0/0/0	0/0/0/0
4	FEC	F	1604[A]	1	-	0/12/100/100	0/0/8/8
4	FEC	F	1604[B]	1	-	0/12/100/100	0/0/8/8
3	SO4	G	1701	-	-	0/0/0/0	0/0/0/0
3	SO4	G	1703	-	-	0/0/0/0	0/0/0/0
4	FEC	G	1704[A]	1	-	0/12/100/100	0/0/8/8
4	FEC	G	1704[B]	1	-	0/12/100/100	0/0/8/8
3	SO4	H	1801	-	-	0/0/0/0	0/0/0/0
3	SO4	H	1802	-	-	0/0/0/0	0/0/0/0
3	SO4	I	1804	-	-	0/0/0/0	0/0/0/0
3	SO4	I	1901	-	-	0/0/0/0	0/0/0/0
3	SO4	I	1902	-	-	0/0/0/0	0/0/0/0
4	FEC	I	1903[A]	1	-	0/12/100/100	0/0/8/8
4	FEC	I	1903[B]	1	-	0/12/100/100	0/0/8/8
3	SO4	J	2001	-	-	0/0/0/0	0/0/0/0
3	SO4	J	2004	-	-	0/0/0/0	0/0/0/0
3	SO4	K	1604	-	-	0/0/0/0	0/0/0/0
3	SO4	K	2101	-	-	0/0/0/0	0/0/0/0
3	SO4	K	2102	-	-	0/0/0/0	0/0/0/0
3	SO4	K	2103	-	-	0/0/0/0	0/0/0/0
4	FEC	K	2104[A]	1	-	0/12/100/100	0/0/8/8
4	FEC	K	2104[B]	1	-	0/12/100/100	0/0/8/8
3	SO4	L	2201	-	-	0/0/0/0	0/0/0/0
3	SO4	L	2204	1	-	0/0/0/0	0/0/0/0
3	SO4	M	2301	-	-	0/0/0/0	0/0/0/0
3	SO4	M	2302	-	-	0/0/0/0	0/0/0/0
3	SO4	M	2303	-	-	0/0/0/0	0/0/0/0
3	SO4	N	1204	-	-	0/0/0/0	0/0/0/0
3	SO4	N	2401	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	N	2402	-	-	0/0/0/0	0/0/0/0
4	FEC	N	2403[A]	1	-	0/12/100/100	0/0/8/8
4	FEC	N	2403[B]	1	-	0/12/100/100	0/0/8/8
3	SO4	O	2501	-	-	0/0/0/0	0/0/0/0
4	FEC	O	2502[A]	1	-	0/12/100/100	0/0/8/8
4	FEC	O	2502[B]	1	-	0/12/100/100	0/0/8/8
3	SO4	P	2601	-	-	0/0/0/0	0/0/0/0
5	GOL	P	2615	-	-	0/4/4/4	0/0/0/0

All (74) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	P	2615	GOL	C3-C2	-7.99	1.21	1.52
3	I	1902	SO4	O3-S	-4.49	1.31	1.47
3	I	1804	SO4	O3-S	-4.49	1.31	1.47
3	A	1001	SO4	O3-S	-4.07	1.32	1.47
3	I	1901	SO4	O3-S	-4.07	1.32	1.47
3	J	2004	SO4	O3-S	-4.07	1.32	1.47
3	M	2301	SO4	O3-S	-4.00	1.33	1.47
3	K	2101	SO4	O3-S	-3.99	1.33	1.47
3	F	1601	SO4	O3-S	-3.96	1.33	1.47
3	C	1304	SO4	O3-S	-3.89	1.33	1.47
3	D	1401	SO4	O3-S	-3.89	1.33	1.47
3	K	2103	SO4	O3-S	-3.85	1.33	1.47
3	L	2201	SO4	O3-S	-3.85	1.33	1.47
3	H	1801	SO4	O3-S	-3.83	1.33	1.47
3	G	1701	SO4	O3-S	-3.82	1.33	1.47
3	P	2601	SO4	O3-S	-3.82	1.33	1.47
3	N	2401	SO4	O3-S	-3.81	1.33	1.47
3	N	1204	SO4	O3-S	-3.80	1.33	1.47
3	O	2501	SO4	O3-S	-3.80	1.33	1.47
