Full wwPDB X-ray Structure Validation Report (i)

May 1, 2016 – 08:09 AM EDT

PDB ID	:	5CHC
Title	:	Crystal structure of the perchlorate reductase PcrAB - substrate analog SeO3 bound - from Azospira suillum PS
Authors	:	Tsai, C.-L.; Tainer, J.A.
Deposited on	:	2015-07-10
Resolution	:	2.38 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:

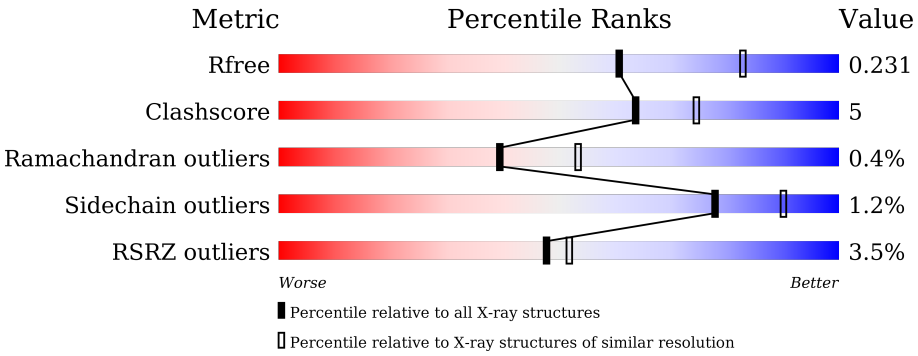
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027457
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027457

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 2.38 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	4019 (2.40-2.36)
Clashscore	102246	4595 (2.40-2.36)
Ramachandran outliers	100387	4520 (2.40-2.36)
Sidechain outliers	100360	4522 (2.40-2.36)
RSRZ outliers	91569	4034 (2.40-2.36)

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	899	2% 88% 12%
1	C	899	5% 87% 12%
1	E	899	4% 86% 12%
2	B	333	% 87% 10%
2	D	333	9% 79% 19%
2	F	333	% 88% 11%

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
10	NA	A	1015	-	-	-	X
10	NA	C	1011	-	-	-	X
10	NA	E	1010	-	-	-	X
13	GOL	E	1006	-	-	-	X
7	EDO	A	1005	-	-	-	X
7	EDO	A	1008	-	-	-	X
7	EDO	A	1009	-	-	-	X
7	EDO	A	1010	-	-	X	X
7	EDO	A	1012	-	-	-	X
7	EDO	A	1019	-	-	-	X
7	EDO	B	407	-	-	-	X
7	EDO	B	408	-	-	X	-
7	EDO	B	409	-	-	-	X
7	EDO	B	410	-	-	X	X
7	EDO	C	1005	-	-	-	X
7	EDO	C	1006	-	-	-	X
7	EDO	C	1007	-	-	-	X
7	EDO	E	1005	-	-	-	X
7	EDO	F	405	-	-	-	X
7	EDO	F	406	-	-	-	X
8	BSY	A	1013	-	-	X	-
8	BSY	C	1009	-	-	X	-
8	BSY	E	1008	-	-	X	-
9	SO3	A	1014	-	-	-	X

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 30958 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.

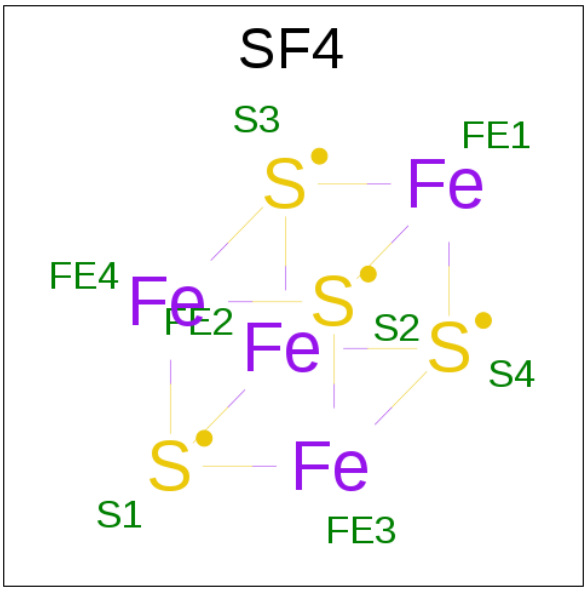
- Molecule 1 is a protein called DMSO reductase family type II enzyme, molybdopterin subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	895	Total	C	N	O	S	0	1	0
			7171	4579	1243	1311	38			
1	C	892	Total	C	N	O	S	0	0	0
			7148	4563	1240	1307	38			
1	E	892	Total	C	N	O	S	0	2	0
			7163	4575	1240	1310	38			

- Molecule 2 is a protein called DMSO reductase family type II enzyme, iron-sulfur subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	329	Total	C	N	O	S	0	0	0
			2564	1627	447	465	25			
2	D	328	Total	C	N	O	S	0	0	0
			2556	1622	446	464	24			
2	F	328	Total	C	N	O	S	0	0	0
			2556	1622	446	464	24			

- Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).

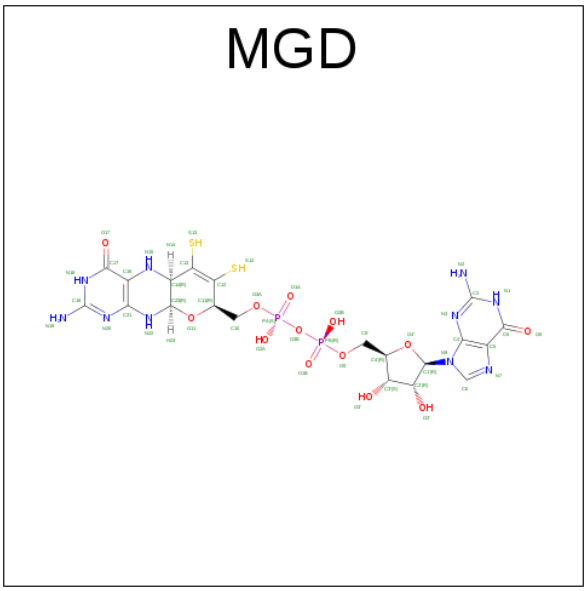


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Fe S 8 4 4	0	0
3	B	1	Total Fe S 8 4 4	0	0
3	B	1	Total Fe S 8 4 4	0	0
3	B	1	Total Fe S 8 4 4	0	0
3	C	1	Total Fe S 8 4 4	0	0
3	D	1	Total Fe S 8 4 4	0	0
3	D	1	Total Fe S 8 4 4	0	0
3	D	1	Total Fe S 8 4 4	0	0
3	E	1	Total Fe S 8 4 4	0	0
3	F	1	Total Fe S 8 4 4	0	0
3	F	1	Total Fe S 8 4 4	0	0
3	F	1	Total Fe S 8 4 4	0	0

- Molecule 4 is MOLYBDENUM ATOM (three-letter code: MO) (formula: Mo).

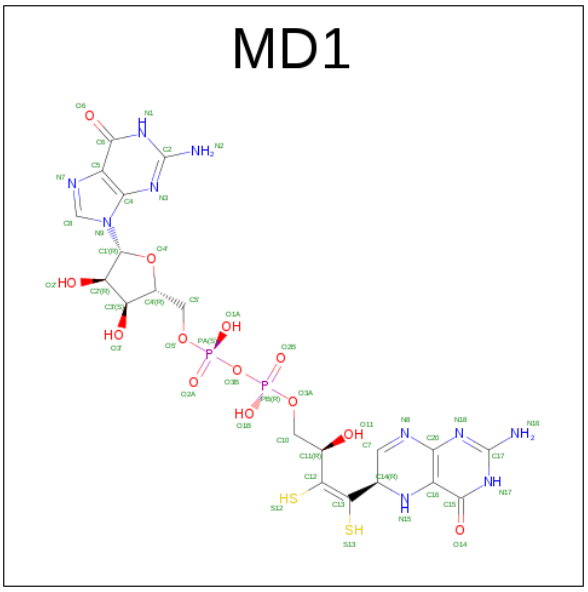
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mo 1 1	0	0
4	C	1	Total Mo 1 1	0	0
4	E	1	Total Mo 1 1	0	0

- Molecule 5 is 2-AMINO-5,6-DIMERCAPTO-7-METHYL-3,7,8A,9-TETRAHYDRO-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-4-ONE GUANOSINE DINUCLEOTIDE (three-letter code: MGD) (formula: $C_{20}H_{26}N_{10}O_{13}P_2S_2$).



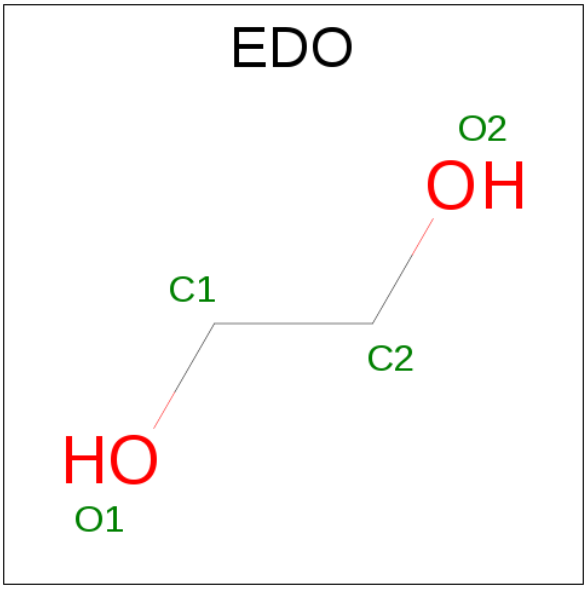
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O P S 47 20 10 13 2 2	0	0
5	C	1	Total C N O P S 47 20 10 13 2 2	0	0
5	E	1	Total C N O P S 47 20 10 13 2 2	0	0

- Molecule 6 is PHOSPHORIC ACID 4-(2-AMINO-4-OXO-3,4,5,6,-TETRAHYDRO-PTERIDIN-6-YL)-2-HYDROXY-3,4-DIMERCAPTO-BUT-3-EN-YL ESTER GUANYLATE ESTER (three-letter code: MD1) (formula: $C_{20}H_{26}N_{10}O_{13}P_2S_2$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
6	C	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
6	E	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		

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

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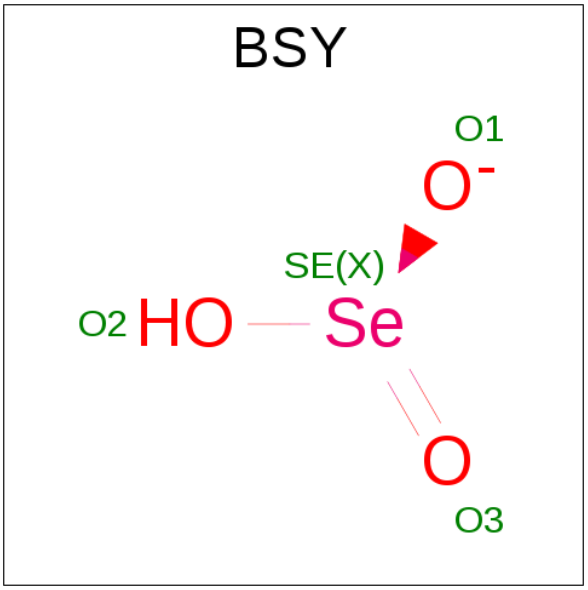
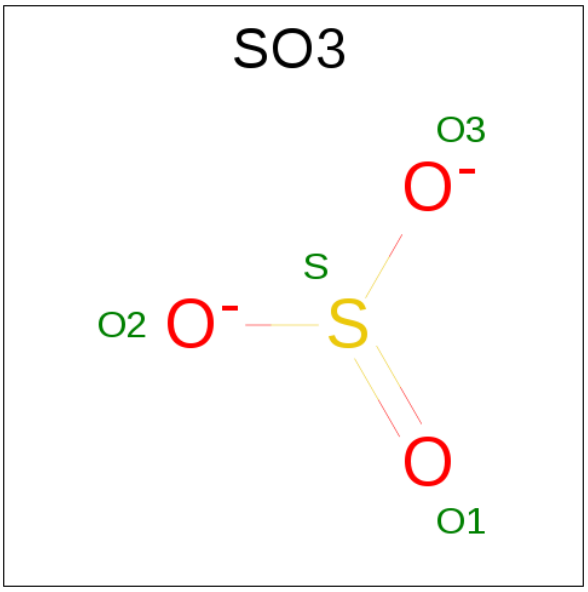
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	F	1	Total C O 4 2 2	0	0
7	F	1	Total C O 4 2 2	0	0

