Full wwPDB X-ray Structure Validation Report ⓘ

Oct 18, 2023 – 12:29 AM EDT

PDB ID	:	1IYX
Title	:	Crystal structure of enolase from Enterococcus hirae
Authors	:	Hosaka, T.; Meguro, T.; Yamato, I.; Shirakihara, Y.
Deposited on	:	2002-09-12
Resolution	:	2.80 Å(reported)

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	:	2.36
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

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 2.80 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	Percentile Ranks	Value
Rfree		0.232
Clashscore		25
Ramachandran outliers		1.2%
Sidechain outliers		6.9%
RSRZ outliers		2.4%

Worse — *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
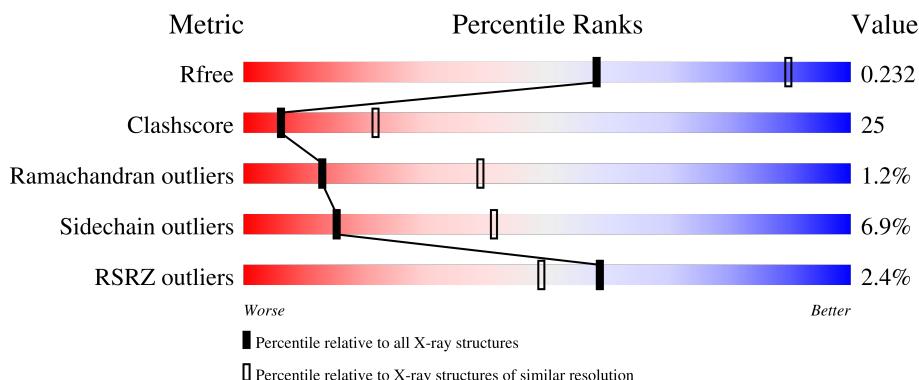
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	432	2% / 63% / 31% / 5%
1	B	432	3% / 58% / 39% / •
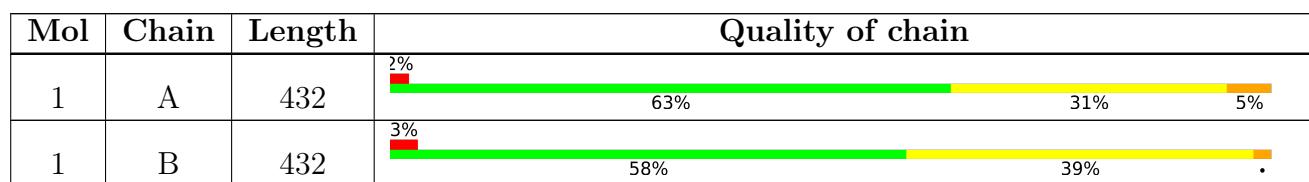
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

WORLDWIDE
wwPDB
PROTEIN DATA BANK

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MG	A	1432	-	-	-	X

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 6718 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 ENOLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	431	Total	C	N	O	S	0	0	0
			3254	2048	534	661	11			
1	B	431	Total	C	N	O	S	0	0	0
			3254	2048	534	661	11			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
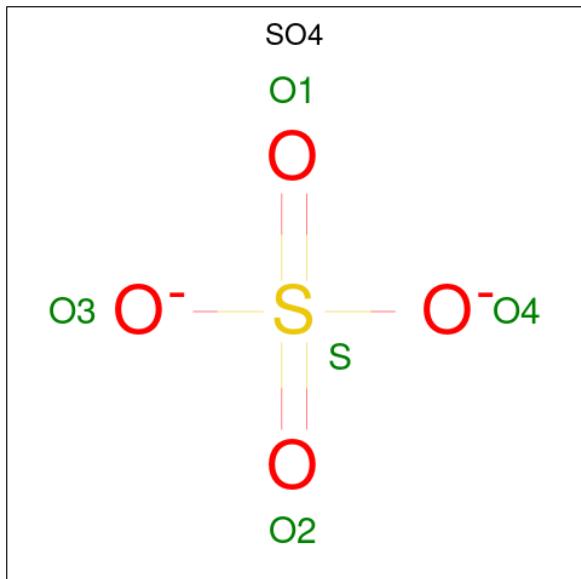
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 5	O 4	S 1	0	0
3	B	1	Total 5	O 4	S 1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).
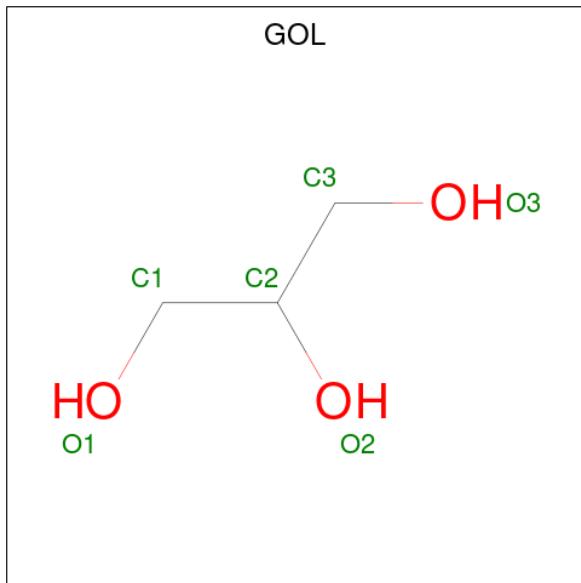
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 6	C 3	O 3	0	0
4	A	1	Total 6	C 3	O 3	0	0
4	A	1	Total 6	C 3	O 3	0	0
4	A	1	Total 6	C 3	O 3	0	0
4	B	1	Total 6	C 3	O 3	0	0
4	B	1	Total 6	C 3	O 3	0	0

- Molecule 5 is water.

