Full wwPDB X-ray Structure Validation Report ⓘ

Jun 7, 2020 – 02:43 am BST

PDB ID	:	6IUM
Title	:	Crystal structure of enoyl-CoA hydratase (ECH) from Ralstonia eutropha H16
Authors	:	Son, H.F.; Kim, K.J.
Deposited on	:	2018-11-29
Resolution	:	2.00 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 ⓘ) were used in the production of this report:

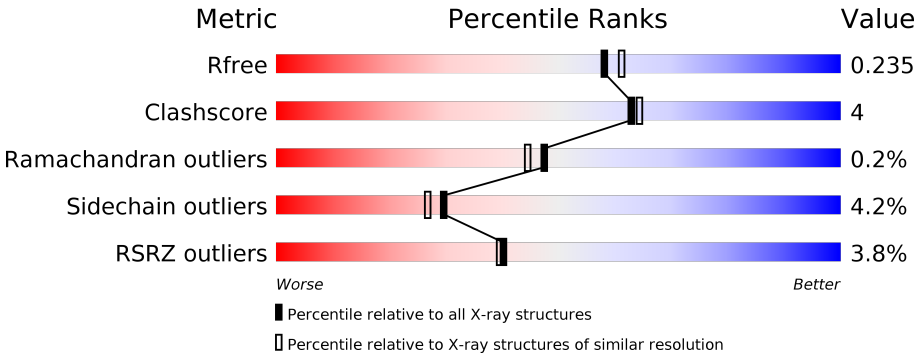
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	701	4% 84% 13%
1	B	701	3% 86% 11%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11602 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.

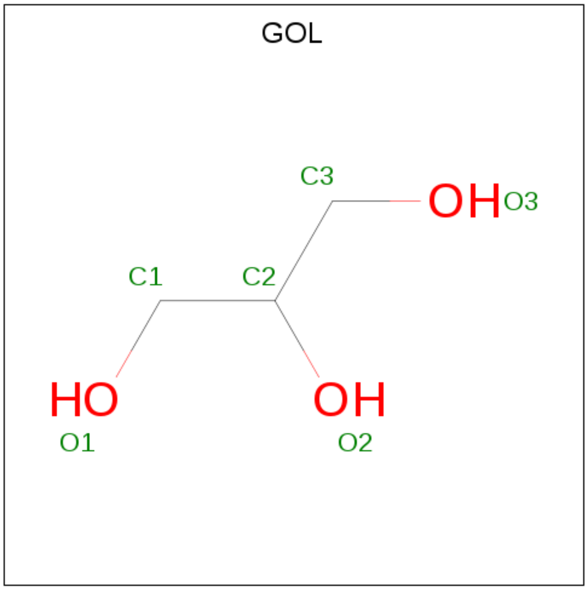
- Molecule 1 is a protein called Enoyl-CoA hydratase/Delta(3)-cis-delta(2)-trans-enoyl-CoA isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	692	Total	C	N	O	S	0	0	0
			5240	3319	917	980	24			
1	A	692	Total	C	N	O	S	0	0	0
			5240	3319	917	980	24			

There are 16 discrepancies between the modelled and reference sequences:

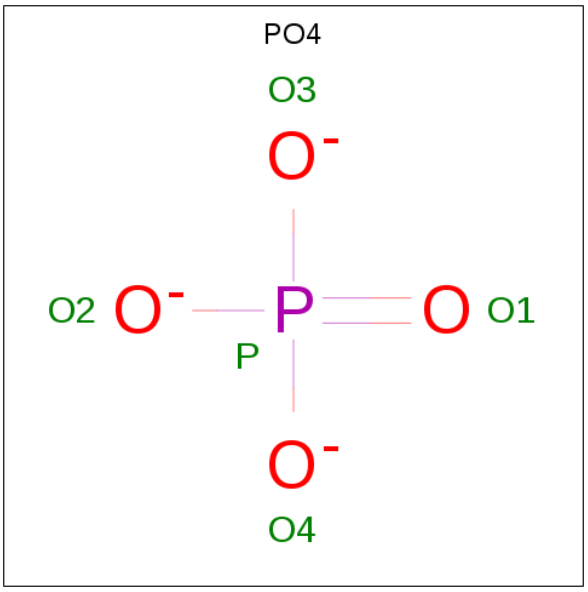
Chain	Residue	Modelled	Actual	Comment	Reference
B	694	LEU	-	expression tag	UNP Q0KBG3
B	695	GLU	-	expression tag	UNP Q0KBG3
B	696	HIS	-	expression tag	UNP Q0KBG3
B	697	HIS	-	expression tag	UNP Q0KBG3
B	698	HIS	-	expression tag	UNP Q0KBG3
B	699	HIS	-	expression tag	UNP Q0KBG3
B	700	HIS	-	expression tag	UNP Q0KBG3
B	701	HIS	-	expression tag	UNP Q0KBG3
A	694	LEU	-	expression tag	UNP Q0KBG3
A	695	GLU	-	expression tag	UNP Q0KBG3
A	696	HIS	-	expression tag	UNP Q0KBG3
A	697	HIS	-	expression tag	UNP Q0KBG3
A	698	HIS	-	expression tag	UNP Q0KBG3
A	699	HIS	-	expression tag	UNP Q0KBG3
A	700	HIS	-	expression tag	UNP Q0KBG3
A	701	HIS	-	expression tag	UNP Q0KBG3

