Full wwPDB X-ray Structure Validation Report ⓘ

Aug 23, 2023 – 08:02 AM EDT

PDB ID	:	3E2Y
Title	:	Crystal structure of mouse kynurenine aminotransferase III in complex with glutamine
Authors	:	Han, Q.; Robinson, R.; Cai, T.; Tagle, D.A.; Li, J.
Deposited on	:	2008-08-06
Resolution	:	2.26 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

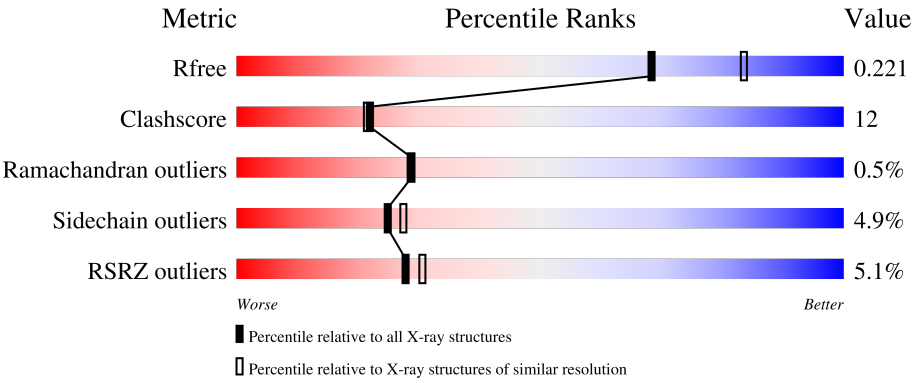
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.26 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	410	4% 79% 19%
1	B	410	6% 80% 17%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PMP	A	457	-	-	X	-
4	GOL	A	459	-	X	X	-
4	GOL	B	459	-	-	X	-

2 Entry composition

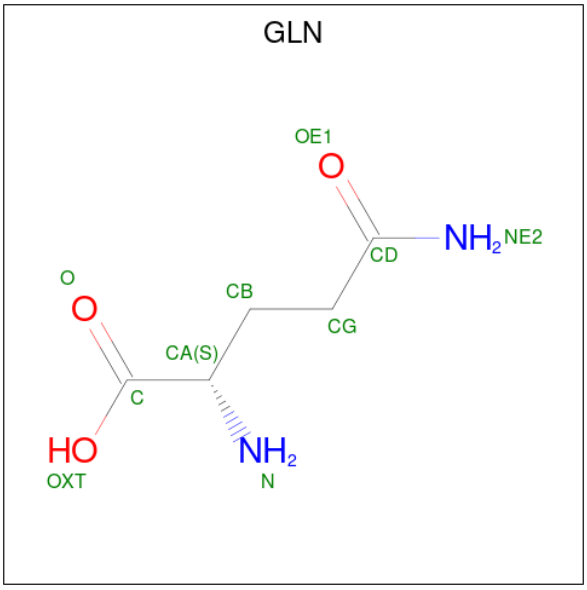
There are 5 unique types of molecules in this entry. The entry contains 6993 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Kynurenine-oxoglutarate transaminase 3.

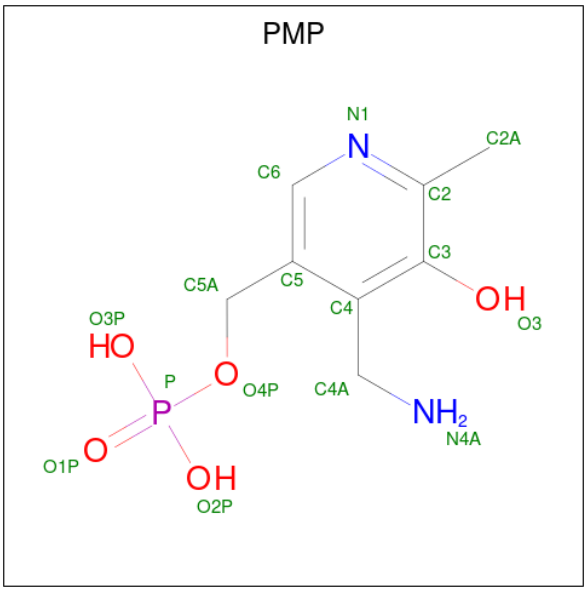
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	410	Total	C	N	O	S	0	0	0
			3253	2100	536	599	18			
1	B	410	Total	C	N	O	S	0	0	0
			3253	2100	536	599	18			

- Molecule 2 is GLUTAMINE (three-letter code: GLN) (formula: $C_5H_{10}N_2O_3$).