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

3 Residue-property plots ⓘ

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: ENOLASE

Chain A:

• Molecule 1: ENOLASE

Chain B:
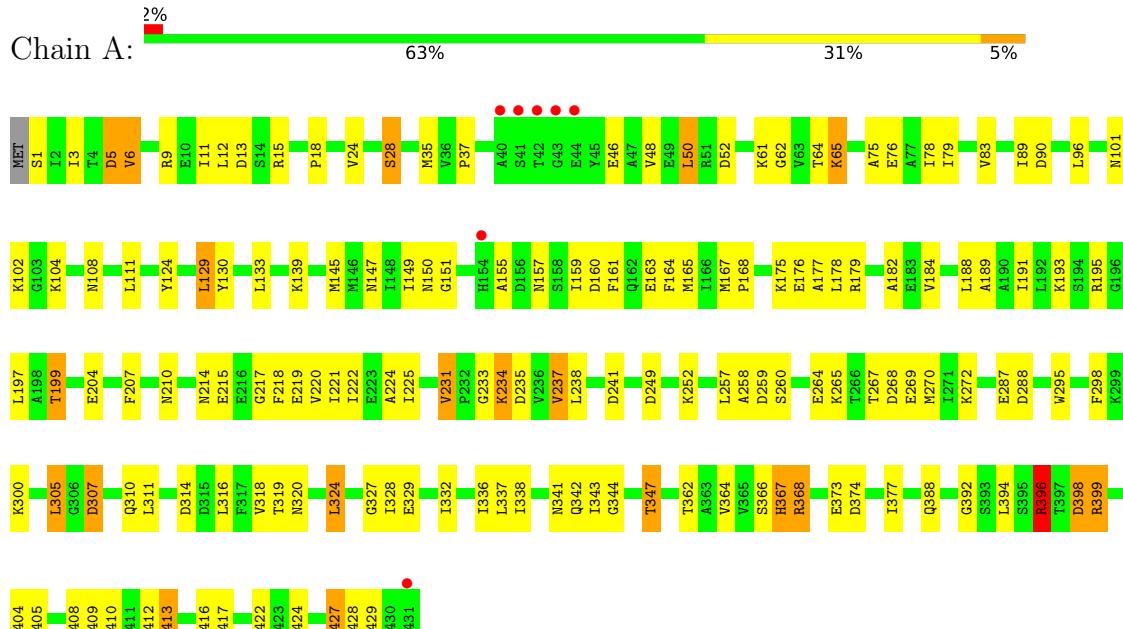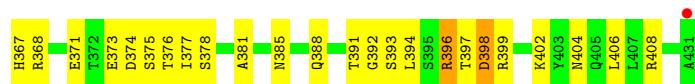
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α, β, γ	153.51Å　　153.51Å　　90.66Å 90.00°　　　90.00°　　　90.00°	Depositor
Resolution (Å)	20.00　–　2.80 19.58　–　2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.80) 100.0 (19.58-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.05 (at 2.79Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.175　,　0.239 0.168　,　0.232	Depositor DCC
R_{free} test set	2554 reflections (9.83%)	wwPDB-VP
Wilson B-factor (Å^2)	41.0	Xtriage
Anisotropy	0.172	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 52.0	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.023 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6718	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% 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: MG, 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	0.34	0/3301	0.60	1/4459 (0.0%)
1	B	0.33	0/3301	0.60	0/4459
All	All	0.33	0/6602	0.60	1/8918 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	396	ARG	NE-CZ-NH1	-5.19	117.70	120.30

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	3254	0	3221	147	0
1	B	3254	0	3221	181	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	24	0	32	0	0
4	B	12	0	16	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	83	0	0	7	0
5	B	79	0	0	10	0
All	All	6718	0	6490	320	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 25.