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 5 4 1	0	0

- Molecule 4 is water.

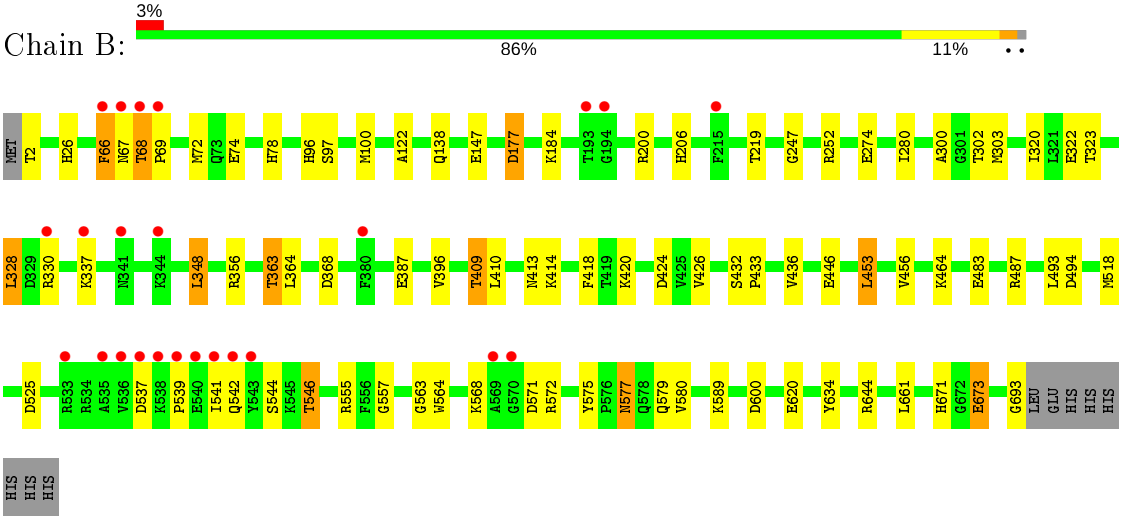
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	523	Total O 523 523	0	0
4	A	528	Total O 528 528	0	0

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.

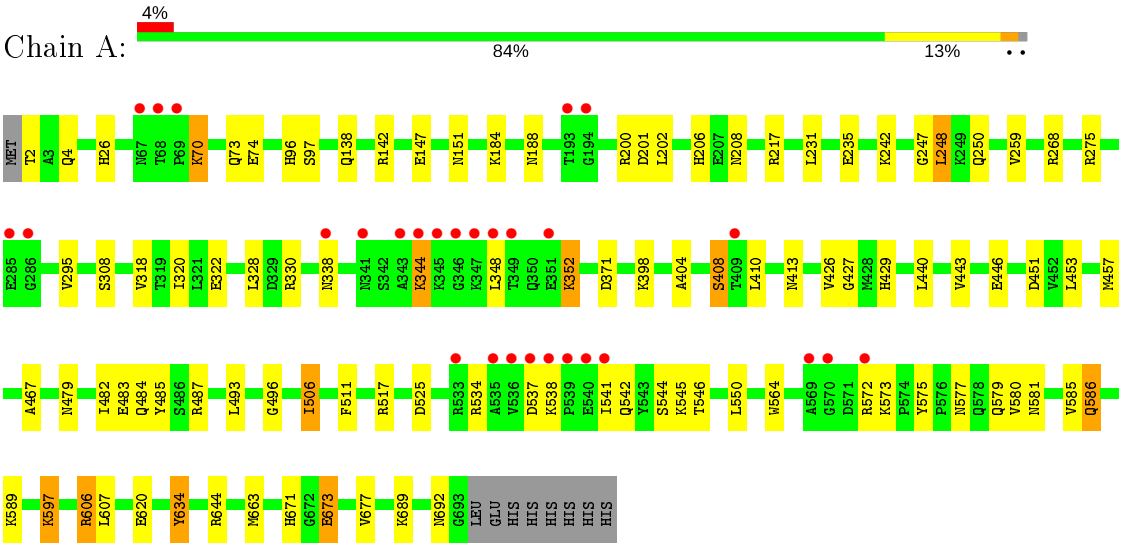
- Molecule 1: Enoyl-CoA hydratase/Delta(3)-cis-delta(2)-trans-enoyl-CoA isomerase