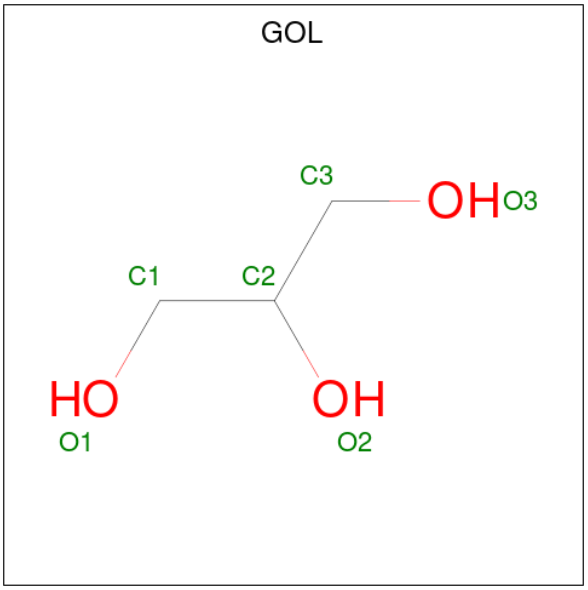
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			10	5	2	3		
2	B	1	Total	C	N	O	0	0
			10	5	2	3		

- Molecule 3 is 4'-DEOXY-4'-AMINOPYRIDOXAL-5'-PHOSPHATE (three-letter code: PMP) (formula: $C_8H_{13}N_2O_5P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			16	8	2	5	1		
3	B	1	Total	C	N	O	P	0	0
			16	8	2	5	1		

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



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

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

- Molecule 5 is water.

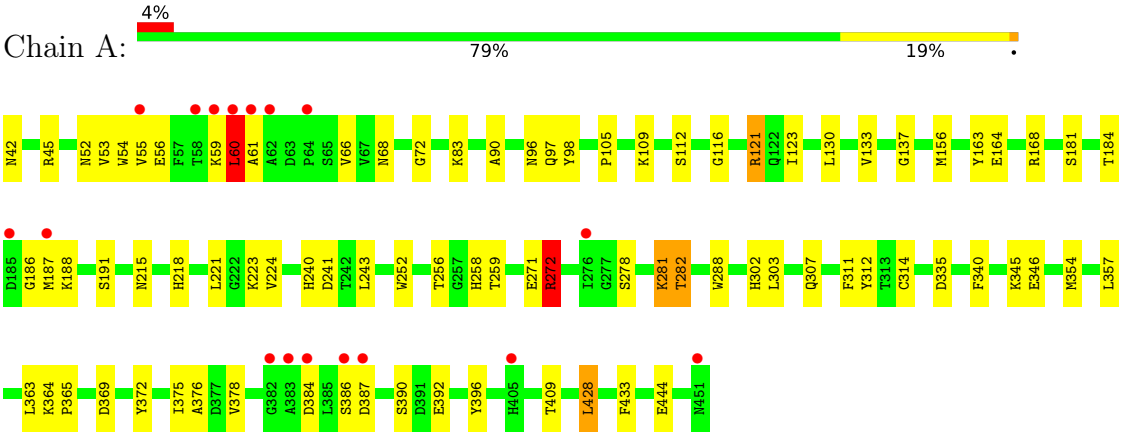
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	216	Total O 216 216	0	0
5	B	195	Total O 195 195	0	0

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.

