Full wwPDB X-ray Structure Validation Report (i)

Jun 15, 2020 – 09:10 am BST

PDB ID	:	4ZQE
Title	:	Crystal structure of DOX-P Reductoisomerase in complex with magnesium
Authors	:	Birkinshaw, R.W.; Brady, R.L.
Deposited on	:	2015-05-10
Resolution	:	1.98 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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 ⓘ

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

The reported resolution of this entry is 1.98 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.
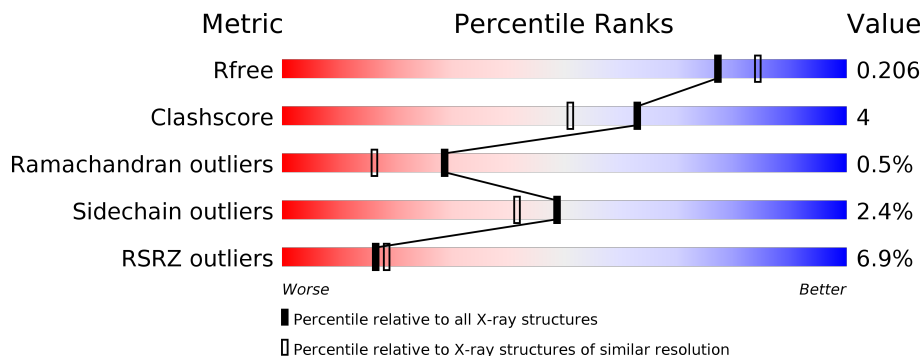
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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	432	
1	B	432	

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	505	-	-	X	-
3	GOL	B	506	-	X	-	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6446 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 1-deoxy-D-xylulose 5-phosphate reductoisomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	400	Total 3007	C 1911	N 512	O 569	S 15	1	2	0
1	B	400	Total 2986	C 1894	N 505	O 572	S 15	0	1	0

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	MET	-	initiating methionine	UNP A0A076U3E6
A	-16	ALA	-	expression tag	UNP A0A076U3E6
A	-15	HIS	-	expression tag	UNP A0A076U3E6
A	-14	HIS	-	expression tag	UNP A0A076U3E6
A	-13	HIS	-	expression tag	UNP A0A076U3E6
A	-12	HIS	-	expression tag	UNP A0A076U3E6
A	-11	HIS	-	expression tag	UNP A0A076U3E6
A	-10	HIS	-	expression tag	UNP A0A076U3E6
A	-9	SER	-	expression tag	UNP A0A076U3E6
A	-8	SER	-	expression tag	UNP A0A076U3E6
A	-7	GLY	-	expression tag	UNP A0A076U3E6
A	-6	LEU	-	expression tag	UNP A0A076U3E6
A	-5	GLU	-	expression tag	UNP A0A076U3E6
A	-4	VAL	-	expression tag	UNP A0A076U3E6
A	-3	LEU	-	expression tag	UNP A0A076U3E6
A	-2	PHE	-	expression tag	UNP A0A076U3E6
A	-1	GLN	-	expression tag	UNP A0A076U3E6
A	0	GLY	-	expression tag	UNP A0A076U3E6
A	1	PRO	-	expression tag	UNP A0A076U3E6
B	-17	MET	-	initiating methionine	UNP A0A076U3E6
B	-16	ALA	-	expression tag	UNP A0A076U3E6
B	-15	HIS	-	expression tag	UNP A0A076U3E6
B	-14	HIS	-	expression tag	UNP A0A076U3E6
B	-13	HIS	-	expression tag	UNP A0A076U3E6
B	-12	HIS	-	expression tag	UNP A0A076U3E6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-11	HIS	-	expression tag	UNP A0A076U3E6
B	-10	HIS	-	expression tag	UNP A0A076U3E6
B	-9	SER	-	expression tag	UNP A0A076U3E6
B	-8	SER	-	expression tag	UNP A0A076U3E6
B	-7	GLY	-	expression tag	UNP A0A076U3E6
B	-6	LEU	-	expression tag	UNP A0A076U3E6
B	-5	GLU	-	expression tag	UNP A0A076U3E6
B	-4	VAL	-	expression tag	UNP A0A076U3E6
B	-3	LEU	-	expression tag	UNP A0A076U3E6
B	-2	PHE	-	expression tag	UNP A0A076U3E6
B	-1	GLN	-	expression tag	UNP A0A076U3E6
B	0	GLY	-	expression tag	UNP A0A076U3E6
B	1	PRO	-	expression tag	UNP A0A076U3E6

