Full wwPDB X-ray Structure Validation Report (i)

Apr 27, 2024 – 11:56 am BST

PDB ID	:	6EUO
Title	:	Crystal structure of APO Fe(II)/alpha-ketoglutarate dependent dioxygenase KDO5
Authors	:	Isabet, T.; Stura, E.; Legrand, P.; Zaparucha, A.; Bastard, K.
Deposited on	:	2017-10-30
Resolution	:	2.30 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

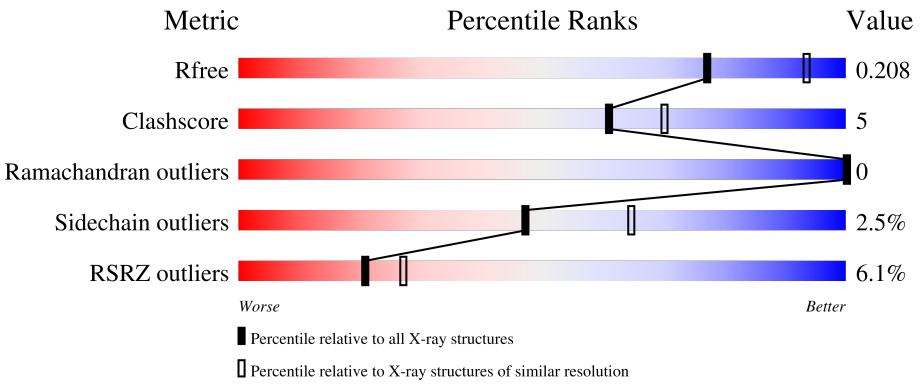
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 of 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	2%, 83%, 10%, 7%
1	B	372	11%, 79%, 11%, 10%
1	C	372	6%, 85%, 10%, 5%
1	D	372	5%, 85%, 8%, 8%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 11693 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.

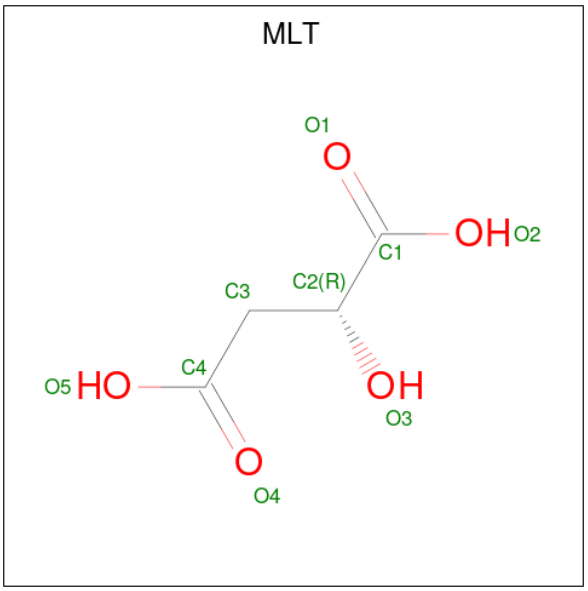
- Molecule 1 is a protein called L-lysine 4-hydroxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	346	2814	1787	482	532	13	0	8	0
1	B	335	2706	1719	459	513	15	0	8	0
1	C	354	2817	1787	482	536	12	0	3	0
1	D	344	2734	1738	466	518	12	0	1	0

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

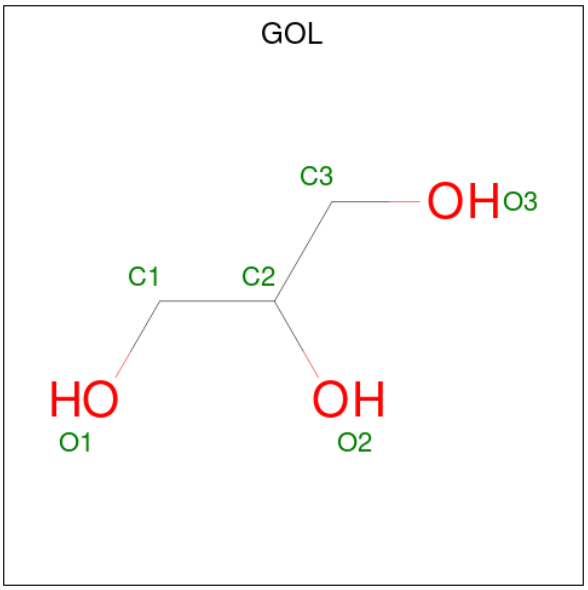
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
2	A	1	1	1	0	0
2	B	1	1	1	0	0
2	C	1	1	1	0	0
2	D	1	1	1	0	0

