Full wwPDB X-ray Structure Validation Report (i)

May 26, 2020 – 10:33 am BST

PDB ID	:	2J6P
Title	:	STRUCTURE OF AS-SB REDUCTASE FROM LEISHMANIA MAJOR
Authors	:	Bisacchi, D.; Zhou, Y.; Rosen, B.P.; Mukhopadhyay, R.; Bordo, D.
Deposited on	:	2006-10-02
Resolution	:	2.15 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.15 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.
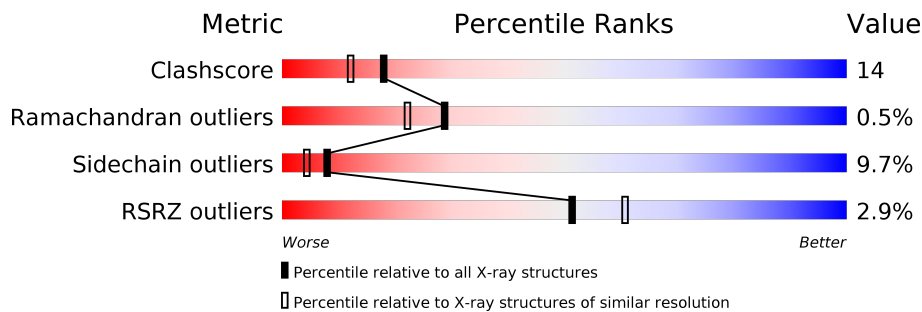
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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 respectively. 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	152	% / 67% / 21% / 6% / · / 5%
1	B	152	2% / 64% / 23% / 5% / · / 5%
1	C	152	2% / 64% / 26% / · / · / 5%
1	D	152	3% / 64% / 23% / 7% / · / 5%
1	E	152	3% / 71% / 17% / 7% / · / 5%
1	F	152	5% / 64% / 22% / 9% / · / 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	A	202	-	-	X	-
3	GOL	B	203	-	-	X	-
3	GOL	C	202	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7503 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 SB(V)-AS(V) REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	145	Total	C	N	O	S	5	1	0
			1157	739	190	219	9			
1	B	145	Total	C	N	O	S	5	2	0
			1161	741	191	220	9			
1	C	145	Total	C	N	O	S	5	0	0
			1155	738	190	219	8			
1	D	145	Total	C	N	O	S	5	0	0
			1155	738	190	219	8			
1	E	145	Total	C	N	O	S	5	2	0
			1161	741	191	220	9			
1	F	145	Total	C	N	O	S	5	2	0
			1161	741	191	220	9			

There are 150 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	128	LYS	-	expression tag	UNP Q6Q1Q5
A	129	LEU	-	expression tag	UNP Q6Q1Q5
A	130	GLY	-	expression tag	UNP Q6Q1Q5
A	131	PRO	-	expression tag	UNP Q6Q1Q5
A	132	GLU	-	expression tag	UNP Q6Q1Q5
A	133	GLN	-	expression tag	UNP Q6Q1Q5
A	134	LYS	-	expression tag	UNP Q6Q1Q5
A	135	LEU	-	expression tag	UNP Q6Q1Q5
A	136	ILE	-	expression tag	UNP Q6Q1Q5
A	137	SER	-	expression tag	UNP Q6Q1Q5
A	138	GLU	-	expression tag	UNP Q6Q1Q5
A	139	GLU	-	expression tag	UNP Q6Q1Q5
A	140	ASP	-	expression tag	UNP Q6Q1Q5
A	141	LEU	-	expression tag	UNP Q6Q1Q5
A	142	ASN	-	expression tag	UNP Q6Q1Q5
A	143	SER	-	expression tag	UNP Q6Q1Q5
A	144	ALA	-	expression tag	UNP Q6Q1Q5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	145	VAL	-	expression tag	UNP Q6Q1Q5
A	146	ASP	-	expression tag	UNP Q6Q1Q5
A	147	HIS	-	expression tag	UNP Q6Q1Q5
A	148	HIS	-	expression tag	UNP Q6Q1Q5
A	149	HIS	-	expression tag	UNP Q6Q1Q5
A	150	HIS	-	expression tag	UNP Q6Q1Q5
A	151	HIS	-	expression tag	UNP Q6Q1Q5
A	152	HIS	-	expression tag	UNP Q6Q1Q5
B	128	LYS	-	expression tag	UNP Q6Q1Q5
B	129	LEU	-	expression tag	UNP Q6Q1Q5
B	130	GLY	-	expression tag	UNP Q6Q1Q5
B	131	PRO	-	expression tag	UNP Q6Q1Q5
B	132	GLU	-	expression tag	UNP Q6Q1Q5
B	133	GLN	-	expression tag	UNP Q6Q1Q5
B	134	LYS	-	expression tag	UNP Q6Q1Q5
B	135	LEU	-	expression tag	UNP Q6Q1Q5
B	136	ILE	-	expression tag	UNP Q6Q1Q5
B	137	SER	-	expression tag	UNP Q6Q1Q5
B	138	GLU	-	expression tag	UNP Q6Q1Q5
B	139	GLU	-	expression tag	UNP Q6Q1Q5
B	140	ASP	-	expression tag	UNP Q6Q1Q5
B	141	LEU	-	expression tag	UNP Q6Q1Q5
B	142	ASN	-	expression tag	UNP Q6Q1Q5
B	143	SER	-	expression tag	UNP Q6Q1Q5
B	144	ALA	-	expression tag	UNP Q6Q1Q5
B	145	VAL	-	expression tag	UNP Q6Q1Q5
B	146	ASP	-	expression tag	UNP Q6Q1Q5
B	147	HIS	-	expression tag	UNP Q6Q1Q5
B	148	HIS	-	expression tag	UNP Q6Q1Q5
B	149	HIS	-	expression tag	UNP Q6Q1Q5
B	150	HIS	-	expression tag	UNP Q6Q1Q5
B	151	HIS	-	expression tag	UNP Q6Q1Q5
B	152	HIS	-	expression tag	UNP Q6Q1Q5
C	128	LYS	-	expression tag	UNP Q6Q1Q5
C	129	LEU	-	expression tag	UNP Q6Q1Q5
C	130	GLY	-	expression tag	UNP Q6Q1Q5
C	131	PRO	-	expression tag	UNP Q6Q1Q5
C	132	GLU	-	expression tag	UNP Q6Q1Q5
C	133	GLN	-	expression tag	UNP Q6Q1Q5
C	134	LYS	-	expression tag	UNP Q6Q1Q5
C	135	LEU	-	expression tag	UNP Q6Q1Q5
C	136	ILE	-	expression tag	UNP Q6Q1Q5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	137	SER	-	expression tag	UNP Q6Q1Q5
C	138	GLU	-	expression tag	UNP Q6Q1Q5
C	139	GLU	-	expression tag	UNP Q6Q1Q5
C	140	ASP	-	expression tag	UNP Q6Q1Q5
C	141	LEU	-	expression tag	UNP Q6Q1Q5
C	142	ASN	-	expression tag	UNP Q6Q1Q5
C	143	SER	-	expression tag	UNP Q6Q1Q5
C	144	ALA	-	expression tag	UNP Q6Q1Q5
C	145	VAL	-	expression tag	UNP Q6Q1Q5
C	146	ASP	-	expression tag	UNP Q6Q1Q5
C	147	HIS	-	expression tag	UNP Q6Q1Q5
C	148	HIS	-	expression tag	UNP Q6Q1Q5
C	149	HIS	-	expression tag	UNP Q6Q1Q5
C	150	HIS	-	expression tag	UNP Q6Q1Q5
C	151	HIS	-	expression tag	UNP Q6Q1Q5
C	152	HIS	-	expression tag	UNP Q6Q1Q5
D	128	LYS	-	expression tag	UNP Q6Q1Q5
D	129	LEU	-	expression tag	UNP Q6Q1Q5
D	130	GLY	-	expression tag	UNP Q6Q1Q5
D	131	PRO	-	expression tag	UNP Q6Q1Q5
D	132	GLU	-	expression tag	UNP Q6Q1Q5
D	133	GLN	-	expression tag	UNP Q6Q1Q5
D	134	LYS	-	expression tag	UNP Q6Q1Q5
D	135	LEU	-	expression tag	UNP Q6Q1Q5
D	136	ILE	-	expression tag	UNP Q6Q1Q5
D	137	SER	-	expression tag	UNP Q6Q1Q5
D	138	GLU	-	expression tag	UNP Q6Q1Q5
D	139	GLU	-	expression tag	UNP Q6Q1Q5
D	140	ASP	-	expression tag	UNP Q6Q1Q5
D	141	LEU	-	expression tag	UNP Q6Q1Q5
D	142	ASN	-	expression tag	UNP Q6Q1Q5
D	143	SER	-	expression tag	UNP Q6Q1Q5
D	144	ALA	-	expression tag	UNP Q6Q1Q5
D	145	VAL	-	expression tag	UNP Q6Q1Q5
D	146	ASP	-	expression tag	UNP Q6Q1Q5
D	147	HIS	-	expression tag	UNP Q6Q1Q5
D	148	HIS	-	expression tag	UNP Q6Q1Q5
D	149	HIS	-	expression tag	UNP Q6Q1Q5
D	150	HIS	-	expression tag	UNP Q6Q1Q5
D	151	HIS	-	expression tag	UNP Q6Q1Q5
D	152	HIS	-	expression tag	UNP Q6Q1Q5
E	128	LYS	-	expression tag	UNP Q6Q1Q5