3	M	2303	SO4	O3-S	-3.79	1.33	1.47
3	G	1703	SO4	O3-S	-3.79	1.33	1.47
3	N	2402	SO4	O3-S	-3.78	1.33	1.47
3	L	2204	SO4	O3-S	-3.71	1.34	1.47
3	K	2102	SO4	O3-S	-3.70	1.34	1.47
3	F	1603	SO4	O3-S	-3.68	1.34	1.47
3	E	1501	SO4	O3-S	-3.67	1.34	1.47
3	K	1604	SO4	O3-S	-3.67	1.34	1.47
3	A	1004	SO4	O3-S	-3.66	1.34	1.47
3	H	1802	SO4	O3-S	-3.66	1.34	1.47
3	B	1201	SO4	O3-S	-3.65	1.34	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1302	SO4	O3-S	-3.59	1.34	1.47
3	M	2302	SO4	O3-S	-3.57	1.34	1.47
3	A	1003	SO4	O3-S	-3.56	1.34	1.47
3	E	1404	SO4	O3-S	-3.56	1.34	1.47
3	J	2001	SO4	O3-S	-3.53	1.34	1.47
5	P	2615	GOL	C1-C2	-3.15	1.40	1.52
5	P	2615	GOL	O2-C2	-2.96	1.34	1.43
4	K	2104[A]	FEC	CMB-C2B	2.02	1.55	1.50
5	P	2615	GOL	O3-C3	3.58	1.57	1.42
5	P	2615	GOL	O1-C1	4.44	1.61	1.42
3	A	1001	SO4	O1-S	4.52	1.62	1.47
3	H	1801	SO4	O1-S	4.74	1.63	1.47
3	O	2501	SO4	O1-S	4.84	1.63	1.47
3	I	1804	SO4	O1-S	4.87	1.63	1.47
3	I	1902	SO4	O1-S	4.89	1.63	1.47
3	M	2301	SO4	O1-S	4.89	1.63	1.47
3	A	1004	SO4	O1-S	4.97	1.64	1.47
3	B	1201	SO4	O1-S	4.98	1.64	1.47
3	L	2201	SO4	O1-S	4.99	1.64	1.47
3	J	2004	SO4	O1-S	5.00	1.64	1.47
3	P	2601	SO4	O1-S	5.00	1.64	1.47
3	K	2101	SO4	O1-S	5.00	1.64	1.47
3	J	2001	SO4	O1-S	5.01	1.64	1.47
3	I	1901	SO4	O1-S	5.01	1.64	1.47
3	C	1302	SO4	O1-S	5.02	1.64	1.47
3	K	2103	SO4	O1-S	5.03	1.64	1.47
3	M	2303	SO4	O1-S	5.12	1.64	1.47
3	E	1501	SO4	O1-S	5.13	1.64	1.47
3	N	2401	SO4	O1-S	5.13	1.64	1.47
3	E	1404	SO4	O1-S	5.14	1.64	1.47
3	F	1603	SO4	O1-S	5.17	1.64	1.47
3	K	1604	SO4	O1-S	5.17	1.64	1.47
3	K	2102	SO4	O1-S	5.17	1.64	1.47
3	L	2204	SO4	O1-S	5.19	1.64	1.47
3	H	1802	SO4	O1-S	5.21	1.65	1.47
3	C	1304	SO4	O1-S	5.23	1.65	1.47
3	D	1401	SO4	O1-S	5.24	1.65	1.47
3	F	1601	SO4	O1-S	5.30	1.65	1.47
3	N	1204	SO4	O1-S	5.43	1.65	1.47
3	M	2302	SO4	O1-S	5.43	1.65	1.47
3	A	1003	SO4	O1-S	5.44	1.65	1.47
3	N	2402	SO4	O1-S	5.44	1.65	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	1703	SO4	O1-S	5.44	1.65	1.47
3	G	1701	SO4	O1-S	5.98	1.67	1.47

All (125) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	2104[B]	FEC	CAA-C3A-C4A	-4.99	121.59	127.01