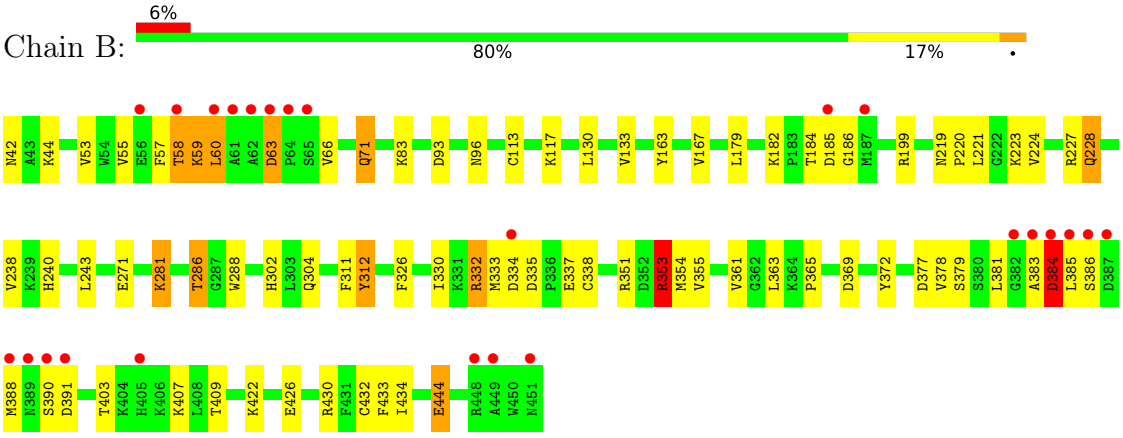
• Molecule 1: Kynurenine-oxoglutarate transaminase 3

Chain A:



• Molecule 1: Kynurenine-oxoglutarate transaminase 3

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	91.57Å 91.57Å 232.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.87 – 2.26 29.58 – 2.26	Depositor EDS
% Data completeness (in resolution range)	95.4 (29.87-2.26) 95.4 (29.58-2.26)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.23 (at 2.26Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.175 , 0.221 0.174 , 0.221	Depositor DCC
R_{free} test set	2273 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	28.4	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 46.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6993	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% 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: PMP, GOL

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	0.96	2/3341 (0.1%)	0.87	3/4539 (0.1%)
1	B	0.95	1/3341 (0.0%)	0.86	5/4539 (0.1%)
All	All	0.95	3/6682 (0.0%)	0.86	8/9078 (0.1%)

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	1	0
1	B	1	2
All	All	2	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	286	THR	CB-OG1	8.00	1.59	1.43
1	A	346	GLU	CG-CD	5.72	1.60	1.51
1	A	345	LYS	CD-CE	5.11	1.64	1.51

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	272	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	A	45	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	B	199	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	B	353	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	A	428	LEU	CB-CG-CD1	5.28	119.98	111.00
1	B	384	ASP	CB-CG-OD2	5.25	123.03	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	63	ASP	CB-CG-OD2	5.14	122.92	118.30
1	B	353	ARG	NE-CZ-NH2	-5.12	117.74	120.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	256	THR	CB
1	B	286	THR	CB

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	383	ALA	Peptide
1	B	384	ASP	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	3253	0	3231	76	0
1	B	3253	0	3231	93	0
2	A	10	0	7	5	0
2	B	10	0	7	3	0
3	A	16	0	10	7	0
3	B	16	0	10	4	0
4	A	12	0	16	12	0
4	B	12	0	16	5	0
5	A	216	0	0	7	0
5	B	195	0	0	9	0
All	All	6993	0	6528	155	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 12.