- Molecule 8 is BISELENITE ION (three-letter code: BSY) (formula: HO_3Se).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total O Se 4 3 1	0	0
8	C	1	Total O Se 4 3 1	0	0
8	E	1	Total O Se 4 3 1	0	0

- Molecule 9 is SULFITE ION (three-letter code: SO3) (formula: O_3S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total O S 4 3 1	0	0
9	C	1	Total O S 4 3 1	0	0
9	E	1	Total O S 4 3 1	0	0

- Molecule 10 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total Na 1 1	0	0
10	A	2	Total Na 2 2	0	0
10	C	2	Total Na 2 2	0	0
10	E	3	Total Na 3 3	0	0

- Molecule 11 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1	Total Zn 1 1	0	0
11	C	1	Total Zn 1 1	0	0

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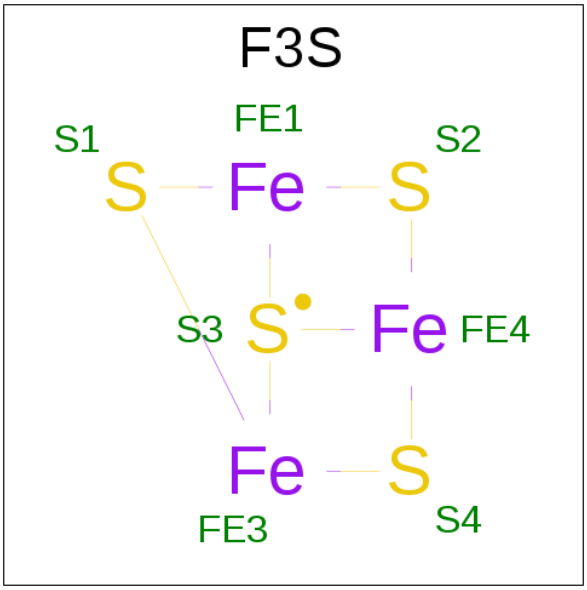
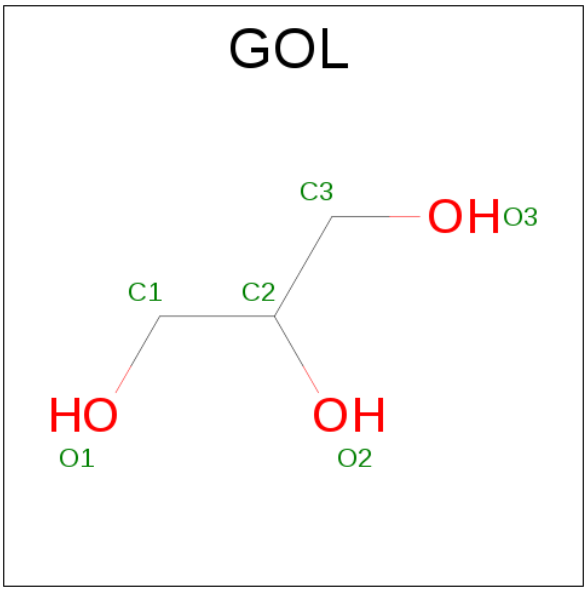
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	E	1	Total Zn 1 1	0	0

- Molecule 12 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	B	1	Total Fe S 7 3 4	0	0
12	D	1	Total Fe S 7 3 4	0	0
12	F	1	Total Fe S 7 3 4	0	0

- Molecule 13 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	E	1	Total C O 6 3 3	0	0

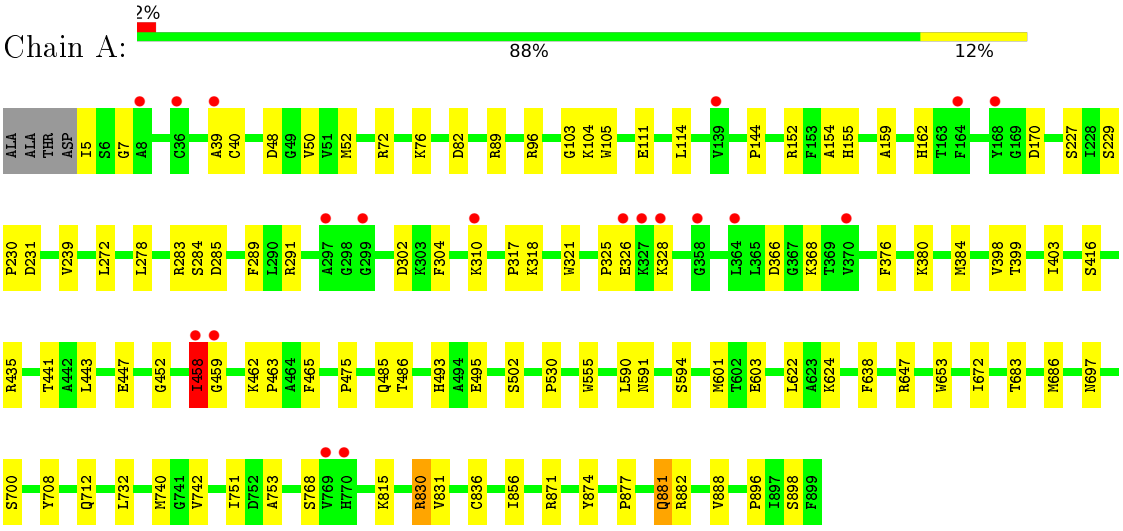
- Molecule 14 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	A	367	Total O 367 367	0	0
14	B	140	Total O 140 140	0	0
14	C	252	Total O 252 252	0	0
14	D	57	Total O 57 57	0	0
14	E	321	Total O 321 321	0	0
14	F	124	Total O 124 124	0	0

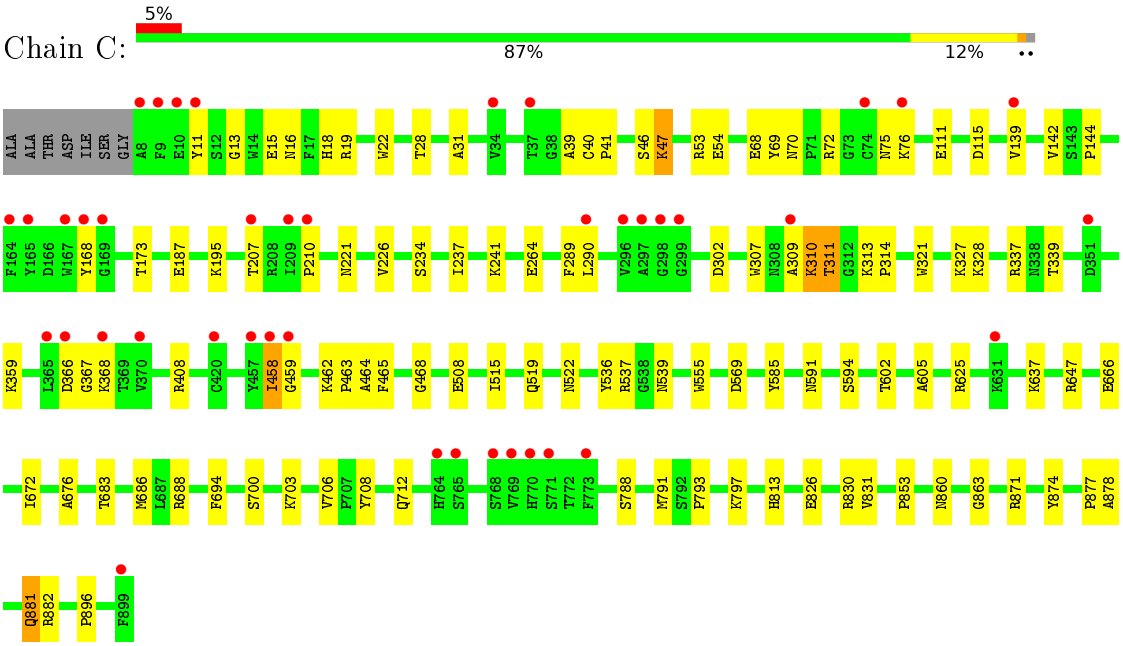
3 Residue-property plots (i)

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.

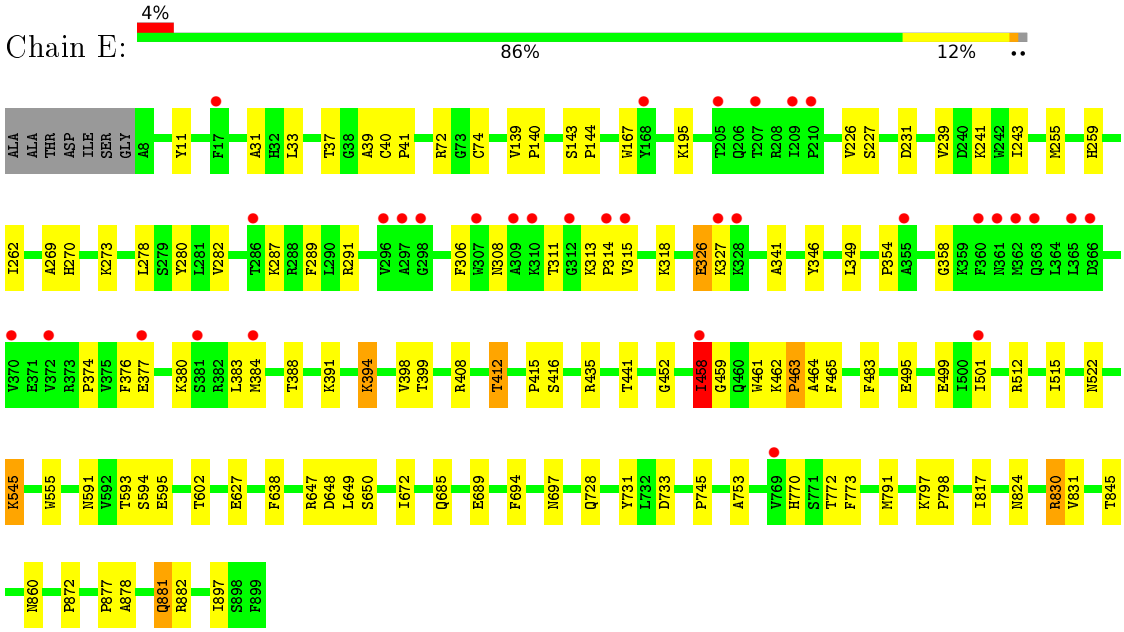
- Molecule 1: DMSO reductase family type II enzyme, molybdopterin subunit