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
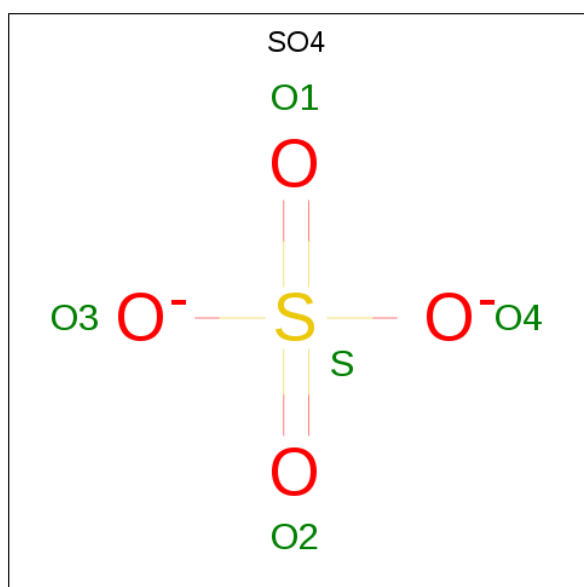
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 5	O 4	S 1	0	0
2	A	1	Total 5	O 4	S 1	0	0
2	A	1	Total 5	O 4	S 1	0	0
2	A	1	Total 5	O 4	S 1	0	0
2	B	1	Total 5	O 4	S 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total 5	O 4	S 1	0	0
2	B	1	Total 5	O 4	S 1	0	0
2	B	1	Total 5	O 4	S 1	0	0
2	B	1	Total 5	O 4	S 1	0	0

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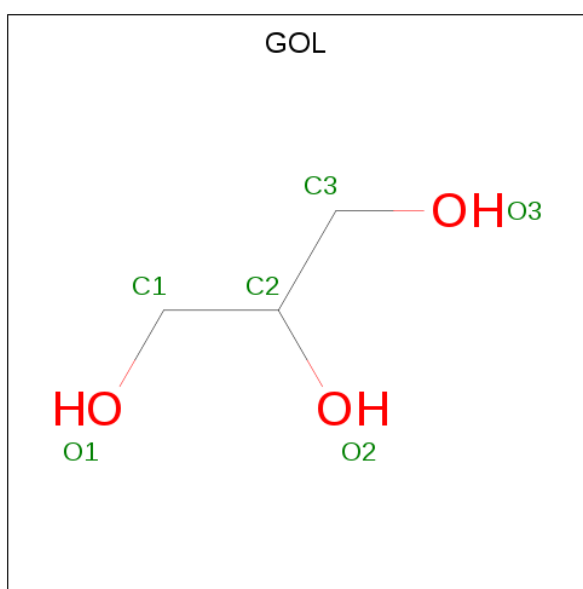
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 6	C 3	O 3	0	0
3	A	1	Total 6	C 3	O 3	0	0
3	B	1	Total 6	C 3	O 3	0	0
3	B	1	Total 6	C 3	O 3	0	0
3	B	1	Total 6	C 3	O 3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	221	Total O 221 221	0	0
4	B	157	Total O 157 157	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: 1-deoxy-D-xylulose 5-phosphate reductoisomerase
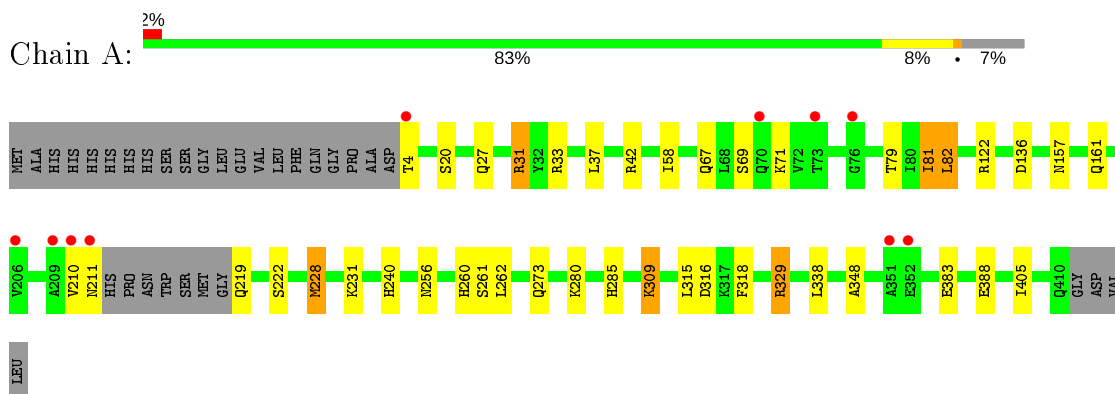
- Molecule 1: 1-deoxy-D-xylulose 5-phosphate reductoisomerase
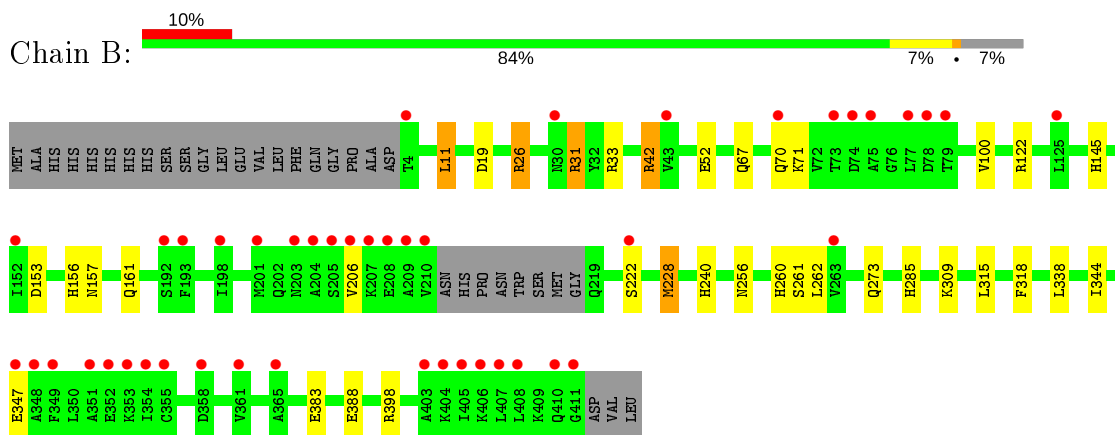
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α, β, γ	133.21Å 133.21Å 77.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.40 – 1.98 44.40 – 1.98	Depositor EDS
% Data completeness (in resolution range)	99.1 (44.40-1.98) 99.2 (44.40-1.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.60 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.171 , 0.195 0.182 , 0.206	Depositor DCC
R_{free} test set	4702 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	28.5	Xtriage
Anisotropy	0.270	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 45.5	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.028 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6446	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% 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 $< \lvert L \rvert >$, $< L^2 >$ 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, 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	1.02	2/3052 (0.1%)	0.95	10/4135 (0.2%)
1	B	0.89	0/3027	0.94	9/4106 (0.2%)
All	All	0.96	2/6079 (0.0%)	0.95	19/8241 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	309	LYS	CE-NZ	-7.99	1.29	1.49
1	A	136	ASP	CB-CG	-5.72	1.39	1.51

