Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 01:46 pm BST

PDB ID	:	6F9P
Title	:	Crystal structure of the Fe(II)/alpha-ketoglutarate dependent dioxygenase KDO5 with Re(II)
Authors	:	Isabet, T.; Stura, E.; Legrand, P.; Zaparucha, A.; Bastard, K.
Deposited on	:	2017-12-15
Resolution	:	2.40 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 ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

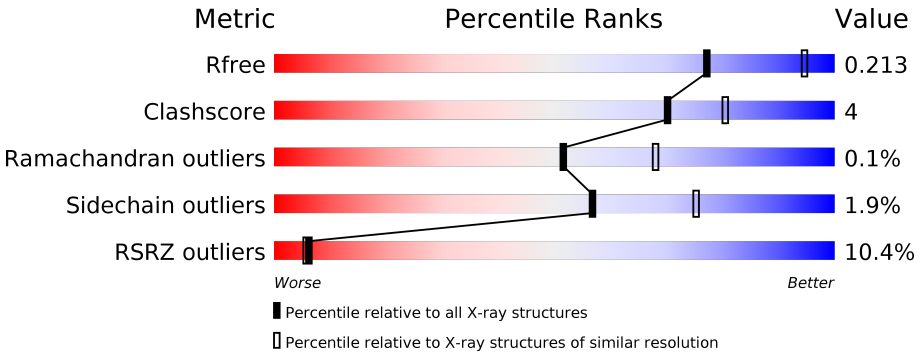
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	372	5% 88% 5% 7%
1	B	372	6% 70% 7% • 22%
1	C	372	17% 81% 8% • 10%
1	D	372	8% 85% 5% • 9%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10635 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 L-lysine 4-hydroxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	347	Total	C	N	O	S	0	1	0
			2756	1752	471	521	12			
1	B	289	Total	C	N	O	S	0	2	0
			2334	1498	397	428	11			
1	C	335	Total	C	N	O	S	0	1	0
			2663	1692	457	502	12			
1	D	339	Total	C	N	O	S	0	0	0
			2684	1706	460	506	12			

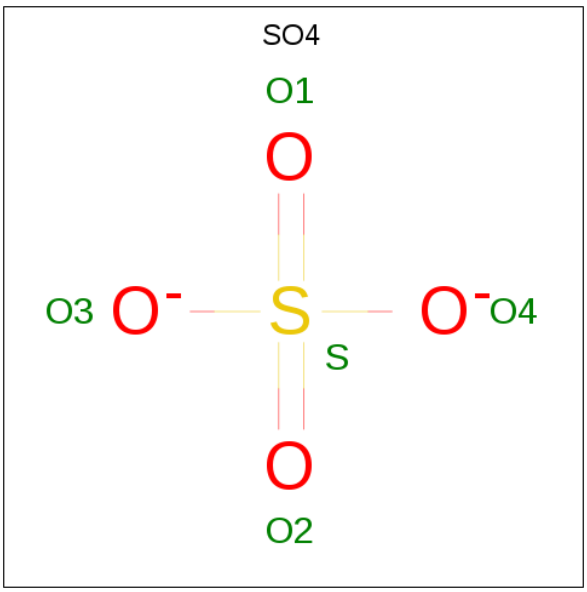
- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Cl	0	0
			1	1		
2	A	1	Total	Cl	0	0
			1	1		
2	D	1	Total	Cl	0	0
			1	1		
2	C	1	Total	Cl	0	0
			1	1		

- Molecule 3 is RHENIUM (three-letter code: RE) (formula: Re).

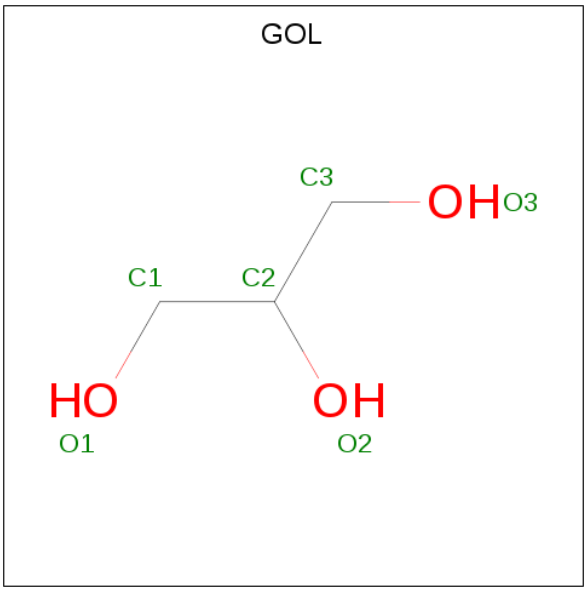
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Re	0	0
			1	1		
3	A	1	Total	Re	0	0
			1	1		
3	D	1	Total	Re	0	0
			1	1		
3	C	1	Total	Re	0	0
			1	1		

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 6 is water.