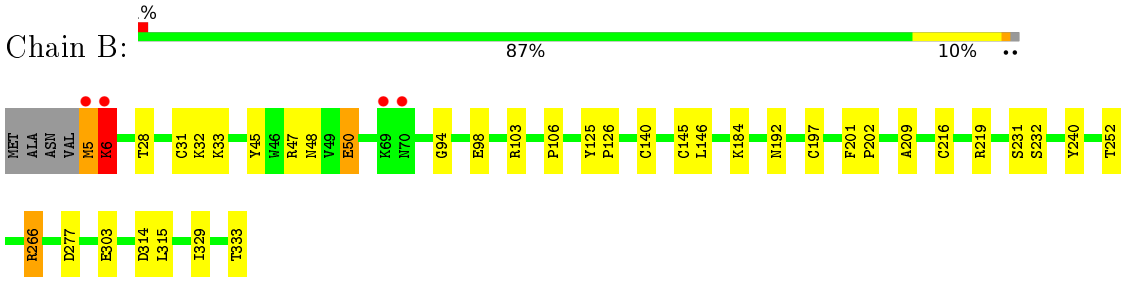
- Molecule 1: DMSO reductase family type II enzyme, molybdopterin subunit



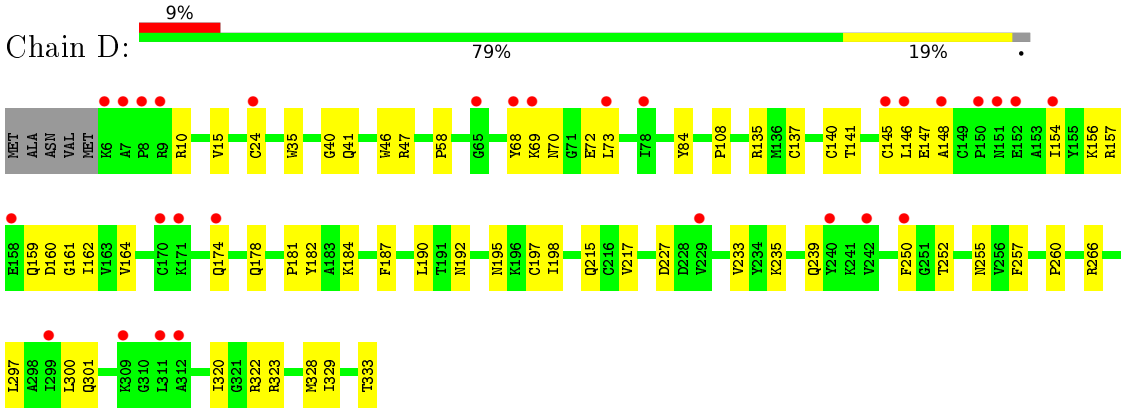
- Molecule 1: DMSO reductase family type II enzyme, molybdopterin subunit



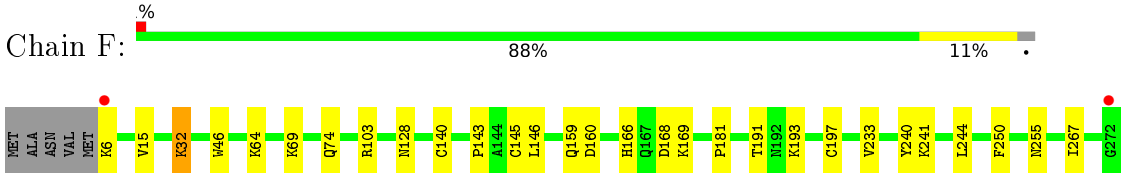
• Molecule 2: DMSO reductase family type II enzyme, iron-sulfur subunit



• Molecule 2: DMSO reductase family type II enzyme, iron-sulfur subunit



• Molecule 2: DMSO reductase family type II enzyme, iron-sulfur subunit




S275
L282
E286
V296
E305
H308
D314
T333

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	133.93Å 176.02Å 193.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.52 – 2.38 48.52 – 2.38	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.52-2.38) 100.0 (48.52-2.38)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.24 (at 2.37Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.170 , 0.227 0.181 , 0.231	Depositor DCC
R_{free} test set	9141 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	32.9	Xtriage
Anisotropy	0.373	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 40.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	30958	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.23% 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: GOL, ZN, BSY, MGD, NA, SF4, EDO, SO3, F3S, MD1, MO

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	0.50	0/7383	0.62	1/10019 (0.0%)
1	C	0.48	0/7357	0.61	0/9984
1	E	0.51	0/7379	0.61	1/10014 (0.0%)
2	B	0.53	0/2632	0.64	1/3567 (0.0%)
2	D	0.44	0/2624	0.57	0/3557
2	F	0.49	0/2624	0.61	0/3557
All	All	0.50	0/29999	0.61	3/40698 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	830	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	E	830	ARG	NE-CZ-NH2	-5.08	117.76	120.30
2	B	5	MET	CA-CB-CG	5.02	121.84	113.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	325	PRO	Peptide