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	31	ARG	NE-CZ-NH2	-12.07	114.26	120.30
1	B	26	ARG	NE-CZ-NH1	11.89	126.25	120.30
1	B	26	ARG	NE-CZ-NH2	-10.80	114.90	120.30
1	B	31	ARG	NE-CZ-NH2	-9.19	115.70	120.30
1	A	33	ARG	NE-CZ-NH1	7.58	124.09	120.30
1	B	122	ARG	NE-CZ-NH2	-7.36	116.62	120.30
1	A	42	ARG	NE-CZ-NH1	6.85	123.72	120.30
1	B	33	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	B	42	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	A	122	ARG	NE-CZ-NH2	-6.23	117.19	120.30
1	A	136	ASP	CB-CG-OD2	-6.15	112.77	118.30
1	B	19	ASP	CB-CG-OD2	5.74	123.47	118.30
1	B	228	MET	CG-SD-CE	-5.70	91.08	100.20
1	A	228	MET	CG-SD-CE	-5.68	91.11	100.20
1	A	122	ARG	CB-CG-CD	-5.42	97.50	111.60
1	B	122	ARG	CB-CG-CD	-5.33	97.74	111.60
1	A	82	LEU	N-CA-CB	5.31	121.02	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	316	ASP	CB-CG-OD1	5.28	123.05	118.30
1	A	329	ARG	NE-CZ-NH1	5.28	122.94	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3007	0	3093	28	7
1	B	2986	0	3042	23	7
2	A	20	0	0	2	0
2	B	25	0	0	3	0
3	A	12	0	16	4	0
3	B	18	0	24	0	0
4	A	221	0	0	8	0
4	B	157	0	0	7	0
All	All	6446	0	6175	52	7

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 4.