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Chain	Residue	Modelled	Actual	Comment	Reference
E	129	LEU	-	expression tag	UNP Q6Q1Q5
E	130	GLY	-	expression tag	UNP Q6Q1Q5
E	131	PRO	-	expression tag	UNP Q6Q1Q5
E	132	GLU	-	expression tag	UNP Q6Q1Q5
E	133	GLN	-	expression tag	UNP Q6Q1Q5
E	134	LYS	-	expression tag	UNP Q6Q1Q5
E	135	LEU	-	expression tag	UNP Q6Q1Q5
E	136	ILE	-	expression tag	UNP Q6Q1Q5
E	137	SER	-	expression tag	UNP Q6Q1Q5
E	138	GLU	-	expression tag	UNP Q6Q1Q5
E	139	GLU	-	expression tag	UNP Q6Q1Q5
E	140	ASP	-	expression tag	UNP Q6Q1Q5
E	141	LEU	-	expression tag	UNP Q6Q1Q5
E	142	ASN	-	expression tag	UNP Q6Q1Q5
E	143	SER	-	expression tag	UNP Q6Q1Q5
E	144	ALA	-	expression tag	UNP Q6Q1Q5
E	145	VAL	-	expression tag	UNP Q6Q1Q5
E	146	ASP	-	expression tag	UNP Q6Q1Q5
E	147	HIS	-	expression tag	UNP Q6Q1Q5
E	148	HIS	-	expression tag	UNP Q6Q1Q5
E	149	HIS	-	expression tag	UNP Q6Q1Q5
E	150	HIS	-	expression tag	UNP Q6Q1Q5
E	151	HIS	-	expression tag	UNP Q6Q1Q5
E	152	HIS	-	expression tag	UNP Q6Q1Q5
F	128	LYS	-	expression tag	UNP Q6Q1Q5
F	129	LEU	-	expression tag	UNP Q6Q1Q5
F	130	GLY	-	expression tag	UNP Q6Q1Q5
F	131	PRO	-	expression tag	UNP Q6Q1Q5
F	132	GLU	-	expression tag	UNP Q6Q1Q5
F	133	GLN	-	expression tag	UNP Q6Q1Q5
F	134	LYS	-	expression tag	UNP Q6Q1Q5
F	135	LEU	-	expression tag	UNP Q6Q1Q5
F	136	ILE	-	expression tag	UNP Q6Q1Q5
F	137	SER	-	expression tag	UNP Q6Q1Q5
F	138	GLU	-	expression tag	UNP Q6Q1Q5
F	139	GLU	-	expression tag	UNP Q6Q1Q5
F	140	ASP	-	expression tag	UNP Q6Q1Q5
F	141	LEU	-	expression tag	UNP Q6Q1Q5
F	142	ASN	-	expression tag	UNP Q6Q1Q5
F	143	SER	-	expression tag	UNP Q6Q1Q5
F	144	ALA	-	expression tag	UNP Q6Q1Q5
F	145	VAL	-	expression tag	UNP Q6Q1Q5

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Chain	Residue	Modelled	Actual	Comment	Reference
F	146	ASP	-	expression tag	UNP Q6Q1Q5
F	147	HIS	-	expression tag	UNP Q6Q1Q5
F	148	HIS	-	expression tag	UNP Q6Q1Q5
F	149	HIS	-	expression tag	UNP Q6Q1Q5
F	150	HIS	-	expression tag	UNP Q6Q1Q5
F	151	HIS	-	expression tag	UNP Q6Q1Q5
F	152	HIS	-	expression tag	UNP Q6Q1Q5

- Molecule 2 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).
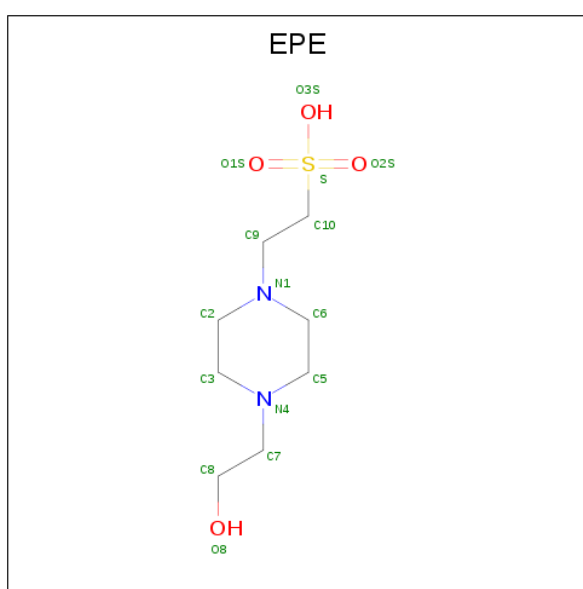
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	1
			15	8	2	4	1		
2	B	1	Total	C	N	O	S	0	1
			15	8	2	4	1		
2	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
2	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).
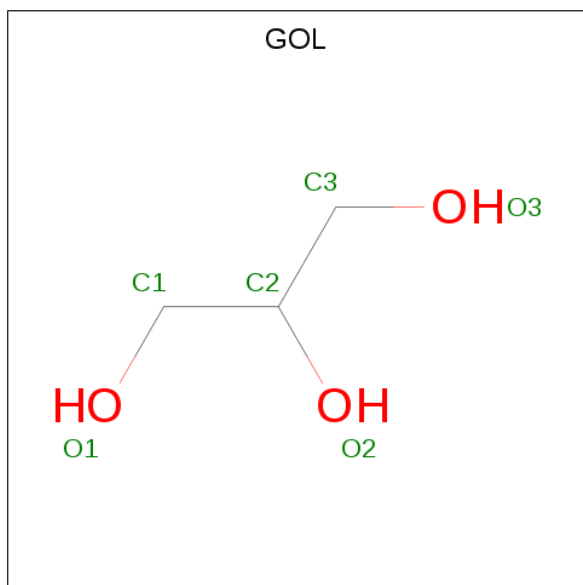
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 6	C 3	O 3	0	0
3	B	1	Total 6	C 3	O 3	0	0
3	B	1	Total 6	C 3	O 3	0	0
3	C	1	Total 6	C 3	O 3	0	0
3	D	1	Total 6	C 3	O 3	0	0
3	E	1	Total 6	C 3	O 3	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