- Molecule 3 is D-MALATE (three-letter code: MLT) (formula: $C_4H_6O_5$).



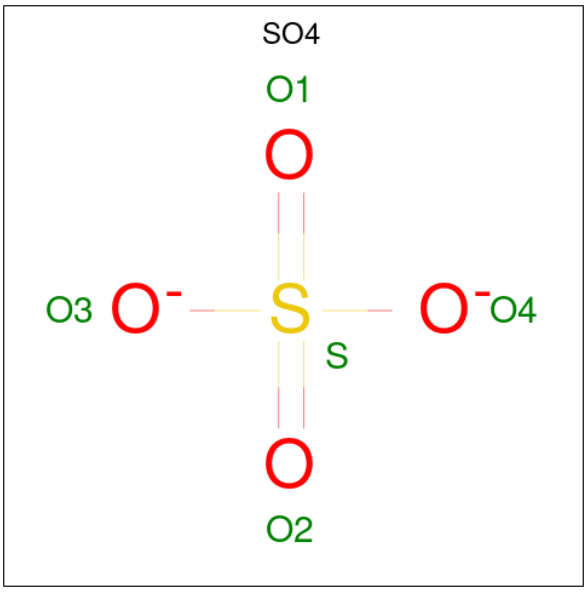
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 9 4 5	0	0
3	B	1	Total C O 9 4 5	0	0
3	C	1	Total C O 9 4 5	0	0
3	D	1	Total C O 9 4 5	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	6	3	3	0	0
			Total	C	O		
4	A	1	6	3	3	0	0
			Total	C	O		
4	B	1	6	3	3	0	0
			Total	C	O		
4	B	1	6	3	3	0	0
			Total	C	O		
4	C	1	6	3	3	0	0
			Total	C	O		
4	C	1	6	3	3	0	0
			Total	C	O		
4	C	1	6	3	3	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 6 is water.

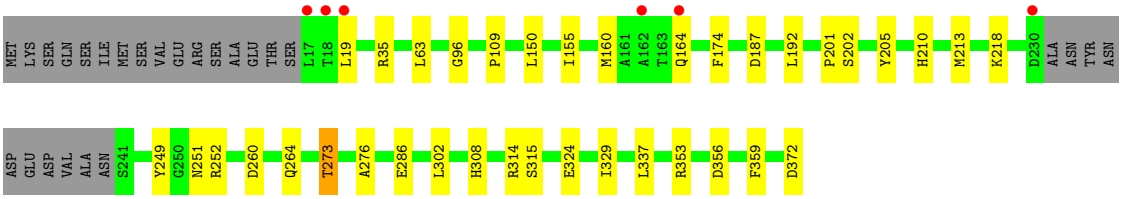
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	172	172	172	0	0
			Total	O		
6	B	105	105	105	0	0
			Total	O		
6	C	117	117	117	0	0
			Total	O		
6	D	131	131	131	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