All (52) 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:58:ILE:O	1:A:81:ILE:O	1.74	1.04
1:B:153[A]:ASP:OD2	4:B:601:HOH:O	2.05	0.74
1:A:20:SER:HA	3:A:505:GOL:H11	1.72	0.70
1:B:26:ARG:NH2	4:B:602:HOH:O	2.26	0.67
1:A:260:HIS:HE1	4:A:626:HOH:O	1.76	0.67
1:B:260:HIS:HE1	4:B:606:HOH:O	1.81	0.62
2:A:501:SO4:O2	4:A:601:HOH:O	2.16	0.62
1:A:240:HIS:HD2	4:A:802:HOH:O	1.84	0.60
1:B:153[B]:ASP:CG	1:B:156:HIS:HD1	2.03	0.60
1:B:145:HIS:HE1	4:B:604:HOH:O	1.86	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:LYS:NZ	3:A:505:GOL:H12	2.18	0.57
1:B:240:HIS:HE1	4:B:655:HOH:O	1.87	0.57
1:A:157:ASN:HD21	1:A:285:HIS:CD2	2.23	0.57
1:B:157:ASN:HD21	1:B:285:HIS:CD2	2.24	0.55
1:B:42:ARG:HD2	2:B:502:SO4:O3	2.06	0.55
1:A:210:VAL:O	1:A:211:ASN:CB	2.55	0.54
1:A:67:GLN:HE21	1:A:71:LYS:NZ	2.05	0.54
1:B:67:GLN:HE21	1:B:71:LYS:NZ	2.06	0.54
1:B:285:HIS:HE1	4:B:728:HOH:O	1.90	0.54
1:A:280:LYS:HZ2	3:A:505:GOL:H12	1.74	0.52
1:A:285:HIS:HE1	4:A:788:HOH:O	1.93	0.52
1:A:157:ASN:HD21	1:A:285:HIS:HD2	1.57	0.51
1:B:157:ASN:HD21	1:B:285:HIS:HD2	1.58	0.51
1:A:280:LYS:HG3	3:A:505:GOL:H12	1.92	0.50
1:B:42:ARG:NH2	2:B:505:SO4:O3	2.38	0.50
1:A:69:SER:HA	1:A:81:ILE:CD1	2.42	0.50
1:A:27:GLN:NE2	4:A:602:HOH:O	2.34	0.49
1:B:240:HIS:HD2	4:B:745:HOH:O	1.93	0.49
1:A:329:ARG:NH2	4:A:606:HOH:O	2.47	0.47
1:B:260:HIS:HD2	1:B:273:GLN:OE1	1.98	0.47
1:A:210:VAL:O	1:A:211:ASN:HB3	2.15	0.47
1:A:256:ASN:ND2	1:A:309:LYS:H	2.14	0.45
1:A:228:MET:HE3	1:A:318:PHE:CD1	2.52	0.45
1:A:260:HIS:HD2	1:A:273:GLN:OE1	1.99	0.45
1:B:256:ASN:ND2	1:B:309:LYS:H	2.15	0.45
1:A:256:ASN:HD21	1:A:309:LYS:H	1.65	0.44
1:B:31:ARG:HG3	2:B:504:SO4:O3	2.17	0.44
1:A:161:GLN:HG2	1:A:285:HIS:CE1	2.53	0.44
1:A:240:HIS:HE1	4:A:637:HOH:O	2.01	0.42
1:A:31:ARG:HG3	2:A:504:SO4:O2	2.19	0.42
1:A:348:ALA:HB2	1:A:405:ILE:HD13	2.02	0.42
1:B:11:LEU:HD22	1:B:100:VAL:HG13	2.01	0.42
1:B:26:ARG:HD3	1:B:52:GLU:OE2	2.20	0.42
1:A:231:LYS:HB2	4:A:725:HOH:O	2.18	0.41
1:A:228:MET:CE	1:A:318:PHE:CD1	3.03	0.41
1:A:37:LEU:O	1:A:58:ILE:HA	2.20	0.41
1:B:228:MET:HE3	1:B:318:PHE:CD1	2.55	0.41
1:B:344:ILE:HD11	1:B:398:ARG:HG3	2.03	0.41
1:B:11:LEU:HD22	1:B:100:VAL:CG1	2.51	0.40
1:B:256:ASN:HD21	1:B:309:LYS:H	1.68	0.40
1:B:161:GLN:HG2	1:B:285:HIS:CE1	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:SER:HA	1:A:81:ILE:HD13	2.03	0.40