Chain B:



- Molecule 1: Enoyl-CoA hydratase/Delta(3)-cis-delta(2)-trans-enoyl-CoA isomerase

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	91.26Å 103.15Å 97.69Å 90.00° 107.02° 90.00°	Depositor
Resolution (Å)	93.41 – 2.00 28.05 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.3 (93.41-2.00) 96.4 (28.05-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	6.14 (at 1.99Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.176 , 0.229 0.186 , 0.235	Depositor DCC
R_{free} test set	5643 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	21.7	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 47.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11602	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% 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, PO4

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	0.90	2/5329 (0.0%)	0.95	18/7188 (0.3%)
1	B	0.91	2/5329 (0.0%)	0.97	15/7188 (0.2%)
All	All	0.91	4/10658 (0.0%)	0.96	33/14376 (0.2%)

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	A	0	4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	235	GLU	CG-CD	6.26	1.61	1.51
1	B	274	GLU	CD-OE1	5.82	1.32	1.25
1	A	620	GLU	CD-OE1	5.16	1.31	1.25
1	B	620	GLU	CD-OE1	5.13	1.31	1.25

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	606	ARG	NE-CZ-NH1	10.26	125.43	120.30
1	B	356	ARG	NE-CZ-NH2	-9.33	115.64	120.30
1	A	606	ARG	NE-CZ-NH2	-9.21	115.69	120.30
1	A	268	ARG	NE-CZ-NH2	-7.98	116.31	120.30
1	B	200	ARG	NE-CZ-NH2	-7.30	116.65	120.30
1	A	217	ARG	NE-CZ-NH1	7.05	123.83	120.30
1	A	268	ARG	NE-CZ-NH1	7.05	123.82	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	275	ARG	NE-CZ-NH1	7.02	123.81	120.30
1	B	600	ASP	CB-CG-OD1	6.82	124.44	118.30
1	B	356	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	B	555	ARG	NE-CZ-NH1	6.21	123.41	120.30
1	B	200	ARG	NE-CZ-NH1	6.11	123.36	120.30
1	A	517	ARG	NE-CZ-NH1	6.11	123.36	120.30
1	A	200	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	B	644	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	A	200	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	A	142	ARG	NE-CZ-NH1	-5.69	117.45	120.30
1	B	555	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	B	644	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	B	487	ARG	NE-CZ-NH2	5.61	123.10	120.30
1	A	217	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	A	451	ASP	CB-CG-OD1	5.47	123.22	118.30
1	B	424	ASP	CB-CG-OD1	5.44	123.20	118.30
1	A	201	ASP	CB-CG-OD2	-5.38	113.46	118.30
1	B	348	LEU	CA-CB-CG	5.37	127.64	115.30
1	B	634	TYR	CA-CB-CG	-5.33	103.27	113.40
1	A	644	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	A	634	TYR	CA-CB-CG	-5.17	103.57	113.40
1	A	248	LEU	CA-CB-CG	5.16	127.16	115.30
1	B	572	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	A	572	ARG	NE-CZ-NH2	5.11	122.86	120.30
1	B	177	ASP	CB-CG-OD2	-5.06	113.74	118.30
1	A	485	TYR	CA-CB-CG	5.05	123.00	113.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2	THR	Peptide
1	A	344	LYS	Peptide
1	A	634	TYR	Sidechain
1	A	692	ASN	Peptide

