Full wwPDB X-ray Structure Validation Report ⓘ

May 2, 2016 – 06:29 PM EDT

PDB ID	:	4YDD
Title	:	Crystal structure of the perchlorate reductase PcrAB from Azospira suillum PS
Authors	:	Tsai, C.-L.; Youngblut, M.D.; Tainer, J.A.
Deposited on	:	2015-02-21
Resolution	:	1.86 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 ①) were used in the production of this report:

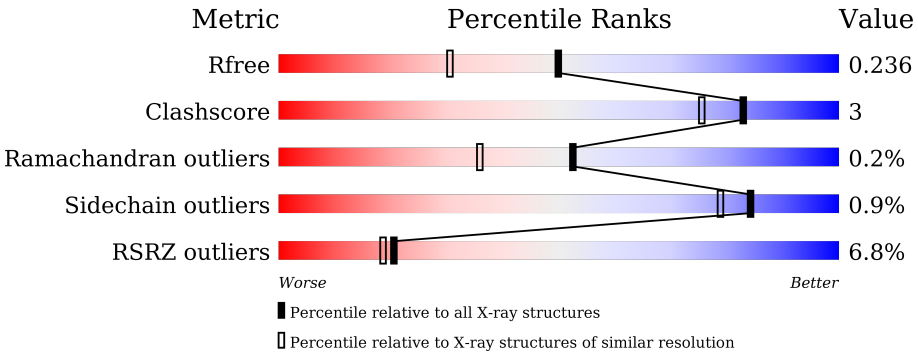
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027457
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.86 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	1745 (1.86-1.86)
Clashscore	102246	1898 (1.86-1.86)
Ramachandran outliers	100387	1875 (1.86-1.86)
Sidechain outliers	100360	1875 (1.86-1.86)
RSRZ outliers	91569	1747 (1.86-1.86)

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	5% 93% 6%
1	C	899	8% 92% 7%
1	E	899	7% 90% 8%
2	B	333	% 93% 5%
2	D	333	19% 88% 10%
2	F	333	2% 94% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	GOL	C	1006	-	-	-	X
11	PEG	C	1008	-	-	-	X
7	EDO	A	1008	-	-	-	X
7	EDO	A	1010	-	-	-	X
7	EDO	B	406	-	-	-	X
7	EDO	C	1005	-	-	-	X
7	EDO	C	1007	-	-	-	X
7	EDO	E	1005	-	-	-	X
7	EDO	E	1006	-	-	-	X
7	EDO	E	1007	-	-	-	X
7	EDO	E	1008	-	-	-	X
7	EDO	E	1010	-	-	-	X

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 61265 atoms, of which 28814 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.

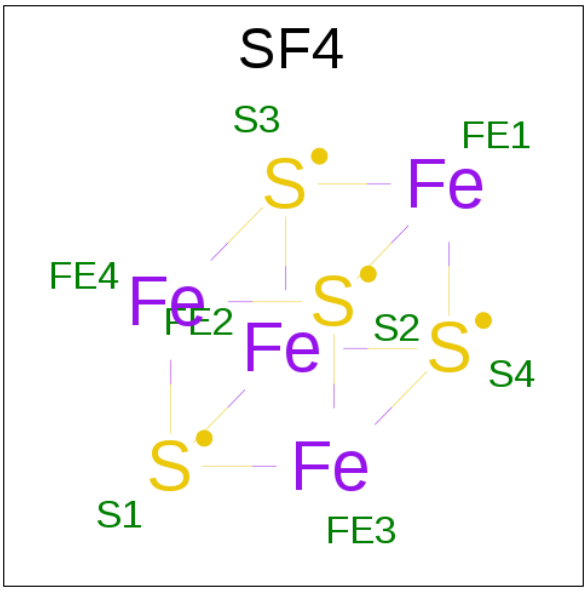
- Molecule 1 is a protein called DMSO reductase family type II enzyme, molybdopterin subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	895	Total	C	H	N	O	S	0	3	0
			14201	4589	7016	1247	1311	38			
1	C	892	Total	C	H	N	O	S	0	0	0
			14110	4563	6962	1240	1307	38			
1	E	892	Total	C	H	N	O	S	0	2	0
			14140	4575	6977	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	H	N	O	S	0	0	0
			5098	1627	2534	447	465	25			
2	D	328	Total	C	H	N	O	S	0	0	0
			5081	1622	2525	446	464	24			
2	F	328	Total	C	H	N	O	S	0	1	0
			5095	1626	2533	447	465	24			

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

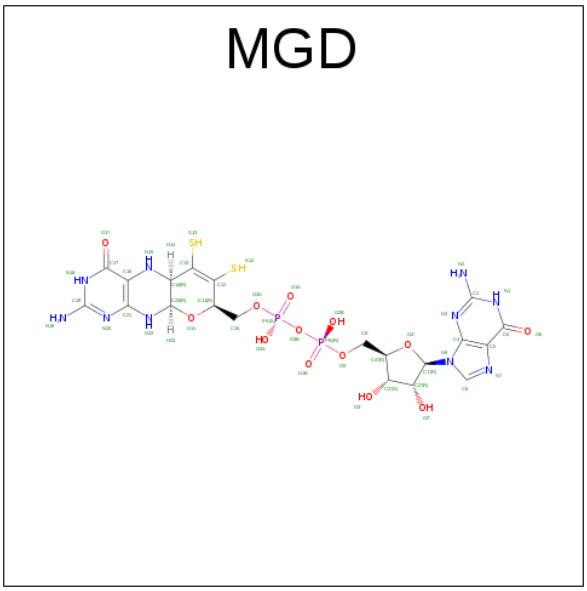


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Fe S 8 4 4	0	0
3	B	1	Total Fe S 8 4 4	0	0
3	B	1	Total Fe S 8 4 4	0	0
3	B	1	Total Fe S 8 4 4	0	0
3	C	1	Total Fe S 8 4 4	0	0
3	D	1	Total Fe S 8 4 4	0	0
3	D	1	Total Fe S 8 4 4	0	0
3	D	1	Total Fe S 8 4 4	0	0
3	E	1	Total Fe S 8 4 4	0	0
3	F	1	Total Fe S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

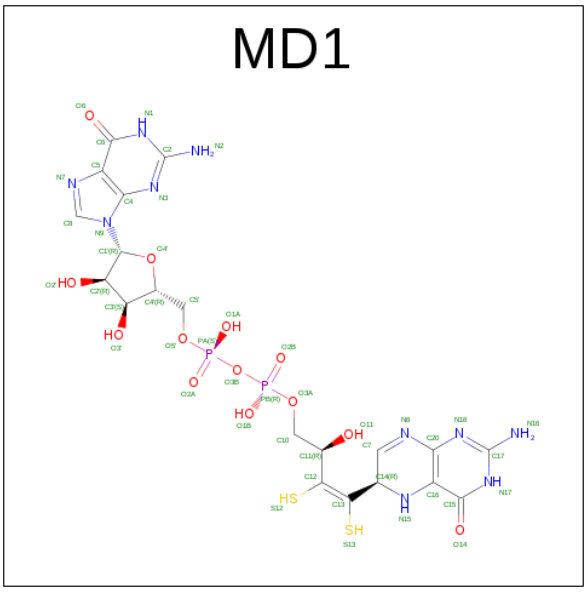
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mo 1 1	0	0
4	C	1	Total Mo 1 1	0	0
4	E	1	Total Mo 1 1	0	0

- 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: $C_{20}H_{26}N_{10}O_{13}P_2S_2$).



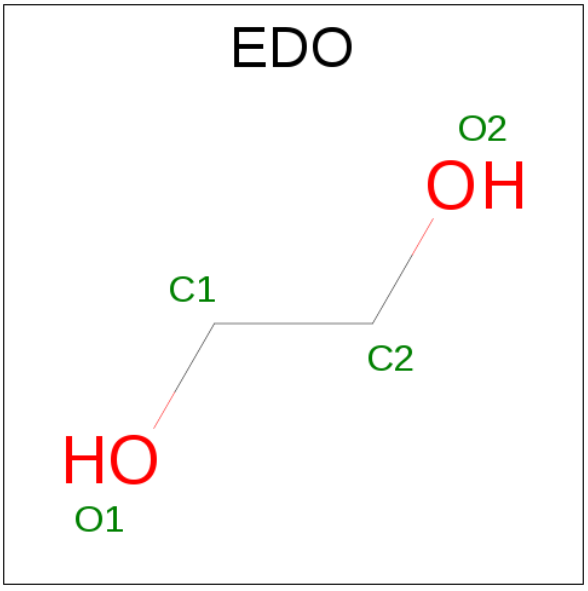
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
5	A	1	Total 70	C 20	H 23	N 10	O 13	P 2	S 2	0	0
5	C	1	Total 70	C 20	H 23	N 10	O 13	P 2	S 2	0	0
5	E	1	Total 70	C 20	H 23	N 10	O 13	P 2	S 2	0	0