4	K	2104[A]	FEC	CAA-C3A-C4A	-4.47	122.16	127.01
4	A	1005[B]	FEC	CAA-C3A-C4A	-4.16	122.49	127.01
4	G	1704[B]	FEC	CAA-C3A-C4A	-3.92	122.75	127.01
4	F	1604[A]	FEC	CAA-C3A-C4A	-3.83	122.85	127.01
4	N	2403[A]	FEC	CAA-C3A-C4A	-3.76	122.92	127.01
4	C	1305[A]	FEC	CAA-C3A-C4A	-3.75	122.94	127.01
4	N	2403[B]	FEC	CAA-C3A-C4A	-3.72	122.96	127.01
4	K	2104[A]	FEC	CMC-C3C-C4C	-3.66	122.31	128.36
4	G	1704[B]	FEC	CMC-C3C-C4C	-3.63	122.36	128.36
4	O	2502[B]	FEC	CMC-C3C-C4C	-3.59	122.43	128.36
4	I	1903[B]	FEC	CAA-C3A-C4A	-3.53	123.18	127.01
4	C	1305[B]	FEC	CMC-C3C-C4C	-3.52	122.55	128.36
4	O	2502[B]	FEC	CAA-C3A-C4A	-3.50	123.21	127.01
4	A	1005[A]	FEC	CAA-C3A-C4A	-3.44	123.28	127.01
4	O	2502[A]	FEC	CAA-C3A-C4A	-3.40	123.31	127.01
4	I	1903[A]	FEC	CAA-C3A-C4A	-3.40	123.32	127.01
4	N	2403[B]	FEC	CAC-C2C-C1C	-3.39	123.33	127.01
4	A	1005[A]	FEC	CMC-C3C-C4C	-3.34	122.83	128.36
4	F	1604[B]	FEC	CMC-C3C-C4C	-3.34	122.84	128.36
4	G	1704[A]	FEC	CAA-C3A-C4A	-3.33	123.39	127.01
4	O	2502[A]	FEC	CMC-C3C-C4C	-3.28	122.94	128.36
4	O	2502[B]	FEC	CAC-C2C-C1C	-3.22	123.51	127.01
4	G	1704[A]	FEC	CMC-C3C-C4C	-3.14	123.17	128.36
4	A	1005[B]	FEC	CMC-C3C-C4C	-3.05	123.31	128.36
4	I	1903[A]	FEC	CMC-C3C-C4C	-3.03	123.35	128.36
4	C	1305[B]	FEC	CAA-C3A-C4A	-3.01	123.74	127.01
4	I	1903[B]	FEC	CMC-C3C-C4C	-2.88	123.60	128.36
4	N	2403[A]	FEC	CMC-C3C-C4C	-2.86	123.63	128.36
4	F	1604[A]	FEC	CMC-C3C-C4C	-2.78	123.77	128.36
4	N	2403[B]	FEC	CMC-C3C-C4C	-2.78	123.77	128.36
4	C	1305[A]	FEC	CMC-C3C-C4C	-2.63	124.00	128.36
4	K	2104[B]	FEC	CMC-C3C-C4C	-2.57	124.11	128.36
4	C	1305[B]	FEC	C4C-CHD-C1D	-2.48	123.94	129.26
4	N	2403[B]	FEC	C4C-CHD-C1D	-2.43	124.03	129.26
4	F	1604[B]	FEC	CAA-C3A-C4A	-2.39	124.42	127.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	1604[A]	FEC	C4C-CHD-C1D	-2.37	124.17	129.26
4	N	2403[A]	FEC	C4C-CHD-C1D	-2.33	124.26	129.26
4	G	1704[A]	FEC	CAC-C2C-C1C	-2.32	124.49	127.01
4	G	1704[A]	FEC	C4C-CHD-C1D	-2.27	124.40	129.26
4	O	2502[A]	FEC	C4C-CHD-C1D	-2.26	124.41	129.26
4	F	1604[B]	FEC	C4C-CHD-C1D	-2.24	124.45	129.26
4	N	2403[B]	FEC	CAB-C3B-C4B	-2.21	120.62	124.58