All (7) 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)
1:A:383[A]:GLU:OE1	1:B:383:GLU:OE2[4_554]	1.40	0.80
1:A:383[A]:GLU:OE2	1:B:383:GLU:OE1[4_554]	1.51	0.69
1:A:383[A]:GLU:CD	1:B:383:GLU:OE2[4_554]	1.65	0.55
1:A:388:GLU:OE2	1:B:388:GLU:OE2[4_554]	1.79	0.41
1:A:383[A]:GLU:CD	1:B:383:GLU:CD[4_554]	1.92	0.28
1:A:383[A]:GLU:OE2	1:B:383:GLU:CD[4_554]	2.04	0.16
1:A:383[A]:GLU:CD	1:B:383:GLU:OE1[4_554]	2.17	0.03

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	398/432 (92%)	390 (98%)	5 (1%)	3 (1%)	19	9
1	B	397/432 (92%)	388 (98%)	8 (2%)	1 (0%)	41	29
All	All	795/864 (92%)	778 (98%)	13 (2%)	4 (0%)	29	16

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	261	SER
1	B	261	SER
1	A	81	ILE
1	A	82	LEU

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	319/349 (91%)	312 (98%)	7 (2%)	52	46
1	B	314/349 (90%)	306 (98%)	8 (2%)	47	39
All	All	633/698 (91%)	618 (98%)	15 (2%)	49	41

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	THR
1	A	79	THR
1	A	219	GLN
1	A	222	SER
1	A	262	LEU
1	A	315	LEU
1	A	338	LEU
1	B	11	LEU
1	B	70	GLN
1	B	206	VAL
1	B	222	SER
1	B	262	LEU
1	B	315	LEU
1	B	338	LEU
1	B	347	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	67	GLN
1	A	203	ASN
1	A	230	ASN
1	A	240	HIS
1	A	248	GLN
1	A	250	GLN

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Mol	Chain	Res	Type
1	A	256	ASN
1	A	260	HIS
1	A	285	HIS
1	A	304	GLN
1	A	410	GLN
1	B	27	GLN
1	B	67	GLN
1	B	145	HIS
1	B	202	GLN
1	B	240	HIS
1	B	248	GLN
1	B	250	GLN
1	B	256	ASN
1	B	260	HIS
1	B	285	HIS
1	B	304	GLN

5.3.3 RNA (i)

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)

14 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	B	506	-	5,5,5	0.51	0	5,5,5	1.71	2 (40%)
2	SO4	A	502	-	4,4,4	0.62	0	6,6,6	1.17	1 (16%)
2	SO4	B	504	-	4,4,4	0.36	0	6,6,6	0.62	0
2	SO4	B	503	-	4,4,4	0.59	0	6,6,6	0.66	0
2	SO4	A	501	-	4,4,4	0.72	0	6,6,6	1.26	1 (16%)
2	SO4	B	501	-	4,4,4	0.25	0	6,6,6	1.36	1 (16%)
3	GOL	B	507	-	5,5,5	0.62	0	5,5,5	0.59	0
2	SO4	B	505	-	4,4,4	0.44	0	6,6,6	0.70	0
2	SO4	A	504	-	4,4,4	0.18	0	6,6,6	0.68	0
2	SO4	B	502	-	4,4,4	0.30	0	6,6,6	0.92	0
3	GOL	A	506	-	5,5,5	0.91	0	5,5,5	3.07	2 (40%)
2	SO4	A	503	-	4,4,4	0.38	0	6,6,6	0.33	0
3	GOL	A	505	-	5,5,5	0.45	0	5,5,5	1.35	1 (20%)
3	GOL	B	508	-	5,5,5	0.77	0	5,5,5	0.85	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	GOL	B	506	-	-	4/4/4/4	-
3	GOL	A	506	-	-	2/4/4/4	-
3	GOL	B	508	-	-	2/4/4/4	-
3	GOL	B	507	-	-	0/4/4/4	-
3	GOL	A	505	-	-	4/4/4/4	-

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	506	GOL	O1-C1-C2	-5.05	85.98	110.20
3	A	506	GOL	O2-C2-C3	4.22	127.72	109.12
3	B	506	GOL	O1-C1-C2	-2.97	95.98	110.20
3	A	505	GOL	O1-C1-C2	2.71	123.18	110.20
2	A	501	SO4	O3-S-O1	2.24	120.99	109.31
3	B	506	GOL	O2-C2-C3	2.09	118.31	109.12
2	B	501	SO4	O4-S-O3	-2.04	100.35	109.06
2	A	502	SO4	O3-S-O1	-2.01	98.80	109.31