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	7171	0	6990	67	0
1	C	7148	0	6960	74	0
1	E	7163	0	6975	77	0
2	B	2564	0	2534	33	0
2	D	2556	0	2526	41	0
2	F	2556	0	2525	22	0
3	A	8	0	0	0	0
3	B	24	0	0	0	0
3	C	8	0	0	0	0
3	D	24	0	0	1	0
3	E	8	0	0	0	0
3	F	24	0	0	0	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
5	A	47	0	21	1	0
5	C	47	0	20	2	0
5	E	47	0	20	1	0
6	A	47	0	22	0	0
6	C	47	0	22	0	0
6	E	47	0	22	3	0
7	A	40	0	60	7	0
7	B	20	0	30	16	0
7	C	16	0	24	1	0
7	D	4	0	6	1	0
7	E	8	0	12	1	0
7	F	8	0	12	0	0
8	A	4	0	0	2	0
8	C	4	0	0	3	0
8	E	4	0	0	2	0
9	A	4	0	0	0	0
9	C	4	0	0	0	0
9	E	4	0	0	0	0
10	A	2	0	0	0	0
10	B	1	0	0	0	0
10	C	2	0	0	0	0
10	E	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	A	1	0	0	0	0
11	C	1	0	0	0	0
11	E	1	0	0	0	0
12	B	7	0	0	0	0
12	D	7	0	0	0	0
12	F	7	0	0	0	0
13	E	6	0	8	0	0
14	A	367	0	0	5	0
14	B	140	0	0	0	0
14	C	252	0	0	5	0
14	D	57	0	0	1	0
14	E	321	0	0	4	0
14	F	124	0	0	2	0
All	All	30958	0	28789	302	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (302) 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:A:881:GLN:HE22	1:A:882:ARG:HE	1.22	0.86
1:E:697:ASN:HD21	7:E:1005:EDO:H11	1.42	0.83
2:F:240:TYR:OH	2:F:314:ASP:OD2	1.96	0.82
1:C:366:ASP:HB2	1:C:368:LYS:H	1.44	0.80
1:C:289:PHE:O	14:C:1101:HOH:O	2.01	0.78
2:D:140:CYS:SG	2:D:252:THR:HG23	2.26	0.75
2:B:216:CYS:HB3	7:B:408:EDO:H22	1.69	0.74
2:B:232:SER:H	7:B:407:EDO:H11	1.52	0.74
1:C:881:GLN:HE22	1:C:882:ARG:HE	1.36	0.73
1:A:231:ASP:OD1	1:A:830:ARG:NH2	2.22	0.72
1:C:19:ARG:NH1	14:C:1102:HOH:O	2.22	0.72
1:C:860:ASN:HD22	1:C:878:ALA:H	1.38	0.72
1:C:16:ASN:OD1	14:C:1102:HOH:O	2.08	0.71
1:C:226:VAL:HG22	1:C:241:LYS:HG2	1.72	0.70
2:F:69:LYS:HD2	2:F:74:GLN:HG3	1.73	0.69
2:B:106:PRO:HD2	7:B:409:EDO:H21	1.74	0.69
1:E:358:GLY:H	1:E:377:GLU:HG3	1.58	0.69
2:D:156:LYS:NZ	2:D:161:GLY:O	2.27	0.68
1:C:195:LYS:NZ	14:C:1106:HOH:O	2.28	0.66
2:B:5:MET:HG3	2:B:6:LYS:N	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:1007:EDO:H11	2:F:103:ARG:HH22	1.62	0.65
1:C:327:LYS:NZ	1:C:328:LYS:O	2.29	0.64
1:A:310:LYS:NZ	14:A:1109:HOH:O	2.31	0.64
2:B:103:ARG:HH21	7:B:409:EDO:H22	1.62	0.64
1:E:797:LYS:HB3	1:E:798:PRO:HD3	1.78	0.64
1:A:111:GLU:OE1	14:A:1101:HOH:O	2.16	0.62
1:E:380:LYS:O	1:E:384:MET:HG2	1.99	0.62
1:C:302:ASP:HB3	1:C:321:TRP:HB3	1.80	0.62
1:C:459:GLY:HA3	8:C:1009:BSY:SE	2.50	0.62
2:B:103:ARG:NH2	7:B:409:EDO:H22	2.15	0.61
2:B:5:MET:HG3	2:B:6:LYS:H	1.66	0.61
2:D:174:GLN:O	2:D:178:GLN:HG3	2.02	0.60
1:A:48:ASP:OD2	14:A:1102:HOH:O	2.16	0.59
2:D:140:CYS:HB3	2:D:252:THR:O	2.02	0.59
1:E:33:LEU:HD13	1:E:143:SER:HB3	1.84	0.59
1:C:366:ASP:CB	1:C:368:LYS:H	2.14	0.59
1:C:187:GLU:HG3	1:C:708:TYR:HB3	1.85	0.59
1:E:227:SER:HB2	1:E:239:VAL:HG11	1.84	0.59
1:E:326:GLU:HG3	1:E:327:LYS:H	1.66	0.59
2:D:73:LEU:HD21	2:D:148:ALA:HB2	1.85	0.58
2:B:5:MET:CG	2:B:6:LYS:H	2.17	0.58
1:E:860:ASN:HD22	1:E:878:ALA:H	1.49	0.58
1:C:464:ALA:HB3	1:C:694:PHE:CE1	2.37	0.58
1:E:791:MET:HG2	1:E:831:VAL:HG12	1.85	0.57
1:E:243:ILE:HG23	1:E:398:VAL:HG11	1.87	0.57
1:E:259:HIS:ND1	1:E:383:LEU:O	2.30	0.57
1:C:515:ILE:HD13	1:C:522:ASN:HB2	1.87	0.56
1:C:366:ASP:N	1:C:367:GLY:HA2	2.21	0.56
1:E:11[A]:TYR:OH	2:F:169:LYS:HE3	2.06	0.56
1:C:54:GLU:HG2	1:C:585:TYR:OH	2.06	0.55
2:F:267:ILE:HB	2:F:275:SER:HB3	1.86	0.55
2:F:305:GLU:HA	2:F:308:MET:HE3	1.88	0.55
1:C:221:ASN:HB2	2:D:320:ILE:HD11	1.87	0.55
1:C:28:THR:HG21	1:C:605:ALA:HA	1.88	0.55
2:B:219:ARG:HA	7:B:408:EDO:H11	1.87	0.54
1:E:278:LEU:HB3	1:E:376:PHE:HB2	1.90	0.54
1:A:272:LEU:HD21	1:A:443:LEU:HA	1.90	0.54
1:C:666:GLU:OE1	1:C:688:ARG:NH2	2.39	0.54
2:D:192:ASN:ND2	14:D:503:HOH:O	2.41	0.54
2:B:32:LYS:HA	7:B:410:EDO:H12	1.89	0.54
2:D:187:PHE:CZ	2:D:192:ASN:HA	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:TRP:CH2	7:A:1010:EDO:H22	2.43	0.54
1:E:269:ALA:O	1:E:273:LYS:HG3	2.08	0.54
1:A:104:LYS:H	7:A:1010:EDO:H11	1.73	0.54
2:B:219:ARG:HG2	7:B:408:EDO:H11	1.90	0.54
2:D:69:LYS:HD2	2:D:70:ASN:N	2.22	0.53
1:E:515:ILE:HD13	1:E:522:ASN:HB2	1.90	0.53
2:D:146:LEU:HG	2:D:154:ILE:O	2.08	0.53
1:E:226:VAL:HG22	1:E:241:LYS:HB3	1.89	0.53
2:F:145:CYS:SG	2:F:146:LEU:N	2.81	0.53
2:F:15:VAL:HG23	2:F:233:VAL:HG12	1.91	0.53
2:D:15:VAL:HG23	2:D:233:VAL:HG12	1.91	0.53
1:C:311:THR:HG22	1:C:313:LYS:HB2	1.91	0.53
1:C:508:GLU:HG3	1:E:897:ILE:HG22	1.91	0.53
2:D:141:THR:HG23	2:D:255:ASN:HD21	1.73	0.53
1:A:289:PHE:HB2	1:A:291:ARG:NH1	2.23	0.52
1:A:366:ASP:OD1	1:A:368:LYS:HG2	2.10	0.52
2:B:216:CYS:CB	7:B:408:EDO:H22	2.38	0.52
2:B:145:CYS:SG	2:B:146:LEU:N	2.82	0.52
2:B:32:LYS:CA	7:B:410:EDO:H12	2.38	0.52
1:E:881:GLN:HE22	1:E:882:ARG:HE	1.56	0.52
1:A:103:GLY:H	7:A:1010:EDO:H12	1.74	0.52
1:A:871:ARG:HB3	1:A:874:TYR:HB3	1.92	0.52
2:B:266:ARG:HD2	2:B:277:ASP:O	2.11	0.51
2:D:41:GLN:NE2	2:D:195:ASN:OD1	2.43	0.51
1:A:624:LYS:HE3	1:A:653:TRP:CD1	2.45	0.51
1:E:195:LYS:HG2	1:E:415:PRO:HD2	1.93	0.51
1:A:170:ASP:O	1:A:458:ILE:HD13	2.10	0.51
2:D:235:LYS:HA	2:D:239:GLN:HB3	1.93	0.51
2:B:303:GLU:HG3	2:B:315:LEU:HD23	1.93	0.51
1:C:290:LEU:O	14:C:1103:HOH:O	2.19	0.51
1:A:459:GLY:HA3	8:A:1013:BSY:O2	2.11	0.51
1:C:462:LYS:HB3	1:C:594:SER:HB3	1.92	0.51
2:F:64:LYS:HG2	2:F:64:LYS:O	2.11	0.51
1:E:638:PHE:CZ	1:E:647:ARG:HD2	2.46	0.51
1:E:461:TRP:O	1:E:463:PRO:HD3	2.11	0.50
1:A:638:PHE:CZ	1:A:647:ARG:HD2	2.47	0.50
2:D:137:CYS:HB3	2:D:197:CYS:SG	2.52	0.50
1:E:306:PHE:CD2	1:E:354:PRO:HB3	2.46	0.50
1:E:731:TYR:CE2	1:E:733:ASP:HB3	2.46	0.50
1:C:13:GLY:HA2	1:C:16:ASN:ND2	2.27	0.50
2:D:135:ARG:NH2	2:D:182:TYR:O	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:PRO:HA	2:D:217:VAL:CG1	2.41	0.49
1:E:280:TYR:O	1:E:374:PRO:HA	2.12	0.49
1:E:311:THR:O	1:E:313:LYS:HD3	2.13	0.49
1:A:740:MET:HB2	1:A:742:VAL:HG22	1.95	0.49
1:E:289:PHE:HB2	1:E:291:ARG:NH1	2.28	0.49
1:C:31:ALA:HB3	1:C:602:THR:HB	1.94	0.49
1:E:231:ASP:OD1	1:E:830:ARG:NH2	2.46	0.49
1:E:40:CYS:SG	1:E:72:ARG:HB3	2.52	0.49
1:A:856:ILE:HG23	1:A:877:PRO:HB3	1.95	0.49
1:C:860:ASN:HB3	1:C:877:PRO:HA	1.94	0.49
2:B:45:TYR:HA	7:B:410:EDO:H11	1.93	0.48
1:C:519:GLN:HB3	1:C:863:GLY:HA3	1.95	0.48
2:B:5:MET:CG	2:B:6:LYS:N	2.71	0.48
2:D:46:TRP:O	2:D:184:LYS:NZ	2.43	0.48
1:A:170:ASP:HB3	1:A:458:ILE:CD1	2.42	0.48
2:B:94:GLY:HA2	2:B:98:GLU:HB2	1.94	0.48
1:A:154:ALA:HB1	1:A:159:ALA:HB3	1.95	0.48
1:E:327:LYS:O	1:E:341:ALA:HB1	2.14	0.48
1:A:416:SER:O	1:A:452:GLY:HA2	2.13	0.48
1:C:791:MET:HG2	1:C:831:VAL:HG12	1.94	0.48
1:E:593:THR:HG23	1:E:595:GLU:H	1.78	0.48
2:F:305:GLU:HA	2:F:308:MET:HB2	1.96	0.48
1:A:283:ARG:HB3	1:A:285:ASP:OD1	2.14	0.47
1:E:462:LYS:HB3	1:E:594:SER:HB3	1.95	0.47
2:F:244:LEU:HD11	2:F:296:VAL:HG21	1.95	0.47
1:A:398:VAL:HG13	7:A:1005:EDO:H12	1.96	0.47
1:A:39:ALA:HA	1:A:591:ASN:OD1	2.15	0.47
1:E:459:GLY:HA3	8:E:1008:BSY:O2	2.14	0.47
1:A:318:LYS:HD3	14:A:1310:HOH:O	2.14	0.47
1:A:485:GLN:CD	1:A:877:PRO:HD2	2.35	0.47
1:C:40:CYS:SG	1:C:72:ARG:HB3	2.54	0.47
1:A:836:CYS:HB2	14:A:1327:HOH:O	2.15	0.47
2:D:10:ARG:HD2	2:D:227:ASP:OD2	2.14	0.47
1:E:31:ALA:HB3	1:E:602:THR:HB	1.97	0.47
1:C:700:SER:OG	1:C:712:GLN:HB2	2.15	0.47
1:A:40:CYS:SG	1:A:72:ARG:HB3	2.55	0.47
1:C:195:LYS:HA	1:C:195:LYS:HD3	1.72	0.47
2:D:328:MET:HG3	2:D:329:ILE:O	2.15	0.47
1:A:155:HIS:CD2	1:A:475:PRO:HD2	2.50	0.47
2:D:266:ARG:N	2:D:266:ARG:HD2	2.30	0.47
2:D:297:LEU:HA	2:D:300:LEU:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:270:HIS:CD2	1:E:349:LEU:HD23	2.50	0.47
1:E:287:LYS:O	1:E:731:TYR:OH	2.23	0.47
2:B:31:CYS:SG	7:B:410:EDO:H21	2.55	0.46
1:C:68:GLU:OE1	1:C:70:ASN:ND2	2.44	0.46
1:C:464:ALA:HB3	1:C:694:PHE:CZ	2.50	0.46
1:C:703:LYS:HB2	1:C:706:VAL:HB	1.97	0.46
2:F:69:LYS:HD2	2:F:74:GLN:CG	2.44	0.46
1:C:683:THR:OG1	1:C:686:MET:HG3	2.14	0.46
1:A:601:MET:CE	1:A:603:GLU:HB3	2.46	0.46
1:A:5:ILE:HG13	1:A:7:GLY:H	1.80	0.46
1:E:860:ASN:HB3	1:E:877:PRO:HA	1.97	0.46
1:A:751:ILE:HG22	1:A:753:ALA:H	1.80	0.46
7:A:1012:EDO:H12	2:B:125:TYR:H	1.81	0.46
2:B:48:ASN:ND2	2:B:50:GLU:HG2	2.31	0.46
2:D:68:TYR:OH	2:D:147:GLU:OE2	2.30	0.46
1:A:683:THR:OG1	1:A:686:MET:HG3	2.16	0.46
1:C:311:THR:O	1:C:313:LYS:HG3	2.15	0.46
1:A:462:LYS:HB3	1:A:594:SER:HB3	1.98	0.46
1:C:813:HIS:CE1	1:C:853:PRO:HB3	2.52	0.45
1:A:302:ASP:HB3	1:A:321:TRP:HB3	1.98	0.45
1:A:162:HIS:HB3	1:A:486:THR:OG1	2.17	0.45
1:A:76:LYS:HD3	1:A:76:LYS:N	2.32	0.45
1:C:327:LYS:HD2	1:C:327:LYS:HA	1.67	0.45
1:C:53:ARG:NH2	2:D:215:GLN:OE1	2.50	0.45
1:E:41:PRO:HA	14:E:1110:HOH:O	2.16	0.45
1:A:170:ASP:HB2	8:A:1013:BSY:O3	2.17	0.45
1:E:408:ARG:O	1:E:412:THR:HB	2.15	0.45
1:E:483:PHE:CD2	1:E:872:PRO:HG3	2.51	0.45
2:B:47:ARG:H	7:B:410:EDO:H22	1.81	0.45
2:D:108:PRO:HG2	7:D:405:EDO:H12	1.99	0.45
1:A:380:LYS:O	1:A:384:MET:HG2	2.16	0.45
1:C:144:PRO:HB2	1:C:672:ILE:HD13	1.99	0.45
1:C:871:ARG:HB3	1:C:874:TYR:HB3	1.99	0.45
5:E:1003:MGD:H2'	5:E:1003:MGD:H8	1.62	0.45
1:E:313:LYS:HB3	1:E:314:PRO:HD2	1.99	0.45
1:E:388:THR:OG1	1:E:391:LYS:HG3	2.17	0.45
2:F:282:LEU:O	2:F:286:GLU:HG3	2.17	0.45
1:A:104:LYS:N	7:A:1010:EDO:H11	2.32	0.45
2:F:191:THR:O	2:F:193:LYS:HG3	2.17	0.45
5:C:1003:MGD:H2'	5:C:1003:MGD:H8	1.68	0.45
1:E:39:ALA:HA	1:E:591:ASN:OD1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:181:PRO:HB2	2:F:250:PHE:CD2	2.52	0.45
2:D:145:CYS:O	2:D:154:ILE:HD12	2.16	0.45
1:E:399:THR:HG23	14:E:1243:HOH:O	2.16	0.45
1:A:399:THR:O	1:A:403:ILE:HG13	2.16	0.45
1:C:826:GLU:OE2	1:C:830:ARG:HD3	2.16	0.45
1:A:441:THR:CG2	1:A:447:GLU:HG2	2.47	0.44
1:A:227:SER:HB2	1:A:239:VAL:HG11	1.99	0.44
1:A:700:SER:OG	1:A:712:GLN:HB2	2.17	0.44
1:A:898:SER:O	1:E:512:ARG:NH1	2.46	0.44
1:C:625:ARG:HA	1:C:625:ARG:HD3	1.70	0.44
2:F:159:GLN:H	2:F:159:GLN:HG3	1.41	0.44
1:A:768:SER:O	5:A:1003:MGD:N18	2.46	0.44
1:E:231:ASP:HB3	1:E:830:ARG:HH21	1.82	0.44
1:A:278:LEU:HB3	1:A:376:PHE:HB2	2.00	0.44
1:E:144:PRO:HB2	1:E:672:ILE:HD13	1.99	0.44
2:B:28:THR:O	7:B:410:EDO:O2	2.27	0.44
2:F:32:LYS:HE3	14:F:611:HOH:O	2.17	0.44
1:C:700:SER:HB2	1:C:708:TYR:CE1	2.53	0.44
1:A:495:GLU:HG2	1:C:896:PRO:HB3	1.98	0.44
1:E:255:MET:HE3	1:E:383:LEU:HD21	2.00	0.44
2:D:58:PRO:HB3	2:D:84:TYR:CD1	2.52	0.43
1:A:144:PRO:HD2	1:A:590:LEU:O	2.18	0.43
1:A:96:ARG:HB2	7:A:1010:EDO:H21	2.01	0.43
1:A:831:VAL:HG11	1:A:888:VAL:HG21	2.00	0.43
1:E:37:THR:HB	1:E:595:GLU:OE1	2.18	0.43
1:A:328:LYS:HD3	1:A:328:LYS:N	2.33	0.43
2:B:231:SER:HB2	7:B:407:EDO:H22	1.99	0.43
1:E:306:PHE:CZ	1:E:315:VAL:HB	2.53	0.43
1:A:82:ASP:OD1	2:B:33:LYS:NZ	2.41	0.43
1:C:337:ARG:HG3	1:C:339:THR:HG23	1.99	0.43
1:A:229:SER:HA	1:A:230:PRO:HD3	1.91	0.43
1:A:435:ARG:CZ	1:A:732:LEU:HD12	2.49	0.43
1:A:815:LYS:HB3	1:A:815:LYS:HE2	1.70	0.43
2:D:162:ILE:HG22	2:D:164:VAL:HG23	1.99	0.43
1:E:416:SER:O	1:E:452:GLY:HA2	2.18	0.43
1:E:627:GLU:HG2	1:E:649:LEU:O	2.19	0.43
1:C:18:HIS:CD2	2:D:198:ILE:HG21	2.53	0.43
1:C:307:TRP:CZ3	1:C:314:PRO:HD3	2.54	0.43
1:C:111:GLU:HG3	1:C:625:ARG:NH2	2.34	0.43
1:C:75:ASN:HB3	2:D:24:CYS:O	2.18	0.43
1:E:318:LYS:HE3	1:E:346:TYR:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:458:ILE:HD13	1:E:459:GLY:H	1.84	0.43
2:F:46:TRP:CE3	2:F:197:CYS:HA	2.53	0.43
1:C:539:ASN:ND2	1:C:569:ASP:HB2	2.34	0.43
1:E:259:HIS:CE1	1:E:384:MET:HA	2.54	0.43
1:E:270:HIS:NE2	1:E:349:LEU:HD23	2.33	0.43
1:A:76:LYS:HD3	1:A:76:LYS:H	1.83	0.43
1:E:167:TRP:O	1:E:545:LYS:NZ	2.51	0.42
1:E:262:ILE:HD12	1:E:383:LEU:HD12	2.01	0.42
1:E:435:ARG:HH21	1:E:745:PRO:HD3	1.83	0.42
2:D:40:GLY:N	2:D:190:LEU:HD12	2.34	0.42
1:A:624:LYS:HE3	1:A:653:TRP:NE1	2.34	0.42
1:A:170:ASP:HB3	1:A:458:ILE:HD12	2.01	0.42
1:C:39:ALA:HA	1:C:591:ASN:OD1	2.19	0.42
2:D:322:ARG:O	2:D:323:ARG:NH1	2.48	0.42
1:E:459:GLY:HA3	8:E:1008:BSY:SE	2.69	0.42
1:E:394:LYS:HD2	1:E:394:LYS:HA	1.70	0.42
1:C:115:ASP:OD1	1:C:625:ARG:HD2	2.19	0.42
1:C:234:SER:O	1:C:237:ILE:HG12	2.18	0.42
1:E:685:GLN:NE2	1:E:689:GLU:OE2	2.44	0.42
2:D:181:PRO:HB2	2:D:250:PHE:CD2	2.54	0.42
2:D:35:TRP:HB3	2:D:46:TRP:CZ3	2.55	0.42
1:E:499:GLU:O	1:E:753:ALA:HB1	2.19	0.42
2:B:209:ALA:HB2	2:B:329:ILE:O	2.20	0.42
1:C:76:LYS:HB2	1:C:76:LYS:HE2	1.88	0.42
6:E:1004:MD1:H11	6:E:1004:MD1:H7	2.02	0.42
1:E:501:ILE:HG22	14:E:1276:HOH:O	2.19	0.42
1:A:697:ASN:HB3	1:A:708:TYR:CE1	2.55	0.42
1:C:11:TYR:O	1:C:15:GLU:HG3	2.19	0.42
1:C:168:TYR:HD2	8:C:1009:BSY:O1	2.03	0.42
1:E:860:ASN:CB	1:E:877:PRO:HA	2.50	0.42
1:A:50:VAL:HB	1:A:52:MET:CE	2.50	0.42
1:C:40:CYS:HA	1:C:41:PRO:HD3	1.86	0.42
1:A:144:PRO:HB2	1:A:672:ILE:HD13	2.02	0.41
1:C:22:TRP:HZ2	2:D:333:THR:HG21	1.85	0.41
1:E:464:ALA:HB3	1:E:694:PHE:CZ	2.54	0.41
1:A:152:ARG:NH1	1:A:475:PRO:HG3	2.35	0.41
2:B:219:ARG:HA	7:B:408:EDO:C1	2.49	0.41
1:E:770:HIS:CG	6:E:1004:MD1:H102	2.56	0.41
1:C:207:THR:HA	5:C:1003:MGD:N20	2.35	0.41
1:E:408:ARG:NH1	14:E:1109:HOH:O	2.35	0.41
1:E:817:ILE:HG13	1:E:845:THR:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:PHE:O	1:A:317:PRO:HD2	2.20	0.41
2:B:201:PHE:CG	2:B:202:PRO:HD3	2.56	0.41
1:C:637:LYS:HA	1:C:647:ARG:O	2.21	0.41
1:C:793:PRO:O	1:C:797:LYS:HG2	2.21	0.41
1:A:114:LEU:HD22	1:A:622:LEU:HD13	2.02	0.41
2:B:140:CYS:HB3	2:B:252:THR:O	2.21	0.41
2:D:159:GLN:H	2:D:159:GLN:CD	2.20	0.41
1:E:824:ASN:HB2	2:F:128:ASN:ND2	2.35	0.41
2:F:140:CYS:O	2:F:143:PRO:HD3	2.21	0.41
1:C:536:TYR:O	1:C:537:ARG:HB2	2.21	0.41
1:E:464:ALA:HB3	1:E:694:PHE:CE1	2.56	0.41
1:C:69:TYR:OH	1:C:187:GLU:HB3	2.20	0.41
1:C:459:GLY:HA3	8:C:1009:BSY:O2	2.21	0.41
2:F:166:HIS:HE1	2:F:168:ASP:HB2	1.86	0.41
1:C:221:ASN:HB2	2:D:320:ILE:CD1	2.49	0.41
1:E:648:ASP:OD1	1:E:650:SER:OG	2.35	0.41
2:D:260:PRO:HB2	2:D:297:LEU:HD21	2.03	0.41
2:B:125:TYR:HA	2:B:126:PRO:HA	1.88	0.41
1:C:264:GLU:OE2	1:C:408:ARG:NH2	2.31	0.41
2:B:184:LYS:HD3	2:B:184:LYS:HA	1.95	0.40
2:B:240:TYR:OH	2:B:314:ASP:OD2	2.28	0.40
1:C:46:SER:O	1:C:47:LYS:HB2	2.21	0.40
2:D:255:ASN:HA	2:D:257:PHE:CE1	2.56	0.40
1:E:139:VAL:HA	1:E:140:PRO:HD2	1.89	0.40
1:C:309:ALA:O	1:C:310:LYS:HB2	2.21	0.40
1:A:896:PRO:HB3	1:E:495:GLU:HG2	2.03	0.40
1:C:15:GLU:OE1	2:D:157:ARG:NH1	2.55	0.40
2:D:47:ARG:HB2	3:D:404:SF4:S4	2.62	0.40
1:E:308:ASN:HD22	1:E:315:VAL:HG21	1.85	0.40
1:E:483:PHE:CG	1:E:872:PRO:HG3	2.56	0.40
2:F:255:ASN:ND2	14:F:512:HOH:O	2.53	0.40
1:A:493:HIS:CE1	1:A:530:PRO:HD3	2.57	0.40
1:C:139:VAL:HB	1:C:142:VAL:HG23	2.02	0.40
1:C:468:GLY:H	1:C:676:ALA:HB2	1.86	0.40
1:E:770:HIS:CE1	6:E:1004:MD1:S12	3.14	0.40
1:E:772:THR:O	1:E:773:PHE:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	894/899 (99%)	861 (96%)	30 (3%)	3 (0%)	46	61
1	C	890/899 (99%)	841 (94%)	44 (5%)	5 (1%)	30	40
1	E	892/899 (99%)	845 (95%)	43 (5%)	4 (0%)	39	53
2	B	327/333 (98%)	314 (96%)	12 (4%)	1 (0%)	46	61
2	D	326/333 (98%)	303 (93%)	23 (7%)	0	100	100
2	F	326/333 (98%)	308 (94%)	18 (6%)	0	100	100
All	All	3655/3696 (99%)	3472 (95%)	170 (5%)	13 (0%)	39	53