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	5240	0	5347	52	0
1	B	5240	0	5347	40	0
2	A	54	0	72	7	0
2	B	12	0	16	0	0
3	A	5	0	0	0	0
4	A	528	0	0	3	0
4	B	523	0	0	6	0
All	All	11602	0	10782	92	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 (92) 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:577:ASN:HD22	1:B:580:VAL:H	1.29	0.79
1:A:577:ASN:HD22	1:A:580:VAL:H	1.31	0.76
1:B:78:HIS:HD2	4:B:1323:HOH:O	1.69	0.76
1:B:413:ASN:HD21	1:B:446:GLU:H	1.31	0.75
1:A:663:MET:HE3	1:A:677:VAL:HG22	1.69	0.74
1:B:78:HIS:CD2	4:B:1323:HOH:O	2.40	0.73
1:A:413:ASN:HD21	1:A:446:GLU:H	1.41	0.69
1:A:597:LYS:O	4:A:901:HOH:O	2.13	0.66
1:A:151:ASN:HB2	2:A:808:GOL:O3	1.96	0.65
1:B:577:ASN:HD21	1:B:579:GLN:HB3	1.60	0.65
1:B:322:GLU:HB2	1:B:328:LEU:HD13	1.78	0.65
1:B:577:ASN:ND2	1:B:580:VAL:H	1.94	0.64
1:B:546:THR:HG23	1:B:564:TRP:HH2	1.62	0.64
1:A:188:ASN:HB2	4:A:1098:HOH:O	1.97	0.63
1:A:96:HIS:HD2	1:A:97:SER:OG	1.82	0.62
1:B:409:THR:OG1	1:B:410:LEU:N	2.33	0.62
1:B:323:THR:O	1:B:364:LEU:HD22	1.99	0.62
1:B:571:ASP:OD2	1:B:575:TYR:OH	2.13	0.62
1:B:303:MET:CE	1:B:303:MET:HA	2.31	0.61
1:B:363:THR:HG21	1:B:368:ASP:HB2	1.82	0.61
1:B:303:MET:HE2	1:B:303:MET:HA	1.83	0.60
1:A:147:GLU:OE2	1:A:206:HIS:HE1	1.84	0.59
1:A:231:LEU:HD22	2:A:804:GOL:C3	2.31	0.59
1:B:518:MET:HG3	4:B:1375:HOH:O	2.02	0.59
1:B:147:GLU:OE2	1:B:206:HIS:HE1	1.87	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:SER:OG	1:A:546:THR:HG22	2.05	0.56
1:A:577:ASN:HD21	1:A:579:GLN:HB3	1.71	0.56
1:A:506:ILE:HG13	1:A:607:LEU:CD1	2.36	0.56
1:A:671:HIS:HA	1:A:673:GLU:OE2	2.06	0.56
1:A:70:LYS:HE2	1:A:73:GLN:NE2	2.22	0.55
1:B:671:HIS:HA	1:B:673:GLU:OE2	2.07	0.55
1:A:408:SER:HB3	1:A:429:HIS:NE2	2.21	0.55
1:B:138:GLN:NE2	1:B:247:GLY:HA3	2.22	0.54
1:B:96:HIS:HD2	1:B:97:SER:OG	1.90	0.54
1:B:544:SER:OG	1:B:546:THR:HB	2.07	0.54
1:A:231:LEU:HD22	2:A:804:GOL:H31	1.90	0.53
1:A:348:LEU:HD12	1:A:352:LYS:HB3	1.91	0.53
1:B:303:MET:HE1	1:B:432:SER:HA	1.90	0.53
1:A:308:SER:OG	1:A:320:ILE:HD11	2.07	0.53
1:A:231:LEU:HD22	2:A:804:GOL:H32	1.91	0.53
1:A:371:ASP:O	1:A:398:LYS:NZ	2.41	0.52
1:B:464:LYS:NZ	4:B:907:HOH:O	2.42	0.51
1:A:371:ASP:HB2	4:A:1232:HOH:O	2.10	0.51
1:A:506:ILE:HG13	1:A:607:LEU:HD12	1.92	0.51
1:A:484:GLN:OE1	1:A:487:ARG:NH1	2.44	0.50