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	506	GOL	O1-C1-C2-O2
3	B	506	GOL	O1-C1-C2-C3
3	A	505	GOL	O1-C1-C2-C3
3	A	505	GOL	C1-C2-C3-O3
3	B	508	GOL	O1-C1-C2-C3
3	B	506	GOL	C1-C2-C3-O3
3	A	506	GOL	O1-C1-C2-C3
3	A	506	GOL	O1-C1-C2-O2
3	A	505	GOL	O1-C1-C2-O2
3	A	505	GOL	O2-C2-C3-O3
3	B	508	GOL	O1-C1-C2-O2
3	B	506	GOL	O2-C2-C3-O3

There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	504	SO4	1	0
2	A	501	SO4	1	0
2	B	505	SO4	1	0
2	A	504	SO4	1	0
2	B	502	SO4	1	0
3	A	505	GOL	4	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	400/432 (92%)	0.06	10 (2%)	57	59	23, 32, 56, 87	1 (0%)
1	B	400/432 (92%)	0.46	45 (11%)	5	5	21, 38, 70, 95	0
All	All	800/864 (92%)	0.26	55 (6%)	16	18	21, 35, 65, 95	1 (0%)

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	407	LEU	8.8
1	B	206	VAL	6.8
1	B	408	LEU	6.4
1	B	351	ALA	4.7
1	B	77	LEU	4.5
1	B	4	THR	4.3
1	B	406	LYS	4.0
1	B	355	CYS	3.8
1	B	349	PHE	3.7
1	B	410	GLN	3.6
1	B	203	ASN	3.3
1	B	354	ILE	3.1
1	B	403	ALA	3.0
1	B	209	ALA	3.0
1	B	208	GLU	3.0
1	B	73	THR	2.9
1	B	198	ILE	2.9
1	B	210	VAL	2.9
1	B	352	GLU	2.9
1	B	411	GLY	2.8
1	B	78	ASP	2.8
1	B	193	PHE	2.7
1	A	211	ASN	2.7
1	A	209	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	351	ALA	2.7
1	A	4	THR	2.6
1	B	204	ALA	2.6
1	B	205	SER	2.6
1	B	263	VAL	2.6
1	B	70	GLN	2.6
1	B	353	LYS	2.6
1	A	70	GLN	2.5
1	B	361	VAL	2.5
1	B	405	ILE	2.5
1	B	348	ALA	2.5
1	B	347	GLU	2.4
1	A	206	VAL	2.4
1	B	201	MET	2.3
1	A	352	GLU	2.3
1	B	74	ASP	2.3
1	B	365	ALA	2.3
1	B	404	LYS	2.3
1	B	75	ALA	2.3
1	B	358	ASP	2.3
1	B	207	LYS	2.2
1	B	192	SER	2.2
1	B	125	LEU	2.2
1	B	43	VAL	2.1
1	B	79	THR	2.1
1	B	30	ASN	2.1
1	A	76	GLY	2.1
1	A	210	VAL	2.1
1	B	222	SER	2.1
1	A	73	THR	2.1
1	B	152	ILE	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	B	506	6/6	0.81	0.20	45,54,58,61	0
2	SO4	B	503	5/5	0.85	0.24	69,73,101,108	0
2	SO4	A	501	5/5	0.88	0.14	38,46,58,92	0
3	GOL	B	507	6/6	0.88	0.17	44,51,53,55	0
3	GOL	A	505	6/6	0.91	0.15	46,47,67,76	0
3	GOL	A	506	6/6	0.92	0.17	38,47,55,55	0
2	SO4	B	505	5/5	0.93	0.33	74,83,86,89	0
2	SO4	A	503	5/5	0.94	0.13	77,79,85,90	0
3	GOL	B	508	6/6	0.95	0.19	40,53,59,61	0
2	SO4	B	501	5/5	0.97	0.11	48,49,63,70	0
2	SO4	B	502	5/5	0.97	0.18	52,54,61,68	0
2	SO4	A	502	5/5	0.97	0.12	43,47,53,62	0
2	SO4	B	504	5/5	0.98	0.14	57,59,65,67	0
2	SO4	A	504	5/5	0.99	0.13	38,47,49,53	0

6.5 Other polymers (i)

There are no such residues in this entry.