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	458	ILE
2	B	6	LYS
1	C	310	LYS
1	C	311	THR
1	C	47	LYS
1	C	458	ILE
1	A	463	PRO
1	E	326	GLU
1	E	458	ILE
1	A	326	GLU
1	E	728	GLN
1	C	463	PRO
1	E	463	PRO

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	767/768 (100%)	760 (99%)	7 (1%)	84 93
1	C	764/768 (100%)	757 (99%)	7 (1%)	84 93
1	E	766/768 (100%)	756 (99%)	10 (1%)	76 89
2	B	278/281 (99%)	272 (98%)	6 (2%)	60 78
2	D	277/281 (99%)	274 (99%)	3 (1%)	80 91
2	F	277/281 (99%)	273 (99%)	4 (1%)	74 88
All	All	3129/3147 (99%)	3092 (99%)	37 (1%)	78 90

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	ARG
1	A	284	SER
1	A	458	ILE
1	A	465	PHE
1	A	502	SER
1	A	555	TRP
1	A	881	GLN
2	B	6	LYS
2	B	50	GLU
2	B	192	ASN
2	B	197	CYS
2	B	266	ARG
2	B	333	THR
1	C	173	THR
1	C	359	LYS
1	C	458	ILE
1	C	465	PHE
1	C	555	TRP
1	C	788	SER
1	C	881	GLN
2	D	72	GLU
2	D	160	ASP
2	D	301	GLN
1	E	74	CYS
1	E	282	VAL
1	E	394	LYS
1	E	412	THR