All (320) 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:149:ILE:HG12	1:A:221:ILE:HD11	1.50	0.94
1:B:2:ILE:HD12	1:B:2:ILE:H	1.34	0.90
1:B:93:MET:HE1	1:B:110:ILE:HA	1.54	0.87
1:B:148:ILE:HG22	1:B:149:ILE:HG12	1.57	0.86
1:A:28:SER:HB3	5:A:2065:HOH:O	1.74	0.86
1:B:1:SER:HB2	1:B:124:TYR:CE1	2.12	0.85
1:A:5:ASP:HB2	5:A:2025:HOH:O	1.76	0.84
1:B:110:ILE:HG13	5:B:2041:HOH:O	1.81	0.80
1:A:75:ALA:O	1:A:79:ILE:HG12	1.81	0.79
1:B:46:GLU:HG3	1:B:342:GLN:HG3	1.63	0.78
1:B:374:ASP:OD1	1:B:376:THR:HG22	1.83	0.78
1:B:8:ALA:H	1:B:71:ASN:HD21	1.29	0.78
1:A:160:ASP:OD2	1:A:260:SER:HB2	1.85	0.77
1:A:90:ASP:OD2	1:A:347:THR:HG22	1.85	0.77
1:A:404:ASN:HD21	1:B:12:LEU:H	1.32	0.77
1:B:52:ASP:CG	1:B:64:THR:HG22	2.07	0.75
1:B:8:ALA:HB2	1:B:22:VAL:HG22	1.69	0.74
1:A:147:ASN:HD21	1:A:150:ASN:HD21	1.33	0.74
1:B:237:VAL:HG21	1:B:284:ILE:HB	1.67	0.74
1:A:257:LEU:HD23	1:A:265:LYS:HD3	1.70	0.74
1:A:427:ASN:H	1:A:427:ASN:HD22	1.36	0.73
1:B:191:ILE:HD11	1:B:227:LYS:HD2	1.68	0.73
1:A:46:GLU:HB2	1:A:318:VAL:HG11	1.70	0.73
1:B:218:PHE:O	1:B:222:ILE:HG12	1.88	0.73
1:A:1:SER:N	5:A:2064:HOH:O	2.21	0.72
1:B:244:SER:HA	1:B:247:PHE:CE1	2.24	0.72
1:A:78:ILE:HD12	1:A:89:ILE:HG23	1.70	0.72
1:B:157:ASN:HB3	1:B:210:ASN:HA	1.73	0.71
1:B:320:ASN:ND2	1:B:323:LYS:H	1.89	0.70
1:A:149:ILE:CG1	1:A:221:ILE:HD11	2.21	0.70
1:B:15:ARG:HH12	1:B:40:ALA:HA	1.56	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:ILE:HA	1:A:214:ASN:ND2	2.08	0.69
1:B:145:MET:HG2	1:B:165:MET:SD	2.33	0.68
1:B:2:ILE:HD12	1:B:2:ILE:N	2.07	0.68
1:B:278:VAL:HG22	1:B:283:ILE:HB	1.76	0.67
1:A:396:ARG:HG2	1:B:396:ARG:HG2	1.75	0.67
1:B:341:ASN:HD21	1:B:368:ARG:HH11	1.41	0.67
1:A:6:VAL:HG12	1:A:79:ILE:HD11	1.75	0.67
1:A:427:ASN:HD22	1:A:427:ASN:N	1.89	0.66
1:A:163:GLU:HG2	1:A:241:ASP:HB3	1.77	0.66
1:B:2:ILE:H	1:B:2:ILE:CD1	2.08	0.66
1:A:324:LEU:O	1:A:328:ILE:HG13	1.95	0.65
1:A:319:THR:HG22	1:A:319:THR:O	1.95	0.65
1:A:341:ASN:HD21	1:A:368:ARG:HG3	1.61	0.65
1:A:167:MET:HB2	1:A:237:VAL:HG12	1.78	0.65
1:A:373:GLU:HG3	5:A:2008:HOH:O	1.96	0.65
1:A:6:VAL:HG11	1:A:75:ALA:HA	1.77	0.65
1:B:106:GLY:O	1:B:110:ILE:HG12	1.97	0.65
1:A:368:ARG:O	1:A:399:ARG:NH1	2.30	0.64
1:B:160:ASP:OD1	1:B:257:LEU:HB3	1.96	0.64
1:A:310:GLN:HE22	1:A:388:GLN:HE22	1.45	0.64
1:A:155:ALA:HB1	1:A:157:ASN:ND2	2.13	0.64
1:B:125:LEU:HD13	4:B:2006:GOL:O3	1.97	0.64
1:B:394:LEU:HD12	1:B:394:LEU:N	2.13	0.64
1:A:409:ILE:O	1:A:413:LEU:HB2	1.98	0.63
1:A:9:ARG:CZ	1:B:408:ARG:HG3	2.29	0.63
1:B:266:THR:HG22	1:B:269:GLU:HG2	1.81	0.63
1:B:52:ASP:OD2	1:B:64:THR:HG22	1.97	0.63
1:B:264:GLU:O	1:B:265:LYS:HD2	1.99	0.62
1:A:241:ASP:HA	1:A:287:GLU:HB3	1.81	0.62
1:A:324:LEU:HD22	1:A:328:ILE:HD11	1.81	0.62
1:B:139:LYS:HE2	5:B:2034:HOH:O	1.99	0.62
1:B:163:GLU:HB3	1:B:241:ASP:HB3	1.82	0.62
1:B:319:THR:O	1:B:319:THR:HG22	1.98	0.62
1:A:102:LYS:HE2	1:A:344:GLY:HA3	1.81	0.61
1:B:337:LEU:HD23	1:B:364:VAL:HB	1.81	0.61
1:A:324:LEU:HG	1:A:336:ILE:HD12	1.83	0.61
1:B:115:ILE:O	1:B:119:ARG:HG3	1.99	0.61
1:B:182:ALA:HA	1:B:394:LEU:HD22	1.83	0.60