All (155) 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:97:GLN:NE2	1:B:286:THR:HG22	1.48	1.27
1:A:240:HIS:O	4:A:458:GOL:H2	1.38	1.19
1:B:221:LEU:HB2	5:B:643:HOH:O	1.45	1.17
1:A:221:LEU:HG	5:A:645:HOH:O	1.51	1.10
1:A:184:THR:HG22	1:A:186:GLY:H	1.21	1.00
1:A:97:GLN:HE21	1:B:286:THR:HG22	1.00	0.97
1:A:218:HIS:CD2	4:A:459:GOL:H2	2.01	0.95
1:A:288:TRP:HE1	1:B:96:ASN:HD22	1.15	0.94
1:B:71:GLN:H	1:B:71:GLN:HE21	1.04	0.92
1:A:97:GLN:HE21	1:B:286:THR:CG2	1.81	0.91
1:A:215:ASN:CB	4:A:459:GOL:H32	2.03	0.89
1:B:71:GLN:H	1:B:71:GLN:NE2	1.72	0.87
1:B:335:ASP:HB3	1:B:337:GLU:OE1	1.76	0.84
1:A:271:GLU:HG2	5:A:567:HOH:O	1.78	0.83
1:A:215:ASN:HB3	4:A:459:GOL:H32	1.60	0.82
1:A:363:LEU:O	1:A:365:PRO:HD3	1.80	0.82
1:A:96:ASN:HD22	1:B:288:TRP:HE1	1.26	0.82
1:B:353:ARG:NH1	1:B:444:GLU:HG3	1.96	0.80
1:A:98:TYR:H	1:B:286:THR:HG23	1.46	0.77
1:B:228:GLN:NE2	1:B:228:GLN:H	1.85	0.74
1:B:228:GLN:H	1:B:228:GLN:HE21	1.32	0.73
1:A:90:ALA:O	1:B:83:LYS:HG2	1.91	0.71
1:A:335:ASP:HB3	5:A:667:HOH:O	1.90	0.71
1:A:281:LYS:NZ	3:A:457:PMP:H4A1	2.05	0.71
2:A:456:GLN:HB3	3:A:457:PMP:HNA2	1.57	0.69
1:B:384:ASP:H	1:B:385:LEU:HG	1.58	0.69
1:A:218:HIS:NE2	4:A:459:GOL:H2	2.10	0.67
1:B:60:LEU:HB3	1:B:403:THR:HG21	1.76	0.66
1:B:71:GLN:HE21	1:B:71:GLN:N	1.86	0.66
1:B:42:ASN:N	5:B:651:HOH:O	2.29	0.66
1:A:184:THR:HG22	1:A:186:GLY:N	2.04	0.66
1:B:384:ASP:CB	1:B:385:LEU:HD23	2.26	0.66
1:A:215:ASN:HB2	4:A:459:GOL:H32	1.76	0.66
1:A:396:TYR:CE2	5:A:522:HOH:O	2.49	0.65
1:A:164:GLU:O	1:A:168:ARG:HG3	1.97	0.65
1:A:281:LYS:HZ1	3:A:457:PMP:H4A1	1.63	0.64
1:B:240:HIS:HB3	4:B:459:GOL:H32	1.78	0.64
1:B:353:ARG:HH11	1:B:444:GLU:HG3	1.62	0.63
2:A:456:GLN:HB3	3:A:457:PMP:N4A	2.12	0.62
1:A:390:SER:OG	1:A:392:GLU:HG3	1.98	0.62
2:A:456:GLN:CB	3:A:457:PMP:HNA2	2.12	0.62
1:A:98:TYR:N	1:B:286:THR:HG23	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:ARG:HD3	5:B:562:HOH:O	2.00	0.62
1:A:53:VAL:O	1:A:56:GLU:HB2	2.01	0.60
1:B:66:VAL:HG11	1:B:409:THR:HG23	1.84	0.60
1:A:215:ASN:HB3	4:A:459:GOL:C3	2.32	0.60
1:A:278:SER:O	1:A:282:THR:HG22	2.02	0.60
1:A:288:TRP:HE1	1:B:96:ASN:ND2	1.94	0.60
1:A:72:GLY:H	2:A:456:GLN:HA	1.67	0.59
1:A:278:SER:O	1:A:282:THR:CG2	2.50	0.59
1:B:117:LYS:HE2	1:B:333:MET:HE1	1.84	0.59
1:B:240:HIS:O	4:B:459:GOL:H32	2.03	0.58
1:B:403:THR:OG1	1:B:409:THR:HG22	2.03	0.58