SO4
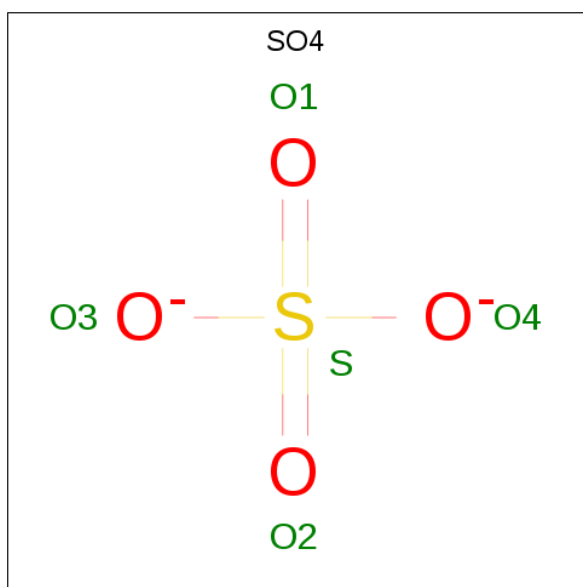
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 5	O 4	S 1	0	1
4	A	1	Total 5	O 4	S 1	0	0
4	B	1	Total 5	O 4	S 1	0	0
4	B	1	Total 5	O 4	S 1	0	1
4	D	1	Total 5	O 4	S 1	0	0
4	D	1	Total 5	O 4	S 1	0	0
4	E	1	Total 5	O 4	S 1	0	0
4	F	1	Total 5	O 4	S 1	0	0
4	F	1	Total 5	O 4	S 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	88	Total 88	O 88	0	0
5	B	83	Total 83	O 83	0	0
5	C	79	Total 79	O 79	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	73	Total 73	O 73	0	0
5	E	48	Total 48	O 48	0	0
5	F	41	Total 41	O 41	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: SB(V)-AS(V) REDUCTASE

Chain A:
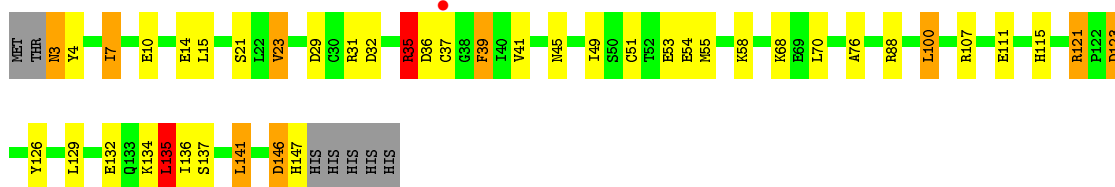
- Molecule 1: SB(V)-AS(V) REDUCTASE

Chain B:
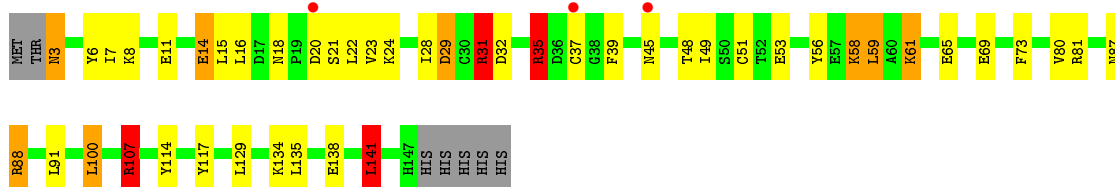
- Molecule 1: SB(V)-AS(V) REDUCTASE

Chain C:
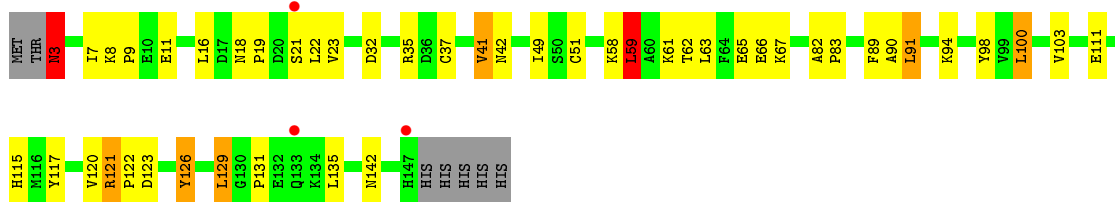
- Molecule 1: SB(V)-AS(V) REDUCTASE

Chain D:
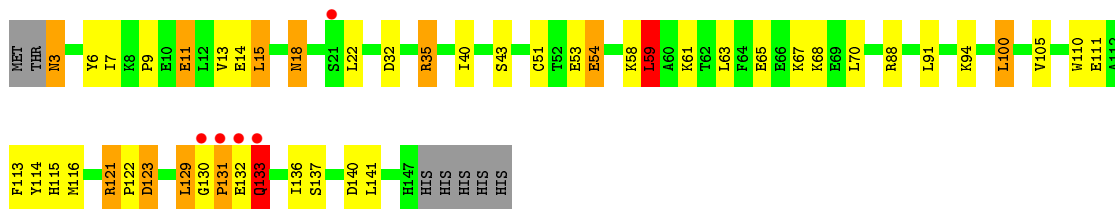
• Molecule 1: SB(V)-AS(V) REDUCTASE

Chain E:

• Molecule 1: SB(V)-AS(V) REDUCTASE

Chain F:
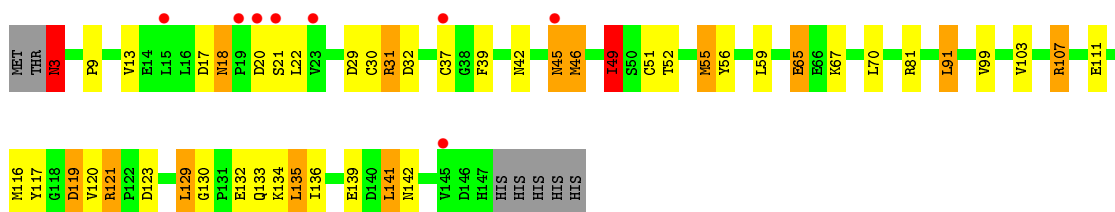
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	111.82Å 111.82Å 177.38Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	65.37 – 2.15 65.41 – 2.15	Depositor EDS
% Data completeness (in resolution range)	100.0 (65.37-2.15) 97.4 (65.41-2.15)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.04 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.190 , 0.241 0.197 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	27.9	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 58.8	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.025 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7503	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.16% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, EPE, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	A	1.79	20/1185 (1.7%)	1.63	15/1603 (0.9%)
1	B	1.78	18/1193 (1.5%)	1.60	17/1614 (1.1%)
1	C	1.64	13/1179 (1.1%)	1.57	11/1595 (0.7%)
1	D	1.69	15/1179 (1.3%)	1.43	13/1595 (0.8%)
1	E	1.48	6/1193 (0.5%)	1.28	13/1614 (0.8%)
1	F	1.45	10/1193 (0.8%)	1.39	13/1614 (0.8%)
All	All	1.64	82/7122 (1.2%)	1.49	82/9635 (0.9%)