4	N	2403[B]	FEC	C1C-CHC-C4B	-2.21	124.52	129.26
4	K	2104[B]	FEC	C4C-CHD-C1D	-2.21	124.53	129.26
4	O	2502[B]	FEC	C4C-CHD-C1D	-2.20	124.54	129.26
4	I	1903[B]	FEC	CAC-C2C-C1C	-2.18	124.64	127.01
4	G	1704[B]	FEC	CMB-C2B-C1B	-2.16	121.68	125.02
4	G	1704[B]	FEC	C4C-CHD-C1D	-2.15	124.64	129.26
4	A	1005[A]	FEC	C4C-CHD-C1D	-2.13	124.69	129.26
4	K	2104[A]	FEC	C4C-CHD-C1D	-2.11	124.74	129.26
4	O	2502[A]	FEC	C1C-CHC-C4B	-2.09	124.78	129.26
4	A	1005[A]	FEC	C1C-CHC-C4B	-2.07	124.83	129.26
4	I	1903[A]	FEC	C4C-CHD-C1D	-2.04	124.88	129.26
4	C	1305[A]	FEC	C4C-CHD-C1D	-2.02	124.92	129.26
4	K	2104[B]	FEC	CAD-CBD-CGD	2.00	116.41	112.75
4	O	2502[A]	FEC	CAB-CBB-CGB	2.04	116.48	112.75
4	A	1005[A]	FEC	CBA-CAA-C3A	2.04	116.19	112.53
4	G	1704[A]	FEC	CMC-C3C-C2C	2.05	129.52	125.24
4	A	1005[B]	FEC	CAA-CBA-CGA	2.07	116.54	112.75
4	N	2403[B]	FEC	C1A-CHA-C4D	2.09	125.76	122.60
4	O	2502[B]	FEC	CBA-CAA-C3A	2.09	116.28	112.53
4	A	1005[B]	FEC	C1A-CHA-C4D	2.10	125.78	122.60
4	C	1305[B]	FEC	C1A-CHA-C4D	2.11	125.80	122.60
4	O	2502[A]	FEC	CMC-C3C-C2C	2.12	129.66	125.24
4	N	2403[A]	FEC	CMA-C2A-C3A	2.15	129.74	125.24
4	N	2403[B]	FEC	CAB-C3B-C2B	2.16	131.79	128.01
4	A	1005[A]	FEC	CMC-C3C-C2C	2.17	129.77	125.24
4	A	1005[A]	FEC	CAD-CBD-CGD	2.17	116.73	112.75
4	K	2104[A]	FEC	CMA-C2A-C3A	2.19	129.81	125.24
4	C	1305[A]	FEC	CMA-C2A-C3A	2.19	129.82	125.24
4	K	2104[A]	FEC	CMC-C3C-C2C	2.24	129.92	125.24
4	F	1604[A]	FEC	CAB-CBB-CGB	2.27	116.91	112.75
4	N	2403[A]	FEC	CAB-CBB-CGB	2.28	116.93	112.75
4	C	1305[A]	FEC	CBA-CAA-C3A	2.32	116.69	112.53
4	O	2502[B]	FEC	CMC-C3C-C2C	2.32	130.09	125.24
4	N	2403[B]	FEC	CAA-CBA-CGA	2.34	117.04	112.75
4	G	1704[A]	FEC	CAB-CBB-CGB	2.35	117.05	112.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	2104[A]	FEC	CAA-CBA-CGA	2.40	117.14	112.75
4	C	1305[B]	FEC	CAA-CBA-CGA	2.41	117.17	112.75
4	N	2403[B]	FEC	CBC-CAC-C2C	2.42	116.87	112.53
4	G	1704[B]	FEC	CAA-CBA-CGA	2.43	117.19	112.75
4	C	1305[B]	FEC	CMC-C3C-C2C	2.44	130.33	125.24
4	N	2403[A]	FEC	CBA-CAA-C3A	2.47	116.96	112.53
4	G	1704[B]	FEC	CMC-C3C-C2C	2.48	130.43	125.24