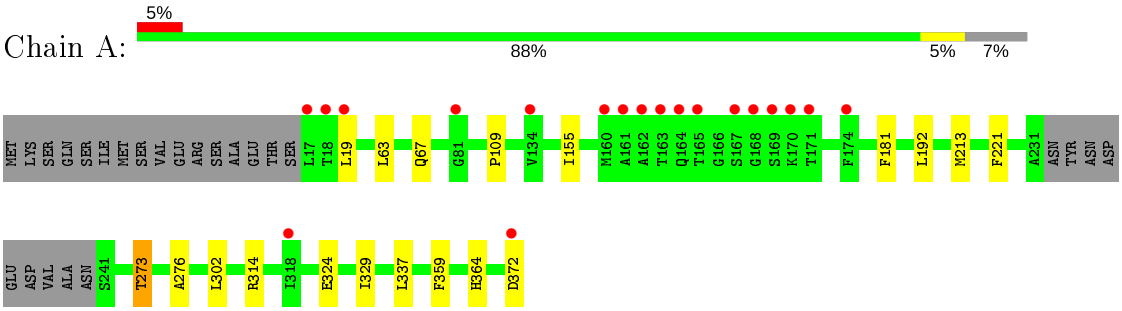
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	60	Total O 60 60	0	0
6	B	31	Total O 31 31	0	0
6	C	32	Total O 32 32	0	0
6	D	46	Total O 46 46	0	0

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 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.

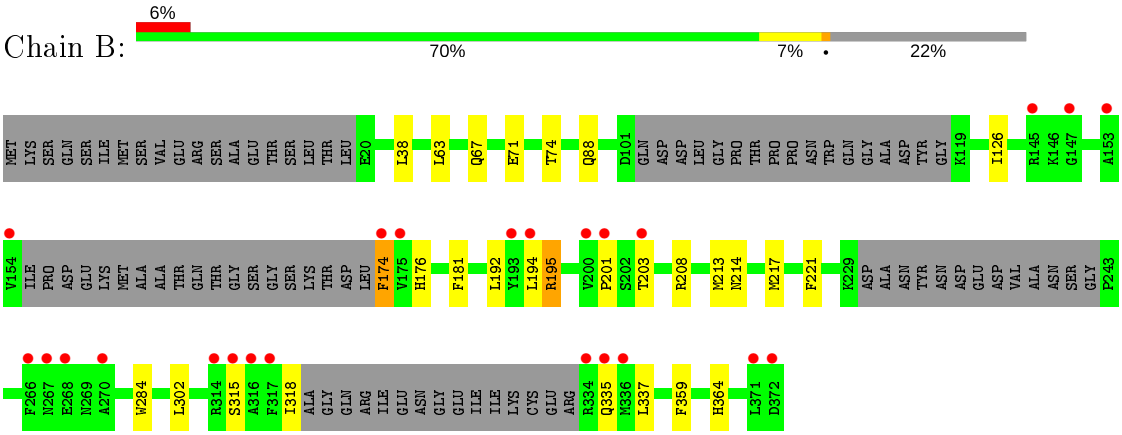
- Molecule 1: L-lysine 4-hydroxylase

Chain A:



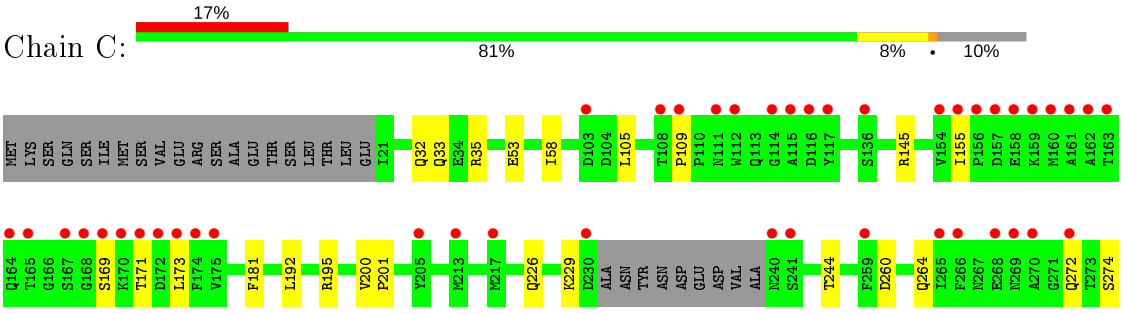
- Molecule 1: L-lysine 4-hydroxylase

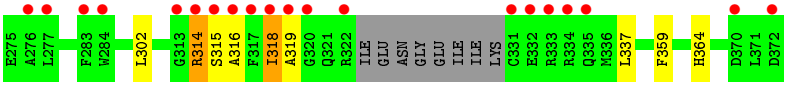
Chain B:



- Molecule 1: L-lysine 4-hydroxylase

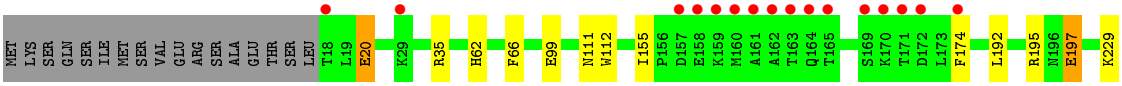
Chain C:

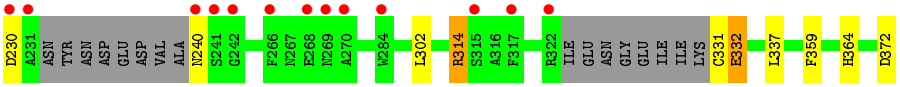




- Molecule 1: L-lysine 4-hydroxylase

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	90.20Å 98.87Å 165.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.43 – 2.40 49.44 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.43-2.40) 100.0 (49.44-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.14 (at 2.39Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.194 , 0.213 0.193 , 0.213	Depositor DCC
R_{free} test set	2925 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	59.2	Xtriage
Anisotropy	0.633	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 60.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	10635	wwPDB-VP
Average B, all atoms (Å^2)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.30% 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, 0.333 respectively for untwinned datasets, and 0.375, 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, CL, SO4, RE

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	0.53	0/2818	0.66	0/3813
1	B	0.49	0/2386	0.69	0/3221
1	C	0.49	0/2724	0.69	1/3686 (0.0%)
1	D	0.49	0/2745	0.67	1/3715 (0.0%)
All	All	0.50	0/10673	0.68	2/14435 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	145	ARG	CG-CD-NE	7.03	126.57	111.80
1	D	314	ARG	N-CA-CB	5.64	120.75	110.60

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	2756	0	2703	15	0
1	B	2334	0	2303	19	0
1	C	2663	0	2599	23	0
1	D	2684	0	2625	19	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	10	0	0	0	0
4	D	5	0	0	0	0
5	D	6	0	8	3	0
6	A	60	0	0	0	0
6	B	31	0	0	0	0
6	C	32	0	0	0	0
6	D	46	0	0	0	0
All	All	10635	0	10238	74	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 4.