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	B	1	0
1	C	1	0
All	All	2	0

All (82) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	31	ARG	CD-NE	-9.42	1.30	1.46
1	C	37	CYS	CB-SG	9.12	1.97	1.82
1	A	4	TYR	CD1-CE1	9.06	1.52	1.39
1	B	3	ASN	N-CA	8.81	1.64	1.46
1	B	51	CYS	CB-SG	-8.57	1.67	1.82
1	E	84	LYS	CD-CE	8.40	1.72	1.51
1	A	14	GLU	CG-CD	8.38	1.64	1.51
1	D	3	ASN	CB-CG	-8.16	1.32	1.51
1	D	54	GLU	CG-CD	8.06	1.64	1.51
1	D	105	VAL	CB-CG2	7.64	1.68	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	14	GLU	CD-OE1	7.56	1.33	1.25
1	D	6	TYR	CE1-CZ	7.52	1.48	1.38
1	F	111	GLU	CD-OE2	7.47	1.33	1.25
1	A	14	GLU	CD-OE2	7.47	1.33	1.25
1	A	68	LYS	CD-CE	7.27	1.69	1.51
1	B	39	PHE	CE2-CZ	7.16	1.50	1.37
1	D	13	VAL	CB-CG1	7.16	1.67	1.52
1	E	84	LYS	CE-NZ	7.05	1.66	1.49
1	F	56	TYR	CE1-CZ	7.00	1.47	1.38
1	E	76	ALA	CA-CB	6.98	1.67	1.52
1	D	114	TYR	CD1-CE1	6.90	1.49	1.39
1	B	53	GLU	CD-OE2	6.87	1.33	1.25
1	D	51	CYS	CB-SG	-6.68	1.70	1.82
1	B	35	ARG	CG-CD	6.55	1.68	1.51
1	A	45	ASN	CB-CG	6.51	1.66	1.51
1	A	4	TYR	CD2-CE2	6.51	1.49	1.39
1	C	90	ALA	CA-CB	6.50	1.66	1.52
1	C	51	CYS	CB-SG	-6.48	1.71	1.82
1	F	31	ARG	CD-NE	-6.34	1.35	1.46
1	D	54	GLU	CD-OE2	6.32	1.32	1.25
1	E	3	ASN	N-CA	6.32	1.58	1.46
1	D	94	LYS	CD-CE	6.26	1.67	1.51
1	A	10	GLU	CG-CD	6.26	1.61	1.51
1	D	53	GLU	CG-CD	6.21	1.61	1.51
1	B	14	GLU	CD-OE2	6.20	1.32	1.25
1	C	103	VAL	CB-CG1	6.19	1.65	1.52
1	B	88	ARG	CZ-NH1	6.17	1.41	1.33
1	A	45	ASN	CG-OD1	6.09	1.37	1.24
1	D	14	GLU	CG-CD	6.06	1.61	1.51
1	A	68	LYS	CB-CG	5.83	1.68	1.52
1	F	45[A]	ASN	CB-CG	5.80	1.64	1.51
1	F	45[B]	ASN	CB-CG	5.80	1.64	1.51
1	F	3	ASN	N-CA	5.71	1.57	1.46
1	A	41	VAL	CB-CG1	5.67	1.64	1.52
1	F	30	CYS	CB-SG	-5.67	1.72	1.81
1	B	11	GLU	CG-CD	5.67	1.60	1.51
1	C	41	VAL	CB-CG1	5.65	1.64	1.52
1	C	121	ARG	CG-CD	5.64	1.66	1.51
1	B	61	LYS	CB-CG	5.55	1.67	1.52
1	C	89	PHE	CE2-CZ	5.52	1.47	1.37
1	A	14	GLU	CD-OE1	5.52	1.31	1.25
1	F	103	VAL	CB-CG1	5.50	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	88	ARG	CZ-NH1	5.48	1.40	1.33
1	A	39	PHE	CE2-CZ	5.46	1.47	1.37
1	B	107	ARG	CD-NE	-5.44	1.37	1.46
1	A	88	ARG	CZ-NH1	5.44	1.40	1.33
1	E	10	GLU	CG-CD	5.43	1.60	1.51
1	C	58	LYS	CD-CE	5.41	1.64	1.51
1	E	14	GLU	CG-CD	5.40	1.60	1.51
1	A	51	CYS	CB-SG	-5.37	1.73	1.81
1	B	138	GLU	CB-CG	5.36	1.62	1.52
1	A	76	ALA	CA-CB	5.32	1.63	1.52
1	C	98	TYR	CD1-CE1	5.30	1.47	1.39
1	C	111	GLU	CD-OE2	5.29	1.31	1.25
1	F	111	GLU	CD-OE1	5.23	1.31	1.25
1	B	117	TYR	CB-CG	-5.22	1.43	1.51
1	F	81	ARG	CB-CG	5.22	1.66	1.52
1	A	53	GLU	CG-CD	5.19	1.59	1.51
1	B	134	LYS	CD-CE	5.12	1.64	1.51
1	C	126	TYR	CD2-CE2	5.10	1.47	1.39
1	B	58	LYS	CB-CG	5.10	1.66	1.52
1	A	3	ASN	CB-CG	5.09	1.62	1.51
1	D	11	GLU	CG-CD	5.08	1.59	1.51
1	C	3	ASN	C-N	-5.06	1.22	1.34
1	B	114	TYR	CD2-CE2	5.05	1.47	1.39
1	D	111	GLU	CB-CG	5.05	1.61	1.52
1	A	23	VAL	CB-CG2	5.04	1.63	1.52
1	D	110	TRP	CB-CG	5.04	1.59	1.50
1	A	55	MET	CB-CG	5.03	1.67	1.51
1	B	73	PHE	CD1-CE1	5.02	1.49	1.39
1	C	89	PHE	CG-CD1	5.02	1.46	1.38
1	A	111	GLU	CG-CD	5.01	1.59	1.51

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	121	ARG	NE-CZ-NH1	-29.43	105.58	120.30
1	A	121	ARG	NE-CZ-NH1	-28.94	105.83	120.30
1	B	31	ARG	NE-CZ-NH2	-21.04	109.78	120.30
1	A	121	ARG	NE-CZ-NH2	20.10	130.35	120.30
1	B	107	ARG	NE-CZ-NH1	-17.61	111.50	120.30
1	C	121	ARG	NE-CZ-NH2	17.31	128.96	120.30
1	F	31	ARG	NE-CZ-NH2	-15.89	112.36	120.30
1	B	31	ARG	NE-CZ-NH1	15.33	127.97	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	121	ARG	NE-CZ-NH1	-15.00	112.80	120.30
1	B	107	ARG	NE-CZ-NH2	14.58	127.59	120.30
1	F	107	ARG	NE-CZ-NH1	14.07	127.34	120.30
1	A	121	ARG	CD-NE-CZ	-13.79	104.29	123.60
1	F	107	ARG	NE-CZ-NH2	-11.61	114.50	120.30
1	F	31	ARG	NE-CZ-NH1	11.27	125.94	120.30
1	C	121	ARG	CD-NE-CZ	-10.99	108.21	123.60
1	F	46	MET	CG-SD-CE	-10.94	82.69	100.20
1	A	68	LYS	CD-CE-NZ	-10.15	88.35	111.70
1	E	107	ARG	NE-CZ-NH1	10.03	125.31	120.30
1	E	88	ARG	NE-CZ-NH1	9.44	125.02	120.30
1	B	3	ASN	N-CA-C	9.27	136.04	111.00
1	E	121	ARG	NE-CZ-NH1	-9.06	115.77	120.30
1	B	100	LEU	CB-CG-CD1	8.51	125.47	111.00
1	A	100	LEU	CB-CG-CD1	8.47	125.40	111.00
1	B	59	LEU	CB-CG-CD2	8.26	125.04	111.00
1	A	88	ARG	NE-CZ-NH2	-8.12	116.24	120.30
1	A	35	ARG	NE-CZ-NH1	7.69	124.14	120.30
1	E	3	ASN	N-CA-C	7.67	131.71	111.00
1	F	55	MET	CG-SD-CE	-7.56	88.11	100.20
1	F	3	ASN	N-CA-C	7.53	131.33	111.00
1	B	81	ARG	NE-CZ-NH1	-7.43	116.58	120.30
1	C	35	ARG	NE-CZ-NH2	-7.38	116.61	120.30
1	E	88	ARG	NE-CZ-NH2	-7.34	116.63	120.30
1	C	59	LEU	CB-CG-CD2	7.28	123.38	111.00
1	C	100	LEU	CB-CG-CD1	7.23	123.29	111.00
1	B	135	LEU	CA-CB-CG	7.14	131.73	115.30
1	F	49	ILE	CG1-CB-CG2	-7.12	95.73	111.40
1	B	31	ARG	CB-CG-CD	-6.97	93.49	111.60
1	B	141	LEU	CB-CG-CD1	6.82	122.60	111.00
1	D	88	ARG	NE-CZ-NH2	-6.59	117.00	120.30
1	F	91	LEU	CA-CB-CG	6.47	130.17	115.30
1	E	107	ARG	CD-NE-CZ	6.40	132.56	123.60
1	C	3	ASN	CB-CA-C	6.37	123.15	110.40
1	E	107	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	B	15	LEU	CB-CG-CD1	-6.23	100.41	111.00
1	A	35	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	E	81	ARG	NE-CZ-NH2	-6.17	117.22	120.30
1	D	100	LEU	CB-CG-CD1	6.07	121.31	111.00
1	E	141	LEU	CB-CG-CD1	6.03	121.26	111.00
1	C	91	LEU	CB-CG-CD1	6.03	121.25	111.00
1	E	84	LYS	CD-CE-NZ	5.99	125.48	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	107	ARG	CD-NE-CZ	5.96	131.95	123.60
1	A	29	ASP	CB-CG-OD2	-5.92	112.97	118.30
1	D	59	LEU	CA-CB-CG	5.91	128.88	115.30
1	B	8	LYS	CD-CE-NZ	5.88	125.21	111.70
1	D	133	GLN	N-CA-C	5.87	126.84	111.00
1	D	35	ARG	CG-CD-NE	-5.83	99.55	111.80
1	A	135	LEU	CB-CG-CD1	-5.77	101.20	111.00
1	F	120	VAL	CB-CA-C	-5.75	100.47	111.40
1	A	7	ILE	CG1-CB-CG2	-5.75	98.75	111.40
1	D	15	LEU	CA-CB-CG	5.68	128.37	115.30
1	A	36	ASP	CB-CG-OD1	5.62	123.36	118.30
1	B	29	ASP	CB-CG-OD2	-5.56	113.29	118.30
1	E	81	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	C	121	ARG	NH1-CZ-NH2	5.50	125.45	119.40
1	D	3	ASN	N-CA-CB	5.50	120.50	110.60
1	E	99	VAL	CG1-CB-CG2	5.44	119.60	110.90
1	C	59	LEU	CA-CB-CG	5.39	127.71	115.30
1	D	100	LEU	CB-CG-CD2	5.39	120.17	111.00
1	E	35	ARG	NE-CZ-NH1	-5.36	117.62	120.30
1	C	35	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	B	134	LYS	CD-CE-NZ	5.33	123.95	111.70
1	A	29	ASP	CB-CG-OD1	5.29	123.07	118.30
1	D	130	GLY	N-CA-C	5.27	126.28	113.10
1	D	133	GLN	CA-C-N	-5.25	105.65	117.20
1	A	123	ASP	CB-CG-OD2	5.21	122.99	118.30
1	D	133	GLN	N-CA-CB	-5.19	101.26	110.60
1	F	91	LEU	CB-CG-CD2	5.14	119.74	111.00
1	B	3	ASN	O-C-N	-5.14	114.47	122.70
1	A	31	ARG	NE-CZ-NH1	-5.11	117.74	120.30
1	B	88	ARG	CB-CG-CD	5.10	124.86	111.60
1	D	116	MET	CG-SD-CE	5.10	108.36	100.20
1	F	121	ARG	NE-CZ-NH2	-5.04	117.78	120.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	3	ASN	CA
1	C	3	ASN	CA