4	C	1305[A]	FEC	CAB-CBB-CGB	2.49	117.31	112.75
4	K	2104[A]	FEC	CAB-CBB-CGB	2.50	117.33	112.75
4	G	1704[A]	FEC	CAA-CBA-CGA	2.52	117.37	112.75
4	O	2502[A]	FEC	CBA-CAA-C3A	2.54	117.08	112.53
4	C	1305[A]	FEC	CAD-CBD-CGD	2.54	117.41	112.75
4	C	1305[B]	FEC	CAB-CBB-CGB	2.55	117.43	112.75
4	O	2502[A]	FEC	CAD-CBD-CGD	2.61	117.53	112.75
4	G	1704[B]	FEC	CAD-CBD-CGD	2.63	117.56	112.75
4	A	1005[B]	FEC	CAC-CBC-CGC	2.68	117.67	112.75
4	F	1604[B]	FEC	CAB-CBB-CGB	2.85	117.97	112.75
4	I	1903[B]	FEC	CBA-CAA-C3A	2.85	117.64	112.53
4	N	2403[B]	FEC	CBA-CAA-C3A	2.85	117.64	112.53
5	P	2615	GOL	O1-C1-C2	2.98	124.62	110.18
4	I	1903[A]	FEC	CBA-CAA-C3A	3.00	117.90	112.53
4	F	1604[A]	FEC	CBA-CAA-C3A	3.07	118.04	112.53
4	G	1704[A]	FEC	CBA-CAA-C3A	3.08	118.04	112.53
4	F	1604[B]	FEC	CBA-CAA-C3A	3.16	118.19	112.53
4	I	1903[B]	FEC	CAB-CBB-CGB	3.20	118.62	112.75
4	G	1704[B]	FEC	CAB-CBB-CGB	3.22	118.65	112.75
4	I	1903[A]	FEC	CAB-CBB-CGB	3.23	118.67	112.75
4	A	1005[B]	FEC	CAB-CBB-CGB	3.56	119.28	112.75
4	A	1005[B]	FEC	CBA-CAA-C3A	3.60	118.98	112.53
4	G	1704[A]	FEC	CBC-CAC-C2C	3.95	119.61	112.53
4	N	2403[A]	FEC	CBC-CAC-C2C	3.95	119.61	112.53
4	I	1903[B]	FEC	CBC-CAC-C2C	4.03	119.76	112.53
4	C	1305[B]	FEC	CBC-CAC-C2C	4.09	119.86	112.53
4	C	1305[B]	FEC	CBA-CAA-C3A	4.14	119.95	112.53
4	I	1903[A]	FEC	CBC-CAC-C2C	4.46	120.53	112.53
4	O	2502[B]	FEC	CBC-CAC-C2C	4.59	120.76	112.53
4	G	1704[B]	FEC	CBC-CAC-C2C	4.83	121.18	112.53
4	C	1305[A]	FEC	CBC-CAC-C2C	4.86	121.25	112.53
4	A	1005[A]	FEC	CBC-CAC-C2C	5.02	121.52	112.53
4	A	1005[B]	FEC	CBC-CAC-C2C	5.11	121.70	112.53
4	O	2502[A]	FEC	CBC-CAC-C2C	5.16	121.78	112.53
4	K	2104[B]	FEC	CBC-CAC-C2C	5.24	121.92	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	2104[A]	FEC	CBC-CAC-C2C	5.38	122.17	112.53
5	P	2615	GOL	O2-C2-C3	6.18	137.00	108.65
4	F	1604[A]	FEC	CBC-CAC-C2C	6.41	124.01	112.53
4	F	1604[B]	FEC	CBC-CAC-C2C	6.75	124.63	112.53
5	P	2615	GOL	O3-C3-C2	8.11	149.53	110.18

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

29 monomers are involved in 182 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1005[A]	FEC	9	0