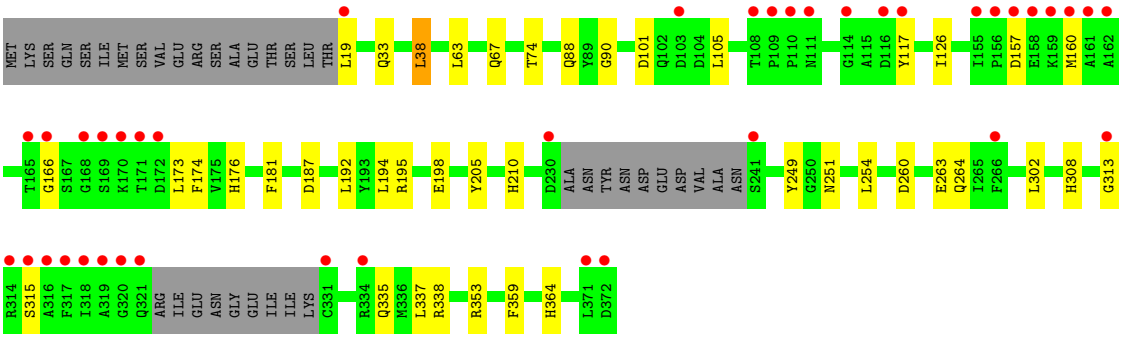
• Molecule 1: L-lysine 4-hydroxylase

Chain A:



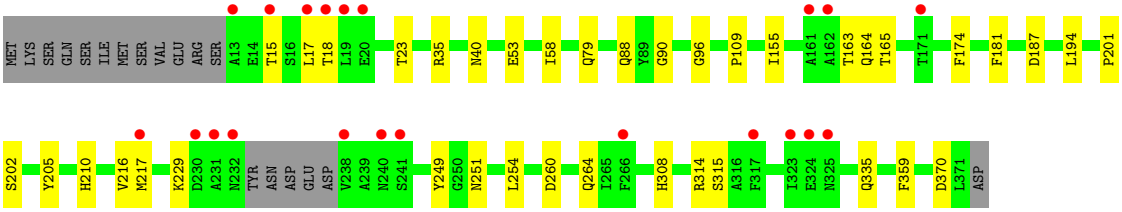
• Molecule 1: L-lysine 4-hydroxylase

Chain B:



• Molecule 1: L-lysine 4-hydroxylase

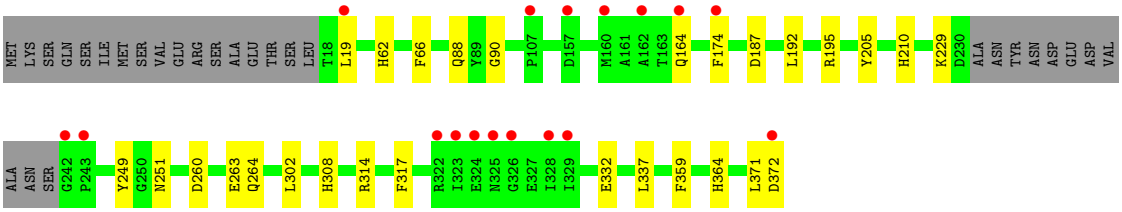
Chain C:



• Molecule 1: L-lysine 4-hydroxylase

Chain D:

5%
85%
8%
8%


MET LYS SER GLN SER ILE MET SER VAL GLU ARG SER ALA GLU THR SER LEU T18 L19 H62 F66 Q88 Y89 G90 P107 D157 M160 A161 A162 T163 Q164 F174 D187 L192 R195 Y205 H210 K229 D230 ALA ASN TYR ASN ASP GLU ASP VAL
ALA ASN SER G242 P243 Y249 G250 N251 D260 E263 Q264 L302 H308 R314 F317 R322 I323 E324 N325 G326 E327 I328 I329 E332 L337 F359 H364 L371 D372

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	91.28Å 98.93Å 166.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	62.20 – 2.30 62.20 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (62.20-2.30) 100.0 (62.20-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.39 (at 2.29Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.169 , 0.205 0.173 , 0.208	Depositor DCC
R_{free} test set	3359 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	49.4	Xtriage
Anisotropy	0.505	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 60.9	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	0.97	EDS
Total number of atoms	11693	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.66% 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 (i)

5.1 Standard geometry (i)

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

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	0.54	0/2878	0.66	0/3892
1	B	0.49	0/2768	0.68	0/3747
1	C	0.48	0/2879	0.66	0/3898
1	D	0.50	0/2796	0.65	0/3784
All	All	0.50	0/11321	0.66	0/15321

There are no bond length outliers.