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Mol	Chain	Res	Type
1	E	441	THR
1	E	458	ILE
1	E	465	PHE
1	E	545	LYS
1	E	555	TRP
1	E	881	GLN
2	F	6	LYS
2	F	32	LYS
2	F	160	ASP
2	F	241	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	639	ASN
1	A	881	GLN
1	C	450	ASN
1	C	860	ASN
1	C	881	GLN
1	E	308	ASN
1	E	881	GLN
2	F	62	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 66 ligands modelled in this entry, 14 are monoatomic - leaving 52 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	SF4	A	1001	1	0,12,12	0.00	-	0,24,24	0.00	-
5	MGD	A	1003	4	41,52,52	5.96	29 (70%)	39,81,81	3.73	17 (43%)
6	MD1	A	1004	4	40,51,51	3.74	15 (37%)	34,78,78	1.56	6 (17%)
7	EDO	A	1005	-	3,3,3	0.61	0	2,2,2	0.11	0
7	EDO	A	1006	-	3,3,3	0.49	0	2,2,2	0.53	0
7	EDO	A	1007	-	3,3,3	0.44	0	2,2,2	0.81	0
7	EDO	A	1008	-	3,3,3	0.62	0	2,2,2	0.46	0
7	EDO	A	1009	-	3,3,3	0.62	0	2,2,2	0.58	0
7	EDO	A	1010	-	3,3,3	1.12	0	2,2,2	1.18	0
7	EDO	A	1011	-	3,3,3	0.50	0	2,2,2	0.48	0
7	EDO	A	1012	-	3,3,3	0.68	0	2,2,2	0.42	0
8	BSY	A	1013	-	0,3,3	0.00	-	1,3,3	3.32	1 (100%)
9	SO3	A	1014	11	1,3,3	0.92	0	0,3,3	0.00	-
7	EDO	A	1018	-	3,3,3	0.53	0	2,2,2	0.60	0
7	EDO	A	1019	-	3,3,3	0.71	0	2,2,2	0.23	0
12	F3S	B	401	2	0,9,9	0.00	-	0,15,15	0.00	-
3	SF4	B	402	2	0,12,12	0.00	-	0,24,24	0.00	-
3	SF4	B	403	2	0,12,12	0.00	-	0,24,24	0.00	-
3	SF4	B	404	2	0,12,12	0.00	-	0,24,24	0.00	-
7	EDO	B	405	-	3,3,3	0.41	0	2,2,2	0.40	0
7	EDO	B	407	-	3,3,3	0.80	0	2,2,2	0.13	0
7	EDO	B	408	-	3,3,3	0.64	0	2,2,2	0.65	0
7	EDO	B	409	-	3,3,3	0.96	0	2,2,2	0.81	0
7	EDO	B	410	-	3,3,3	0.38	0	2,2,2	0.38	0
3	SF4	C	1001	1	0,12,12	0.00	-	0,24,24	0.00	-
5	MGD	C	1003	4	41,52,52	5.88	28 (68%)	39,81,81	4.25	17 (43%)
6	MD1	C	1004	4	40,51,51	3.62	15 (37%)	34,78,78	1.45	7 (20%)
7	EDO	C	1005	-	3,3,3	0.74	0	2,2,2	0.34	0
7	EDO	C	1006	-	3,3,3	0.63	0	2,2,2	0.13	0
7	EDO	C	1007	-	3,3,3	0.50	0	2,2,2	1.33	0
7	EDO	C	1008	-	3,3,3	0.48	0	2,2,2	0.50	0
8	BSY	C	1009	-	0,3,3	0.00	-	1,3,3	4.71	1 (100%)
9	SO3	C	1010	11	1,3,3	0.65	0	0,3,3	0.00	-
12	F3S	D	401	2	0,9,9	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	SF4	D	402	2	0,12,12	0.00	-	0,24,24	0.00	-
3	SF4	D	403	2	0,12,12	0.00	-	0,24,24	0.00	-
3	SF4	D	404	2	0,12,12	0.00	-	0,24,24	0.00	-
7	EDO	D	405	-	3,3,3	0.48	0	2,2,2	0.23	0
3	SF4	E	1001	1	0,12,12	0.00	-	0,24,24	0.00	-
5	MGD	E	1003	4	41,52,52	5.93	25 (60%)	39,81,81	4.02	15 (38%)
6	MD1	E	1004	4	40,51,51	3.50	15 (37%)	34,78,78	1.47	6 (17%)
7	EDO	E	1005	-	3,3,3	0.69	0	2,2,2	0.43	0
13	GOL	E	1006	-	5,5,5	0.50	0	5,5,5	0.83	0
7	EDO	E	1007	-	3,3,3	0.44	0	2,2,2	0.93	0
8	BSY	E	1008	-	0,3,3	0.00	-	1,3,3	3.76	1 (100%)
9	SO3	E	1009	11	1,3,3	0.88	0	0,3,3	0.00	-
12	F3S	F	401	2	0,9,9	0.00	-	0,15,15	0.00	-
3	SF4	F	402	2	0,12,12	0.00	-	0,24,24	0.00	-
3	SF4	F	403	2	0,12,12	0.00	-	0,24,24	0.00	-
3	SF4	F	404	2	0,12,12	0.00	-	0,24,24	0.00	-
7	EDO	F	405	-	3,3,3	0.49	0	2,2,2	0.36	0
7	EDO	F	406	-	3,3,3	0.81	0	2,2,2	0.23	0

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	SF4	A	1001	1	-	0/0/48/48	0/6/5/5
5	MGD	A	1003	4	-	0/18/66/66	0/6/6/6
6	MD1	A	1004	4	-	0/21/59/59	0/5/5/5
7	EDO	A	1005	-	-	0/1/1/1	0/0/0/0
7	EDO	A	1006	-	-	0/1/1/1	0/0/0/0
7	EDO	A	1007	-	-	0/1/1/1	0/0/0/0
7	EDO	A	1008	-	-	0/1/1/1	0/0/0/0
7	EDO	A	1009	-	-	0/1/1/1	0/0/0/0
7	EDO	A	1010	-	-	0/1/1/1	0/0/0/0
7	EDO	A	1011	-	-	0/1/1/1	0/0/0/0
7	EDO	A	1012	-	-	0/1/1/1	0/0/0/0
8	BSY	A	1013	-	-	0/0/0/0	0/0/0/0
9	SO3	A	1014	11	-	0/0/0/0	0/0/0/0
7	EDO	A	1018	-	-	0/1/1/1	0/0/0/0
7	EDO	A	1019	-	-	0/1/1/1	0/0/0/0
12	F3S	B	401	2	-	0/0/24/24	0/0/3/3
3	SF4	B	402	2	-	0/0/48/48	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SF4	B	403	2	-	0/0/48/48	0/6/5/5
3	SF4	B	404	2	-	0/0/48/48	0/6/5/5
7	EDO	B	405	-	-	0/1/1/1	0/0/0/0
7	EDO	B	407	-	-	0/1/1/1	0/0/0/0
7	EDO	B	408	-	-	0/1/1/1	0/0/0/0
7	EDO	B	409	-	-	0/1/1/1	0/0/0/0
7	EDO	B	410	-	-	0/1/1/1	0/0/0/0
3	SF4	C	1001	1	-	0/0/48/48	0/6/5/5
5	MGD	C	1003	4	-	0/18/66/66	0/6/6/6
6	MD1	C	1004	4	-	0/21/59/59	0/5/5/5
7	EDO	C	1005	-	-	0/1/1/1	0/0/0/0
7	EDO	C	1006	-	-	0/1/1/1	0/0/0/0
7	EDO	C	1007	-	-	0/1/1/1	0/0/0/0
7	EDO	C	1008	-	-	0/1/1/1	0/0/0/0
8	BSY	C	1009	-	-	0/0/0/0	0/0/0/0
9	SO3	C	1010	11	-	0/0/0/0	0/0/0/0
12	F3S	D	401	2	-	0/0/24/24	0/0/3/3
3	SF4	D	402	2	-	0/0/48/48	0/6/5/5
3	SF4	D	403	2	-	0/0/48/48	0/6/5/5
3	SF4	D	404	2	-	0/0/48/48	0/6/5/5
7	EDO	D	405	-	-	0/1/1/1	0/0/0/0
3	SF4	E	1001	1	-	0/0/48/48	0/6/5/5
5	MGD	E	1003	4	-	0/18/66/66	0/6/6/6
6	MD1	E	1004	4	-	0/21/59/59	0/5/5/5
7	EDO	E	1005	-	-	0/1/1/1	0/0/0/0
13	GOL	E	1006	-	-	0/4/4/4	0/0/0/0
7	EDO	E	1007	-	-	0/1/1/1	0/0/0/0
8	BSY	E	1008	-	-	0/0/0/0	0/0/0/0
9	SO3	E	1009	11	-	0/0/0/0	0/0/0/0
12	F3S	F	401	2	-	0/0/24/24	0/0/3/3
3	SF4	F	402	2	-	0/0/48/48	0/6/5/5
3	SF4	F	403	2	-	0/0/48/48	0/6/5/5
3	SF4	F	404	2	-	0/0/48/48	0/6/5/5
7	EDO	F	405	-	-	0/1/1/1	0/0/0/0
7	EDO	F	406	-	-	0/1/1/1	0/0/0/0