- 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	H	N	O	P	S	0	0
			71	20	24	10	13	2	2		
6	C	1	Total	C	H	N	O	P	S	0	0
			71	20	24	10	13	2	2		
6	E	1	Total	C	H	N	O	P	S	0	0
			71	20	24	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	H	O	0	0
			10	2	6	2		

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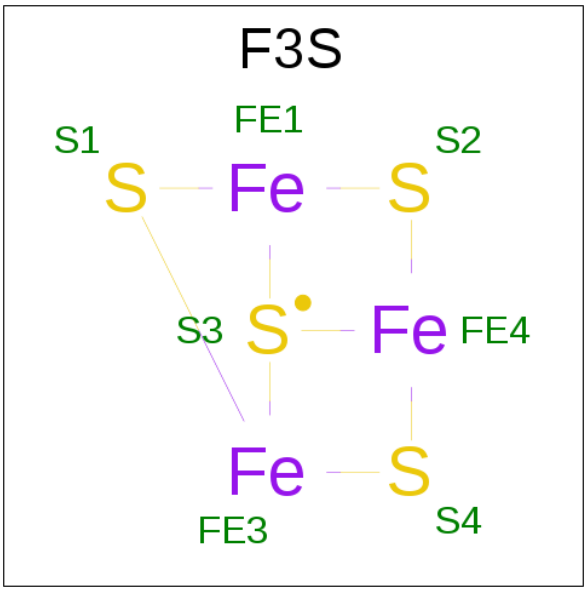
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C H O 10 2 6 2	0	0
7	A	1	Total C H O 10 2 6 2	0	0
7	A	1	Total C H O 10 2 6 2	0	0
7	A	1	Total C H O 10 2 6 2	0	0
7	A	1	Total C H O 10 2 6 2	0	0
7	B	1	Total C H O 10 2 6 2	0	0
7	B	1	Total C H O 10 2 6 2	0	0
7	C	1	Total C H O 10 2 6 2	0	0
7	C	1	Total C H O 10 2 6 2	0	0
7	D	1	Total C H O 10 2 6 2	0	0
7	E	1	Total C H O 10 2 6 2	0	0
7	E	1	Total C H O 10 2 6 2	0	0
7	E	1	Total C H O 10 2 6 2	0	0
7	E	1	Total C H O 10 2 6 2	0	0
7	E	1	Total C H O 10 2 6 2	0	0
7	E	1	Total C H O 10 2 6 2	0	0
7	F	1	Total C H O 10 2 6 2	0	0

- Molecule 8 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).

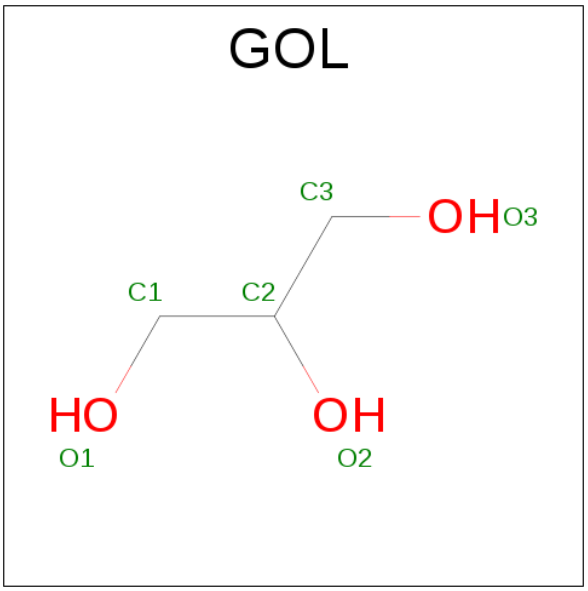


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total Fe S 7 3 4	0	0
8	D	1	Total Fe S 7 3 4	0	0
8	F	1	Total Fe S 7 3 4	0	0

- Molecule 9 is SODIUM ION (three-letter code: NA) (formula: Na).

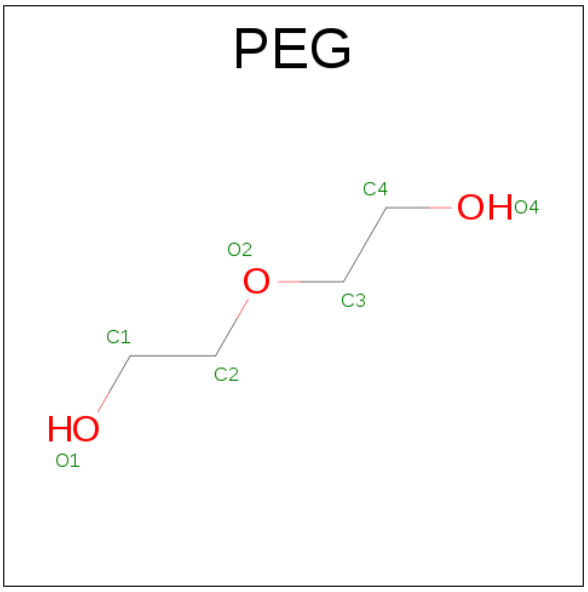
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total Na 1 1	0	0

- Molecule 10 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	C	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 11 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	C	1	Total	C	H	O	0	0
			17	4	10	3		

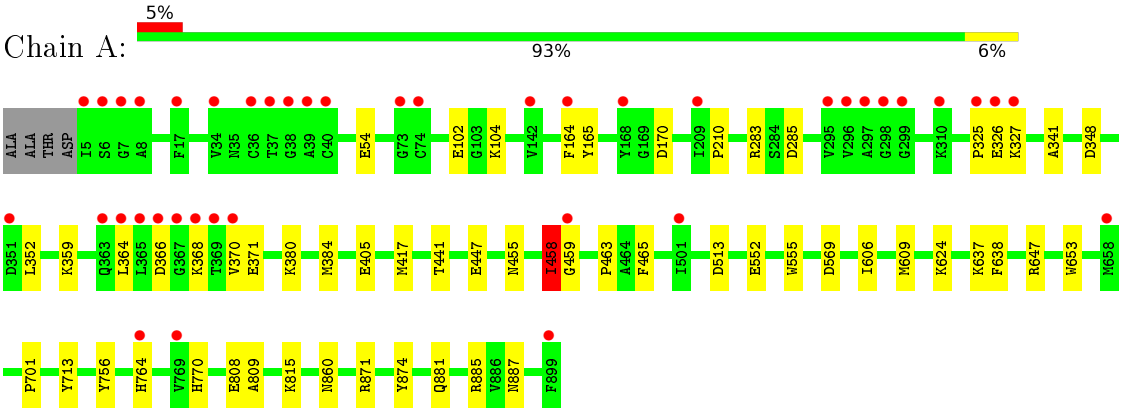
- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	738	Total O 738 738	0	0
12	B	357	Total O 358 358	0	1
12	C	575	Total O 576 576	0	1
12	D	140	Total O 141 141	0	1
12	E	681	Total O 681 681	0	0
12	F	291	Total O 291 291	0	0

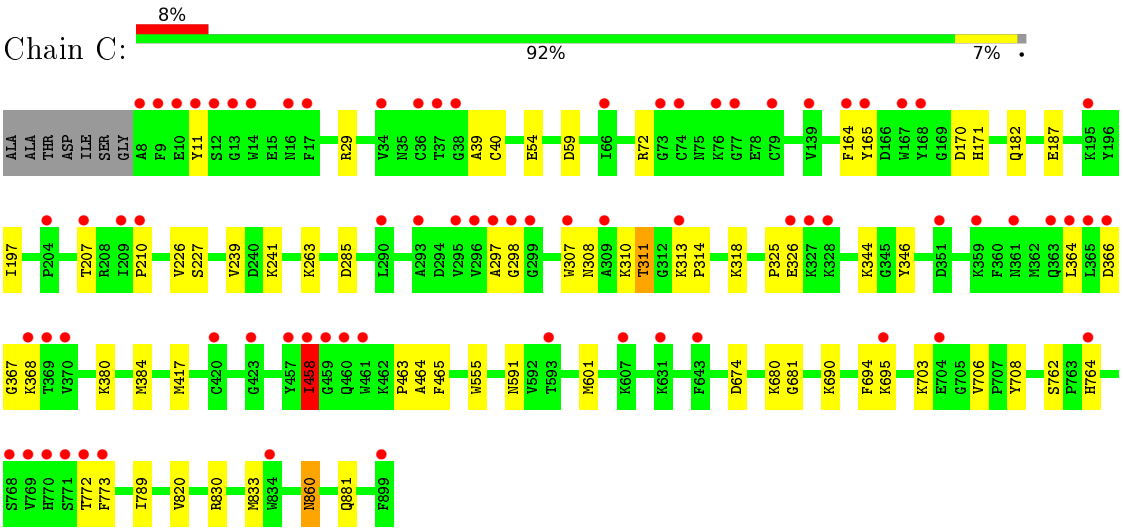
3 Residue-property plots (i)

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.