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1157	0	1144	25	0
1	B	1161	0	1146	40	0
1	C	1155	0	1144	32	0
1	D	1155	0	1144	31	0
1	E	1161	0	1146	29	0
1	F	1161	0	1146	38	0
2	A	15	0	14	1	0
2	B	15	0	13	1	0
2	C	15	0	18	0	0
2	D	15	0	17	0	0
3	A	6	0	7	5	0
3	B	12	0	16	11	0
3	C	6	0	8	5	0
3	D	6	0	8	2	0
3	E	6	0	8	1	0
4	A	10	0	0	0	0
4	B	10	0	0	0	0
4	D	10	0	0	0	0
4	E	5	0	0	0	0
4	F	10	0	0	0	0
5	A	88	0	0	1	0
5	B	83	0	0	1	0
5	C	79	0	0	9	0
5	D	73	0	0	2	0
5	E	48	0	0	1	0
5	F	41	0	0	1	0
All	All	7503	0	6979	190	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 14.

All (190) 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:B:107:ARG:HD2	3:B:203:GOL:H12	1.19	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:8:LYS:HE2	3:C:202:GOL:H2	1.14	1.11
1:B:107:ARG:CD	3:B:203:GOL:H12	1.90	1.01
1:B:107:ARG:HD2	3:B:203:GOL:C1	1.96	0.95
1:A:115:HIS:NE2	3:C:202:GOL:H11	1.81	0.95
1:B:107:ARG:HH21	3:B:203:GOL:H32	1.32	0.93
5:C:320:HOH:O	3:E:201:GOL:H12	1.69	0.92
1:A:107:ARG:HE	3:A:202:GOL:H12	1.30	0.91
1:E:35:ARG:HH12	1:E:45[B]:ASN:HD21	1.21	0.89
1:A:115:HIS:NE2	3:C:202:GOL:H31	1.88	0.88
1:B:107:ARG:HH21	3:B:203:GOL:C3	1.87	0.88
3:C:202:GOL:H12	5:C:365:HOH:O	1.74	0.88
1:B:87:ASN:HB3	1:F:55:MET:HE2	1.53	0.87
1:C:8:LYS:HE2	3:C:202:GOL:C2	2.05	0.85
1:B:107:ARG:NH2	3:B:203:GOL:H32	1.91	0.84
1:B:107:ARG:CD	3:B:203:GOL:C1	2.57	0.82
1:F:29:ASP:OD1	1:F:31:ARG:HD3	1.80	0.82
1:D:132:GLU:C	1:D:133:GLN:CG	2.49	0.79
1:D:131:PRO:HG2	1:D:132:GLU:H	1.49	0.78
1:D:136:ILE:HD11	1:D:140:ASP:CB	2.13	0.78
1:A:107:ARG:HE	3:A:202:GOL:C1	1.96	0.77
1:C:18:ASN:OD1	1:C:19:PRO:HD2	1.85	0.77
1:D:132:GLU:C	1:D:133:GLN:HG3	2.05	0.77
1:C:18:ASN:HB3	1:C:21:SER:HB2	1.67	0.77
5:C:326:HOH:O	1:E:111:GLU:HB2	1.85	0.76
1:F:129:LEU:HD12	1:F:141:LEU:HD11	1.69	0.74
1:C:41:VAL:O	1:C:42:ASN:HB2	1.86	0.73
1:A:39:PHE:CZ	1:A:135:LEU:HD21	2.23	0.73
1:D:121:ARG:HH12	1:D:123:ASP:CG	1.91	0.72
1:F:132:GLU:OE1	1:F:134:LYS:HE2	1.90	0.72
1:E:121:ARG:NH1	1:E:123:ASP:OD1	2.24	0.70
1:A:39:PHE:HZ	1:A:135:LEU:CD2	2.05	0.69
1:A:107:ARG:NE	3:A:202:GOL:H12	2.07	0.69
1:B:29:ASP:OD1	1:B:31:ARG:CD	2.40	0.69
1:B:29:ASP:OD1	1:B:31:ARG:HD3	1.93	0.69
1:A:39:PHE:CZ	1:A:135:LEU:CD2	2.76	0.69
1:E:35:ARG:NH1	1:E:45[B]:ASN:HD21	1.91	0.69
1:C:9:PRO:HG3	5:C:340:HOH:O	1.91	0.68
1:D:136:ILE:HD11	1:D:140:ASP:HB3	1.74	0.68
1:D:136:ILE:HD11	1:D:140:ASP:HB2	1.74	0.68
1:F:9:PRO:O	1:F:13:VAL:HG13	1.93	0.68
1:E:35:ARG:HD3	1:E:35:ARG:C	2.14	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:TYR:HB2	3:B:203:GOL:H31	1.76	0.67
3:A:202:GOL:H31	1:C:115:HIS:NE2	2.10	0.66
1:A:146:ASP:O	1:A:147:HIS:CB	2.44	0.66
1:D:35:ARG:NH2	1:D:43:SER:OG	2.28	0.66
1:C:41:VAL:O	1:C:42:ASN:CB	2.44	0.66
1:B:87:ASN:CB	1:F:55:MET:HE2	2.26	0.65
1:A:136:ILE:HD13	1:A:141:LEU:HD13	1.79	0.65
1:B:35:ARG:HD3	1:B:45[A]:ASN:ND2	2.11	0.65
1:F:3:ASN:C	1:F:3:ASN:HD22	2.01	0.64
1:D:136:ILE:CD1	1:D:140:ASP:HB2	2.28	0.64
1:B:107:ARG:HD3	3:B:203:GOL:O1	1.98	0.63
1:F:18:ASN:ND2	1:F:20:ASP:HB3	2.13	0.63
1:B:24:LYS:HD3	1:B:69:GLU:OE1	1.99	0.62
1:D:54:GLU:HG3	5:D:365:HOH:O	1.98	0.62
3:A:202:GOL:H31	1:C:115:HIS:CE1	2.34	0.62
1:E:116:MET:HG2	1:E:117:TYR:CD1	2.36	0.61
1:C:142:ASN:OD1	1:E:129:LEU:HD12	2.01	0.61
1:D:131:PRO:CG	1:D:132:GLU:H	2.15	0.60
1:C:18:ASN:OD1	1:C:19:PRO:CD	2.49	0.59
1:E:37[B]:CYS:HB2	5:E:330:HOH:O	2.02	0.59
2:A:201[A]:EPE:H71	5:B:375:HOH:O	2.00	0.59
1:A:39:PHE:CE1	1:A:135:LEU:HD21	2.38	0.59
5:A:377:HOH:O	2:B:201[B]:EPE:H71	2.03	0.59
1:F:18:ASN:HD22	1:F:20:ASP:H	1.51	0.59
1:B:107:ARG:HD3	3:B:203:GOL:C1	2.33	0.58
1:D:123:ASP:N	1:D:123:ASP:OD1	2.34	0.57
1:F:29:ASP:OD1	1:F:31:ARG:CD	2.53	0.57
1:F:17:ASP:CG	1:F:121:ARG:HH22	2.07	0.57
1:C:129:LEU:HD22	1:E:142:ASN:OD1	2.04	0.57
1:B:129:LEU:HD22	1:B:141:LEU:HD11	1.85	0.57
1:B:107:ARG:NH2	3:B:203:GOL:C3	2.58	0.57
1:C:61:LYS:HE3	1:C:65:GLU:OE1	2.05	0.57
1:F:37[B]:CYS:HB2	5:F:323:HOH:O	2.05	0.57
1:B:29:ASP:OD1	1:B:31:ARG:HD2	2.05	0.56
1:F:52:THR:OG1	1:F:55:MET:HE3	2.06	0.56
1:D:133:GLN:NE2	1:F:119:ASP:OD2	2.38	0.56
1:B:80:VAL:HG22	1:F:49:ILE:HG12	1.87	0.56
1:D:115:HIS:CD2	3:D:202:GOL:H32	2.40	0.56
1:C:3:ASN:HB2	5:C:372:HOH:O	2.05	0.56
1:A:121:ARG:HH12	1:A:123:ASP:CG	2.10	0.55