4	A	1005[B]	FEC	8	0
3	C	1302	SO4	1	0
4	C	1305[A]	FEC	8	0
4	C	1305[B]	FEC	9	0
3	D	1401	SO4	1	0
3	E	1404	SO4	0	1
4	F	1604[A]	FEC	8	0
4	F	1604[B]	FEC	10	0
3	G	1701	SO4	1	0
4	G	1704[A]	FEC	8	0
4	G	1704[B]	FEC	7	0
3	H	1802	SO4	1	0
3	I	1804	SO4	4	0
4	I	1903[A]	FEC	12	0
4	I	1903[B]	FEC	11	0
3	J	2004	SO4	0	6
3	K	1604	SO4	1	0
4	K	2104[A]	FEC	10	0
4	K	2104[B]	FEC	7	0
3	L	2204	SO4	3	8
3	M	2302	SO4	1	0
3	N	1204	SO4	2	0
4	N	2403[A]	FEC	9	0
4	N	2403[B]	FEC	12	0
4	O	2502[A]	FEC	7	0
4	O	2502[B]	FEC	12	0
3	P	2601	SO4	1	0
5	P	2615	GOL	4	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, 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	170/179 (94%)	-0.16	6 (3%)	48	61	17, 26, 40, 66	0
1	B	170/179 (94%)	-0.32	5 (2%)	55	67	17, 25, 40, 55	0
1	C	170/179 (94%)	-0.19	6 (3%)	48	61	17, 26, 41, 85	0
1	D	170/179 (94%)	-0.11	7 (4%)	41	55	17, 26, 40, 55	0
1	E	170/179 (94%)	-0.19	4 (2%)	62	74	17, 26, 40, 57	0
1	F	171/179 (95%)	-0.25	6 (3%)	48	61	17, 26, 43, 76	0
1	G	169/179 (94%)	-0.27	4 (2%)	62	74	17, 25, 40, 55	0
1	H	170/179 (94%)	-0.27	5 (2%)	55	67	17, 26, 41, 55	0
1	I	170/179 (94%)	-0.25	2 (1%)	81	89	17, 25, 40, 55	0
1	J	170/179 (94%)	-0.24	4 (2%)	62	74	17, 26, 41, 55	0
1	K	169/179 (94%)	-0.26	2 (1%)	81	89	17, 26, 41, 55	0
1	L	170/179 (94%)	-0.15	2 (1%)	81	89	17, 26, 39, 55	0
1	M	169/179 (94%)	-0.26	4 (2%)	62	74	17, 25, 40, 55	0
1	N	170/179 (94%)	-0.30	2 (1%)	81	89	17, 25, 38, 55	0
1	O	169/179 (94%)	-0.15	5 (2%)	54	66	17, 25, 41, 74	0
1	P	170/179 (94%)	-0.29	4 (2%)	62	74	17, 26, 41, 55	0
All	All	2717/2864 (94%)	-0.23	68 (2%)	61	73	17, 26, 41, 85	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	166	THR	6.0
1	A	166	THR	5.7
1	N	166	THR	5.5
1	E	166	THR	4.9
1	O	166	THR	4.8

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Mol	Chain	Res	Type	RSRZ
1	O	173	THR	4.8
1	J	3	GLY	4.7
1	F	3	GLY	4.6
1	J	166	THR	4.3
1	D	7	ASP	4.2
1	I	166	THR	4.2
1	H	166	THR	4.1
1	D	166	THR	4.1
1	A	3	GLY	4.0
1	F	166	THR	4.0
1	G	168	SER	3.7
1	F	2	ALA	3.5
1	D	4	ASN	3.4
1	A	168	SER	3.3
1	C	167	ALA	3.3