There are no bond angle outliers.

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	2814	0	2744	33	0
1	B	2706	0	2622	25	0
1	C	2817	0	2757	22	0
1	D	2734	0	2671	22	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	9	0	4	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	9	0	4	2	0
3	C	9	0	4	0	0
3	D	9	0	4	0	0
4	A	12	0	16	4	0
4	B	12	0	16	1	0
4	C	18	0	24	0	0
5	A	5	0	0	0	0
5	C	5	0	0	0	0
5	D	5	0	0	0	0
6	A	172	0	0	1	0
6	B	105	0	0	0	0
6	C	117	0	0	0	0
6	D	131	0	0	0	0
All	All	11693	0	10866	100	0

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

All (100) 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:88:GLN:HE21	1:B:90:GLY:H	1.23	0.85
1:C:251:ASN:HD22	1:C:254:LEU:H	1.25	0.84
1:A:273:THR:HG22	1:A:276:ALA:H	1.40	0.84
1:D:88:GLN:HE21	1:D:90:GLY:H	1.25	0.84
1:B:251:ASN:HD22	1:B:254:LEU:H	1.26	0.84
1:C:88:GLN:HE21	1:C:90:GLY:H	1.24	0.83
1:B:67:GLN:HB2	1:C:40:ASN:HD22	1.55	0.71
1:B:166:GLY:H	3:B:402:MLT:H32	1.55	0.71
1:A:353:ARG:HA	4:A:403:GOL:H32	1.74	0.68
1:B:353:ARG:HA	4:B:404:GOL:H2	1.76	0.68
1:A:260:ASP:H	1:A:264:GLN:HE21	1.44	0.66
1:D:249:TYR:OH	1:D:308:HIS:HD2	1.79	0.65
1:D:260:ASP:H	1:D:264:GLN:HE21	1.45	0.65
1:C:260:ASP:H	1:C:264:GLN:HE21	1.45	0.64
1:B:249:TYR:OH	1:B:308:HIS:HD2	1.82	0.63
1:A:249:TYR:OH	1:A:308:HIS:HD2	1.81	0.63
1:B:260:ASP:H	1:B:264:GLN:HE21	1.45	0.63
1:C:249:TYR:OH	1:C:308:HIS:HD2	1.82	0.62
1:D:205:TYR:OH	1:D:210:HIS:HE1	1.84	0.60
1:A:205:TYR:OH	1:A:210:HIS:HE1	1.85	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:THR:CG2	1:A:276:ALA:H	2.13	0.58
1:B:205:TYR:OH	1:B:210:HIS:HE1	1.87	0.57
1:A:356:ASP:OD1	4:A:404:GOL:H12	2.05	0.57
1:C:205:TYR:OH	1:C:210:HIS:HE1	1.87	0.56
1:C:88:GLN:HE21	1:C:90:GLY:N	2.01	0.56