1:A:184:THR:CG2	1:A:186:GLY:H	2.07	0.58
1:B:384:ASP:HB2	1:B:385:LEU:HD23	1.85	0.57
1:A:54:TRP:CH2	2:A:456:GLN:OXT	2.58	0.57
1:B:42:ASN:N	5:B:468:HOH:O	2.37	0.56
1:B:430:ARG:NH2	2:B:457:GLN:OXT	2.27	0.56
1:A:164:GLU:OE2	1:A:168:ARG:NH1	2.40	0.55
1:B:60:LEU:HD23	1:B:63:ASP:HB3	1.88	0.55
1:A:133:VAL:HG21	1:B:133:VAL:HG21	1.90	0.54
1:B:182:LYS:HE3	5:B:630:HOH:O	2.06	0.54
1:B:184:THR:HG22	1:B:186:GLY:H	1.72	0.54
4:A:459:GOL:H11	5:A:666:HOH:O	2.08	0.54
1:A:97:GLN:HE22	1:B:286:THR:H	1.57	0.53
1:A:241:ASP:OD1	1:A:272:ARG:NH2	2.41	0.53
1:A:97:GLN:HE22	1:B:286:THR:HG22	1.60	0.53
1:B:351:ARG:O	1:B:355:VAL:HG13	2.09	0.53
1:A:302:HIS:ND1	1:B:42:ASN:HB3	2.24	0.53
1:B:334:ASP:HB3	5:B:585:HOH:O	2.09	0.52
1:A:357:LEU:CD2	1:A:444:GLU:HG3	2.40	0.52
1:A:384:ASP:HB3	5:A:641:HOH:O	2.08	0.52
1:B:130:LEU:HD13	1:B:304:GLN:HG2	1.93	0.51
1:B:332:ARG:O	1:B:338:CYS:HB2	2.09	0.51
1:B:117:LYS:HD3	1:B:333:MET:HE3	1.93	0.51
1:A:218:HIS:HD2	4:A:459:GOL:H2	1.67	0.51
1:A:363:LEU:HD22	1:A:378:VAL:HG12	1.93	0.51
1:B:60:LEU:O	1:B:409:THR:HG21	2.11	0.51
1:B:385:LEU:HB3	1:B:388:MET:HE3	1.93	0.50
1:B:184:THR:HG22	1:B:186:GLY:N	2.26	0.50
3:B:456:PMP:N4A	2:B:457:GLN:N	2.60	0.49
1:B:238:VAL:HG21	4:B:458:GOL:H32	1.95	0.49
1:B:221:LEU:HD11	1:B:223:LYS:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:384:ASP:H	1:B:385:LEU:CG	2.25	0.49
1:B:179:LEU:CD1	1:B:221:LEU:HD21	2.43	0.49
1:A:258:HIS:HD2	5:A:623:HOH:O	1.96	0.48
1:A:281:LYS:HZ2	3:A:457:PMP:H4A1	1.78	0.48
1:B:55:VAL:O	1:B:58:THR:HG22	2.13	0.48
1:B:281:LYS:HE2	3:B:456:PMP:N4A	2.28	0.48
1:B:334:ASP:HA	5:B:585:HOH:O	2.13	0.48
1:B:354:MET:HG3	1:B:433:PHE:HB3	1.96	0.48
1:B:219:ASN:OD1	1:B:220:PRO:HA	2.14	0.47
1:B:66:VAL:CG1	1:B:409:THR:HG23	2.43	0.47
1:B:184:THR:HG22	1:B:185:ASP:N	2.28	0.47
1:B:60:LEU:CD2	1:B:63:ASP:HB3	2.45	0.47
1:A:105:PRO:O	1:A:109:LYS:HB3	2.15	0.47
1:A:130:LEU:HD23	1:A:303:LEU:HB3	1.96	0.47
1:B:334:ASP:CA	5:B:585:HOH:O	2.63	0.47
1:B:384:ASP:H	1:B:385:LEU:CD2	2.28	0.46
1:A:354:MET:HG3	1:A:433:PHE:HB3	1.96	0.46
1:A:98:TYR:H	1:B:286:THR:CG2	2.23	0.46
1:B:240:HIS:O	4:B:459:GOL:H11	2.15	0.46
1:B:363:LEU:O	1:B:365:PRO:HD3	2.15	0.46
1:A:96:ASN:ND2	1:B:288:TRP:HE1	2.05	0.45
1:A:311:PHE:HE2	1:A:314:CYS:HG	1.65	0.45
1:A:66:VAL:HG11	1:A:409:THR:HG23	1.99	0.45