1:A:413:LEU:O	1:A:416:VAL:HG22	2.02	0.60
1:B:74:ILE:HG21	1:B:93:MET:HE3	1.82	0.60
1:B:167:MET:CE	1:B:239:ALA:HB2	2.31	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:ASN:H	1:A:427:ASN:ND2	1.99	0.60
1:B:78:ILE:HD12	1:B:89:ILE:HG23	1.84	0.60
1:A:52:ASP:CG	1:A:64:THR:HG22	2.22	0.60
1:B:167:MET:HE2	1:B:239:ALA:HB2	1.83	0.59
1:A:215:GLU:O	1:A:219:GLU:HG3	2.02	0.59
1:B:184:VAL:HG11	1:B:225:ILE:HD13	1.85	0.59
1:B:378:SER:HB3	1:B:406:LEU:CD1	2.33	0.58
1:A:318:VAL:HG12	1:A:318:VAL:O	2.03	0.58
1:A:18:PRO:HG2	1:A:61:LYS:O	2.04	0.58
1:A:46:GLU:HB2	1:A:318:VAL:CG1	2.34	0.58
1:A:101:ASN:O	1:A:102:LYS:HB2	2.04	0.57
1:A:52:ASP:OD1	1:A:64:THR:HG22	2.05	0.57
1:A:12:LEU:H	1:B:404:ASN:HD21	1.52	0.57
1:A:37:PRO:HG2	1:A:341:ASN:HD22	1.69	0.57
1:B:18:PRO:HG2	1:B:61:LYS:O	2.05	0.57
4:B:2006:GOL:H32	5:B:2083:HOH:O	2.04	0.57
1:B:266:THR:HG22	1:B:269:GLU:CD	2.25	0.56
1:B:392:GLY:HA3	1:B:399:ARG:HG3	1.86	0.56
1:B:1:SER:HB3	5:B:2058:HOH:O	2.04	0.56
1:B:217:GLY:O	1:B:220:VAL:HG12	2.05	0.56
1:B:266:THR:HG22	1:B:269:GLU:OE1	2.05	0.56
1:A:160:ASP:H	1:A:214:ASN:HD21	1.53	0.56
1:A:188:LEU:HD12	1:A:207:PHE:CD2	2.40	0.56
1:B:171:ALA:HB2	1:B:180:MET:HE3	1.88	0.56
1:B:393:SER:C	1:B:394:LEU:HD12	2.26	0.56
1:A:6:VAL:CG1	1:A:75:ALA:HA	2.36	0.55
1:B:255:TYR:CD2	1:B:270:MET:HG3	2.41	0.55
1:A:182:ALA:HA	1:A:394:LEU:HD22	1.88	0.55
1:B:180:MET:O	1:B:184:VAL:HG23	2.06	0.55
1:A:404:ASN:ND2	1:B:12:LEU:H	2.03	0.55
1:B:299:LYS:HB2	1:B:332:ILE:HG22	1.88	0.55
1:A:189:ALA:HB2	1:A:207:PHE:CZ	2.42	0.54
1:B:237:VAL:CG2	1:B:284:ILE:HB	2.36	0.54
1:B:248:TYR:HD2	1:B:255:TYR:CE1	2.25	0.54
1:B:340:VAL:HG23	1:B:341:ASN:H	1.72	0.54
1:B:341:ASN:H	1:B:341:ASN:HD22	1.55	0.54
1:B:266:THR:CG2	1:B:269:GLU:HG2	2.38	0.54
1:B:44:GLU:O	1:B:45:TYR:HB2	2.08	0.54
1:A:257:LEU:HD21	1:A:270:MET:CE	2.38	0.54
1:B:318:VAL:HG23	1:B:342:GLN:NE2	2.23	0.54
1:A:217:GLY:O	1:A:220:VAL:HG12	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:ILE:O	1:B:225:ILE:HG12	2.08	0.54
1:A:161:PHE:HB2	1:A:164:PHE:HE1	1.73	0.53
1:A:46:GLU:CD	1:A:342:GLN:HE21	2.12	0.53
1:A:111:LEU:HD22	1:A:341:ASN:HA	1.90	0.53
1:B:42:THR:HG23	1:B:46:GLU:CD	2.29	0.53
1:B:213:SER:HB3	1:B:216:GLU:HG3	1.90	0.53
1:B:266:THR:HG22	1:B:269:GLU:CG	2.39	0.53
1:B:45:TYR:CE1	1:B:323:LYS:HE2	2.42	0.53
1:B:322:GLN:O	1:B:326:GLU:HG3	2.08	0.53
1:B:213:SER:HB3	1:B:216:GLU:CG	2.38	0.53
1:A:405:GLN:HE21	1:A:408:ARG:HH21	1.56	0.52
1:B:139:LYS:H	1:B:385:ASN:HD21	1.58	0.52
1:A:151:GLY:HA2	1:A:155:ALA:HB3	1.91	0.52
1:A:234:LYS:NZ	1:A:234:LYS:HA	2.24	0.52
1:A:396:ARG:HB3	1:A:398:ASP:OD1	2.09	0.52
1:B:268:ASP:HB3	5:B:2074:HOH:O	2.10	0.52
1:A:257:LEU:HD21	1:A:270:MET:HE3	1.90	0.52
1:B:42:THR:HG22	1:B:43:GLY:N	2.25	0.52
1:B:237:VAL:HG22	1:B:238:LEU:H	1.75	0.52
1:B:300:LYS:O	1:B:304:VAL:HG12	2.10	0.52
1:B:337:LEU:HD22	1:B:366:SER:HB3	1.92	0.52
1:B:46:GLU:CG	1:B:342:GLN:HG3	2.37	0.51
1:A:48:VAL:HG22	1:A:101:ASN:HB3	1.92	0.51
1:B:238:LEU:O	1:B:284:ILE:HG22	2.10	0.51
1:B:299:LYS:CA	1:B:332:ILE:HG22	2.39	0.51