1:E:35:ARG:HD3	1:E:35:ARG:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:LEU:HA	1:B:22:LEU:HD13	1.89	0.55
1:F:46:MET:CA	1:F:46:MET:HE2	2.33	0.54
1:B:61:LYS:O	1:B:65:GLU:HG3	2.08	0.53
1:D:136:ILE:CD1	1:D:140:ASP:CB	2.85	0.53
1:C:120:VAL:HG13	1:C:121:ARG:HG2	1.91	0.53
1:F:65:GLU:OE1	1:F:65:GLU:CA	2.57	0.53
1:B:87:ASN:HB3	1:F:55:MET:CE	2.34	0.52
1:E:121:ARG:HH12	1:E:123:ASP:CG	2.12	0.52
1:D:59:LEU:HD22	1:D:63:LEU:HG	1.91	0.52
1:E:35:ARG:HH12	1:E:45[B]:ASN:ND2	2.01	0.52
1:D:121:ARG:N	1:D:122:PRO:CD	2.73	0.52
1:B:28:ILE:N	1:B:28:ILE:HD12	2.24	0.52
1:D:121:ARG:NH1	1:D:123:ASP:OD1	2.44	0.51
1:B:18:ASN:HB3	1:B:21:SER:HB2	1.92	0.51
1:C:41:VAL:HB	1:C:126:TYR:CD1	2.45	0.51
1:E:116:MET:HG2	1:E:117:TYR:CE1	2.46	0.51
1:F:46:MET:HG3	1:F:51:CYS:SG	2.51	0.51
1:D:18:ASN:OD1	1:D:18:ASN:C	2.49	0.51
1:D:9:PRO:HG3	5:D:326:HOH:O	2.11	0.51
1:F:18:ASN:HD21	1:F:20:ASP:HB3	1.76	0.51
1:A:121:ARG:NH1	1:A:123:ASP:OD1	2.35	0.50
1:D:63:LEU:HD22	1:D:68:LYS:HG3	1.93	0.50
1:B:20:ASP:O	1:B:23:VAL:HG22	2.12	0.50
1:C:121:ARG:HD3	5:C:347:HOH:O	2.11	0.50
1:F:17:ASP:OD2	1:F:121:ARG:NH2	2.44	0.50
1:B:48:THR:O	1:B:88:ARG:NH2	2.44	0.49
1:C:41:VAL:HB	1:C:126:TYR:CE1	2.47	0.49
1:C:94:LYS:NZ	5:C:303:HOH:O	2.46	0.49
1:E:18:ASN:OD1	1:E:19:PRO:HD2	2.12	0.49
1:C:59:LEU:HD22	1:C:63:LEU:HG	1.96	0.48
1:F:46:MET:N	1:F:46:MET:HE2	2.29	0.48
1:F:116:MET:SD	1:F:117:TYR:CE1	3.07	0.48
1:E:70:LEU:HD23	1:E:104:TYR:CE2	2.48	0.48
1:D:15:LEU:HD11	1:D:70:LEU:HD22	1.96	0.48
1:E:35:ARG:NH1	1:E:45[B]:ASN:ND2	2.60	0.47
1:A:54:GLU:OE2	1:A:58:LYS:HE3	2.15	0.47
1:C:41:VAL:HG12	5:C:302:HOH:O	2.14	0.47
1:C:82:ALA:N	1:C:83:PRO:HD2	2.30	0.47
1:F:139:GLU:O	1:F:142:ASN:HB2	2.15	0.47
1:A:35:ARG:HH11	1:A:35:ARG:HB3	1.79	0.46
1:D:132:GLU:O	1:D:133:GLN:HG3	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:65:GLU:HA	1:F:65:GLU:OE1	2.16	0.46
1:A:49:ILE:HD13	1:A:49:ILE:HG21	1.69	0.46
1:A:35:ARG:CB	1:A:35:ARG:HH11	2.29	0.46
1:E:75:CYS:SG	1:E:78:SER:HA	2.56	0.46
1:D:131:PRO:HG2	1:D:133:GLN:H	1.80	0.46
1:F:121:ARG:NH1	1:F:123:ASP:OD2	2.49	0.46
1:C:49:ILE:HD13	1:C:49:ILE:HG21	1.32	0.46
1:D:61:LYS:O	1:D:65:GLU:HG3	2.16	0.45
1:D:121:ARG:N	1:D:122:PRO:HD3	2.32	0.45
1:E:66:GLU:O	1:E:67:LYS:HB2	2.16	0.45
1:C:121:ARG:HH12	1:C:123:ASP:CG	2.19	0.45
1:C:16:LEU:O	1:C:22:LEU:HD22	2.17	0.44
1:D:40:ILE:HD11	1:D:113:PHE:CE2	2.53	0.44
1:E:49:ILE:HG21	1:E:49:ILE:HD13	1.33	0.44
1:A:15:LEU:HD11	1:A:70:LEU:HD22	2.00	0.44
1:F:129:LEU:CD1	1:F:141:LEU:HD11	2.43	0.44
1:A:121:ARG:HD2	1:A:121:ARG:HH11	0.85	0.43
1:C:121:ARG:N	1:C:122:PRO:CD	2.80	0.43
1:D:129:LEU:HD23	1:D:129:LEU:HA	1.81	0.43
1:C:62:THR:O	1:C:66:GLU:HG3	2.18	0.43
1:C:7:ILE:HG13	1:C:11:GLU:HB2	1.99	0.43
1:D:7:ILE:HG13	1:D:11:GLU:HB2	2.01	0.43
1:E:9:PRO:HD2	1:E:10:GLU:OE1	2.19	0.43
1:F:39:PHE:HE1	1:F:135:LEU:HD11	1.84	0.43
1:B:49:ILE:HG21	1:B:49:ILE:HD13	1.53	0.42
1:B:58:LYS:HE2	5:C:303:HOH:O	2.19	0.42
1:B:56:TYR:HE1	1:B:88:ARG:NH1	2.17	0.42
1:C:82:ALA:HB3	1:C:83:PRO:HD3	2.00	0.42
1:A:132:GLU:HB2	1:A:134:LYS:HG3	2.02	0.42
1:E:18:ASN:HA	1:E:19:PRO:HD3	1.92	0.42
1:C:61:LYS:O	1:C:65:GLU:HG3	2.20	0.42
1:E:116:MET:SD	1:E:117:TYR:CE1	3.12	0.42
1:D:136:ILE:HG13	1:D:137:SER:O	2.20	0.42
1:F:130:GLY:O	1:F:133:GLN:N	2.36	0.42
1:B:87:ASN:ND2	1:F:55:MET:HE1	2.35	0.42
1:F:136:ILE:HD13	1:F:141:LEU:HD13	2.01	0.42
1:C:117:TYR:HA	1:C:120:VAL:HG12	2.02	0.42
1:B:20:ASP:OD2	1:B:24:LYS:HE3	2.20	0.42
1:F:117:TYR:HB3	1:F:121:ARG:HB2	2.02	0.41
1:F:22:LEU:HA	1:F:22:LEU:HD23	1.92	0.41
1:D:115:HIS:CG	3:D:202:GOL:H32	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:123:ASP:OD1	1:C:123:ASP:N	2.53	0.41
1:F:49:ILE:HG21	1:F:49:ILE:HD13	1.24	0.41
1:B:87:ASN:CB	1:F:55:MET:CE	2.96	0.41
1:A:7:ILE:HG21	1:A:7:ILE:HD13	1.74	0.40
1:A:126:TYR:CZ	1:A:137:SER:HB3	2.57	0.40
1:B:7:ILE:HD13	1:B:7:ILE:HG21	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	144/152 (95%)	139 (96%)	4 (3%)	1 (1%)	22	15
1	B	145/152 (95%)	141 (97%)	4 (3%)	0	100	100
1	C	143/152 (94%)	138 (96%)	4 (3%)	1 (1%)	22	15
1	D	143/152 (94%)	136 (95%)	5 (4%)	2 (1%)	11	5
1	E	145/152 (95%)	139 (96%)	6 (4%)	0	100	100
1	F	145/152 (95%)	134 (92%)	11 (8%)	0	100	100
All	All	865/912 (95%)	827 (96%)	34 (4%)	4 (0%)	29	22