All (74) 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:D:155:ILE:CG1	1:D:155:ILE:CD1	1.79	1.55
1:D:155:ILE:HD12	1:D:155:ILE:O	1.58	1.03
1:C:173:LEU:HB2	1:C:314:ARG:NH1	1.76	1.01
1:A:273:THR:HG22	1:A:276:ALA:H	1.38	0.86
1:A:213:MET:HE2	1:A:221:PHE:HE2	1.43	0.81
1:A:213:MET:CE	1:A:221:PHE:HE2	1.97	0.77
1:B:213:MET:HE2	1:B:221:PHE:HE2	1.47	0.77
1:C:173:LEU:HB2	1:C:314:ARG:HH12	1.47	0.76
1:D:155:ILE:CD1	1:D:155:ILE:O	2.33	0.76
1:B:213:MET:CE	1:B:221:PHE:HE2	1.98	0.75
1:D:112:TRP:H	1:D:155:ILE:HD11	1.51	0.75
1:D:111:ASN:HA	1:D:155:ILE:HD13	1.73	0.70
1:D:174:PHE:HA	5:D:403:GOL:C3	2.22	0.69
1:C:226:GLN:HB2	1:C:272:GLN:OE1	1.95	0.67
1:C:260:ASP:H	1:C:264:GLN:HE21	1.43	0.66
1:C:32:GLN:OE1	1:C:35:ARG:NH1	2.29	0.65
1:B:194:LEU:HB2	1:B:335:GLN:HG3	1.80	0.64
1:D:112:TRP:N	1:D:155:ILE:HD11	2.13	0.63
1:C:314:ARG:HE	1:C:318:ILE:HD11	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:169:SER:O	1:C:316:ALA:HB1	2.00	0.61
1:D:174:PHE:HA	5:D:403:GOL:H32	1.84	0.60
1:B:174:PHE:N	1:B:315:SER:HG	1.99	0.60
1:A:273:THR:CG2	1:A:276:ALA:H	2.14	0.56
1:A:314:ARG:HH21	1:A:314:ARG:HG2	1.70	0.56
1:A:213:MET:HE2	1:A:221:PHE:CE2	2.34	0.55
1:C:173:LEU:HB2	1:C:314:ARG:HH11	1.70	0.55
1:D:112:TRP:N	1:D:155:ILE:CD1	2.71	0.54
1:B:63:LEU:O	1:B:67:GLN:HG2	2.08	0.53
1:B:213:MET:HE2	1:B:221:PHE:CE2	2.37	0.53
1:A:109:PRO:HG2	1:A:155:ILE:HD13	1.91	0.52
1:A:213:MET:CE	1:A:221:PHE:CE2	2.87	0.52
1:C:109:PRO:HG2	1:C:155:ILE:HD13	1.92	0.52
1:B:213:MET:CE	1:B:221:PHE:CE2	2.87	0.52
1:D:192:LEU:HD23	1:D:337:LEU:HD12	1.93	0.51
1:C:105:LEU:HD22	1:C:195:ARG:CZ	2.41	0.50
1:A:192:LEU:HD23	1:A:337:LEU:HD12	1.94	0.49
1:B:192:LEU:HD23	1:B:337:LEU:HD12	1.95	0.49
1:B:214:ASN:OD1	1:B:217[B]:MET:HG2	2.12	0.49
1:C:171:THR:O	1:C:316:ALA:HB2	2.13	0.49
1:B:38:LEU:HD22	1:B:126:ILE:HG12	1.95	0.48
1:C:200:VAL:HG21	1:C:318:ILE:HG12	1.96	0.48
1:D:20:GLU:HG2	1:D:20:GLU:O	2.15	0.47
1:A:324:GLU:HB3	1:A:329:ILE:CD1	2.44	0.47
1:A:192:LEU:HB2	1:A:302:LEU:HD12	1.97	0.46
1:C:201:PRO:HD2	1:C:315:SER:HB2	1.97	0.46
1:D:62:HIS:O	1:D:66:PHE:HD2	1.98	0.46
1:D:174:PHE:HA	5:D:403:GOL:H31	1.98	0.45
1:C:315:SER:O	1:C:316:ALA:HB3	2.16	0.45
1:B:195:ARG:HB2	1:B:335:GLN:HG2	1.97	0.45
1:B:213:MET:HE1	1:B:221:PHE:HE2	1.79	0.45
1:D:192:LEU:HB2	1:D:302:LEU:HD12	1.99	0.45
1:D:197:GLU:HB3	1:D:331:CYS:SG	2.57	0.44
1:D:195:ARG:HD3	1:D:332:GLU:HB3	1.98	0.44
1:D:229:LYS:HD3	1:D:364:HIS:HB2	1.99	0.44
1:B:213:MET:HE1	1:B:221:PHE:CE2	2.52	0.44
1:D:155:ILE:CB	1:D:155:ILE:CD1	2.81	0.44
1:A:63:LEU:HD13	1:B:74:THR:HG21	1.99	0.44
1:C:53:GLU:HA	1:C:58:ILE:HD11	1.99	0.43
1:B:174:PHE:HD2	1:B:284:TRP:HH2	1.64	0.43
1:B:201:PRO:HG2	1:B:318:ILE:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:318:ILE:HG22	1:C:319:ALA:N	2.33	0.43
1:C:260:ASP:H	1:C:264:GLN:NE2	2.14	0.43
1:B:181:PHE:HB2	1:B:364:HIS:HD2	1.84	0.43
1:C:192:LEU:HD23	1:C:337:LEU:HD12	2.00	0.43
1:A:67:GLN:NE2	1:C:33:GLN:HG3	2.34	0.43
1:C:314:ARG:HG3	1:C:314:ARG:HH11	1.84	0.43
1:C:192:LEU:HB2	1:C:302:LEU:HD12	2.01	0.42
1:D:35:ARG:HD3	1:D:99:GLU:HG3	2.01	0.42
1:A:213:MET:HE1	1:A:221:PHE:CE2	2.54	0.42
1:A:181:PHE:HB2	1:A:364:HIS:HD2	1.84	0.42
1:B:192:LEU:HB2	1:B:302:LEU:HD12	2.01	0.41
1:C:181:PHE:CG	1:C:229:LYS:HA	2.56	0.41
1:B:88:GLN:O	1:B:208:ARG:HG3	2.21	0.41
1:C:181:PHE:HB2	1:C:364:HIS:HD2	1.85	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	344/372 (92%)	338 (98%)	6 (2%)	0	100	100
1	B	281/372 (76%)	275 (98%)	6 (2%)	0	100	100
1	C	330/372 (89%)	321 (97%)	8 (2%)	1 (0%)	41	55
1	D	333/372 (90%)	326 (98%)	7 (2%)	0	100	100
All	All	1288/1488 (87%)	1260 (98%)	27 (2%)	1 (0%)	51	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	318	ILE