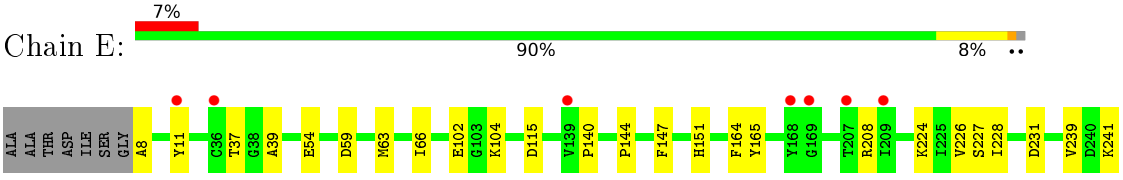
- Molecule 1: DMSO reductase family type II enzyme, molybdopterin subunit

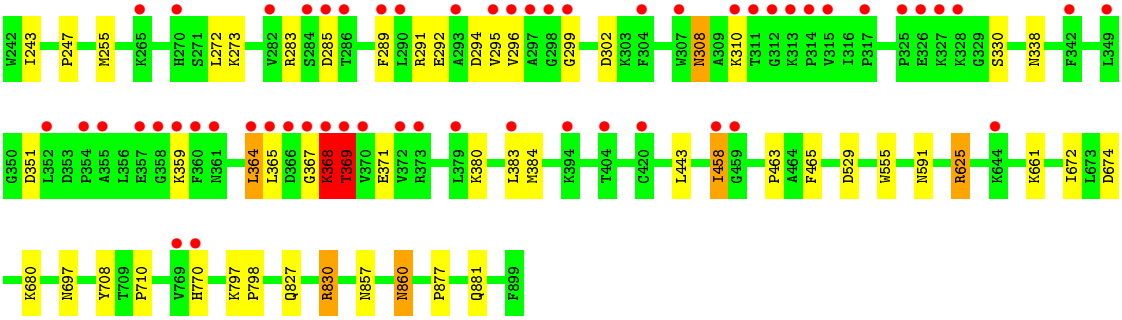


- Molecule 1: DMSO reductase family type II enzyme, molybdopterin subunit

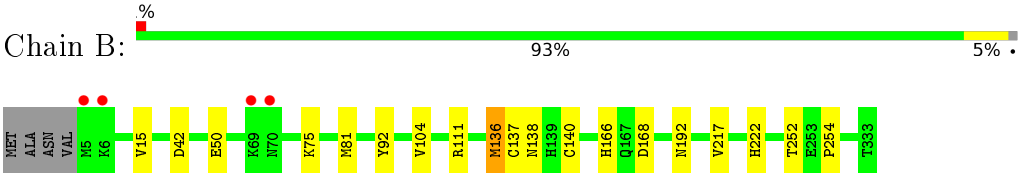


- Molecule 1: DMSO reductase family type II enzyme, molybdopterin subunit

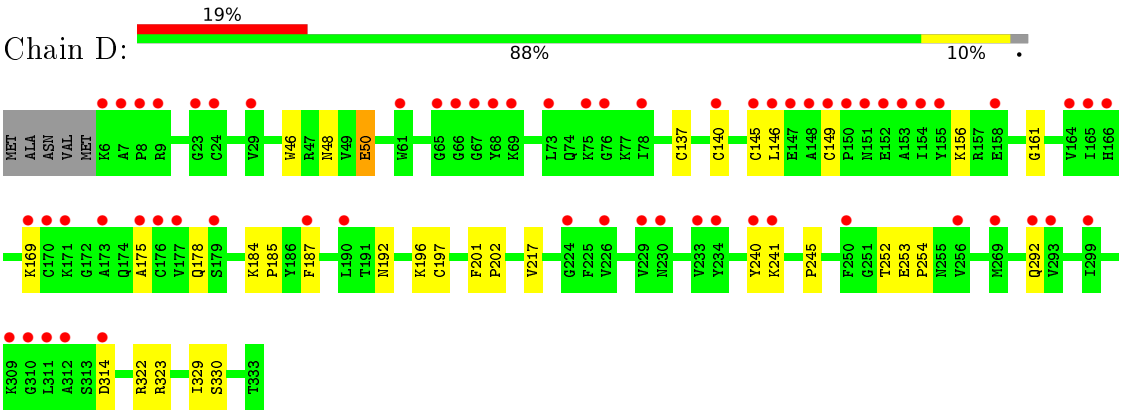




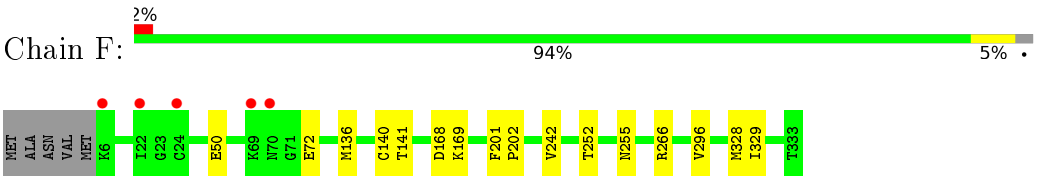
• Molecule 2: DMSO reductase family type II enzyme, iron-sulfur subunit



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



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



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	132.83Å 175.50Å 193.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.35 – 1.86 48.35 – 1.86	Depositor EDS
% Data completeness (in resolution range)	98.9 (48.35-1.86) 98.9 (48.35-1.86)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.23 (at 1.86Å)	Xtriage
Refinement program	PHENIX (dev_2299: ???)	Depositor
R, R_{free}	0.201 , 0.237 0.201 , 0.236	Depositor DCC
R_{free} test set	36317 reflections (5.01%)	DCC
Wilson B-factor (Å^2)	23.1	Xtriage
Anisotropy	0.444	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 39.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	61265	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.04% 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, PEG, MGD, NA, SF4, EDO, 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	0.51	0/7403	0.65	1/10045 (0.0%)
1	C	0.47	0/7357	0.64	0/9984
1	E	0.50	0/7379	0.68	6/10014 (0.1%)
2	B	0.55	0/2632	0.68	1/3567 (0.0%)
2	D	0.42	0/2624	0.61	0/3557
2	F	0.50	0/2633	0.66	0/3569
All	All	0.50	0/30028	0.65	8/40736 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	830	ARG	NE-CZ-NH2	-9.26	115.67	120.30
1	E	625	ARG	NE-CZ-NH2	-6.33	117.14	120.30
1	E	830	ARG	NE-CZ-NH1	6.24	123.42	120.30
2	B	81	MET	CG-SD-CE	-6.03	90.56	100.20
1	E	625	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	A	569	ASP	CB-CG-OD1	5.51	123.26	118.30
1	E	59	ASP	CB-CG-OD1	5.06	122.86	118.30
1	E	529	ASP	CB-CG-OD2	-5.04	113.76	118.30

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	7185	7016	7016	32	0
1	C	7148	6962	6960	44	0
1	E	7163	6977	6975	53	0
2	B	2564	2534	2534	11	0
2	D	2556	2525	2525	24	0
2	F	2562	2533	2533	10	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	23	21	0	0
5	C	47	23	21	1	0
5	E	47	23	21	1	0
6	A	47	24	22	5	0
6	C	47	24	21	4	0
6	E	47	24	21	4	0
7	A	24	36	36	1	0
7	B	8	12	12	0	0
7	C	8	12	12	0	0
7	D	4	6	6	0	0
7	E	24	36	36	0	0
7	F	4	6	6	0	0
8	B	7	0	0	0	0
8	D	7	0	0	1	0
8	F	7	0	0	0	0
9	B	1	0	0	0	0
10	C	6	8	8	0	0
11	C	7	10	10	1	0
12	A	738	0	0	7	1
12	B	358	0	0	2	2
12	C	576	0	0	3	0
12	D	141	0	0	0	0
12	E	681	0	0	7	2
12	F	291	0	0	2	1
All	All	32451	28814	28796	179	3

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 3.