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	146	ASP
1	D	131	PRO
1	D	133	GLN
1	C	131	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	127/133 (96%)	118 (93%)	9 (7%)	14	9
1	B	128/133 (96%)	118 (92%)	10 (8%)	12	7
1	C	126/133 (95%)	117 (93%)	9 (7%)	14	9
1	D	126/133 (95%)	114 (90%)	12 (10%)	8	4
1	E	128/133 (96%)	112 (88%)	16 (12%)	4	1
1	F	128/133 (96%)	111 (87%)	17 (13%)	4	1
All	All	763/798 (96%)	690 (90%)	73 (10%)	8	4

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	21	SER
1	A	23	VAL
1	A	32	ASP
1	A	35	ARG
1	A	100	LEU
1	A	129	LEU
1	A	135	LEU
1	A	141	LEU
1	B	3	ASN
1	B	14	GLU
1	B	31	ARG
1	B	32	ASP
1	B	35	ARG
1	B	59	LEU
1	B	91	LEU
1	B	100	LEU
1	B	107	ARG
1	B	141	LEU
1	C	3	ASN
1	C	23	VAL
1	C	32	ASP

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Mol	Chain	Res	Type
1	C	59	LEU
1	C	67	LYS
1	C	91	LEU
1	C	100	LEU
1	C	129	LEU
1	C	135	LEU
1	D	3	ASN
1	D	18	ASN
1	D	22	LEU
1	D	32	ASP
1	D	58	LYS
1	D	59	LEU
1	D	67	LYS
1	D	91	LEU
1	D	100	LEU
1	D	123	ASP
1	D	129	LEU
1	D	141	LEU
1	E	3	ASN
1	E	14	GLU
1	E	23	VAL
1	E	32	ASP
1	E	35	ARG
1	E	59	LEU
1	E	67	LYS
1	E	70	LEU
1	E	99	VAL
1	E	107	ARG
1	E	119	ASP
1	E	120	VAL
1	E	129	LEU
1	E	135	LEU
1	E	137	SER
1	E	141	LEU
1	F	3	ASN
1	F	18	ASN
1	F	21	SER
1	F	32	ASP
1	F	42	ASN
1	F	49	ILE
1	F	59	LEU
1	F	65	GLU

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Mol	Chain	Res	Type
1	F	67	LYS
1	F	70	LEU
1	F	91	LEU
1	F	99	VAL
1	F	107	ARG
1	F	119	ASP
1	F	129	LEU
1	F	135	LEU
1	F	141	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	45	ASN
1	B	87	ASN
1	C	3	ASN
1	C	45	ASN
1	D	3	ASN
1	E	133	GLN
1	F	3	ASN
1	F	18	ASN
1	F	93	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 ⓘ

19 ligands are modelled in this entry.

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	GOL	C	202	-	5,5,5	0.75	0	5,5,5	2.12	3 (60%)
4	SO4	A	204	-	4,4,4	0.25	0	6,6,6	1.84	2 (33%)
4	SO4	B	205[A]	-	4,4,4	0.35	0	6,6,6	0.50	0
2	EPE	A	201[A]	-	15,15,15	1.20	1 (6%)	18,20,20	2.45	8 (44%)
4	SO4	F	201	-	4,4,4	0.26	0	6,6,6	0.51	0
3	GOL	B	203	-	5,5,5	0.99	0	5,5,5	1.20	0
4	SO4	A	203[B]	-	4,4,4	0.58	0	6,6,6	0.59	0
4	SO4	F	202	-	4,4,4	0.81	0	6,6,6	1.09	0
4	SO4	E	202	-	4,4,4	0.31	0	6,6,6	0.83	0
4	SO4	D	204	-	4,4,4	0.75	0	6,6,6	0.59	0
4	SO4	B	204	-	4,4,4	0.36	0	6,6,6	0.62	0
2	EPE	D	201	-	15,15,15	1.14	2 (13%)	18,20,20	1.99	6 (33%)
3	GOL	B	202	-	5,5,5	0.50	0	5,5,5	0.82	0
3	GOL	D	202	-	5,5,5	0.45	0	5,5,5	0.49	0
4	SO4	D	203	-	4,4,4	0.42	0	6,6,6	1.52	1 (16%)
3	GOL	E	201	-	5,5,5	0.85	0	5,5,5	1.81	1 (20%)
2	EPE	B	201[B]	-	15,15,15	1.20	1 (6%)	18,20,20	2.85	9 (50%)
3	GOL	A	202	-	5,5,5	1.33	1 (20%)	5,5,5	1.69	1 (20%)
2	EPE	C	201	-	15,15,15	1.07	0	18,20,20	2.07	6 (33%)

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	GOL	C	202	-	-	2/4/4/4	-
2	EPE	A	201[A]	-	-	7/9/19/19	0/1/1/1
3	GOL	B	203	-	-	2/4/4/4	-
2	EPE	D	201	-	-	0/9/19/19	0/1/1/1
3	GOL	B	202	-	-	4/4/4/4	-
3	GOL	D	202	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	E	201	-	-	1/4/4/4	-
2	EPE	B	201[B]	-	-	4/9/19/19	0/1/1/1
3	GOL	A	202	-	-	2/4/4/4	-
2	EPE	C	201	-	-	0/9/19/19	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	201[A]	EPE	C10-S	3.71	1.82	1.77
2	B	201[B]	EPE	C10-S	3.71	1.82	1.77
3	A	202	GOL	O2-C2	-2.30	1.36	1.43
2	D	201	EPE	C2-N1	2.08	1.52	1.46
2	D	201	EPE	C9-N1	2.07	1.52	1.47