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	300/322 (93%)	296 (99%)	4 (1%)	69	84
1	B	256/322 (80%)	250 (98%)	6 (2%)	50	70
1	C	290/322 (90%)	286 (99%)	4 (1%)	67	82
1	D	292/322 (91%)	284 (97%)	8 (3%)	44	65
All	All	1138/1288 (88%)	1116 (98%)	22 (2%)	57	75

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	LEU
1	A	273	THR
1	A	359	PHE
1	A	372	ASP
1	B	71	GLU
1	B	174	PHE
1	B	176	HIS
1	B	195	ARG
1	B	203	THR
1	B	359	PHE
1	C	244	THR
1	C	274	SER
1	C	314	ARG
1	C	359	PHE
1	D	20	GLU
1	D	197	GLU
1	D	230	ASP
1	D	240	ASN
1	D	314	ARG
1	D	332	GLU
1	D	359	PHE
1	D	372	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	67	GLN
1	B	40	ASN
1	B	184	ASN
1	C	264	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
4	SO4	A	404	-	4,4,4	0.19	0	6,6,6	0.20	0
4	SO4	D	404	-	4,4,4	0.21	0	6,6,6	0.16	0
4	SO4	A	403	-	4,4,4	0.34	0	6,6,6	0.27	0
5	GOL	D	403	-	5,5,5	0.15	0	5,5,5	0.35	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
5	GOL	D	403	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	403	GOL	3	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	347/372 (93%)	0.22	19 (5%) 25 24	49, 67, 112, 139	0
1	B	289/372 (77%)	0.55	24 (8%) 11 10	55, 76, 119, 175	0
1	C	335/372 (90%)	1.08	64 (19%) 1 0	52, 87, 166, 189	0
1	D	339/372 (91%)	0.42	29 (8%) 10 9	55, 78, 141, 170	0
All	All	1310/1488 (88%)	0.57	136 (10%) 6 6	49, 76, 137, 189	0

All (136) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	171	THR	10.8
1	C	165	THR	10.4
1	C	160	MET	9.5
1	C	162	ALA	9.3
1	C	168	GLY	8.2
1	C	161	ALA	8.1
1	C	317	PHE	7.9
1	C	316	ALA	7.8
1	C	173	LEU	7.7
1	C	156	PRO	7.7
1	A	19	LEU	7.6
1	C	331	CYS	7.3
1	C	167	SER	7.3
1	C	164	GLN	7.2
1	B	317	PHE	7.2
1	C	318	ILE	7.2
1	A	161	ALA	6.9
1	B	316	ALA	6.9
1	A	17	LEU	6.7
1	C	163	THR	6.7
1	D	162	ALA	6.4