1:B:71:GLN:NE2	1:B:71:GLN:N	2.54	0.45
1:A:61:ALA:HB3	1:A:68:ASN:HD22	1.82	0.45
1:A:357:LEU:HD21	1:A:444:GLU:HG3	1.99	0.45
1:B:281:LYS:HE2	3:B:456:PMP:HNA1	1.83	0.44
1:A:59:LYS:O	1:A:60:LEU:C	2.56	0.44
1:B:117:LYS:CE	1:B:333:MET:CE	2.96	0.44
1:B:384:ASP:HB3	1:B:385:LEU:HD23	1.99	0.44
1:A:221:LEU:HD12	1:A:375:ILE:CD1	2.48	0.44
1:B:60:LEU:HD13	5:B:541:HOH:O	2.18	0.44
1:B:163:TYR:O	1:B:167:VAL:HG13	2.18	0.44
1:B:384:ASP:N	1:B:385:LEU:HG	2.30	0.44
1:A:61:ALA:HB3	1:A:68:ASN:ND2	2.32	0.43
1:A:191:SER:HB3	1:A:223:LYS:HA	2.00	0.43
1:A:137:GLY:CA	1:B:311:PHE:HD2	2.32	0.43
1:A:156:MET:O	4:A:459:GOL:O2	2.33	0.43
1:B:326:PHE:O	1:B:330:ILE:HG13	2.18	0.43
1:B:351:ARG:HB2	1:B:433:PHE:CE1	2.54	0.43
1:A:83:LYS:HE3	1:B:93:ASP:OD2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:432:CYS:SG	1:B:434:ILE:HG22	2.58	0.43
1:A:42:ASN:HB3	1:B:302:HIS:CE1	2.53	0.43
1:B:384:ASP:HB3	1:B:385:LEU:HA	2.00	0.43
1:A:224:VAL:HG23	1:A:369:ASP:HB2	2.01	0.43
1:A:363:LEU:HB3	1:A:376:ALA:HB1	2.01	0.43
1:A:307:GLN:NE2	1:A:311:PHE:CZ	2.87	0.42
1:B:422:LYS:O	1:B:426:GLU:HB3	2.19	0.42
1:A:281:LYS:NZ	3:A:457:PMP:C4A	2.79	0.42
1:B:353:ARG:HH11	1:B:444:GLU:CG	2.31	0.42
1:B:377:ASP:OD1	1:B:379:SER:OG	2.35	0.42
1:A:218:HIS:ND1	1:A:221:LEU:HB2	2.34	0.42
1:B:281:LYS:HZ3	1:B:281:LYS:HG2	1.63	0.42
1:A:252:TRP:CE3	1:A:340:PHE:HB3	2.55	0.42
1:B:117:LYS:HE2	1:B:333:MET:CE	2.48	0.42
1:B:224:VAL:HG23	1:B:369:ASP:HB2	2.01	0.42
3:B:456:PMP:HNA2	2:B:457:GLN:N	2.18	0.41
1:B:271:GLU:H	1:B:271:GLU:CD	2.23	0.41
1:B:351:ARG:HB2	1:B:433:PHE:CZ	2.55	0.41
1:A:52:ASN:HD22	1:A:55:VAL:H	1.67	0.41
1:B:240:HIS:O	4:B:459:GOL:C2	2.69	0.41
1:A:163:TYR:CE2	4:A:459:GOL:H31	2.56	0.41
1:B:58:THR:HG23	1:B:58:THR:O	2.21	0.41
1:A:66:VAL:CG1	1:A:409:THR:HG23	2.50	0.41
1:A:112:SER:HB2	1:A:123:ILE:O	2.20	0.41
1:A:137:GLY:HA2	1:B:311:PHE:HD2	1.85	0.41
1:B:57:PHE:C	1:B:59:LYS:H	2.25	0.41
1:B:363:LEU:HD23	1:B:381:LEU:HD13	2.02	0.40
1:B:53:VAL:HG13	1:B:57:PHE:CE2	2.56	0.40
1:A:163:TYR:HE2	4:A:459:GOL:H31	1.86	0.40
1:A:116:GLY:HA2	1:A:121:ARG:O	2.21	0.40
1:A:137:GLY:HA2	1:B:311:PHE:CD2	2.56	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	408/410 (100%)	393 (96%)	14 (3%)	1 (0%)	47 55
1	B	408/410 (100%)	390 (96%)	15 (4%)	3 (1%)	22 21
All	All	816/820 (100%)	783 (96%)	29 (4%)	4 (0%)	29 29