All (179) 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:E:369:THR:O	12:E:1101:HOH:O	2.01	0.78
1:E:231:ASP:OD1	1:E:830:ARG:NH2	2.21	0.74
1:A:405:GLU:OE2	12:A:1101:HOH:O	2.06	0.73
1:E:368:LYS:O	1:E:369:THR:OG1	2.05	0.73
1:C:680:LYS:O	1:C:695:LYS:HE3	1.90	0.72
2:B:42:ASP:OD1	12:B:501:HOH:O	2.08	0.71
1:E:710:PRO:O	12:E:1102:HOH:O	2.11	0.69
2:F:168:ASP:OD1	12:F:501:HOH:O	2.12	0.67
6:E:1004:MD1:C11	6:E:1004:MD1:H7	2.25	0.67
1:E:273:LYS:O	12:E:1103:HOH:O	2.14	0.66
1:E:310:LYS:NZ	1:E:351:ASP:OD1	2.29	0.65
1:C:364:LEU:O	12:C:1101:HOH:O	2.15	0.63
1:C:366:ASP:N	1:C:367:GLY:HA2	2.13	0.63
1:C:11:TYR:CE1	2:D:169:LYS:HE3	2.33	0.62
6:A:1004:MD1:C11	6:A:1004:MD1:H7	2.31	0.61
6:A:1004:MD1:H11	6:A:1004:MD1:H7	1.84	0.60
1:C:308:ASN:O	1:C:310:LYS:N	2.32	0.59
1:E:380:LYS:O	1:E:384:MET:HG2	2.03	0.59
1:E:294:ASP:HB3	1:E:364:LEU:HD21	1.85	0.59
1:A:325:PRO:O	1:A:326:GLU:HB3	2.03	0.58
1:E:797:LYS:HB3	1:E:798:PRO:HD3	1.87	0.57
1:A:359:LYS:CE	1:A:371:GLU:OE2	2.53	0.57
2:D:196:LYS:HD2	3:D:402:SF4:S3	2.46	0.56
6:C:1004:MD1:H11	6:C:1004:MD1:H7	1.88	0.56
1:C:325:PRO:O	1:C:326:GLU:HB2	2.06	0.56
6:E:1004:MD1:H11	6:E:1004:MD1:H7	1.88	0.55
1:A:756:TYR:O	1:A:885[B]:ARG:HD3	2.07	0.55
2:D:175:ALA:HA	2:D:178:GLN:HE21	1.72	0.55
1:A:170:ASP:HB3	1:A:458:ILE:HD13	1.87	0.54
1:E:63:MET:HB2	1:E:66:ILE:HD11	1.88	0.53
1:A:352:LEU:O	12:A:1102:HOH:O	2.18	0.53
1:E:368:LYS:CG	1:E:369:THR:H	2.22	0.53
2:B:140:CYS:HB3	2:B:252:THR:O	2.10	0.52
2:D:187:PHE:CZ	2:D:192:ASN:HA	2.45	0.51
2:D:240:TYR:OH	2:D:314:ASP:OD2	2.23	0.51
1:C:366:ASP:OD1	1:C:368:LYS:N	2.40	0.51
1:E:860:ASN:N	1:E:860:ASN:HD22	2.07	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:175:ALA:HA	2:D:178:GLN:NE2	2.26	0.51
1:C:674:ASP:O	1:C:680:LYS:HD3	2.11	0.50
1:C:170:ASP:HB3	1:C:458:ILE:HD13	1.92	0.50
1:E:115:ASP:OD1	1:E:625:ARG:HD2	2.12	0.50
1:E:860:ASN:HB3	1:E:877:PRO:HA	1.94	0.50
1:A:770:HIS:CE1	6:A:1004:MD1:S12	3.04	0.50
1:A:283:ARG:HB3	1:A:285:ASP:OD1	2.11	0.50
1:C:307:TRP:CZ3	1:C:314:PRO:HG3	2.46	0.49
2:D:140:CYS:HB3	2:D:252:THR:O	2.12	0.49
1:A:764:HIS:HE2	6:A:1004:MD1:H15	1.59	0.49
1:C:681:GLY:HA3	1:C:695:LYS:HE3	1.95	0.49
1:C:680:LYS:O	1:C:695:LYS:CE	2.59	0.49
1:A:327:LYS:O	1:A:341:ALA:HB1	2.13	0.48
6:C:1004:MD1:C11	6:C:1004:MD1:H7	2.42	0.48
1:A:364:LEU:HD11	1:A:370:VAL:CG1	2.43	0.48
1:A:380:LYS:O	1:A:384:MET:HG2	2.13	0.48
1:E:308:ASN:HD22	1:E:308:ASN:C	2.17	0.48
1:E:359:LYS:HE2	1:E:371:GLU:OE2	2.13	0.48
1:A:441:THR:HG21	1:A:447:GLU:OE2	2.14	0.47
2:D:48:ASN:ND2	2:D:50:GLU:HG2	2.28	0.47
2:F:141:THR:HG22	12:F:526:HOH:O	2.13	0.47
2:D:46:TRP:O	2:D:184:LYS:NZ	2.36	0.47
1:E:302:ASP:OD1	12:E:1104:HOH:O	2.20	0.47
1:E:292:GLU:HG2	1:E:299:GLY:HA3	1.96	0.47
1:E:294:ASP:O	1:E:364:LEU:HD22	2.13	0.47
1:A:102:GLU:OE2	1:A:104:LYS:NZ	2.48	0.47
1:A:348:ASP:OD1	12:A:1103:HOH:O	2.20	0.47
1:C:860:ASN:HD22	1:C:860:ASN:N	2.13	0.47
1:C:464:ALA:HB3	1:C:694:PHE:CE1	2.49	0.46
1:E:115:ASP:OD1	1:E:625:ARG:CD	2.63	0.46
1:C:210:PRO:HA	2:D:217:VAL:CG1	2.45	0.46
1:C:311:THR:O	1:C:313:LYS:HG3	2.15	0.46
1:A:210:PRO:HA	2:B:217:VAL:CG1	2.46	0.46
6:E:1004:MD1:C11	6:E:1004:MD1:C7	2.94	0.46
1:C:366:ASP:OD1	1:C:368:LYS:HG3	2.16	0.46
1:E:226:VAL:HG22	1:E:241:LYS:HG2	1.98	0.46
1:C:764:HIS:HE2	6:C:1004:MD1:H15	1.64	0.46
1:C:366:ASP:N	1:C:367:GLY:CA	2.79	0.45
1:A:606:ILE:HD11	1:A:609:MET:CE	2.47	0.45
1:A:808:GLU:OE2	1:A:815:LYS:HD2	2.17	0.45
1:E:147:PHE:CE2	1:E:151:HIS:CE1	3.05	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:294:ASP:O	1:E:365:LEU:HB2	2.17	0.45
2:D:145:CYS:SG	2:D:146:LEU:N	2.89	0.45
1:E:368:LYS:C	1:E:369:THR:OG1	2.55	0.45
1:E:661:LYS:NZ	12:E:1128:HOH:O	2.49	0.45
1:C:197:ILE:HG12	1:C:417:MET:HG2	1.99	0.44
2:D:156:LYS:NZ	2:D:161:GLY:O	2.46	0.44
7:A:1010:EDO:H22	2:B:111:ARG:HG2	2.00	0.44
1:C:170:ASP:HB3	1:C:458:ILE:CD1	2.47	0.44
2:D:184:LYS:N	2:D:185:PRO:CD	2.81	0.44
1:C:171:HIS:HB3	12:C:1193:HOH:O	2.18	0.44
1:C:187:GLU:HG3	1:C:708:TYR:HB3	1.99	0.44
1:C:285:ASP:N	1:C:285:ASP:OD1	2.51	0.44
2:F:136:MET:HB2	2:F:136:MET:HE2	1.71	0.44
1:E:308:ASN:O	1:E:310:LYS:N	2.50	0.43
1:E:368:LYS:HG2	1:E:369:THR:H	1.82	0.43
1:E:39:ALA:HA	1:E:591:ASN:OD1	2.18	0.43
2:F:201:PHE:CG	2:F:202:PRO:HD3	2.53	0.43
1:C:59:ASP:HB2	1:C:690:LYS:HE2	1.99	0.43
1:E:285:ASP:N	1:E:285:ASP:OD1	2.52	0.43
1:A:459:GLY:HA3	12:A:1110:HOH:O	2.17	0.43
1:A:164:PHE:CD1	1:A:165:TYR:N	2.87	0.43
1:E:283:ARG:HB3	1:E:285:ASP:OD1	2.18	0.43
1:E:289:PHE:HB2	1:E:291:ARG:NH1	2.33	0.43
1:E:674:ASP:O	1:E:680:LYS:HD3	2.18	0.43
6:A:1004:MD1:C11	6:A:1004:MD1:C7	2.95	0.43
1:E:368:LYS:CG	1:E:369:THR:N	2.81	0.43
1:E:697:ASN:HB3	1:E:708:TYR:CE1	2.53	0.43
2:F:266:ARG:N	2:F:266:ARG:HD2	2.34	0.43
2:B:166:HIS:CE1	2:B:168:ASP:HB2	2.54	0.43
2:D:137:CYS:CB	2:D:197:CYS:HB3	2.49	0.43
2:D:292:GLN:CD	2:D:292:GLN:H	2.22	0.43
1:E:102:GLU:OE1	1:E:104:LYS:HE2	2.18	0.43
2:D:196:LYS:HG2	2:D:197:CYS:N	2.34	0.43
1:A:624:LYS:HE3	1:A:653:TRP:CD1	2.54	0.42
1:A:860:ASN:HD22	1:A:860:ASN:N	2.17	0.42
6:C:1004:MD1:C11	6:C:1004:MD1:C7	2.97	0.42
1:A:637:LYS:HA	1:A:647:ARG:O	2.19	0.42
2:D:149:CYS:HA	8:D:401:F3S:S4	2.58	0.42
1:C:318:LYS:HB3	1:C:346:TYR:CE2	2.55	0.42
1:C:29:ARG:HG2	1:C:601:MET:HG3	2.01	0.42
1:C:11:TYR:HE1	2:D:169:LYS:HE3	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:247:PRO:HD3	1:E:827:GLN:OE1	2.19	0.42
1:E:224:LYS:NZ	12:E:1106:HOH:O	2.30	0.42
1:E:295:VAL:HG12	1:E:296:VAL:HG23	2.00	0.42
1:A:701:PRO:HD3	1:A:713:TYR:CE1	2.55	0.42
1:C:40:CYS:SG	1:C:72:ARG:HB3	2.60	0.42
2:F:140:CYS:HB3	2:F:252:THR:O	2.20	0.42
1:A:417:MET:HG3	1:A:455:ASN:HD22	1.85	0.42
1:A:552:GLU:OE2	12:A:1105:HOH:O	2.22	0.42
2:D:240:TYR:O	2:D:241:LYS:HB3	2.19	0.42
1:E:227:SER:HB2	1:E:239:VAL:HG11	2.01	0.42
2:D:329:ILE:O	2:D:330:SER:C	2.58	0.41
2:B:92:TYR:CD1	2:B:104:VAL:HG11	2.55	0.41
1:C:39:ALA:HA	1:C:591:ASN:OD1	2.19	0.41
2:D:322:ARG:O	2:D:323:ARG:NH1	2.51	0.41
1:A:359:LYS:HE3	1:A:371:GLU:OE2	2.20	0.41
2:D:137:CYS:HB3	2:D:197:CYS:HB3	2.02	0.41
1:E:272:LEU:HD21	1:E:443:LEU:HA	2.03	0.41
1:E:8:ALA:N	12:E:1145:HOH:O	2.53	0.41
6:E:1004:MD1:O11	6:E:1004:MD1:H7	2.20	0.41
1:E:11[A]:TYR:CZ	2:F:169:LYS:HE3	2.56	0.41
1:E:37:THR:HG21	1:E:208:ARG:NH1	2.35	0.41
1:C:164:PHE:CD1	1:C:165:TYR:N	2.88	0.41
1:C:297:ALA:HA	1:C:298:GLY:HA2	1.83	0.41
1:E:330:SER:O	1:E:338:ASN:ND2	2.50	0.41
2:B:15:VAL:HB	2:B:222:HIS:HB2	2.02	0.41
12:A:1568:HOH:O	2:B:42:ASP:HB3	2.20	0.41
1:C:344:LYS:HE2	1:C:344:LYS:HB3	1.90	0.41
2:F:242:VAL:HA	2:F:296:VAL:HG13	2.03	0.41
2:F:141:THR:HG23	2:F:255:ASN:OD1	2.21	0.41
1:A:366:ASP:O	1:A:368:LYS:N	2.49	0.41
2:B:136:MET:HG2	2:B:137:CYS:O	2.20	0.41
1:C:789:ILE:O	1:C:820:VAL:HA	2.21	0.41
1:E:770:HIS:CE1	5:E:1003:MGD:S13	3.14	0.41
1:E:367:GLY:O	1:E:368:LYS:CB	2.68	0.41
2:D:201:PHE:CG	2:D:202:PRO:HD3	2.55	0.41
1:E:228:ILE:HA	1:E:243:ILE:O	2.21	0.41
1:A:513:ASP:OD1	12:A:1104:HOH:O	2.22	0.41
2:B:138:ASN:HB3	2:B:254:PRO:HB3	2.02	0.41
1:C:226:VAL:HG22	1:C:241:LYS:HG2	2.03	0.41
1:C:772:THR:HG22	1:C:773:PHE:CD2	2.56	0.41
1:C:464:ALA:HB3	1:C:694:PHE:CZ	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:703:LYS:HB2	1:C:706:VAL:HB	2.02	0.40
1:C:762:SER:HA	1:C:833:MET:O	2.21	0.40
1:A:809:ALA:HA	1:A:887:ASN:O	2.21	0.40
1:C:182:GLN:OE1	11:C:1008:PEG:H22	2.21	0.40
2:D:245:PRO:HB2	2:D:254:PRO:HG2	2.03	0.40
1:E:164:PHE:CD1	1:E:165:TYR:N	2.90	0.40
1:E:255:MET:HE3	1:E:383:LEU:HD21	2.02	0.40
2:F:328:MET:HG3	2:F:329:ILE:O	2.21	0.40
1:A:638:PHE:CZ	1:A:647:ARG:HD2	2.56	0.40
1:A:871:ARG:HB3	1:A:874:TYR:HB3	2.03	0.40
1:E:857:ASN:C	1:E:857:ASN:OD1	2.60	0.40
1:E:140:PRO:HB3	1:E:147:PHE:CD1	2.56	0.40
1:E:226:VAL:HG22	1:E:241:LYS:CG	2.52	0.40
2:B:75:LYS:HE2	12:B:555:HOH:O	2.21	0.40
1:C:207:THR:HA	5:C:1003:MGD:N20	2.36	0.40
1:C:227:SER:HB2	1:C:239:VAL:HG11	2.04	0.40
1:C:263:LYS:HE3	12:C:1129:HOH:O	2.20	0.40
1:C:380:LYS:O	1:C:384:MET:HG2	2.22	0.40
1:E:144:PRO:HB2	1:E:672:ILE:HD13	2.03	0.40