1:A:151:ASN:CB	2:A:808:GOL:O3	2.57	0.50
1:A:453:LEU:O	1:A:457:MET:HG2	2.12	0.50
1:B:280:ILE:HD13	1:B:453:LEU:HD13	1.92	0.50
1:A:70:LYS:CE	1:A:73:GLN:HE22	2.24	0.50
1:A:427:GLY:HA3	1:A:443:VAL:HB	1.93	0.50
1:A:506:ILE:HD12	1:A:511:PHE:CD1	2.46	0.49
1:A:506:ILE:CD1	1:A:511:PHE:CD1	2.95	0.49
1:A:242:LYS:NZ	1:A:250:GLN:HE22	2.11	0.49
1:A:586:GLN:O	1:A:589:LYS:HB3	2.13	0.49
1:B:494:ASP:OD1	1:B:544:SER:OG	2.26	0.48
1:A:663:MET:HE1	1:A:677:VAL:HG13	1.97	0.47
1:A:493:LEU:HD12	1:A:546:THR:HG21	1.97	0.47
1:A:322:GLU:HB2	1:A:328:LEU:HD13	1.96	0.47
1:B:433:PRO:HG2	1:B:436:VAL:HB	1.97	0.47
1:B:525:ASP:OD1	1:B:525:ASP:N	2.47	0.47
1:B:302:THR:HG23	4:B:1234:HOH:O	2.14	0.46
1:A:206:HIS:CD2	1:A:208:ASN:H	2.33	0.46
1:A:581:ASN:O	1:A:585:VAL:HG23	2.16	0.46
1:B:68:THR:HG22	1:B:69:PRO:HD2	1.98	0.46
1:A:479:ASN:HA	1:A:482:ILE:HG22	1.97	0.45
1:B:493:LEU:HD12	1:B:546:THR:HG21	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:GLN:NE2	1:A:247:GLY:HA3	2.31	0.45
1:A:404:ALA:HA	1:A:426:VAL:O	2.17	0.45
1:A:70:LYS:HE3	1:A:73:GLN:HE22	1.82	0.44
1:A:525:ASP:OD1	1:A:525:ASP:N	2.49	0.44
1:A:577:ASN:ND2	1:A:580:VAL:H	2.06	0.44
1:A:483:GLU:OE1	1:A:534:ARG:NH2	2.51	0.43
1:B:387:GLU:HA	1:B:418:PHE:CD2	2.53	0.43
1:A:70:LYS:CE	1:A:73:GLN:NE2	2.82	0.43
1:A:689:LYS:O	2:A:809:GOL:O2	2.31	0.43
1:A:550:LEU:HD22	1:A:564:TRP:CE2	2.54	0.43
1:B:537:ASP:CB	1:B:539:PRO:HD2	2.49	0.43
1:A:573:LYS:HD3	1:A:575:TYR:CE1	2.55	0.42
1:B:66:PHE:O	1:B:67:ASN:CB	2.67	0.42
1:B:26:HIS:HE1	1:B:74:GLU:O	2.02	0.42
1:A:295:VAL:O	1:A:318:VAL:HA	2.20	0.42
1:B:100:MET:HA	1:B:122:ALA:O	2.19	0.42
1:A:506:ILE:HG13	1:A:607:LEU:HD13	2.01	0.41
1:B:557:GLY:HA2	1:B:563:GLY:HA3	2.02	0.41
1:A:26:HIS:HE1	1:A:74:GLU:O	2.04	0.41
1:B:693:GLY:HA2	4:B:1171:HOH:O	2.20	0.41
1:A:151:ASN:HA	2:A:808:GOL:H32	2.02	0.41
1:B:300:ALA:HB2	1:B:320:ILE:HG21	2.04	0.41
1:B:252:ARG:HA	1:B:252:ARG:HD2	1.91	0.40
1:B:426:VAL:HG11	1:B:456:VAL:HG21	2.04	0.40
1:B:546:THR:HG23	1:B:564:TRP:CH2	2.49	0.40
1:A:440:LEU:O	1:A:467:ALA:HA	2.22	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	690/701 (98%)	668 (97%)	19 (3%)	3 (0%)	34 30
1	B	690/701 (98%)	671 (97%)	19 (3%)	0	100 100
All	All	1380/1402 (98%)	1339 (97%)	38 (3%)	3 (0%)	47 44