1	K	166	THR	3.3
1	E	3	GLY	3.3
1	M	168	SER	3.3
1	E	4	ASN	3.3
1	C	168	SER	3.2
1	M	166	THR	3.2
1	C	4	ASN	3.1
1	J	168	SER	3.1
1	L	168	SER	3.1
1	P	166	THR	3.1
1	G	166	THR	3.1
1	C	3	GLY	3.1
1	C	7	ASP	3.0
1	D	3	GLY	3.0
1	H	4	ASN	2.9
1	A	165	GLY	2.9
1	B	168	SER	2.9
1	L	166	THR	2.9
1	D	167	ALA	2.8
1	D	168	SER	2.7
1	H	168	SER	2.7
1	M	165	GLY	2.7
1	J	4	ASN	2.7
1	I	168	SER	2.6
1	H	7	ASP	2.6
1	K	168	SER	2.6
1	E	168	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	168	SER	2.5
1	A	27	ILE	2.5
1	N	3	GLY	2.4
1	B	166	THR	2.4
1	D	10	ALA	2.4
1	O	168	SER	2.4
1	B	167	ALA	2.4
1	B	169	LYS	2.4
1	O	90	VAL	2.3
1	P	168	SER	2.3
1	A	167	ALA	2.2
1	F	7	ASP	2.2
1	F	4	ASN	2.1
1	G	167	ALA	2.1
1	B	4	ASN	2.1
1	G	81	LYS	2.1
1	H	27	ILE	2.1
1	O	27	ILE	2.1
1	P	6	GLU	2.0
1	M	4	ASN	2.0
1	P	79	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	SO4	G	1701	5/5	0.78	0.31	5.30	74,74,74,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	SO4	J	2001	5/5	0.91	0.17	2.31	66,67,67,69	0
5	GOL	P	2615	6/6	0.89	0.21	2.01	27,31,47,67	0
3	SO4	O	2501	5/5	0.85	0.21	1.97	70,70,71,71	0
3	SO4	E	1501	5/5	0.92	0.22	1.74	67,68,68,68	0
3	SO4	H	1801	5/5	0.91	0.21	1.72	54,54,55,56	0
3	SO4	N	2401	5/5	0.90	0.17	1.37	62,63,63,63	0
3	SO4	P	2601	5/5	0.91	0.19	1.14	62,62,63,63	0
4	FEC	F	1604[B]	49/49	0.95	0.19	1.09	17,19,26,27	49
3	SO4	I	1901	5/5	0.91	0.18	0.99	61,61,62,63	0
3	SO4	F	1601	5/5	0.87	0.24	0.86	66,66,67,67	0
3	SO4	D	1401	5/5	0.89	0.16	0.77	58,59,60,60	0
4	FEC	K	2104[B]	49/49	0.96	0.20	0.70	10,19,26,27	49
4	FEC	G	1704[B]	49/49	0.96	0.21	0.69	10,19,26,27	49
4	FEC	F	1604[A]	49/49	0.95	0.19	0.66	16,19,26,27	49
4	FEC	G	1704[A]	49/49	0.96	0.21	0.64	16,19,26,27	49
4	FEC	N	2403[B]	49/49	0.96	0.20	0.59	11,19,24,29	49
3	SO4	L	2201	5/5	0.91	0.17	0.58	64,64,65,65	0
4	FEC	N	2403[A]	49/49	0.96	0.20	0.58	16,19,26,27	49
3	SO4	K	2101	5/5	0.93	0.17	0.57	51,53,53,54	0
4	FEC	K	2104[A]	49/49	0.96	0.20	0.54	16,19,25,27	49
4	FEC	O	2502[B]	49/49	0.97	0.18	0.46	15,19,25,32	49
4	FEC	O	2502[A]	49/49	0.97	0.18	0.42	16,19,26,28	49
4	FEC	C	1305[B]	49/49	0.96	0.18	0.31	13,20,25,31	49