All (3) 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)
12:B:791:HOH:O	12:E:1471:HOH:O[4_477]	2.04	0.16
12:B:808:HOH:O	12:E:1633:HOH:O[4_477]	2.06	0.14
12:A:1703:HOH:O	12:F:578:HOH:O[2_874]	2.08	0.12

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	896/899 (100%)	864 (96%)	30 (3%)	2 (0%)	52 36
1	C	890/899 (99%)	851 (96%)	36 (4%)	3 (0%)	46 29
1	E	892/899 (99%)	854 (96%)	34 (4%)	4 (0%)	39 22
2	B	327/333 (98%)	316 (97%)	11 (3%)	0	100 100
2	D	326/333 (98%)	314 (96%)	12 (4%)	0	100 100
2	F	327/333 (98%)	316 (97%)	11 (3%)	0	100 100
All	All	3658/3696 (99%)	3515 (96%)	134 (4%)	9 (0%)	52 36

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	311	THR
1	C	458	ILE
1	E	369	THR
1	A	458	ILE
1	E	368	LYS
1	E	458	ILE
1	C	463	PRO
1	A	463	PRO
1	E	463	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	769/768 (100%)	764 (99%)	5 (1%)	88 84
1	C	764/768 (100%)	757 (99%)	7 (1%)	84 79
1	E	766/768 (100%)	756 (99%)	10 (1%)	76 65
2	B	278/281 (99%)	275 (99%)	3 (1%)	80 72
2	D	277/281 (99%)	275 (99%)	2 (1%)	88 84
2	F	278/281 (99%)	276 (99%)	2 (1%)	88 84
All	All	3132/3147 (100%)	3103 (99%)	29 (1%)	84 79

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	GLU
1	A	458	ILE
1	A	465	PHE
1	A	555	TRP
1	A	881	GLN
2	B	50	GLU
2	B	136	MET
2	B	192	ASN
1	C	54	GLU
1	C	458	ILE
1	C	465	PHE
1	C	555	TRP
1	C	830	ARG
1	C	860	ASN
1	C	881	GLN
2	D	50	GLU
2	D	253	GLU
1	E	54	GLU
1	E	308	ASN
1	E	364	LEU
1	E	368	LYS
1	E	369	THR
1	E	458	ILE
1	E	465	PHE
1	E	555	TRP
1	E	860	ASN
1	E	881	GLN
2	F	50	GLU
2	F	72	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	166	HIS
2	D	178	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 45 ligands modelled in this entry, 4 are monoatomic - leaving 41 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	5.94	25 (60%)	37,81,81	1.98	8 (21%)
6	MD1	A	1004	4	40,51,51	4.46	14 (35%)	33,78,78	1.37	3 (9%)
7	EDO	A	1005	-	3,3,3	0.48	0	2,2,2	0.15	0
7	EDO	A	1006	-	3,3,3	0.44	0	2,2,2	0.53	0
7	EDO	A	1007	-	3,3,3	0.47	0	2,2,2	0.43	0
7	EDO	A	1008	-	3,3,3	0.40	0	2,2,2	0.75	0
7	EDO	A	1009	-	3,3,3	0.51	0	2,2,2	0.68	0
7	EDO	A	1010	-	3,3,3	0.62	0	2,2,2	0.67	0
8	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	0.46	0	2,2,2	1.01	0
7	EDO	B	406	-	3,3,3	0.72	0	2,2,2	0.33	0
3	SF4	C	1001	1	0,12,12	0.00	-	0,24,24	0.00	-
5	MGD	C	1003	4	41,52,52	6.19	25 (60%)	37,81,81	2.37	7 (18%)
6	MD1	C	1004	4	40,51,51	4.63	12 (30%)	33,78,78	1.03	1 (3%)
7	EDO	C	1005	-	3,3,3	0.85	0	2,2,2	0.67	0
10	GOL	C	1006	-	5,5,5	0.49	0	5,5,5	0.31	0
7	EDO	C	1007	-	3,3,3	0.50	0	2,2,2	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	PEG	C	1008	-	6,6,6	0.60	0	5,5,5	0.57	0
8	F3S	D	401	2	0,9,9	0.00	-	0,15,15	0.00	-
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	0.45	0
3	SF4	E	1001	1	0,12,12	0.00	-	0,24,24	0.00	-
5	MGD	E	1003	4	41,52,52	6.26	25 (60%)	37,81,81	2.38	10 (27%)
6	MD1	E	1004	4	40,51,51	4.12	15 (37%)	33,78,78	1.67	7 (21%)
7	EDO	E	1005	-	3,3,3	0.72	0	2,2,2	0.54	0
7	EDO	E	1006	-	3,3,3	0.98	0	2,2,2	0.42	0
7	EDO	E	1007	-	3,3,3	0.63	0	2,2,2	0.26	0
7	EDO	E	1008	-	3,3,3	0.31	0	2,2,2	0.66	0
7	EDO	E	1009	-	3,3,3	0.56	0	2,2,2	0.48	0
7	EDO	E	1010	-	3,3,3	0.64	0	2,2,2	0.14	0
8	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	0.32	0	2,2,2	0.59	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	-	0/18/59/59	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
8	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
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	406	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-	0/18/59/59	0/5/5/5
7	EDO	C	1005	-	-	0/1/1/1	0/0/0/0
10	GOL	C	1006	-	-	0/4/4/4	0/0/0/0
7	EDO	C	1007	-	-	0/1/1/1	0/0/0/0
11	PEG	C	1008	-	-	0/4/4/4	0/0/0/0
8	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	-	0/18/59/59	0/5/5/5
7	EDO	E	1005	-	-	0/1/1/1	0/0/0/0
7	EDO	E	1006	-	-	0/1/1/1	0/0/0/0
7	EDO	E	1007	-	-	0/1/1/1	0/0/0/0
7	EDO	E	1008	-	-	0/1/1/1	0/0/0/0
7	EDO	E	1009	-	-	0/1/1/1	0/0/0/0
7	EDO	E	1010	-	-	0/1/1/1	0/0/0/0
8	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