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Mol	Chain	Res	Type	RSRZ
1	C	117	TYR	6.3
1	A	168	GLY	6.1
1	C	372	ASP	6.0
1	D	169	SER	5.9
1	C	155	ILE	5.8
1	D	160	MET	5.7
1	A	162	ALA	5.6
1	D	171	THR	5.5
1	C	314	ARG	5.5
1	B	315	SER	5.5
1	C	268	GLU	5.4
1	C	112	TRP	5.4
1	B	372	ASP	5.3
1	B	147	GLY	5.2
1	C	270	ALA	5.2
1	D	161	ALA	5.1
1	A	160	MET	5.1
1	D	174	PHE	5.1
1	B	334	ARG	5.0
1	C	320	GLY	5.0
1	D	165	THR	4.9
1	C	109	PRO	4.9
1	C	116	ASP	4.9
1	D	170	LYS	4.9
1	C	172	ASP	4.8
1	D	270	ALA	4.7
1	B	154	VAL	4.6
1	A	171	THR	4.6
1	D	163	THR	4.6
1	A	18	THR	4.5
1	D	241	SER	4.5
1	B	200	VAL	4.4
1	B	270	ALA	4.4
1	B	314	ARG	4.4
1	A	165	THR	4.3
1	C	266	PHE	4.3
1	C	230	ASP	4.3
1	B	371	LEU	4.3
1	C	174	PHE	4.3
1	C	334	ARG	4.1
1	C	315	SER	4.0
1	C	319	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	164	GLN	3.9
1	D	315	SER	3.9
1	C	159	LYS	3.9
1	C	154	VAL	3.9
1	A	170	LYS	3.8
1	A	164	GLN	3.7
1	C	115	ALA	3.7
1	C	333	ARG	3.7
1	C	284	TRP	3.7
1	C	241	SER	3.6
1	B	335	GLN	3.6
1	C	240	ASN	3.5
1	D	18	THR	3.5
1	D	240	ASN	3.4
1	C	157	ASP	3.4
1	D	268	GLU	3.4
1	C	114	GLY	3.3
1	A	167	SER	3.3
1	D	242	GLY	3.3
1	B	268	GLU	3.2
1	C	272	GLN	3.2
1	C	335	GLN	3.2
1	A	174	PHE	3.2
1	C	269	ASN	3.1
1	C	175	VAL	3.1
1	C	277	LEU	3.1
1	D	322	ARG	3.0
1	C	217	MET	3.0
1	B	145	ARG	2.9
1	D	231	ALA	2.9
1	B	336	MET	2.8
1	A	163	THR	2.8
1	C	213	MET	2.8
1	C	169	SER	2.8
1	C	103	ASP	2.7
1	C	322	ARG	2.7
1	C	158	GLU	2.6
1	D	230	ASP	2.6
1	C	259	PHE	2.6
1	D	158	GLU	2.6
1	D	317	PHE	2.6
1	D	157	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	193	TYR	2.6
1	B	194	LEU	2.5
1	B	266	PHE	2.5
1	A	169	SER	2.5
1	B	174	PHE	2.5
1	A	81	GLY	2.5
1	B	175	VAL	2.5
1	C	111	ASN	2.5
1	C	313	GLY	2.4
1	D	269	ASN	2.4
1	B	153	ALA	2.4
1	C	108	THR	2.4
1	D	172	ASP	2.3
1	C	276	ALA	2.3
1	C	170	LYS	2.3
1	A	372	ASP	2.3
1	C	370	ASP	2.3
1	B	201	PRO	2.3
1	D	29	LYS	2.2
1	D	266	PHE	2.2
1	C	283	PHE	2.2
1	D	284	TRP	2.2
1	A	134	VAL	2.1
1	C	332	GLU	2.1
1	D	159	LYS	2.1
1	B	203	THR	2.1
1	C	205	TYR	2.1
1	C	265	ILE	2.1
1	A	318	ILE	2.1
1	B	267	ASN	2.1
1	C	136	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

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, 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	B-factors(Å^2)	Q<0.9
5	GOL	D	403	6/6	0.64	0.22	103,108,108,109	0
2	CL	B	401	1/1	0.82	0.14	92,92,92,92	1
4	SO4	A	404	5/5	0.84	0.44	156,158,158,159	0
4	SO4	D	404	5/5	0.91	0.11	134,135,136,137	0
4	SO4	A	403	5/5	0.93	0.12	111,113,115,115	0
3	RE	D	402	1/1	0.93	0.06	108,108,108,108	1
2	CL	C	401	1/1	0.94	0.15	116,116,116,116	1
2	CL	D	401	1/1	0.95	0.34	103,103,103,103	1
3	RE	B	402	1/1	0.97	0.10	101,101,101,101	1
2	CL	A	401	1/1	0.98	0.18	92,92,92,92	0
3	RE	C	402	1/1	0.98	0.07	119,119,119,119	1
3	RE	A	402	1/1	0.99	0.16	76,76,76,76	1

6.5 Other polymers

There are no such residues in this entry.