1:A:182:ALA:CA	1:A:394:LEU:HD22	2.40	0.51
1:B:1:SER:CB	5:B:2058:HOH:O	2.58	0.51
1:A:405:GLN:NE2	1:A:408:ARG:HH21	2.08	0.51
1:A:147:ASN:HD21	1:A:150:ASN:ND2	2.05	0.51
1:B:140:VAL:H	1:B:385:ASN:ND2	2.08	0.51
1:B:187:ALA:HB1	1:B:227:LYS:CG	2.40	0.51
1:B:188:LEU:HD23	1:B:207:PHE:HD1	1.76	0.51
1:B:115:ILE:HG22	1:B:119:ARG:HD2	1.91	0.50
1:A:160:ASP:OD2	1:A:260:SER:CB	2.57	0.50
1:A:324:LEU:HD22	1:A:328:ILE:CD1	2.40	0.50
1:A:408:ARG:NH1	1:B:35:MET:HE3	2.26	0.50
1:A:257:LEU:CD2	1:A:265:LYS:HD3	2.39	0.50
1:A:35:MET:HB2	1:A:374:ASP:HB2	1.94	0.50
1:A:327:GLY:CA	1:A:332:ILE:HG12	2.41	0.50
1:A:188:LEU:HD21	1:A:220:VAL:HG22	1.93	0.50
1:B:154:HIS:O	1:B:155:ALA:HB2	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:LYS:HG3	1:B:253:GLY:N	2.27	0.50
1:A:11:ILE:O	1:A:18:PRO:HA	2.12	0.49
1:A:249:ASP:HB3	1:A:252:LYS:HB2	1.94	0.49
1:B:148:ILE:HG23	1:B:188:LEU:HD22	1.93	0.49
1:A:3:ILE:HG23	1:A:24:VAL:HG13	1.93	0.49
1:A:160:ASP:N	1:A:214:ASN:HD21	2.09	0.49
1:A:398:ASP:HB3	1:B:397:THR:OG1	2.12	0.49
1:A:188:LEU:HD23	1:A:224:ALA:HB2	1.93	0.49
1:A:257:LEU:N	1:A:257:LEU:HD22	2.27	0.49
1:B:111:LEU:HD22	1:B:341:ASN:HA	1.94	0.49
1:B:15:ARG:NH1	1:B:40:ALA:HA	2.26	0.49
1:B:212:GLY:O	1:B:213:SER:HB2	2.12	0.49
1:A:221:ILE:O	1:A:225:ILE:HG12	2.12	0.49
1:B:108:ASN:OD1	1:B:108:ASN:N	2.46	0.49
1:A:264:GLU:O	1:A:265:LYS:HD2	2.13	0.48
1:A:337:LEU:HD12	1:A:364:VAL:HB	1.94	0.48
1:B:299:LYS:HD3	1:B:330:LYS:O	2.13	0.48
1:A:218:PHE:O	1:A:222:ILE:HG12	2.13	0.48
1:B:241:ASP:HA	1:B:287:GLU:HB3	1.94	0.48
1:A:108:ASN:OD1	1:A:108:ASN:N	2.46	0.48
1:A:300:LYS:HD3	5:A:2034:HOH:O	2.12	0.48
1:B:318:VAL:HG22	1:B:318:VAL:O	2.13	0.48
1:B:257:LEU:HD12	1:B:262:GLU:HB2	1.95	0.48
1:A:90:ASP:HB2	1:A:347:THR:HG21	1.96	0.48
1:A:159:ILE:HA	1:A:214:ASN:HD21	1.78	0.48
1:B:293:ASN:O	1:B:295:TRP:HD1	1.96	0.48
1:A:265:LYS:HB2	1:A:270:MET:HE3	1.96	0.47
1:A:319:THR:CG2	1:A:343:ILE:HB	2.43	0.47
1:B:160:ASP:N	1:B:214:ASN:OD1	2.48	0.47
1:B:160:ASP:OD2	1:B:259:ASP:HB2	2.14	0.47
1:B:367:HIS:HB3	1:B:391:THR:HA	1.96	0.47
1:A:318:VAL:HG13	1:A:342:GLN:NE2	2.29	0.47
1:A:413:LEU:HB3	1:A:417:ALA:HB2	1.94	0.47
1:A:46:GLU:HG3	1:A:342:GLN:HG3	1.96	0.47
1:B:147:ASN:OD1	1:B:206:GLY:HA3	2.14	0.47
1:B:187:ALA:HB1	1:B:227:LYS:HG3	1.97	0.47
1:B:97:ASP:OD2	1:B:102:LYS:HA	2.14	0.47
1:B:255:TYR:HE2	1:B:267:THR:HB	1.80	0.47
1:B:332:ILE:C	1:B:332:ILE:HD12	2.35	0.47
1:A:341:ASN:HD21	1:A:368:ARG:CG	2.28	0.47
1:B:293:ASN:O	1:B:295:TRP:N	2.43	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:GLN:HE21	1:A:405:GLN:HA	1.78	0.47
1:B:224:ALA:HA	1:B:227:LYS:HG2	1.97	0.46
1:B:115:ILE:CG2	1:B:119:ARG:HD2	2.45	0.46
1:B:207:PHE:HB3	1:B:209:PRO:HD3	1.97	0.46
1:B:327:GLY:HA3	1:B:332:ILE:HD11	1.96	0.46
1:A:46:GLU:OE2	1:A:342:GLN:NE2	2.47	0.46
1:B:249:ASP:O	1:B:252:LYS:O	2.34	0.46
1:B:128:PRO:HG2	1:B:131:HIS:HB2	1.98	0.46
1:B:290:LEU:CD2	1:B:301:LEU:HD22	2.45	0.46
1:B:271:ILE:O	1:B:275:GLU:HB2	2.16	0.46
1:A:399:ARG:N	1:A:399:ARG:HD2	2.30	0.46
1:A:179:ARG:HG3	1:B:58:TYR:CE2	2.51	0.45