All (116) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1003	MGD	C2'-C1'	-14.85	1.30	1.53
5	E	1003	MGD	C2'-C1'	-14.73	1.30	1.53
5	A	1003	MGD	C2'-C1'	-13.78	1.31	1.53
6	C	1004	MD1	C2'-C1'	-11.49	1.35	1.53
6	A	1004	MD1	C2'-C1'	-10.83	1.36	1.53
5	E	1003	MGD	C23-C14	-10.24	1.45	1.53
6	E	1004	MD1	C2'-C1'	-10.08	1.37	1.53
5	C	1003	MGD	C23-C14	-9.88	1.46	1.53
5	A	1003	MGD	C3'-C4'	-8.71	1.29	1.53
5	E	1003	MGD	C3'-C4'	-8.56	1.30	1.53
5	C	1003	MGD	C3'-C4'	-8.52	1.30	1.53
5	A	1003	MGD	C23-C14	-8.11	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1003	MGD	O11-C23	-6.22	1.34	1.43
6	C	1004	MD1	C16-C20	-5.98	1.32	1.41
5	A	1003	MGD	O11-C23	-5.65	1.35	1.43
6	A	1004	MD1	C16-C20	-5.64	1.33	1.41
6	E	1004	MD1	C16-C20	-5.63	1.33	1.41
5	E	1003	MGD	O11-C23	-5.26	1.36	1.43
6	C	1004	MD1	C6-N1	-5.23	1.29	1.36
6	A	1004	MD1	O4'-C4'	-5.02	1.33	1.45
6	C	1004	MD1	O4'-C4'	-4.94	1.33	1.45
6	E	1004	MD1	O4'-C4'	-4.07	1.35	1.45
6	E	1004	MD1	C6-N1	-3.50	1.31	1.36
6	C	1004	MD1	O3'-C3'	-3.30	1.35	1.43
6	A	1004	MD1	C15-C16	-3.05	1.37	1.41
6	E	1004	MD1	O3'-C3'	-3.04	1.35	1.43
6	E	1004	MD1	C15-C16	-2.96	1.37	1.41
6	A	1004	MD1	C15-N17	-2.87	1.32	1.36
5	C	1003	MGD	O17-C17	-2.41	1.18	1.24
6	A	1004	MD1	C4-N3	-2.39	1.32	1.35
6	A	1004	MD1	C6-N1	-2.26	1.33	1.36
5	A	1003	MGD	O17-C17	-2.19	1.19	1.24
6	A	1004	MD1	O3'-C3'	-2.19	1.37	1.43
5	E	1003	MGD	O6-C6	-2.18	1.19	1.24
6	C	1004	MD1	O14-C15	-2.09	1.19	1.24
6	E	1004	MD1	O14-C15	-2.08	1.19	1.24
6	E	1004	MD1	PB-O3A	2.02	1.67	1.59
5	E	1003	MGD	C13-C12	2.48	1.51	1.35
5	A	1003	MGD	C13-C12	2.54	1.52	1.35
5	C	1003	MGD	C13-C12	2.75	1.53	1.35
6	A	1004	MD1	C20-N8	2.89	1.45	1.38
6	C	1004	MD1	C20-N8	3.00	1.46	1.38
6	E	1004	MD1	C20-N8	3.02	1.46	1.38
6	E	1004	MD1	C2-N3	3.06	1.37	1.33
5	E	1003	MGD	C21-N20	3.47	1.40	1.34
5	E	1003	MGD	C6-N1	3.56	1.41	1.36
5	C	1003	MGD	C6-N1	3.71	1.41	1.36
5	C	1003	MGD	C21-N20	3.74	1.41	1.34
5	C	1003	MGD	C17-C16	3.97	1.47	1.41
5	E	1003	MGD	C2'-C3'	3.99	1.64	1.53
5	A	1003	MGD	C2'-C3'	4.02	1.64	1.53
5	C	1003	MGD	C2'-C3'	4.13	1.64	1.53
6	C	1004	MD1	C16-N15	4.15	1.47	1.38
6	A	1004	MD1	C16-N15	4.23	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	1003	MGD	C17-C16	4.24	1.47	1.41
5	C	1003	MGD	C2-N1	4.44	1.43	1.36
5	A	1003	MGD	C23-N22	4.47	1.53	1.44
5	A	1003	MGD	C6-N1	4.53	1.43	1.36
5	C	1003	MGD	O4'-C4'	4.53	1.55	1.45
5	A	1003	MGD	C17-C16	4.55	1.47	1.41
5	A	1003	MGD	C2-N1	4.69	1.43	1.36
5	A	1003	MGD	C21-N20	4.81	1.43	1.34
5	A	1003	MGD	O4'-C4'	4.85	1.56	1.45
6	E	1004	MD1	C16-N15	4.89	1.48	1.38
5	E	1003	MGD	O4'-C4'	4.94	1.56	1.45
5	A	1003	MGD	C6-C5	5.13	1.50	1.40
5	E	1003	MGD	C2-N1	5.26	1.44	1.36
5	E	1003	MGD	C23-N22	5.44	1.55	1.44
5	C	1003	MGD	C6-C5	5.47	1.51	1.40
5	C	1003	MGD	C23-N22	5.49	1.55	1.44
5	E	1003	MGD	C6-C5	5.99	1.52	1.40
6	E	1004	MD1	C17-N16	6.32	1.41	1.32
5	C	1003	MGD	C2-N2	6.74	1.42	1.32
5	A	1003	MGD	C19-N19	6.95	1.42	1.32
5	A	1003	MGD	C4-N3	7.03	1.46	1.35
5	A	1003	MGD	C17-N18	7.11	1.46	1.36
5	A	1003	MGD	C2-N2	7.26	1.43	1.32
6	A	1004	MD1	C17-N16	7.28	1.43	1.32
6	C	1004	MD1	C17-N16	7.45	1.43	1.32
5	C	1003	MGD	C4-N3	7.48	1.47	1.35
5	C	1003	MGD	C17-N18	7.51	1.47	1.36
5	E	1003	MGD	C19-N19	7.66	1.43	1.32
5	E	1003	MGD	C17-N18	7.68	1.47	1.36
5	A	1003	MGD	O4'-C1'	7.71	1.52	1.41
5	E	1003	MGD	C4-N3	7.97	1.48	1.35
5	C	1003	MGD	C19-N19	7.98	1.44	1.32
5	E	1003	MGD	C2-N2	8.10	1.44	1.32
5	C	1003	MGD	O4'-C1'	8.19	1.52	1.41
5	E	1003	MGD	O4'-C1'	8.26	1.53	1.41
6	C	1004	MD1	C2-N2	9.11	1.45	1.32
5	E	1003	MGD	C14-N15	9.41	1.56	1.45
5	C	1003	MGD	C16-C21	9.52	1.59	1.41
5	C	1003	MGD	C19-N18	9.61	1.51	1.36
5	A	1003	MGD	O11-C11	9.67	1.57	1.43
5	C	1003	MGD	C2-N3	9.67	1.45	1.33
5	E	1003	MGD	C16-C21	9.71	1.59	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1003	MGD	C2-N3	9.75	1.45	1.33
6	E	1004	MD1	C2-N2	9.93	1.47	1.32
5	A	1003	MGD	C14-N15	10.02	1.57	1.45
5	A	1003	MGD	C19-N20	10.22	1.45	1.33
5	E	1003	MGD	C2-N3	10.29	1.45	1.33
5	A	1003	MGD	C16-C21	10.47	1.61	1.41
5	C	1003	MGD	C14-N15	10.52	1.58	1.45
5	E	1003	MGD	O11-C11	10.67	1.59	1.43
5	C	1003	MGD	O11-C11	10.68	1.59	1.43
5	A	1003	MGD	C19-N18	10.89	1.53	1.36
6	A	1004	MD1	C2-N2	11.02	1.48	1.32
6	E	1004	MD1	O4'-C1'	11.09	1.57	1.41
5	E	1003	MGD	C19-N18	11.11	1.53	1.36
5	E	1003	MGD	C19-N20	11.55	1.47	1.33
5	C	1003	MGD	C19-N20	12.40	1.48	1.33
6	A	1004	MD1	O4'-C1'	12.86	1.59	1.41
6	E	1004	MD1	C7-N8	12.87	1.42	1.27
6	A	1004	MD1	C7-N8	14.02	1.43	1.27
6	C	1004	MD1	C7-N8	14.33	1.43	1.27
6	C	1004	MD1	O4'-C1'	14.78	1.62	1.41