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	537	ASP
1	A	538	LYS
1	A	496	GLY

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	544/553 (98%)	524 (96%)	20 (4%)	34 32
1	B	544/553 (98%)	518 (95%)	26 (5%)	25 22
All	All	1088/1106 (98%)	1042 (96%)	46 (4%)	30 27

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	2	THR
1	B	66	PHE
1	B	68	THR
1	B	72	MET
1	B	177	ASP
1	B	184	LYS
1	B	219	THR
1	B	328	LEU
1	B	330	ARG
1	B	337	LYS
1	B	348	LEU
1	B	363	THR
1	B	396	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	409	THR
1	B	414	LYS
1	B	420	LYS
1	B	453	LEU
1	B	483	GLU
1	B	541	ILE
1	B	542	GLN
1	B	546	THR
1	B	568	LYS
1	B	577	ASN
1	B	589	LYS
1	B	661	LEU
1	B	673	GLU
1	A	4	GLN
1	A	70	LYS
1	A	184	LYS
1	A	202	LEU
1	A	248	LEU
1	A	259	VAL
1	A	330	ARG
1	A	338	ASN
1	A	344	LYS
1	A	352	LYS
1	A	408	SER
1	A	410	LEU
1	A	506	ILE
1	A	541	ILE
1	A	542	GLN
1	A	545	LYS
1	A	586	GLN
1	A	597	LYS
1	A	606	ARG
1	A	673	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	B	18	ASN
1	B	26	HIS
1	B	78	HIS
1	B	96	HIS
1	B	138	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	187	GLN
1	B	206	HIS
1	B	250	GLN
1	B	310	ASN
1	B	413	ASN
1	B	577	ASN
1	B	658	ASN
1	A	18	ASN
1	A	26	HIS
1	A	73	GLN
1	A	96	HIS
1	A	138	GLN
1	A	206	HIS
1	A	250	GLN
1	A	310	ASN
1	A	413	ASN
1	A	577	ASN
1	A	671	HIS

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

12 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	$\#\|Z\| > 2$
2	GOL	B	801	-	5,5,5	0.64	0	5,5,5	1.04	0
2	GOL	A	807	-	5,5,5	0.76	0	5,5,5	0.99	0
2	GOL	A	808	-	5,5,5	0.68	0	5,5,5	1.50	1 (20%)
3	PO4	A	810	-	4,4,4	1.17	0	6,6,6	0.82	0
2	GOL	B	802	-	5,5,5	1.11	0	5,5,5	1.37	1 (20%)
2	GOL	A	802	-	5,5,5	0.59	0	5,5,5	0.97	0
2	GOL	A	806	-	5,5,5	0.67	0	5,5,5	0.47	0
2	GOL	A	801	-	5,5,5	0.52	0	5,5,5	1.06	0
2	GOL	A	805	-	5,5,5	1.01	0	5,5,5	1.01	1 (20%)
2	GOL	A	809	-	5,5,5	1.05	0	5,5,5	1.86	1 (20%)
2	GOL	A	803	-	5,5,5	0.31	0	5,5,5	0.52	0
2	GOL	A	804	-	5,5,5	0.79	0	5,5,5	1.55	1 (20%)

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
2	GOL	B	801	-	-	1/4/4/4	-
2	GOL	A	807	-	-	0/4/4/4	-
2	GOL	A	808	-	-	4/4/4/4	-
2	GOL	B	802	-	-	4/4/4/4	-
2	GOL	A	802	-	-	2/4/4/4	-
2	GOL	A	806	-	-	2/4/4/4	-
2	GOL	A	801	-	-	0/4/4/4	-
2	GOL	A	805	-	-	4/4/4/4	-
2	GOL	A	809	-	-	2/4/4/4	-
2	GOL	A	803	-	-	0/4/4/4	-
2	GOL	A	804	-	-	4/4/4/4	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	809	GOL	C3-C2-C1	3.59	125.67	111.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	808	GOL	O1-C1-C2	-3.10	95.35	110.20
2	A	804	GOL	O3-C3-C2	2.69	123.10	110.20
2	B	802	GOL	O1-C1-C2	2.21	120.80	110.20
2	A	805	GOL	O3-C3-C2	2.19	120.68	110.20