1:A:195:ARG:HB3	1:A:197:LEU:HD23	1.97	0.45
1:A:427:ASN:ND2	1:A:428:LEU:HD13	2.32	0.45
1:B:52:ASP:OD1	1:B:64:THR:HG22	2.16	0.45
1:A:184:VAL:HG11	1:A:225:ILE:HD13	1.99	0.45
1:B:237:VAL:HG22	1:B:238:LEU:N	2.31	0.45
1:A:231:VAL:HG23	1:A:233:GLY:H	1.81	0.45
1:B:319:THR:HG22	1:B:343:ILE:HB	1.99	0.45
1:B:332:ILE:O	1:B:333:ALA:HB2	2.17	0.45
1:B:399:ARG:HD2	1:B:399:ARG:N	2.31	0.45
1:A:264:GLU:C	1:A:265:LYS:HD2	2.37	0.44
1:A:392:GLY:HA3	1:A:399:ARG:HG3	1.99	0.44
1:B:184:VAL:CG1	1:B:225:ILE:HD13	2.47	0.44
1:B:320:ASN:ND2	1:B:323:LYS:N	2.62	0.44
1:A:6:VAL:HG13	1:A:75:ALA:CB	2.47	0.44
1:A:288:ASP:OD2	1:A:314:ASP:HB3	2.17	0.44
1:A:341:ASN:ND2	1:A:368:ARG:HG3	2.30	0.44
1:B:92:ALA:HB2	5:B:2011:HOH:O	2.17	0.44
1:B:159:ILE:HA	1:B:214:ASN:OD1	2.18	0.44
1:B:8:ALA:H	1:B:71:ASN:ND2	2.07	0.44
1:B:248:TYR:CD2	1:B:255:TYR:CE1	3.04	0.44
1:B:316:LEU:HD22	1:B:317:PHE:CE1	2.52	0.44
1:A:37:PRO:HG2	1:A:341:ASN:ND2	2.32	0.44
1:A:338:ILE:N	1:A:338:ILE:HD12	2.32	0.44
1:A:130:TYR:HE2	1:A:412:GLN:HE21	1.66	0.44
1:A:157:ASN:HB3	1:A:210:ASN:HA	1.99	0.44
1:B:291:ASP:C	1:B:293:ASN:H	2.21	0.44
1:B:365:VAL:CG2	1:B:377:ILE:HB	2.47	0.44
1:A:217:GLY:O	1:A:221:ILE:HG12	2.18	0.44
1:B:74:ILE:HD13	1:B:93:MET:CE	2.47	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340:VAL:HG23	1:B:341:ASN:N	2.33	0.44
1:B:365:VAL:HG11	1:B:381:ALA:HB2	2.00	0.44
1:B:398:ASP:HB2	1:B:399:ARG:HH11	1.82	0.44
1:B:288:ASP:OD1	1:B:314:ASP:HB3	2.18	0.43
1:A:129:LEU:HD22	1:A:133:LEU:HG	2.01	0.43
1:A:145:MET:HB3	1:A:145:MET:HE2	1.79	0.43
1:A:179:ARG:CG	1:B:58:TYR:CE2	3.01	0.43
1:A:191:ILE:O	1:A:195:ARG:HB2	2.18	0.43
1:B:174:PHE:CE1	1:B:406:LEU:HD23	2.53	0.43
1:A:307:ASP:OD1	1:A:429:LYS:HB3	2.18	0.43
1:B:320:ASN:HD22	1:B:323:LYS:CG	2.31	0.43
1:B:337:LEU:HD23	1:B:337:LEU:HA	1.89	0.43
1:A:269:GLU:O	1:A:272:LYS:HB3	2.19	0.43
1:B:266:THR:O	1:B:269:GLU:HG2	2.18	0.43
1:B:278:VAL:O	1:B:278:VAL:HG12	2.19	0.43
1:B:287:GLU:HG3	1:B:312:VAL:HG22	2.00	0.43
1:B:362:THR:HG21	1:B:388:GLN:NE2	2.33	0.43
1:A:204:GLU:HG3	1:A:367:HIS:HE1	1.83	0.43
1:B:105:LEU:HB2	1:B:110:ILE:HD11	1.99	0.43
1:B:374:ASP:O	1:B:402:LYS:HE3	2.18	0.43
1:A:265:LYS:HA	1:A:269:GLU:OE2	2.19	0.43
1:B:28:SER:N	5:B:2058:HOH:O	2.26	0.43
1:B:368:ARG:O	1:B:371:GLU:HG2	2.18	0.43
1:B:375:SER:O	1:B:378:SER:HB2	2.18	0.43
1:B:261:GLY:C	1:B:263:GLY:H	2.21	0.43
1:A:184:VAL:CG1	1:A:225:ILE:HD13	2.49	0.42
1:A:257:LEU:HD22	1:A:257:LEU:H	1.83	0.42
1:A:413:LEU:HD12	1:A:413:LEU:HA	1.84	0.42
1:B:48:VAL:CG2	1:B:101:ASN:ND2	2.82	0.42
1:B:110:ILE:CD1	5:B:2041:HOH:O	2.67	0.42
1:B:225:ILE:HD12	1:B:236:VAL:HG11	2.02	0.42
1:B:398:ASP:HB2	1:B:399:ARG:NH1	2.34	0.42
1:B:368:ARG:HD2	1:B:368:ARG:HA	1.81	0.42
1:A:168:PRO:CG	1:A:177:ALA:HB1	2.50	0.42
1:A:422:LEU:C	1:A:424:SER:H	2.22	0.42
1:B:210:ASN:O	1:B:211:LEU:HD23	2.20	0.42
1:A:405:GLN:NE2	1:A:405:GLN:HA	2.34	0.42
1:B:44:GLU:C	1:B:46:GLU:H	2.23	0.42
1:A:147:ASN:HA	1:A:165:MET:HG2	2.02	0.42
1:A:319:THR:HG22	1:A:343:ILE:HB	2.01	0.42
1:A:405:GLN:HE21	1:A:408:ARG:NH2	2.16	0.42