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	1003	MGD	C4'-O4'-C1'	-9.56	99.51	109.64
5	E	1003	MGD	C4'-O4'-C1'	-8.12	101.04	109.64
5	A	1003	MGD	C4'-O4'-C1'	-6.02	103.27	109.64
5	E	1003	MGD	C1'-N9-C4	-5.67	120.48	126.81
5	A	1003	MGD	C1'-N9-C4	-5.60	120.56	126.81
5	C	1003	MGD	C1'-N9-C4	-4.89	121.34	126.81
6	A	1004	MD1	C4'-O4'-C1'	-4.77	104.58	109.64
6	E	1004	MD1	N16-C17-N18	-4.21	114.90	120.29
6	E	1004	MD1	C4'-O4'-C1'	-3.76	105.65	109.64
6	C	1004	MD1	O11-C11-C12	-3.16	105.00	111.16
5	A	1003	MGD	C16-N15-C14	-2.73	111.52	118.60
5	E	1003	MGD	O11-C23-C14	-2.57	107.20	108.96
6	E	1004	MD1	O11-C11-C12	-2.50	106.30	111.16
5	E	1003	MGD	C16-N15-C14	-2.44	112.25	118.60
6	A	1004	MD1	O11-C11-C12	-2.43	106.43	111.16
6	E	1004	MD1	C16-N15-C14	-2.33	112.56	118.60
6	E	1004	MD1	O4'-C1'-N9	-2.15	104.04	108.11
5	A	1003	MGD	O3'-C3'-C2'	-2.01	105.35	111.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	1003	MGD	O4'-C4'-C3'	2.06	109.33	105.16
6	E	1004	MD1	O4'-C4'-C3'	2.07	109.36	105.16
5	C	1003	MGD	O4'-C4'-C3'	2.11	109.43	105.16
5	E	1003	MGD	C21-C16-N15	2.34	121.84	118.83
5	A	1003	MGD	O4'-C1'-N9	2.45	112.74	108.11
5	C	1003	MGD	N19-C19-N18	2.46	120.65	117.82
5	A	1003	MGD	C21-C16-N15	2.56	122.12	118.83
5	E	1003	MGD	O4'-C1'-N9	2.81	113.42	108.11
6	A	1004	MD1	N2-C2-N1	2.82	121.07	117.82
5	A	1003	MGD	C17-C16-C21	2.99	117.24	114.61
5	C	1003	MGD	O4'-C1'-N9	3.10	113.96	108.11
6	E	1004	MD1	N16-C17-N17	3.13	121.43	117.82
5	E	1003	MGD	N19-C19-N18	3.42	121.76	117.82
5	E	1003	MGD	C17-C16-C21	3.48	117.68	114.61
5	A	1003	MGD	C16-C21-N22	4.35	122.32	118.19
5	C	1003	MGD	C17-C16-C21	4.42	118.50	114.61
5	C	1003	MGD	C16-C21-N22	5.01	122.95	118.19
5	E	1003	MGD	C16-C21-N22	5.58	123.49	118.19

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1004	MD1	5	0
7	A	1010	EDO	1	0
5	C	1003	MGD	1	0
6	C	1004	MD1	4	0
11	C	1008	PEG	1	0
8	D	401	F3S	1	0
3	D	402	SF4	1	0
5	E	1003	MGD	1	0
6	E	1004	MD1	4	0

5.7 Other polymers (i)

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%)	0.24	41 (4%) 36 34	13, 24, 42, 64	0
1	C	892/899 (99%)	0.56	74 (8%) 14 14	15, 30, 52, 86	0
1	E	892/899 (99%)	0.43	63 (7%) 19 17	13, 25, 55, 76	0
2	B	329/333 (98%)	-0.04	4 (1%) 81 81	14, 20, 32, 55	0
2	D	328/333 (98%)	1.24	62 (18%) 2 1	21, 46, 62, 85	0
2	F	328/333 (98%)	0.27	5 (1%) 76 76	14, 26, 43, 58	0
All	All	3664/3696 (99%)	0.43	249 (6%) 20 18	13, 26, 53, 86	0

All (249) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	8	ALA	10.3
1	C	9	PHE	7.2
2	D	146	LEU	5.9
1	A	5	ILE	5.5
2	D	250	PHE	5.5
2	D	73	LEU	5.4
1	E	369	THR	5.3
2	B	5	MET	5.2
2	D	6	LYS	4.8
1	E	364	LEU	4.7
2	D	312	ALA	4.7
1	E	314	PRO	4.7
2	F	6	LYS	4.7
1	E	370	VAL	4.7
1	E	310	LYS	4.6
2	B	6	LYS	4.4
1	C	17	PHE	4.4
2	D	154	ILE	4.3
1	C	366	ASP	4.3