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	808	GOL	O1-C1-C2-O2
2	A	808	GOL	O1-C1-C2-C3
2	A	808	GOL	C1-C2-C3-O3
2	A	808	GOL	O2-C2-C3-O3
2	B	802	GOL	O1-C1-C2-O2
2	B	802	GOL	O1-C1-C2-C3
2	B	802	GOL	C1-C2-C3-O3
2	A	802	GOL	O1-C1-C2-C3
2	A	806	GOL	C1-C2-C3-O3
2	A	805	GOL	O1-C1-C2-C3
2	A	805	GOL	C1-C2-C3-O3
2	A	809	GOL	O1-C1-C2-C3
2	A	804	GOL	C1-C2-C3-O3
2	B	802	GOL	O2-C2-C3-O3
2	B	801	GOL	C1-C2-C3-O3
2	A	804	GOL	O1-C1-C2-C3
2	A	802	GOL	O1-C1-C2-O2
2	A	806	GOL	O2-C2-C3-O3
2	A	809	GOL	O1-C1-C2-O2
2	A	804	GOL	O1-C1-C2-O2
2	A	805	GOL	O2-C2-C3-O3
2	A	804	GOL	O2-C2-C3-O3
2	A	805	GOL	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	808	GOL	3	0
2	A	809	GOL	1	0
2	A	804	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	692/701 (98%)	-0.16	29 (4%)	36	35	11, 26, 58, 109	0
1	B	692/701 (98%)	-0.26	24 (3%)	44	43	11, 26, 54, 118	0
All	All	1384/1402 (98%)	-0.21	53 (3%)	40	39	11, 26, 56, 118	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	538	LYS	8.5
1	A	536	VAL	5.9
1	A	343	ALA	5.6
1	A	346	GLY	5.5
1	B	194	GLY	5.3
1	A	344	LYS	4.7
1	A	535	ALA	4.5
1	B	67	ASN	4.5
1	B	539	PRO	4.3
1	A	345	LYS	4.3
1	A	347	LYS	4.3
1	A	341	ASN	4.2
1	B	69	PRO	4.1
1	A	540	GLU	4.0
1	A	538	LYS	4.0
1	A	569	ALA	4.0
1	A	348	LEU	3.8
1	B	537	ASP	3.8
1	B	541	ILE	3.6
1	A	69	PRO	3.6
1	A	570	GLY	3.5
1	B	570	GLY	3.5
1	B	193	THR	3.5
1	B	215	PHE	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	330	ARG	3.4
1	A	286	GLY	3.3
1	B	569	ALA	3.3
1	A	194	GLY	3.2
1	B	536	VAL	3.2
1	A	533	ARG	3.1
1	A	539	PRO	3.0
1	B	66	PHE	2.9
1	A	68	THR	2.9
1	A	285	GLU	2.8
1	A	541	ILE	2.8
1	B	543	TYR	2.8
1	B	535	ALA	2.7
1	A	537	ASP	2.6
1	B	344	LYS	2.6
1	B	68	THR	2.5
1	B	341	ASN	2.5
1	B	533	ARG	2.5
1	A	67	ASN	2.5
1	A	349	THR	2.4
1	B	540	GLU	2.4
1	B	337	LYS	2.3
1	A	409	THR	2.2
1	A	338	ASN	2.2
1	B	542	GLN	2.1
1	A	351	GLU	2.0
1	A	572	ARG	2.0
1	A	193	THR	2.0
1	B	380	PHE	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
2	GOL	A	807	6/6	0.75	0.26	43,49,51,58	0
2	GOL	A	806	6/6	0.76	0.23	48,56,59,67	0
2	GOL	A	809	6/6	0.78	0.28	32,47,51,53	0
2	GOL	B	801	6/6	0.81	0.16	49,55,56,57	0
2	GOL	A	804	6/6	0.83	0.33	39,49,53,53	0
2	GOL	A	808	6/6	0.85	0.18	35,39,42,42	0
2	GOL	B	802	6/6	0.86	0.20	29,51,53,55	0
2	GOL	A	802	6/6	0.93	0.10	28,35,44,45	0
2	GOL	A	803	6/6	0.93	0.16	46,49,51,63	0
2	GOL	A	805	6/6	0.93	0.22	25,37,44,46	0
3	PO4	A	810	5/5	0.94	0.16	63,70,76,82	0
2	GOL	A	801	6/6	0.96	0.11	19,27,30,33	0

6.5 Other polymers

There are no such residues in this entry.