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	LEU
1	B	312	TYR
1	B	58	THR
1	B	391	ASP

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	358/358 (100%)	341 (95%)	17 (5%)	26 29
1	B	358/358 (100%)	340 (95%)	18 (5%)	24 26
All	All	716/716 (100%)	681 (95%)	35 (5%)	25 27

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	LEU
1	A	121	ARG
1	A	181	SER
1	A	187	MET
1	A	188	LYS
1	A	243	LEU
1	A	256	THR
1	A	259	THR
1	A	272	ARG

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Mol	Chain	Res	Type
1	A	281	LYS
1	A	282	THR
1	A	312	TYR
1	A	364	LYS
1	A	372	TYR
1	A	386	SER
1	A	387	ASP
1	A	428	LEU
1	B	44	LYS
1	B	59	LYS
1	B	60	LEU
1	B	71	GLN
1	B	113	CYS
1	B	228	GLN
1	B	243	LEU
1	B	281	LYS
1	B	312	TYR
1	B	332	ARG
1	B	353	ARG
1	B	361	VAL
1	B	372	TYR
1	B	378	VAL
1	B	386	SER
1	B	390	SER
1	B	407	LYS
1	B	444	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	ASN
1	A	52	ASN
1	A	96	ASN
1	A	97	GLN
1	A	122	GLN
1	A	258	HIS
1	A	307	GLN
1	A	341	ASN
1	A	405	HIS
1	B	52	ASN
1	B	71	GLN
1	B	94	ASN

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Mol	Chain	Res	Type
1	B	96	ASN
1	B	97	GLN
1	B	228	GLN
1	B	231	GLN
1	B	307	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

8 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	$\#\|Z\| > 2$
4	GOL	A	459	-	5,5,5	1.21	0	5,5,5	2.22	4 (80%)
4	GOL	B	459	-	5,5,5	0.38	0	5,5,5	0.27	0
3	PMP	B	456	-	16,16,16	0.86	1 (6%)	21,23,23	1.02	2 (9%)
2	GLN	A	456	-	8,9,9	1.95	1 (12%)	10,11,11	0.47	0
4	GOL	B	458	-	5,5,5	0.37	0	5,5,5	0.65	0
4	GOL	A	458	-	5,5,5	0.55	0	5,5,5	0.52	0
2	GLN	B	457	-	8,9,9	0.64	0	10,11,11	0.97	1 (10%)
3	PMP	A	457	-	16,16,16	0.94	1 (6%)	21,23,23	0.98	2 (9%)

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	A	459	-	-	4/4/4/4	-
4	GOL	B	459	-	-	0/4/4/4	-
3	PMP	B	456	-	-	1/8/8/8	0/1/1/1
2	GLN	A	456	-	-	2/9/9/9	-
4	GOL	B	458	-	-	2/4/4/4	-
4	GOL	A	458	-	-	2/4/4/4	-
2	GLN	B	457	-	-	2/9/9/9	-
3	PMP	A	457	-	-	0/8/8/8	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	456	GLN	OXT-C	-5.32	1.13	1.30
3	B	456	PMP	C2-N1	2.05	1.37	1.33
3	A	457	PMP	C2-N1	2.04	1.37	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	456	PMP	C6-C5-C4	3.08	120.30	118.12
4	A	459	GOL	O1-C1-C2	3.01	124.63	110.20
4	A	459	GOL	O3-C3-C2	2.61	122.72	110.20
3	A	457	PMP	C6-C5-C4	2.49	119.88	118.12
2	B	457	GLN	OXT-C-CA	2.31	121.25	113.38
4	A	459	GOL	O2-C2-C1	-2.15	99.65	109.12
3	A	457	PMP	C5-C6-N1	-2.07	120.36	123.82
3	B	456	PMP	C5-C6-N1	-2.06	120.39	123.82
4	A	459	GOL	O2-C2-C3	-2.01	100.25	109.12