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Mol	Chain	Res	Type	RSRZ
1	E	298	GLY	4.3
1	E	365	LEU	4.2
1	C	298	GLY	4.2
2	D	170	CYS	4.2
1	A	6	SER	4.2
2	D	152	GLU	4.1
2	D	153	ALA	4.1
1	C	11	TYR	4.0
1	C	297	ALA	4.0
1	E	313	LYS	3.9
2	D	179	SER	3.9
2	D	78	ILE	3.8
1	C	37	THR	3.7
1	A	297	ALA	3.7
1	E	282	VAL	3.7
1	A	7	GLY	3.7
1	E	360	PHE	3.7
1	C	370	VAL	3.6
1	A	327	LYS	3.6
1	A	8	ALA	3.6
1	C	769	VAL	3.6
1	C	365	LEU	3.6
2	D	7	ALA	3.5
2	D	150	PRO	3.5
2	D	240	TYR	3.5
1	C	313	LYS	3.5
1	E	366	ASP	3.5
1	E	315	VAL	3.4
1	E	296	VAL	3.4
1	C	351	ASP	3.3
1	E	359	LYS	3.3
1	C	770	HIS	3.3
1	A	299	GLY	3.3
2	D	69	LYS	3.3
1	C	12	SER	3.3
2	D	311	LEU	3.3
2	D	75	LYS	3.3
2	D	24	CYS	3.3
2	D	234	TYR	3.3
2	D	148	ALA	3.3
2	D	145	CYS	3.2
1	C	899	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
2	D	67	GLY	3.2
2	D	76	GLY	3.2
2	D	299	ILE	3.2
1	C	368	LYS	3.2
1	E	328	LYS	3.1
1	C	459	GLY	3.1
1	C	10	GLU	3.1
1	C	293	ALA	3.1
1	C	74	CYS	3.1
1	E	327	LYS	3.1
1	C	309	ALA	3.1
1	C	168	TYR	3.1
2	D	310	GLY	3.1
1	C	461	TRP	3.0
1	E	11[A]	TYR	3.0
1	E	368	LYS	3.0
1	C	164	PHE	3.0
1	C	14	TRP	3.0
2	D	176	CYS	3.0
1	C	34	VAL	3.0
1	E	355	ALA	3.0
1	C	364	LEU	3.0
1	E	367	GLY	3.0
1	C	458	ILE	2.9
2	D	171	LYS	2.9
2	D	8	PRO	2.9
1	C	66	ILE	2.9
2	D	165	ILE	2.9
2	D	229	VAL	2.9
1	E	325	PRO	2.9
2	D	147	GLU	2.9
1	A	326	GLU	2.9
1	C	773	PHE	2.9
1	C	764	HIS	2.9
1	A	364	LEU	2.8
1	C	38	GLY	2.8
2	D	140	CYS	2.8
2	D	9	ARG	2.8
1	E	361	ASN	2.8
1	C	327	LYS	2.8
1	E	286	THR	2.8
1	C	290	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	207	THR	2.8
1	C	369	THR	2.8
2	D	309	LYS	2.8
1	C	209	ILE	2.8
2	D	68	TYR	2.7
2	D	155	TYR	2.7
2	D	166	HIS	2.7
1	A	368	LYS	2.7
2	B	69	LYS	2.7
1	A	459	GLY	2.7
2	D	177	VAL	2.7
1	C	195	LYS	2.7
1	A	367	GLY	2.6
1	C	36	CYS	2.6
1	E	209	ILE	2.6
1	A	36	CYS	2.6
1	E	299	GLY	2.6
1	E	317	PRO	2.6
1	E	342	PHE	2.6
2	D	190	LEU	2.6
1	A	298	GLY	2.6
1	E	304	PHE	2.6
2	D	293	VAL	2.6
1	A	366	ASP	2.6
2	D	314	ASP	2.6
1	A	142	VAL	2.6
1	E	295	VAL	2.6
1	C	167	TRP	2.5
1	C	834	TRP	2.5
1	C	13	GLY	2.5
2	D	66	GLY	2.5
2	F	24	CYS	2.5
1	C	299	GLY	2.5
2	D	23	GLY	2.5
1	E	307	TRP	2.5
1	E	297	ALA	2.5
1	C	607	LYS	2.5
1	E	352	LEU	2.5
2	D	158	GLU	2.5
2	D	164	VAL	2.5
1	C	363	GLN	2.5
1	C	460	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	379	LEU	2.5
1	C	768	SER	2.5
1	C	423	GLY	2.4
1	A	295	VAL	2.4
1	A	370	VAL	2.4
2	D	233	VAL	2.4
1	E	311	THR	2.4
1	E	383	LEU	2.4
1	E	459	GLY	2.4
2	F	70	ASN	2.4
1	C	77	GLY	2.4
1	E	285	ASP	2.4
1	E	312	GLY	2.4
1	C	359	LYS	2.4
1	C	204	PRO	2.4
1	C	296	VAL	2.4
2	D	29	VAL	2.4
1	A	39	ALA	2.3
2	D	173	ALA	2.3
1	A	369	THR	2.3
2	D	224	GLY	2.3
1	C	210	PRO	2.3
2	D	149	CYS	2.3
1	C	631	LYS	2.3
1	E	644	LYS	2.3
1	E	289	PHE	2.3
1	E	354	PRO	2.3
1	C	457	TYR	2.3
1	C	771	SER	2.3
1	C	295	VAL	2.3
1	E	293	ALA	2.3
1	A	899	PHE	2.3
2	D	256	VAL	2.3
1	E	404	THR	2.3
2	D	230	ASN	2.3
1	A	365	LEU	2.3
1	E	326	GLU	2.2
1	E	265	LYS	2.2
1	A	73	GLY	2.2
1	A	40	CYS	2.2
1	A	363	GLN	2.2
1	A	17	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	643	PHE	2.2
1	A	658	MET	2.2
1	C	361	ASN	2.2
1	C	420	CYS	2.2
2	D	269	MET	2.2
2	D	151	ASN	2.2
1	E	290	LEU	2.2
2	D	241	LYS	2.2
2	F	69	LYS	2.2
1	E	270	HIS	2.2
2	D	61	TRP	2.2
1	C	165	TYR	2.2
2	D	187	PHE	2.2
1	C	695	LYS	2.2
1	E	207	THR	2.1
2	D	65	GLY	2.1
1	A	168	TYR	2.1
1	A	769	VAL	2.1
1	C	328	LYS	2.1
2	F	22	ILE	2.1
1	C	307	TRP	2.1
1	E	168	TYR	2.1
1	A	325	PRO	2.1
1	E	372	VAL	2.1
1	E	769	VAL	2.1
1	E	358	GLY	2.1
1	C	79	CYS	2.1
1	C	593	THR	2.1
1	A	501	ILE	2.1
1	E	349	LEU	2.1
2	D	175	ALA	2.1
2	D	292	GLN	2.1
1	C	73	GLY	2.1
2	D	226	VAL	2.1
1	A	209	ILE	2.1
1	E	420	CYS	2.1
2	B	70	ASN	2.1
1	C	76	LYS	2.1
1	E	458	ILE	2.1
1	A	38	GLY	2.1
1	A	74	CYS	2.1
1	E	169	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	37	THR	2.0
1	A	351	ASP	2.0
1	C	16	ASN	2.0
1	A	296	VAL	2.0
2	D	169	LYS	2.0
1	C	326	GLU	2.0
1	C	704	GLU	2.0
1	C	772	THR	2.0
1	E	284	SER	2.0
1	A	310	LYS	2.0
1	A	764	HIS	2.0
1	A	34	VAL	2.0
1	C	139	VAL	2.0
1	E	139	VAL	2.0
1	A	164	PHE	2.0
1	E	357	GLU	2.0
1	E	394	LYS	2.0
1	E	770	HIS	2.0
1	E	36	CYS	2.0
1	E	373	ARG	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
10	GOL	C	1006	6/6	0.73	0.35	12.35	37,47,56,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
7	EDO	E	1005	4/4	0.90	0.15	6.46	16,20,23,23	0
7	EDO	E	1007	4/4	0.79	0.19	6.25	25,30,35,35	0
7	EDO	E	1008	4/4	0.88	0.19	6.10	26,31,35,41	0
7	EDO	A	1008	4/4	0.86	0.20	5.62	30,36,41,42	0
7	EDO	E	1010	4/4	0.79	0.27	4.63	34,41,43,45	0
7	EDO	A	1010	4/4	0.84	0.28	4.40	21,27,30,33	0
7	EDO	E	1006	4/4	0.69	0.23	4.08	25,30,34,36	0
7	EDO	B	406	4/4	0.77	0.26	3.22	32,39,40,42	0
7	EDO	C	1007	4/4	0.94	0.12	2.51	17,22,26,27	0
7	EDO	C	1005	4/4	0.60	0.20	2.44	27,33,38,42	0
11	PEG	C	1008	7/7	0.78	0.22	2.01	32,39,42,42	0
7	EDO	A	1009	4/4	0.89	0.19	1.94	29,35,41,50	0
7	EDO	A	1005	4/4	0.92	0.14	1.51	18,25,32,32	0
7	EDO	A	1007	4/4	0.95	0.13	0.95	22,27,28,33	0
5	MGD	E	1003	47/47	0.94	0.19	0.76	15,21,29,31	0
5	MGD	C	1003	47/47	0.94	0.23	0.61	20,22,27,30	0
6	MD1	A	1004	47/47	0.97	0.17	0.60	15,17,22,23	0
5	MGD	A	1003	47/47	0.96	0.17	0.34	13,16,19,23	0
9	NA	B	407	1/1	0.87	0.10	0.15	35,35,35,35	0
6	MD1	E	1004	47/47	0.96	0.15	0.08	12,16,21,23	0
6	MD1	C	1004	47/47	0.96	0.17	0.03	17,20,24,26	0
3	SF4	F	404	8/8	0.97	0.11	-0.10	17,18,20,23	0
3	SF4	B	402	8/8	0.98	0.08	-0.37	15,16,19,20	0
7	EDO	B	405	4/4	0.96	0.08	-0.48	16,19,19,20	0
7	EDO	F	405	4/4	0.98	0.09	-0.58	16,19,21,21	0
3	SF4	F	403	8/8	0.98	0.13	-0.65	18,21,24,25	0
7	EDO	A	1006	4/4	0.96	0.10	-0.73	24,29,32,32	0
7	EDO	D	405	4/4	0.94	0.11	-0.92	26,31,35,35	0
3	SF4	B	404	8/8	0.98	0.09	-0.98	12,13,14,15	0
3	SF4	D	403	8/8	0.95	0.11	-1.53	30,35,39,40	0
8	F3S	B	401	7/7	0.98	0.05	-1.63	19,20,22,22	0
3	SF4	F	402	8/8	0.95	0.08	-1.64	19,22,23,25	0
3	SF4	D	402	8/8	0.87	0.09	-1.65	32,42,49,51	0
3	SF4	D	404	8/8	0.87	0.12	-1.89	29,38,39,42	0
8	F3S	F	401	7/7	0.97	0.05	-1.91	21,22,23,24	0
3	SF4	A	1001	8/8	0.99	0.13	-1.98	13,14,17,19	0
3	SF4	C	1001	8/8	0.98	0.14	-1.98	24,25,27,27	0
3	SF4	B	403	8/8	0.98	0.10	-2.17	12,14,15,17	0
3	SF4	E	1001	8/8	0.98	0.09	-2.22	13,15,15,15	0
8	F3S	D	401	7/7	0.91	0.08	-2.99	45,47,55,57	0
4	MO	A	1002	1/1	0.99	0.06	-3.41	20,20,20,20	0
4	MO	E	1002	1/1	0.99	0.08	-3.66	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	MO	C	1002	1/1	0.99	0.08	-4.73	24,24,24,24	0
7	EDO	E	1009	4/4	0.85	0.38	-	30,36,40,42	0

6.5 Other polymers (i)

There are no such residues in this entry.