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:SER:HB3	1:A:124:TYR:CZ	2.55	0.42
1:A:6:VAL:HG12	1:A:79:ILE:CD1	2.46	0.42
1:A:199:THR:HG23	1:A:199:THR:O	2.19	0.42
1:B:274:TYR:O	1:B:278:VAL:HG23	2.20	0.42
1:A:176:GLU:OE1	1:A:179:ARG:NH1	2.45	0.41
1:B:155:ALA:HB1	1:B:157:ASN:ND2	2.35	0.41
1:B:179:ARG:HD3	1:B:183:GLU:OE2	2.20	0.41
1:A:76:GLU:HG2	5:A:2027:HOH:O	2.19	0.41
1:A:237:VAL:HG13	1:A:238:LEU:N	2.35	0.41
1:B:158:SER:OG	1:B:212:GLY:HA2	2.21	0.41
1:B:272:LYS:O	1:B:276:GLU:N	2.53	0.41
1:B:299:LYS:CB	1:B:332:ILE:HG22	2.50	0.41
1:B:394:LEU:N	1:B:394:LEU:CD1	2.83	0.41
1:A:18:PRO:HG3	1:A:62:GLY:HA2	2.02	0.41
1:B:227:LYS:HE3	1:B:227:LYS:HB2	1.95	0.41
1:B:320:ASN:HD22	1:B:323:LYS:HG2	1.84	0.41
1:A:50:LEU:HD13	1:A:65:LYS:HB3	2.03	0.41
1:A:195:ARG:HG2	1:A:197:LEU:CD2	2.51	0.41
1:A:327:GLY:HA2	1:A:332:ILE:HG12	2.02	0.41
1:B:42:THR:CG2	1:B:43:GLY:N	2.84	0.41
1:B:48:VAL:HG23	1:B:101:ASN:ND2	2.35	0.41
1:A:305:LEU:HD12	1:A:305:LEU:HA	1.90	0.41
1:B:160:ASP:OD1	1:B:260:SER:HB3	2.20	0.41
1:A:366:SER:OG	1:A:367:HIS:N	2.54	0.41
1:A:377:ILE:HG12	5:A:2058:HOH:O	2.21	0.41
1:B:148:ILE:HG23	1:B:188:LEU:CD2	2.50	0.41
1:B:318:VAL:O	1:B:318:VAL:HG13	2.21	0.41
1:B:377:ILE:HG23	5:B:2057:HOH:O	2.20	0.41
1:B:398:ASP:OD2	1:B:399:ARG:NH1	2.46	0.41
1:A:175:LYS:HB2	1:A:410:GLU:OE2	2.21	0.41
1:B:179:ARG:O	1:B:183:GLU:HG3	2.21	0.41
1:B:340:VAL:O	1:B:343:ILE:HG22	2.19	0.41
1:B:396:ARG:O	1:B:399:ARG:HB2	2.21	0.41
1:A:13:ASP:OD2	1:A:13:ASP:C	2.60	0.41
1:B:35:MET:HB2	1:B:374:ASP:HB2	2.02	0.41
1:B:167:MET:HE3	1:B:239:ALA:HB2	2.01	0.41
1:A:234:LYS:HA	1:A:234:LYS:HZ3	1.84	0.40
1:A:398:ASP:C	1:A:399:ARG:HD2	2.41	0.40
1:B:187:ALA:O	1:B:191:ILE:HG12	2.21	0.40
1:B:299:LYS:HA	1:B:332:ILE:HG22	2.03	0.40
1:A:168:PRO:HG2	1:A:177:ALA:HB1	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:THR:HG23	1:B:46:GLU:OE2	2.22	0.40
1:A:231:VAL:HG13	1:A:235:ASP:OD2	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	429/432 (99%)	392 (91%)	34 (8%)	3 (1%)	22	53
1	B	429/432 (99%)	383 (89%)	39 (9%)	7 (2%)	9	31
All	All	858/864 (99%)	775 (90%)	73 (8%)	10 (1%)	13	39