4	FEC	A	1005[B]	49/49	0.97	0.20	0.27	14,19,25,27	49
4	FEC	C	1305[A]	49/49	0.96	0.18	0.27	16,19,26,27	49
4	FEC	A	1005[A]	49/49	0.97	0.20	0.17	16,19,26,27	49
3	SO4	M	2301	5/5	0.94	0.15	0.13	51,51,52,53	0
4	FEC	I	1903[A]	49/49	0.97	0.18	0.05	16,19,26,28	49
4	FEC	I	1903[B]	49/49	0.97	0.18	0.01	16,19,26,29	49
3	SO4	B	1201	5/5	0.93	0.14	-0.05	66,66,67,67	0
3	SO4	A	1001	5/5	0.96	0.15	-0.18	53,54,54,55	0
3	SO4	I	1902	5/5	0.96	0.13	-1.62	36,37,38,38	0
2	FE	D	200	1/1	0.97	0.05	-2.12	33,33,33,33	0
2	FE	N	200	1/1	0.97	0.06	-2.21	28,28,28,28	0
2	FE	K	200	1/1	0.99	0.05	-2.44	29,29,29,29	0
2	FE	M	200	1/1	0.99	0.06	-2.54	27,27,27,27	0
2	FE	L	200	1/1	0.99	0.06	-2.56	29,29,29,29	0
2	FE	I	200	1/1	1.00	0.06	-2.62	28,28,28,28	0
2	FE	A	200	1/1	0.99	0.03	-2.67	30,30,30,30	0
2	FE	H	200	1/1	0.99	0.05	-3.14	28,28,28,28	0
2	FE	C	200	1/1	0.99	0.04	-3.32	32,32,32,32	0
2	FE	O	200	1/1	0.98	0.04	-4.00	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	FE	G	200	1/1	0.99	0.03	-4.08	29,29,29,29	0
2	FE	J	200	1/1	0.99	0.04	-4.23	30,30,30,30	0
2	FE	B	200	1/1	0.99	0.04	-4.73	28,28,28,28	0
2	FE	E	200	1/1	0.99	0.02	-4.81	31,31,31,31	0
2	FE	F	200	1/1	0.97	0.03	-5.12	31,31,31,31	0
2	FE	P	200	1/1	0.99	0.04	-5.36	31,31,31,31	0
3	SO4	A	1004	5/5	0.97	0.12	-	66,66,67,67	5
3	SO4	N	1204	5/5	0.86	0.19	-	73,73,74,75	0
3	SO4	C	1302	5/5	0.93	0.35	-	73,73,73,75	0
3	SO4	I	1804	5/5	0.83	0.30	-	36,37,38,38	0
3	SO4	K	2102	5/5	0.88	0.18	-	78,78,78,79	0
3	SO4	F	1603	5/5	0.89	0.29	-	78,78,78,79	0
3	SO4	N	2402	5/5	0.91	0.32	-	73,73,74,75	0
3	SO4	G	1703	5/5	0.86	0.25	-	73,73,74,75	0
3	SO4	L	2204	5/5	0.95	0.37	-	78,78,78,79	1
3	SO4	C	1304	5/5	0.82	0.34	-	58,59,60,60	5
3	SO4	E	1404	5/5	0.89	0.22	-	65,65,67,67	0
3	SO4	J	2004	5/5	0.97	0.27	-	61,61,62,63	2
3	SO4	H	1802	5/5	0.84	0.37	-	72,72,73,73	0
3	SO4	M	2302	5/5	0.84	0.46	-	73,73,73,74	0
3	SO4	K	2103	5/5	0.79	0.23	-	69,69,69,71	0
3	SO4	K	1604	5/5	0.90	0.15	-	78,78,78,79	0
3	SO4	M	2303	5/5	0.82	0.40	-	62,63,63,63	0
3	SO4	A	1003	5/5	0.94	0.17	-	73,73,73,74	0

6.5 Other polymers [i](#)

There are no such residues in this entry.