All (127) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	1003	MGD	C23-C14	-21.24	1.37	1.53
5	A	1003	MGD	C23-C14	-20.42	1.38	1.53
5	C	1003	MGD	C23-C14	-20.41	1.38	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1003	MGD	C2'-C3'	-10.29	1.25	1.53
5	A	1003	MGD	C2'-C3'	-9.98	1.26	1.53
5	E	1003	MGD	C2'-C3'	-9.88	1.26	1.53
6	E	1004	MD1	C5-C6	-8.40	1.37	1.53
6	A	1004	MD1	C5-C6	-8.38	1.37	1.53
6	C	1004	MD1	C5-C6	-8.35	1.37	1.53
6	E	1004	MD1	C4-N9	-8.00	1.37	1.47
6	A	1004	MD1	C4-N9	-7.89	1.37	1.47
6	C	1004	MD1	C4-N9	-7.65	1.37	1.47
5	A	1003	MGD	O4'-C4'	-7.00	1.29	1.45
5	C	1003	MGD	O4'-C4'	-6.97	1.29	1.45
5	E	1003	MGD	O4'-C4'	-6.28	1.30	1.45
6	E	1004	MD1	C2'-C1'	-6.09	1.34	1.53
6	C	1004	MD1	C2'-C1'	-6.01	1.34	1.53
6	A	1004	MD1	C2'-C1'	-5.79	1.35	1.53
6	E	1004	MD1	C14-N15	-5.55	1.42	1.47
6	A	1004	MD1	C14-N15	-5.40	1.42	1.47
6	E	1004	MD1	O4'-C4'	-5.02	1.33	1.45
6	C	1004	MD1	O4'-C4'	-5.01	1.33	1.45
6	A	1004	MD1	O4'-C4'	-4.89	1.33	1.45
6	C	1004	MD1	C14-N15	-4.70	1.42	1.47
6	C	1004	MD1	C8-N9	-3.04	1.37	1.47
6	A	1004	MD1	C8-N9	-2.96	1.37	1.47
6	E	1004	MD1	C8-N9	-2.96	1.37	1.47
6	C	1004	MD1	C16-C20	-2.85	1.37	1.41
5	C	1003	MGD	O11-C23	-2.58	1.40	1.43
6	C	1004	MD1	O3'-C3'	-2.54	1.37	1.43
6	A	1004	MD1	O3'-C3'	-2.41	1.37	1.43
6	E	1004	MD1	C16-C20	-2.34	1.37	1.41
6	E	1004	MD1	C15-C16	-2.30	1.38	1.41
6	C	1004	MD1	C15-C16	-2.23	1.38	1.41
6	A	1004	MD1	C16-C20	-2.23	1.38	1.41
5	A	1003	MGD	O11-C23	-2.23	1.40	1.43
6	A	1004	MD1	C2-N3	-2.06	1.34	1.43
5	A	1003	MGD	C5-C4	-2.05	1.35	1.40
6	E	1004	MD1	O3'-C3'	-2.02	1.38	1.43
5	C	1003	MGD	O3'-C3'	2.09	1.47	1.43
5	C	1003	MGD	C8-N7	2.10	1.38	1.34
6	E	1004	MD1	C15-N17	2.11	1.36	1.33
5	E	1003	MGD	C8-N7	2.18	1.38	1.34
6	A	1004	MD1	C13-C12	2.20	1.41	1.34
6	C	1004	MD1	C13-C12	2.22	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	1004	MD1	C13-C12	2.23	1.41	1.34
5	A	1003	MGD	O3'-C3'	2.26	1.48	1.43
5	C	1003	MGD	C21-N22	2.28	1.42	1.35
6	A	1004	MD1	C14-C7	2.33	1.57	1.50
6	C	1004	MD1	C15-N17	2.39	1.37	1.33
5	A	1003	MGD	C21-N22	2.43	1.43	1.35
5	A	1003	MGD	C21-N20	2.53	1.39	1.34
5	C	1003	MGD	C21-N20	2.63	1.39	1.34
5	A	1003	MGD	C2'-C1'	2.66	1.57	1.53
5	C	1003	MGD	C13-C12	2.67	1.52	1.35
5	E	1003	MGD	C16-N15	2.69	1.44	1.38
5	E	1003	MGD	C21-N20	2.71	1.39	1.34
5	A	1003	MGD	C13-C12	2.79	1.53	1.35
5	A	1003	MGD	C2-N1	2.89	1.40	1.35
5	E	1003	MGD	C13-C12	2.90	1.54	1.35
5	E	1003	MGD	C2'-C1'	2.91	1.58	1.53
5	A	1003	MGD	C8-N7	2.95	1.40	1.34
5	C	1003	MGD	C16-N15	2.96	1.44	1.38
5	C	1003	MGD	C17-C16	3.00	1.45	1.41
6	E	1004	MD1	C17-N16	3.11	1.40	1.34
5	C	1003	MGD	C2'-C1'	3.14	1.58	1.53
5	C	1003	MGD	C2-N1	3.22	1.41	1.35
6	C	1004	MD1	C17-N16	3.30	1.41	1.34
6	A	1004	MD1	C17-N16	3.44	1.41	1.34
5	E	1003	MGD	C17-C16	3.58	1.46	1.41
5	A	1003	MGD	C16-N15	3.63	1.46	1.38
5	E	1003	MGD	O2'-C2'	3.71	1.51	1.43
6	E	1004	MD1	C16-N15	3.71	1.46	1.38
5	C	1003	MGD	O2'-C2'	3.72	1.51	1.43
5	C	1003	MGD	C2-N2	3.73	1.42	1.34
5	A	1003	MGD	C2-N2	3.87	1.42	1.34
5	E	1003	MGD	C2-N2	3.95	1.42	1.34
5	A	1003	MGD	O2'-C2'	3.97	1.52	1.43
6	C	1004	MD1	C16-N15	4.00	1.46	1.38
5	E	1003	MGD	C2-N1	4.01	1.43	1.35
6	A	1004	MD1	C16-N15	4.28	1.47	1.38
5	A	1003	MGD	C23-N22	4.35	1.53	1.44
5	A	1003	MGD	C17-C16	4.42	1.47	1.41
5	E	1003	MGD	C19-N19	4.53	1.43	1.34
5	C	1003	MGD	C23-N22	4.58	1.54	1.44
5	A	1003	MGD	C19-N19	4.62	1.43	1.34
5	A	1003	MGD	C6-N1	4.92	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1003	MGD	C19-N19	4.93	1.44	1.34
5	C	1003	MGD	C6-N1	5.06	1.42	1.33
5	E	1003	MGD	C6-N1	5.11	1.42	1.33
5	E	1003	MGD	C23-N22	5.18	1.55	1.44
5	A	1003	MGD	C4-N3	5.20	1.44	1.35
5	C	1003	MGD	C3'-C4'	5.24	1.67	1.53
5	E	1003	MGD	C3'-C4'	5.24	1.67	1.53
5	A	1003	MGD	C6-C5	5.34	1.52	1.41
5	C	1003	MGD	C6-C5	5.39	1.52	1.41
5	A	1003	MGD	C3'-C4'	5.45	1.67	1.53
5	E	1003	MGD	C6-C5	5.64	1.52	1.41
5	E	1003	MGD	C4-N3	5.72	1.44	1.35
5	C	1003	MGD	C4-N3	5.92	1.45	1.35
5	C	1003	MGD	O4'-C1'	6.20	1.50	1.41
5	E	1003	MGD	C14-N15	6.61	1.53	1.45
5	C	1003	MGD	C19-N20	6.73	1.48	1.35
5	E	1003	MGD	O4'-C1'	6.87	1.51	1.41
5	C	1003	MGD	C17-N18	7.21	1.46	1.33
5	A	1003	MGD	O4'-C1'	7.23	1.51	1.41
5	E	1003	MGD	C17-N18	7.33	1.46	1.33
5	A	1003	MGD	C19-N20	7.38	1.49	1.35
5	E	1003	MGD	C19-N20	7.47	1.49	1.35
5	C	1003	MGD	C14-N15	7.47	1.54	1.45
6	E	1004	MD1	O4'-C1'	7.57	1.60	1.42
6	A	1004	MD1	O4'-C1'	7.68	1.61	1.42
6	C	1004	MD1	O4'-C1'	7.86	1.61	1.42
5	A	1003	MGD	C17-N18	7.88	1.47	1.33
5	A	1003	MGD	C14-N15	8.14	1.55	1.45
5	E	1003	MGD	O11-C11	10.19	1.58	1.43
5	A	1003	MGD	C19-N18	10.30	1.54	1.35
5	A	1003	MGD	O11-C11	10.92	1.59	1.43
5	C	1003	MGD	C19-N18	10.96	1.56	1.35
6	E	1004	MD1	C7-N8	11.07	1.40	1.27
5	C	1003	MGD	C16-C21	11.09	1.62	1.41
5	E	1003	MGD	C19-N18	11.26	1.56	1.35
5	C	1003	MGD	O11-C11	11.67	1.60	1.43
5	E	1003	MGD	C16-C21	11.96	1.63	1.41
5	A	1003	MGD	C16-C21	12.31	1.64	1.41
6	C	1004	MD1	C7-N8	12.41	1.41	1.27
6	A	1004	MD1	C7-N8	13.78	1.43	1.27

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1003	MGD	N3-C2-N1	-7.02	118.01	127.56
5	C	1003	MGD	C4'-O4'-C1'	-7.02	102.21	109.64
5	C	1003	MGD	N3-C2-N1	-6.02	119.36	127.56
5	E	1003	MGD	N3-C2-N1	-5.80	119.67	127.56
5	E	1003	MGD	C4'-O4'-C1'	-4.34	105.05	109.64
5	A	1003	MGD	C6-C5-C4	-4.31	115.93	120.86
5	C	1003	MGD	N18-C19-N20	-3.99	118.99	125.51
5	E	1003	MGD	C5-C6-N1	-3.90	118.43	123.52
5	A	1003	MGD	N18-C19-N20	-3.62	119.60	125.51
6	C	1004	MD1	O11-C11-C12	-3.59	104.16	111.16
5	C	1003	MGD	C5-C6-N1	-3.53	118.90	123.52
5	A	1003	MGD	C4'-O4'-C1'	-3.42	106.02	109.64
5	A	1003	MGD	C5-C6-N1	-3.38	119.11	123.52
6	A	1004	MD1	N17-C17-N18	-3.34	120.06	125.51
5	E	1003	MGD	N18-C19-N20	-3.15	120.37	125.51
6	A	1004	MD1	O11-C11-C12	-3.13	105.06	111.16
6	C	1004	MD1	N17-C17-N18	-2.94	120.71	125.51
6	E	1004	MD1	O6-C6-N1	-2.92	118.97	122.80
5	C	1003	MGD	C6-C5-C4	-2.86	117.59	120.86
6	E	1004	MD1	N17-C17-N18	-2.64	121.20	125.51
5	A	1003	MGD	O3'-C3'-C4'	-2.52	103.48	111.01
5	C	1003	MGD	C21-C16-N15	-2.35	115.80	118.83
5	A	1003	MGD	C21-C16-N15	-2.26	115.91	118.83
6	C	1004	MD1	O6-C6-N1	-2.18	119.93	122.80
5	E	1003	MGD	C6-C5-C4	-2.15	118.40	120.86
6	C	1004	MD1	C8-N9-C4	2.03	107.09	104.78
6	A	1004	MD1	N16-C17-N18	2.14	120.73	117.20
5	E	1003	MGD	C19-N20-C21	2.15	119.46	114.63
5	E	1003	MGD	N19-C19-N18	2.19	120.82	117.20
5	E	1003	MGD	C2'-C3'-C4'	2.23	107.20	102.64
5	C	1003	MGD	C19-N20-C21	2.39	120.00	114.63
5	A	1003	MGD	N22-C21-N20	2.45	120.52	116.62
6	E	1004	MD1	C8-N9-C4	2.49	107.62	104.78
6	C	1004	MD1	C15-N17-C17	2.54	118.86	115.88
5	A	1003	MGD	C2'-C3'-C4'	2.60	107.95	102.64
6	A	1004	MD1	C8-N9-C4	2.62	107.76	104.78
5	C	1003	MGD	O4'-C1'-N9	2.72	113.25	108.11
6	C	1004	MD1	N16-C17-N17	2.83	121.88	117.20
6	E	1004	MD1	N16-C17-N17	2.86	121.91	117.20
5	A	1003	MGD	C19-N20-C21	2.89	121.11	114.63
5	C	1003	MGD	N2-C2-N1	2.91	122.00	117.20
6	C	1004	MD1	C4-C5-N7	2.93	107.25	102.67
5	C	1003	MGD	C2'-C1'-N9	3.12	121.82	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	1003	MGD	C2'-C1'-N9	3.14	121.87	113.47
6	E	1004	MD1	C15-N17-C17	3.24	119.68	115.88
5	A	1003	MGD	N19-C19-N18	3.30	122.65	117.20
8	A	1013	BSY	O2-SE-O3	3.32	107.54	100.38
5	C	1003	MGD	N22-C21-N20	3.40	122.04	116.62
6	A	1004	MD1	C4-C5-N7	3.44	108.04	102.67
5	C	1003	MGD	N19-C19-N18	3.45	122.89	117.20
5	A	1003	MGD	C17-C16-C21	3.46	117.65	114.61
6	E	1004	MD1	C4-C5-N7	3.51	108.14	102.67
5	A	1003	MGD	C2'-C1'-N9	3.51	122.87	113.47
5	E	1003	MGD	N22-C21-N20	3.67	122.46	116.62
8	E	1008	BSY	O2-SE-O3	3.76	108.49	100.38
5	C	1003	MGD	O11-C23-C14	3.76	111.53	108.96
5	E	1003	MGD	N2-C2-N1	3.89	123.61	117.20
6	A	1004	MD1	C15-N17-C17	4.02	120.59	115.88
5	E	1003	MGD	C17-N18-C19	4.29	120.91	115.88
5	A	1003	MGD	C17-N18-C19	4.34	120.97	115.88
5	A	1003	MGD	N2-C2-N1	4.38	124.43	117.20
5	E	1003	MGD	C6-N1-C2	4.59	121.27	115.88
5	C	1003	MGD	C17-C16-C21	4.65	118.70	114.61
8	C	1009	BSY	O2-SE-O3	4.71	110.56	100.38
5	C	1003	MGD	C6-N1-C2	5.08	121.83	115.88
5	E	1003	MGD	C17-C16-C21	5.15	119.15	114.61
5	C	1003	MGD	C17-N18-C19	5.26	122.05	115.88
5	A	1003	MGD	C6-N1-C2	5.81	122.69	115.88
5	A	1003	MGD	C1'-N9-C4	17.09	145.88	126.81
5	E	1003	MGD	C1'-N9-C4	20.36	149.52	126.81
5	C	1003	MGD	C1'-N9-C4	20.38	149.55	126.81