1:A:353:ARG:HG2	4:A:403:GOL:H11	1.88	0.55
1:B:88:GLN:HE21	1:B:90:GLY:N	2.01	0.54
1:A:205:TYR:OH	1:A:210:HIS:CE1	2.61	0.53
1:B:88:GLN:NE2	1:B:90:GLY:H	2.02	0.53
1:A:164:GLN:HE22	1:A:174[B]:PHE:H	1.57	0.53
1:A:109:PRO:HG2	1:A:155:ILE:HD13	1.91	0.52
1:D:88:GLN:HE21	1:D:90:GLY:N	2.00	0.52
1:D:192:LEU:HD23	1:D:337:LEU:HD12	1.93	0.51
1:C:205:TYR:OH	1:C:210:HIS:CE1	2.63	0.51
1:D:205:TYR:OH	1:D:210:HIS:CE1	2.63	0.51
1:B:205:TYR:OH	1:B:210:HIS:CE1	2.64	0.51
1:C:109:PRO:HG2	1:C:155:ILE:HD13	1.93	0.51
1:C:88:GLN:NE2	1:C:90:GLY:H	2.02	0.51
1:B:338:ARG:HH12	3:B:402:MLT:H2	1.76	0.50
1:B:38:LEU:HD22	1:B:126:ILE:HG12	1.93	0.50
1:A:252:ARG:HD2	6:A:538:HOH:O	2.12	0.50
1:C:163:THR:OG1	1:C:165:THR:HG22	2.11	0.50
1:D:88:GLN:NE2	1:D:90:GLY:H	2.02	0.50
1:B:249:TYR:OH	1:B:308:HIS:CD2	2.65	0.49
1:A:324:GLU:HB3	1:A:329:ILE:CD1	2.42	0.49
1:D:249:TYR:OH	1:D:308:HIS:CD2	2.63	0.49
1:C:164:GLN:HE22	1:C:174:PHE:H	1.59	0.49
1:D:164:GLN:HE22	1:D:174:PHE:H	1.59	0.49
1:C:249:TYR:OH	1:C:308:HIS:CD2	2.65	0.48
1:A:192:LEU:HD23	1:A:337:LEU:HD12	1.95	0.48
1:A:249:TYR:OH	1:A:308:HIS:CD2	2.64	0.48
1:A:314:ARG:HH11	1:A:314:ARG:HG2	1.78	0.48
1:B:63:LEU:O	1:B:67:GLN:HG2	2.14	0.48
1:C:251:ASN:ND2	1:C:254:LEU:H	2.03	0.47
1:A:164:GLN:HE22	1:A:174[A]:PHE:H	1.60	0.47
1:D:195:ARG:HD3	1:D:332:GLU:HB3	1.95	0.47
1:B:173:LEU:HD23	1:B:313:GLY:HA2	1.96	0.47
1:C:53:GLU:HA	1:C:58:ILE:HD11	1.95	0.47
1:B:192:LEU:HD23	1:B:337:LEU:HD12	1.97	0.46
1:A:187:ASP:OD1	1:A:308:HIS:HE1	1.98	0.46
1:A:210:HIS:HD2	1:A:286:GLU:OE2	1.99	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:187:ASP:OD1	1:D:308:HIS:HE1	2.00	0.45
1:C:201:PRO:HD2	1:C:315:SER:HB2	2.00	0.44
1:C:187:ASP:OD1	1:C:308:HIS:HE1	1.99	0.44