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	201[B]	EPE	C5-C6-N1	-6.76	96.76	110.64
2	B	201[B]	EPE	C6-C5-N4	-5.20	99.98	110.64
2	A	201[A]	EPE	C6-C5-N4	-4.90	100.58	110.64
2	C	201	EPE	O2S-S-C10	4.58	112.44	106.92
2	B	201[B]	EPE	O2S-S-C10	4.31	112.11	106.92
2	A	201[A]	EPE	O3S-S-C10	4.15	112.47	105.77
2	B	201[B]	EPE	C5-N4-C3	4.13	118.13	108.83
2	D	201	EPE	O3S-S-C10	3.93	112.12	105.77
2	A	201[A]	EPE	O1S-S-C10	3.89	111.60	106.92
3	E	201	GOL	O2-C2-C1	-3.88	92.03	109.12
2	C	201	EPE	C5-N4-C3	3.85	117.50	108.83
2	D	201	EPE	C6-C5-N4	3.78	118.39	110.64
2	D	201	EPE	C5-N4-C3	3.55	116.81	108.83
2	B	201[B]	EPE	C7-N4-C3	3.33	119.75	111.23
2	A	201[A]	EPE	C5-C6-N1	-3.22	104.04	110.64
3	C	202	GOL	O2-C2-C3	3.21	123.25	109.12
3	A	202	GOL	O2-C2-C3	-3.18	95.13	109.12
4	A	204	SO4	O3-S-O1	-3.16	92.80	109.31
2	A	201[A]	EPE	C5-N4-C3	3.11	115.82	108.83
2	A	201[A]	EPE	C7-N4-C5	2.84	118.51	111.23
2	C	201	EPE	O3S-S-C10	2.73	110.18	105.77
2	C	201	EPE	O3S-S-O2S	-2.72	104.63	111.27
4	A	204	SO4	O3-S-O2	2.69	123.34	109.31
3	C	202	GOL	O3-C3-C2	2.63	122.81	110.20
4	D	203	SO4	O3-S-O1	-2.59	95.78	109.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	201[A]	EPE	O3S-S-O2S	-2.54	105.06	111.27
2	B	201[B]	EPE	C7-N4-C5	2.44	117.47	111.23
2	C	201	EPE	C7-N4-C3	2.40	117.36	111.23
2	C	201	EPE	C6-N1-C2	2.32	114.04	108.83
2	D	201	EPE	O1S-S-C10	-2.30	104.15	106.92
2	D	201	EPE	O2S-S-C10	2.21	109.58	106.92
2	B	201[B]	EPE	O1S-S-C10	2.14	109.49	106.92
2	B	201[B]	EPE	C6-N1-C2	2.12	113.59	108.83
2	A	201[A]	EPE	C7-N4-C3	2.08	116.55	111.23
2	B	201[B]	EPE	C8-C7-N4	-2.06	105.98	113.40
3	C	202	GOL	O2-C2-C1	-2.05	100.09	109.12
2	D	201	EPE	C6-N1-C2	2.03	113.41	108.83

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	201[A]	EPE	C10-C9-N1-C2
2	A	201[A]	EPE	C9-C10-S-O2S
2	A	201[A]	EPE	C9-C10-S-O3S
3	B	203	GOL	O1-C1-C2-O2
3	B	203	GOL	O1-C1-C2-C3
3	B	202	GOL	O1-C1-C2-C3
3	B	202	GOL	C1-C2-C3-O3
3	E	201	GOL	C1-C2-C3-O3
3	A	202	GOL	O1-C1-C2-C3
3	C	202	GOL	O1-C1-C2-C3
3	B	202	GOL	O1-C1-C2-O2
3	B	202	GOL	O2-C2-C3-O3
3	A	202	GOL	O1-C1-C2-O2
2	B	201[B]	EPE	N4-C7-C8-O8
3	C	202	GOL	O1-C1-C2-O2
2	B	201[B]	EPE	C8-C7-N4-C5
2	A	201[A]	EPE	C10-C9-N1-C6
2	B	201[B]	EPE	C10-C9-N1-C2
2	B	201[B]	EPE	C10-C9-N1-C6
2	A	201[A]	EPE	C8-C7-N4-C5
2	A	201[A]	EPE	C9-C10-S-O1S
2	A	201[A]	EPE	C8-C7-N4-C3

There are no ring outliers.

7 monomers are involved in 26 short contacts:

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	202	GOL	5	0
2	A	201[A]	EPE	1	0
3	B	203	GOL	11	0
3	D	202	GOL	2	0
3	E	201	GOL	1	0
2	B	201[B]	EPE	1	0
3	A	202	GOL	5	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	145/152 (95%)	-0.13	1 (0%)	87	91	16, 27, 52, 65	2 (1%)
1	B	145/152 (95%)	-0.05	3 (2%)	63	71	18, 29, 52, 62	3 (2%)
1	C	145/152 (95%)	-0.00	3 (2%)	63	71	17, 29, 57, 68	1 (0%)
1	D	145/152 (95%)	0.02	5 (3%)	45	53	18, 32, 60, 82	1 (0%)
1	E	145/152 (95%)	-0.10	5 (3%)	45	53	21, 36, 56, 67	3 (2%)
1	F	145/152 (95%)	0.34	8 (5%)	25	34	24, 44, 72, 84	3 (2%)
All	All	870/912 (95%)	0.01	25 (2%)	51	61	16, 33, 60, 84	13 (1%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	21	SER	4.3
1	B	37[A]	CYS	3.9
1	E	21	SER	3.8
1	E	37[A]	CYS	3.8
1	C	21	SER	3.6
1	D	132	GLU	3.5
1	F	37[A]	CYS	3.4
1	F	45[A]	ASN	3.3
1	D	133	GLN	3.3
1	F	20	ASP	3.0
1	B	45[A]	ASN	2.9
1	F	23	VAL	2.6
1	A	37[A]	CYS	2.6
1	E	64	PHE	2.5
1	E	45[A]	ASN	2.5
1	D	131	PRO	2.5
1	B	20	ASP	2.3
1	F	145	VAL	2.3
1	C	147	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	22	LEU	2.2
1	D	130	GLY	2.2
1	F	19	PRO	2.1
1	F	15	LEU	2.0
1	C	133	GLN	2.0
1	D	21	SER	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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	C	202	6/6	0.87	0.17	41,53,58,60	0
3	GOL	D	202	6/6	0.92	0.13	51,54,55,57	0
3	GOL	B	203	6/6	0.93	0.19	40,47,52,62	0
3	GOL	A	202	6/6	0.93	0.16	35,39,45,55	0
4	SO4	D	204	5/5	0.94	0.17	49,55,61,61	0
3	GOL	E	201	6/6	0.94	0.14	47,50,54,60	0
3	GOL	B	202	6/6	0.94	0.11	46,56,58,61	0
4	SO4	F	202	5/5	0.95	0.10	45,45,50,53	0
4	SO4	A	204	5/5	0.98	0.13	45,51,52,56	0
4	SO4	D	203	5/5	0.98	0.13	38,44,50,50	0
4	SO4	B	204	5/5	0.98	0.13	41,44,48,51	0
2	EPE	B	201[B]	15/15	0.98	0.17	17,22,23,25	15
2	EPE	A	201[A]	15/15	0.98	0.17	15,19,23,24	15
4	SO4	A	203[B]	5/5	0.99	0.13	14,15,16,20	5
2	EPE	D	201	15/15	0.99	0.10	22,29,34,35	0
2	EPE	C	201	15/15	0.99	0.11	19,29,34,34	0
4	SO4	B	205[A]	5/5	1.00	0.13	12,12,13,17	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SO4	E	202	5/5	1.00	0.11	26,26,28,31	0
4	SO4	F	201	5/5	1.00	0.13	26,29,30,31	0

6.5 Other polymers (i)

There are no such residues in this entry.