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	396	ARG
1	B	159	ILE
1	B	158	SER
1	B	213	SER
1	B	292	GLU
1	B	306	GLY
1	A	83	VAL
1	B	251	GLU
1	B	396	ARG
1	A	258	ALA

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	341/342 (100%)	305 (89%)	36 (11%)	6	20
1	B	341/342 (100%)	330 (97%)	11 (3%)	39	73
All	All	682/684 (100%)	635 (93%)	47 (7%)	15	41

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ASP
1	A	6	VAL
1	A	15	ARG
1	A	28	SER
1	A	50	LEU
1	A	65	LYS
1	A	96	LEU
1	A	104	LYS
1	A	129	LEU
1	A	139	LYS
1	A	178	LEU
1	A	193	LYS
1	A	199	THR
1	A	231	VAL
1	A	234	LYS
1	A	237	VAL
1	A	259	ASP
1	A	267	THR
1	A	268	ASP
1	A	295	TRP
1	A	298	PHE
1	A	305	LEU
1	A	307	ASP
1	A	311	LEU
1	A	316	LEU
1	A	320	ASN
1	A	324	LEU
1	A	329	GLU
1	A	347	THR
1	A	362	THR
1	A	367	HIS
1	A	368	ARG
1	A	398	ASP

Continued from previous page...

Mol	Chain	Res	Type
1	A	399	ARG
1	A	413	LEU
1	A	427	ASN
1	B	1	SER
1	B	50	LEU
1	B	139	LYS
1	B	231	VAL
1	B	298	PHE
1	B	312	VAL
1	B	324	LEU
1	B	341	ASN
1	B	365	VAL
1	B	373	GLU
1	B	398	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
1	A	69	ASN
1	A	86	GLN
1	A	150	ASN
1	A	186	HIS
1	A	214	ASN
1	A	341	ASN
1	A	342	GLN
1	A	388	GLN
1	A	404	ASN
1	A	405	GLN
1	A	412	GLN
1	A	427	ASN
1	B	69	ASN
1	B	71	ASN
1	B	72	ASN
1	B	131	HIS
1	B	150	ASN
1	B	320	ASN
1	B	341	ASN
1	B	342	GLN
1	B	385	ASN
1	B	404	ASN
1	B	412	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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	B	2006	-	5,5,5	0.17	0	5,5,5	0.40	0
4	GOL	A	2002	-	5,5,5	0.14	0	5,5,5	0.46	0
4	GOL	A	2003	-	5,5,5	0.16	0	5,5,5	0.44	0
3	SO4	B	1001	-	4,4,4	0.26	0	6,6,6	0.09	0
3	SO4	A	1002	-	4,4,4	0.24	0	6,6,6	0.10	0
4	GOL	A	2005	-	5,5,5	0.17	0	5,5,5	0.46	0
4	GOL	A	2001	-	5,5,5	0.17	0	5,5,5	0.42	0
4	GOL	B	2004	-	5,5,5	0.20	0	5,5,5	0.49	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	B	2006	-	-	2/4/4/4	-
4	GOL	A	2002	-	-	2/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	2003	-	-	0/4/4/4	-
4	GOL	A	2005	-	-	0/4/4/4	-
4	GOL	A	2001	-	-	2/4/4/4	-
4	GOL	B	2004	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2002	GOL	O1-C1-C2-C3
4	A	2002	GOL	O1-C1-C2-O2
4	B	2006	GOL	O1-C1-C2-C3
4	B	2004	GOL	O1-C1-C2-O2
4	A	2001	GOL	O1-C1-C2-C3
4	B	2006	GOL	O1-C1-C2-O2
4	A	2001	GOL	O1-C1-C2-O2
4	B	2004	GOL	O1-C1-C2-C3

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	2006	GOL	2	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 (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	431/432 (99%)	-0.63	7 (1%) 72	66	13, 31, 60, 92	0
1	B	431/432 (99%)	-0.46	14 (3%) 47	37	14, 35, 80, 111	0
All	All	862/864 (99%)	-0.55	21 (2%) 59	49	13, 33, 73, 111	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	42	THR	5.9
1	B	41	SER	4.8
1	A	42	THR	4.5
1	B	251	GLU	4.4
1	A	41	SER	4.1
1	B	40	ALA	4.0
1	B	154	HIS	3.7
1	B	250	LYS	3.1
1	B	153	SER	3.0
1	B	44	GLU	2.7
1	A	40	ALA	2.6
1	A	43	GLY	2.5
1	B	252	LYS	2.5
1	B	43	GLY	2.4
1	B	210	ASN	2.4
1	A	154	HIS	2.1
1	A	44	GLU	2.1
1	B	194	SER	2.1
1	B	431	ALA	2.1
1	B	55	LYS	2.1
1	A	431	ALA	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides 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, 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
2	MG	A	1432	1/1	0.76	0.42	58,58,58,58	0
4	GOL	B	2006	6/6	0.81	0.40	77,83,87,99	0
4	GOL	B	2004	6/6	0.85	0.29	47,60,61,62	0
4	GOL	A	2003	6/6	0.86	0.28	57,63,65,68	0
4	GOL	A	2002	6/6	0.90	0.25	46,50,52,59	0
4	GOL	A	2001	6/6	0.90	0.22	60,64,67,69	0
2	MG	B	1432	1/1	0.92	0.13	57,57,57,57	0
4	GOL	A	2005	6/6	0.92	0.21	40,47,48,52	0
3	SO4	A	1002	5/5	0.97	0.12	44,47,57,59	0
3	SO4	B	1001	5/5	0.98	0.13	52,53,53,56	0

6.5 Other polymers ⓘ

There are no such residues in this entry.