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	457	GLN	N-CA-CB-CG
2	B	457	GLN	C-CA-CB-CG
4	A	458	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	A	458	GOL	O2-C2-C3-O3
4	A	459	GOL	O1-C1-C2-C3
4	A	459	GOL	C1-C2-C3-O3
4	A	459	GOL	O2-C2-C3-O3
2	A	456	GLN	CA-CB-CG-CD
4	B	458	GOL	O1-C1-C2-C3
4	A	459	GOL	O1-C1-C2-O2
4	B	458	GOL	O1-C1-C2-O2
3	B	456	PMP	C5-C4-C4A-N4A
2	A	456	GLN	OXT-C-CA-N

There are no ring outliers.

8 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	459	GOL	11	0
4	B	459	GOL	4	0
3	B	456	PMP	4	0
2	A	456	GLN	5	0
4	B	458	GOL	1	0
4	A	458	GOL	1	0
2	B	457	GLN	3	0
3	A	457	PMP	7	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

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	410/410 (100%)	-0.13	17 (4%)	37	40	15, 22, 47, 70	0
1	B	410/410 (100%)	-0.00	25 (6%)	21	23	15, 25, 59, 88	0
All	All	820/820 (100%)	-0.07	42 (5%)	28	30	15, 24, 54, 88	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	386	SER	8.4
1	B	64	PRO	7.2
1	B	61	ALA	6.9
1	B	387	ASP	6.2
1	B	385	LEU	5.9
1	B	389	ASN	5.9
1	A	61	ALA	5.9
1	B	62	ALA	5.7
1	B	384	ASP	5.5
1	A	60	LEU	4.8
1	B	391	ASP	4.7
1	B	58	THR	4.5
1	B	187	MET	4.2
1	A	386	SER	4.1
1	B	388	MET	4.0
1	A	62	ALA	3.9
1	A	384	ASP	3.8
1	A	382	GLY	3.7
1	B	60	LEU	3.5
1	A	387	ASP	3.4
1	B	390	SER	3.3
1	B	382	GLY	3.2
1	A	58	THR	3.0
1	A	451	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	185	ASP	2.9
1	B	334	ASP	2.9
1	A	383	ALA	2.8
1	A	187	MET	2.7
1	B	56	GLU	2.7
1	A	55	VAL	2.7
1	B	383	ALA	2.6
1	A	59	LYS	2.5
1	A	64	PRO	2.4
1	B	449	ALA	2.4
1	B	451	ASN	2.4
1	B	65	SER	2.3
1	A	405	HIS	2.3
1	B	63	ASP	2.2
1	A	185	ASP	2.2
1	B	448	ARG	2.1
1	B	405	HIS	2.1
1	A	276	ILE	2.0

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

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

6.3 Carbohydrates (i)

There are no 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, 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
4	GOL	B	459	6/6	0.66	0.21	20,20,20,20	0
4	GOL	A	458	6/6	0.67	0.20	20,20,20,20	0
2	GLN	B	457	10/10	0.78	0.25	21,26,28,29	0
2	GLN	A	456	10/10	0.80	0.25	16,22,31,33	0
4	GOL	B	458	6/6	0.90	0.15	39,45,48,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GOL	A	459	6/6	0.92	0.19	16,25,28,31	0
3	PMP	A	457	16/16	0.96	0.16	20,24,26,31	0
3	PMP	B	456	16/16	0.97	0.11	21,22,24,27	0

6.5 Other polymers (i)

There are no such residues in this entry.