1:A:213[A]:MET:HG3	1:A:218:LYS:HE2	1.99	0.44
1:A:164:GLN:NE2	1:A:174[B]:PHE:HD1	2.15	0.44
1:B:187:ASP:OD1	1:B:308:HIS:HE1	2.00	0.44
1:B:251:ASN:ND2	1:B:254:LEU:H	2.05	0.44
1:D:19:LEU:HD12	1:D:19:LEU:H	1.83	0.44
1:A:150:LEU:HD21	4:A:404:GOL:H32	2.01	0.43
1:B:194:LEU:HD12	1:B:335:GLN:HG2	1.99	0.43
1:D:314:ARG:HD2	1:D:317:PHE:HE1	1.84	0.43
1:A:164:GLN:HE22	1:A:174[B]:PHE:HD1	1.67	0.43
1:C:260:ASP:H	1:C:264:GLN:NE2	2.15	0.42
1:C:216:VAL:HG12	1:C:217:MET:HE1	2.02	0.42
1:A:192:LEU:HB2	1:A:302:LEU:HD12	2.02	0.42
1:A:201:PRO:HD2	1:A:315:SER:HB2	2.02	0.42
1:C:194:LEU:HD12	1:C:335:GLN:HG2	2.01	0.41
1:D:229:LYS:HD3	1:D:364:HIS:HB2	2.01	0.41
1:B:157:ASP:HB3	1:B:160:MET:HB2	2.02	0.41
1:D:164:GLN:NE2	1:D:174:PHE:H	2.19	0.41
1:A:35:ARG:HD3	1:A:96:GLY:O	2.20	0.41
1:D:192:LEU:HB2	1:D:302:LEU:HD12	2.02	0.41
1:C:181:PHE:CG	1:C:229:LYS:HA	2.56	0.41
1:D:62:HIS:O	1:D:66:PHE:HD2	2.04	0.41
1:A:260:ASP:H	1:A:264:GLN:NE2	2.14	0.41
1:B:105:LEU:HD12	1:B:195:ARG:CZ	2.51	0.41
1:C:35:ARG:HD3	1:C:96:GLY:O	2.21	0.41
1:B:192:LEU:HB2	1:B:302:LEU:HD12	2.03	0.40
1:B:181:PHE:HB2	1:B:364:HIS:HD2	1.87	0.40
1:A:63:LEU:HD13	1:B:74:THR:HG21	2.03	0.40
1:A:324:GLU:HB3	1:A:329:ILE:HD11	2.03	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	350/372 (94%)	345 (99%)	5 (1%)	0	100	100
1	B	337/372 (91%)	329 (98%)	8 (2%)	0	100	100
1	C	353/372 (95%)	342 (97%)	11 (3%)	0	100	100
1	D	341/372 (92%)	331 (97%)	10 (3%)	0	100	100
All	All	1381/1488 (93%)	1347 (98%)	34 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	307/322 (95%)	301 (98%)	6 (2%)	55	72
1	B	295/322 (92%)	284 (96%)	11 (4%)	34	48
1	C	307/322 (95%)	298 (97%)	9 (3%)	42	58
1	D	297/322 (92%)	293 (99%)	4 (1%)	69	82
All	All	1206/1288 (94%)	1176 (98%)	30 (2%)	47	65