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

18 monomers are involved in 41 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1003	MGD	1	0
7	A	1005	EDO	1	0
7	A	1010	EDO	5	0
7	A	1012	EDO	1	0
8	A	1013	BSY	2	0
7	B	407	EDO	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	408	EDO	5	0
7	B	409	EDO	3	0
7	B	410	EDO	6	0
5	C	1003	MGD	2	0
7	C	1007	EDO	1	0
8	C	1009	BSY	3	0
3	D	404	SF4	1	0
7	D	405	EDO	1	0
5	E	1003	MGD	1	0
6	E	1004	MD1	3	0
7	E	1005	EDO	1	0
8	E	1008	BSY	2	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	895/899 (99%)	-0.09	19 (2%) 67 70	19, 32, 51, 66	0
1	C	892/899 (99%)	0.05	41 (4%) 36 41	21, 37, 58, 96	0
1	E	892/899 (99%)	-0.04	33 (3%) 45 49	18, 33, 61, 77	0
2	B	329/333 (98%)	-0.34	4 (1%) 81 83	20, 27, 41, 88	0
2	D	328/333 (98%)	0.56	29 (8%) 12 14	26, 52, 70, 92	0
2	F	328/333 (98%)	-0.15	2 (0%) 90 91	22, 35, 53, 65	0
All	All	3664/3696 (99%)	-0.01	128 (3%) 48 52	18, 34, 60, 96	0

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	9	PHE	9.6
1	C	8	ALA	8.4
2	B	5	MET	7.2
2	B	6	LYS	4.4
1	C	298	GLY	4.3
2	D	6	LYS	4.1
2	D	7	ALA	4.1
1	C	11	TYR	4.0
1	E	315	VAL	3.5
1	C	297	ALA	3.5
1	E	362	MET	3.5
1	C	34	VAL	3.4
1	E	366	ASP	3.4
1	E	365	LEU	3.4
1	C	366	ASP	3.3
1	A	327	LYS	3.3
2	D	311	LEU	3.2
1	E	314	PRO	3.2
1	A	8	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
2	D	8	PRO	3.2
1	E	361	ASN	3.1
1	E	327	LYS	3.1
1	C	351	ASP	3.1
1	A	370	VAL	3.0
1	C	207	THR	3.0
1	C	458	ILE	3.0
1	C	770	HIS	3.0
1	E	286	THR	3.0
1	A	358	GLY	3.0
1	C	769	VAL	3.0
1	E	297	ALA	2.9
1	E	296	VAL	2.9
2	D	73	LEU	2.9
2	D	154	ILE	2.9
1	E	370	VAL	2.9
2	D	240	TYR	2.9
1	C	10	GLU	2.8
2	D	170	CYS	2.8
1	C	37	THR	2.8
1	A	310	LYS	2.8
2	D	68	TYR	2.8
1	E	309	ALA	2.7
1	E	381	SER	2.7
1	C	296	VAL	2.7
1	A	364	LEU	2.7
1	E	501	ILE	2.7
1	A	328	LYS	2.7
1	C	168	TYR	2.6
1	E	312	GLY	2.6
1	E	298	GLY	2.6
1	C	459	GLY	2.6
1	C	773	PHE	2.6
1	C	309	ALA	2.6
2	D	146	LEU	2.6
2	D	9	ARG	2.5
1	A	769	VAL	2.5
1	A	458	ILE	2.5
1	C	74	CYS	2.5
2	D	145	CYS	2.5
1	E	209	ILE	2.5
1	E	168	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	363	GLN	2.5
1	A	326	GLU	2.5
1	A	297	ALA	2.5
1	C	209	ILE	2.5
1	A	36	CYS	2.5
1	C	139	VAL	2.4
1	C	210	PRO	2.4
1	A	299	GLY	2.4
2	D	69	LYS	2.4
1	A	39	ALA	2.4
2	D	250	PHE	2.4
1	E	360	PHE	2.4
1	C	368	LYS	2.4
2	D	148	ALA	2.4
1	C	768	SER	2.4
1	E	372	VAL	2.4
1	C	165	TYR	2.3
1	A	139	VAL	2.3
2	D	78	ILE	2.3
2	B	70	ASN	2.3
2	F	272	GLY	2.3
2	D	150	PRO	2.3
2	D	312	ALA	2.3
1	C	365	LEU	2.3
2	D	309	LYS	2.3
2	D	229	VAL	2.3
2	D	158	GLU	2.3
1	E	769	VAL	2.3
1	C	765	SER	2.3
2	D	65	GLY	2.2
1	C	764	HIS	2.2
1	E	377	GLU	2.2
2	D	242	VAL	2.2
1	E	307	TRP	2.2
1	C	899	PHE	2.2
1	A	770	HIS	2.2
1	C	290	LEU	2.2
1	A	459	GLY	2.2
2	F	6	LYS	2.2
1	C	299	GLY	2.2
1	E	310	LYS	2.1
1	C	164	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	210	PRO	2.1
2	D	171	LYS	2.1
1	C	169	GLY	2.1
2	D	151	ASN	2.1
1	C	370	VAL	2.1
2	D	299	ILE	2.1
1	C	76	LYS	2.1
2	B	69	LYS	2.1
2	D	174	GLN	2.1
2	D	152	GLU	2.1
1	E	458	ILE	2.1
1	E	207	THR	2.1
1	E	328	LYS	2.1
1	A	168	TYR	2.1
1	E	17	PHE	2.1
1	E	384	MET	2.0
1	E	205	THR	2.0
1	C	457	TYR	2.0
2	D	24	CYS	2.0
1	C	631	LYS	2.0
1	A	164	PHE	2.0
1	C	167	TRP	2.0
1	C	420	CYS	2.0
1	C	771	SER	2.0
1	E	355	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
7	EDO	A	1010	4/4	0.69	0.47	11.96	33,35,36,40	0
7	EDO	B	409	4/4	0.79	0.25	10.46	26,28,32,33	0
7	EDO	A	1008	4/4	0.85	0.27	9.55	31,36,38,40	0
7	EDO	B	407	4/4	0.77	0.26	8.98	29,36,39,43	0
7	EDO	F	406	4/4	0.83	0.22	6.85	28,28,37,41	0
7	EDO	C	1007	4/4	0.85	0.19	6.71	26,32,34,44	0
13	GOL	E	1006	6/6	0.77	0.30	5.68	37,42,45,46	0
7	EDO	C	1006	4/4	0.86	0.26	5.35	47,49,50,52	0
7	EDO	C	1005	4/4	0.85	0.21	4.99	31,39,40,45	0
7	EDO	A	1012	4/4	0.93	0.26	4.78	24,24,27,39	0
7	EDO	F	405	4/4	0.98	0.15	4.69	25,27,30,30	0
7	EDO	A	1009	4/4	0.73	0.23	3.84	33,38,41,43	0
7	EDO	E	1005	4/4	0.82	0.23	3.52	34,35,40,43	0
10	NA	E	1010	1/1	0.99	0.18	3.17	19,19,19,19	0
7	EDO	B	410	4/4	0.95	0.23	3.10	25,30,31,31	0
10	NA	C	1011	1/1	0.99	0.24	2.99	27,27,27,27	0
10	NA	A	1015	1/1	0.96	0.18	2.80	23,23,23,23	0
7	EDO	A	1019	4/4	0.94	0.12	2.22	26,28,29,34	0
9	SO3	A	1014	4/4	0.91	0.15	2.10	50,54,61,82	0
7	EDO	A	1005	4/4	0.92	0.15	2.02	27,28,34,35	0
10	NA	B	406	1/1	0.94	0.13	1.70	44,44,44,44	0
7	EDO	A	1018	4/4	0.83	0.22	1.64	44,44,45,47	0
7	EDO	B	408	4/4	0.93	0.20	1.60	27,30,30,32	0
9	SO3	E	1009	4/4	0.91	0.13	1.32	52,52,70,86	0
8	BSY	A	1013	4/4	0.96	0.27	1.06	31,35,43,64	4
7	EDO	A	1007	4/4	0.95	0.13	0.67	28,31,33,35	0
7	EDO	B	405	4/4	0.98	0.11	0.65	22,22,24,24	0
7	EDO	A	1006	4/4	0.93	0.16	0.57	35,36,39,39	0
7	EDO	A	1011	4/4	0.96	0.12	0.54	28,28,32,32	0
8	BSY	E	1008	4/4	0.97	0.23	0.51	34,35,38,59	4
5	MGD	C	1003	47/47	0.97	0.24	0.34	18,27,32,35	0
5	MGD	A	1003	47/47	0.98	0.19	0.12	17,24,28,30	0
5	MGD	E	1003	47/47	0.96	0.19	0.11	19,28,33,36	0
6	MD1	A	1004	47/47	0.98	0.16	-0.02	20,27,31,35	0
7	EDO	E	1007	4/4	0.92	0.10	-0.04	38,42,43,43	0
6	MD1	E	1004	47/47	0.98	0.16	-0.08	19,25,32,34	0
3	SF4	F	404	8/8	0.98	0.11	-0.13	26,28,30,31	0
6	MD1	C	1004	47/47	0.97	0.17	-0.27	22,28,33,35	0
3	SF4	B	404	8/8	0.99	0.11	-0.40	22,23,24,26	0
3	SF4	B	402	8/8	0.98	0.08	-0.52	21,25,27,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
9	SO3	C	1010	4/4	0.88	0.12	-0.59	60,65,68,83	0
3	SF4	D	403	8/8	0.98	0.14	-0.62	40,42,48,52	0
10	NA	E	1011	1/1	0.97	0.11	-0.69	25,25,25,25	0
7	EDO	D	405	4/4	0.97	0.10	-0.88	30,32,34,36	0
3	SF4	E	1001	8/8	0.99	0.13	-1.01	21,25,28,29	0
8	BSY	C	1009	4/4	0.98	0.23	-1.27	33,35,39,51	4
3	SF4	F	403	8/8	0.98	0.13	-1.27	25,31,35,39	0
3	SF4	A	1001	8/8	0.99	0.15	-1.46	21,23,27,27	0
3	SF4	D	404	8/8	0.97	0.10	-1.46	38,45,52,53	0
3	SF4	C	1001	8/8	0.98	0.15	-1.51	32,34,36,38	0
3	SF4	B	403	8/8	0.99	0.12	-2.39	18,25,28,32	0
12	F3S	F	401	7/7	0.98	0.04	-2.61	29,33,35,36	0
12	F3S	B	401	7/7	0.99	0.05	-2.66	27,29,30,32	0
3	SF4	D	402	8/8	0.94	0.06	-2.87	37,49,57,58	0
12	F3S	D	401	7/7	0.96	0.05	-3.23	52,58,67,67	0
3	SF4	F	402	8/8	0.98	0.07	-3.24	31,34,36,37	0
4	MO	E	1002	1/1	0.99	0.10	-4.41	34,34,34,34	0
4	MO	A	1002	1/1	1.00	0.10	-4.56	35,35,35,35	0
4	MO	C	1002	1/1	1.00	0.12	-5.40	35,35,35,35	0
10	NA	A	1016	1/1	0.94	0.12	-	46,46,46,46	0
11	ZN	C	1013	1/1	0.94	0.07	-	82,82,82,82	0
10	NA	C	1012	1/1	0.96	0.18	-	42,42,42,42	0
7	EDO	C	1008	4/4	0.90	0.26	-	37,40,43,47	0
11	ZN	A	1017	1/1	0.99	0.03	-	57,57,57,57	0
10	NA	E	1012	1/1	0.87	0.18	-	48,48,48,48	0
11	ZN	E	1013	1/1	0.98	0.08	-	52,52,52,52	0

6.5 Other polymers (i)

There are no such residues in this entry.