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	LEU
1	A	160	MET
1	A	202	SER
1	A	273	THR
1	A	359	PHE
1	A	372	ASP
1	B	19	LEU
1	B	33	GLN
1	B	38	LEU
1	B	101	ASP

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Mol	Chain	Res	Type
1	B	117	TYR
1	B	174	PHE
1	B	176	HIS
1	B	198	GLU
1	B	263	GLU
1	B	315	SER
1	B	359	PHE
1	C	15	THR
1	C	17	LEU
1	C	18	THR
1	C	23	THR
1	C	79	GLN
1	C	202	SER
1	C	314	ARG
1	C	359	PHE
1	C	370	ASP
1	D	263	GLU
1	D	359	PHE
1	D	371	LEU
1	D	372	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	164	GLN
1	A	184	ASN
1	A	210	HIS
1	A	251	ASN
1	A	264	GLN
1	A	298	ASN
1	A	308	HIS
1	B	88	GLN
1	B	184	ASN
1	B	210	HIS
1	B	251	ASN
1	B	264	GLN
1	B	267	ASN
1	B	298	ASN
1	B	308	HIS
1	C	40	ASN
1	C	88	GLN

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Mol	Chain	Res	Type
1	C	164	GLN
1	C	184	ASN
1	C	210	HIS
1	C	251	ASN
1	C	264	GLN
1	C	298	ASN
1	C	308	HIS
1	C	347	HIS
1	D	40	ASN
1	D	51	ASN
1	D	88	GLN
1	D	164	GLN
1	D	184	ASN
1	D	210	HIS
1	D	251	ASN
1	D	264	GLN
1	D	308	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 4 are monoatomic - leaving 14 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	GOL	C	403	-	5,5,5	0.09	0	5,5,5	0.41	0
4	GOL	A	404	-	5,5,5	0.07	0	5,5,5	0.33	0
4	GOL	C	404	-	5,5,5	0.05	0	5,5,5	0.16	0
3	MLT	D	402	2	8,8,8	1.05	0	10,10,10	1.56	3 (30%)
3	MLT	C	402	-	8,8,8	1.11	0	10,10,10	1.48	2 (20%)
3	MLT	A	402	2	8,8,8	1.13	0	10,10,10	1.54	1 (10%)
3	MLT	B	402	-	8,8,8	1.02	0	10,10,10	1.48	2 (20%)
5	SO4	D	403	-	4,4,4	0.17	0	6,6,6	0.24	0
5	SO4	A	405	-	4,4,4	0.37	0	6,6,6	0.39	0
4	GOL	B	403	-	5,5,5	0.09	0	5,5,5	0.14	0
4	GOL	C	405	-	5,5,5	0.05	0	5,5,5	0.29	0
4	GOL	B	404	-	5,5,5	0.07	0	5,5,5	0.15	0
4	GOL	A	403	-	5,5,5	0.11	0	5,5,5	0.30	0
5	SO4	C	406	-	4,4,4	0.27	0	6,6,6	0.19	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
4	GOL	C	403	-	-	2/4/4/4	-
4	GOL	A	404	-	-	0/4/4/4	-
4	GOL	C	404	-	-	0/4/4/4	-
3	MLT	D	402	2	-	5/8/8/8	-
3	MLT	C	402	-	-	6/8/8/8	-
3	MLT	A	402	2	-	4/8/8/8	-
3	MLT	B	402	-	-	4/8/8/8	-
4	GOL	B	403	-	-	0/4/4/4	-
4	GOL	C	405	-	-	0/4/4/4	-
4	GOL	B	404	-	-	0/4/4/4	-
4	GOL	A	403	-	-	0/4/4/4	-

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	402	MLT	O2-C1-C2	3.22	119.79	112.72
3	B	402	MLT	O2-C1-C2	3.08	119.49	112.72
3	D	402	MLT	O5-C4-C3	2.49	122.05	114.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	402	MLT	O2-C1-C2	2.30	117.78	112.72
3	B	402	MLT	O1-C1-C2	-2.12	118.40	122.54
3	D	402	MLT	O4-C4-C3	-2.08	116.14	122.80
3	D	402	MLT	O2-C1-C2	2.07	117.27	112.72
3	C	402	MLT	O3-C2-C1	-2.02	104.98	110.36

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	402	MLT	C1-C2-C3-C4
3	B	402	MLT	O3-C2-C3-C4
3	C	402	MLT	O1-C1-C2-O3
3	C	402	MLT	O2-C1-C2-O3
3	C	402	MLT	O2-C1-C2-C3
3	D	402	MLT	O1-C1-C2-O3
3	D	402	MLT	O2-C1-C2-O3
4	C	403	GOL	O1-C1-C2-C3
3	C	402	MLT	O3-C2-C3-C4
3	B	402	MLT	O1-C1-C2-O3
3	C	402	MLT	O1-C1-C2-C3
4	C	403	GOL	O1-C1-C2-O2
3	C	402	MLT	C1-C2-C3-C4
3	B	402	MLT	O2-C1-C2-O3
3	D	402	MLT	O2-C1-C2-C3
3	A	402	MLT	O1-C1-C2-O3
3	A	402	MLT	O2-C1-C2-O3
3	A	402	MLT	O1-C1-C2-C3
3	A	402	MLT	O2-C1-C2-C3
3	D	402	MLT	O1-C1-C2-C3
3	D	402	MLT	O3-C2-C3-C4

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	404	GOL	2	0
3	B	402	MLT	2	0
4	B	404	GOL	1	0
4	A	403	GOL	2	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	346/372 (93%)	-0.18	6 (1%)	70	76	36, 52, 89, 131	0
1	B	335/372 (90%)	0.44	40 (11%)	4	6	41, 66, 140, 177	0
1	C	354/372 (95%)	0.11	21 (5%)	22	28	41, 71, 132, 170	0
1	D	344/372 (92%)	0.09	17 (4%)	29	36	41, 65, 130, 190	0
All	All	1379/1488 (92%)	0.12	84 (6%)	21	27	36, 62, 130, 190	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	162	ALA	11.5
1	B	316	ALA	9.3
1	B	160	MET	9.2
1	D	323	ILE	8.8
1	C	19	LEU	7.4
1	A	17	LEU	7.3
1	B	320	GLY	7.2
1	B	372	ASP	6.8
1	A	18	THR	6.4
1	D	324	GLU	6.2
1	C	238	VAL	6.1
1	B	161	ALA	6.0
1	B	172	ASP	5.7
1	B	331	CYS	5.7
1	B	117	TYR	5.6
1	D	329	ILE	5.4
1	A	19	LEU	5.2
1	B	321	GLN	5.0
1	D	326	GLY	4.8
1	C	241	SER	4.7
1	B	318	ILE	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	116	ASP	4.4
1	B	171	THR	4.4
1	B	169	SER	4.4
1	C	266	PHE	4.4
1	B	319	ALA	4.3
1	B	110	PRO	4.3
1	B	159	LYS	4.2
1	D	242	GLY	4.0
1	C	171	THR	3.9
1	D	325	ASN	3.9
1	B	158	GLU	3.8
1	B	371	LEU	3.7
1	B	155	ILE	3.7
1	D	19	LEU	3.5
1	B	165	THR	3.5
1	C	17	LEU	3.4
1	B	109	PRO	3.4
1	C	13	ALA	3.3
1	B	103	ASP	3.3
1	B	230	ASP	3.2
1	B	315	SER	3.2
1	C	324	GLU	3.2
1	B	314	ARG	3.2
1	B	19	LEU	3.2
1	D	322	ARG	3.1
1	C	15	THR	3.1
1	C	217	MET	3.0
1	C	231	ALA	3.0
1	D	107	PRO	3.0
1	B	334	ARG	2.9
1	D	164	GLN	2.9
1	C	317	PHE	2.8
1	B	241	SER	2.8
1	C	325	ASN	2.8
1	B	313	GLY	2.7
1	B	266	PHE	2.7
1	B	166	GLY	2.6
1	B	114	GLY	2.5
1	C	323	ILE	2.4
1	B	168	GLY	2.4
1	B	156	PRO	2.4
1	C	240	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	160	MET	2.3
1	D	372	ASP	2.3
1	B	317	PHE	2.3
1	C	230	ASP	2.3
1	C	18	THR	2.2
1	B	111	ASN	2.2
1	B	157	ASP	2.2
1	A	164	GLN	2.2
1	C	232	ASN	2.2
1	D	174	PHE	2.2
1	C	161	ALA	2.2
1	D	328	ILE	2.2
1	D	157	ASP	2.1
1	B	108	THR	2.1
1	B	170	LYS	2.1
1	D	243	PRO	2.1
1	D	162	ALA	2.1
1	C	20	GLU	2.0
1	A	230	ASP	2.0
1	A	162	ALA	2.0
1	C	162	ALA	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides 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	MLT	B	402	9/9	0.73	0.17	123,125,128,128	0
4	GOL	A	403	6/6	0.79	0.30	81,89,91,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GOL	C	405	6/6	0.80	0.25	134,136,137,137	0
3	MLT	D	402	9/9	0.85	0.28	90,92,98,101	0
5	SO4	C	406	5/5	0.85	0.13	130,130,131,131	0
4	GOL	B	403	6/6	0.87	0.18	81,86,87,90	0
4	GOL	C	403	6/6	0.87	0.29	69,80,83,83	0
4	GOL	A	404	6/6	0.89	0.34	68,81,86,88	0
4	GOL	C	404	6/6	0.89	0.27	89,91,93,95	0
4	GOL	B	404	6/6	0.91	0.16	92,94,95,96	0
5	SO4	D	403	5/5	0.95	0.10	108,110,111,112	0
3	MLT	A	402	9/9	0.96	0.17	72,79,83,88	0
3	MLT	C	402	9/9	0.96	0.26	109,112,114,115	0
5	SO4	A	405	5/5	0.97	0.10	80,80,83,85	0
2	FE	D	401	1/1	0.98	0.17	65,65,65,65	0
2	FE	C	401	1/1	0.99	0.17	68,68,68,68	0
2	FE	B	401	1/1	0.99	0.23	60,60,60,60	0
2	FE	A	401	1/1	1.00	0.17	50,50,50,50	0

6.5 Other polymers (i)

There are no such residues in this entry.