Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:52 PM GMT

PDB ID	:	1HOZ
Title	:	CRYSTAL STRUCTURE OF AN INOSINE-ADENOSINE-GUANOSINE-PREFERRING NUCLEOSIDE HYDROLASE FROM TRYPANOSOMA VIVAX
Authors	:	Versees, W.; Decanniere, K.; Pelle, R.; Depoorter, J.; Parkin, D.W.; Steyaert, J.
Deposited on	:	2000-12-12
Resolution	:	1.60 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

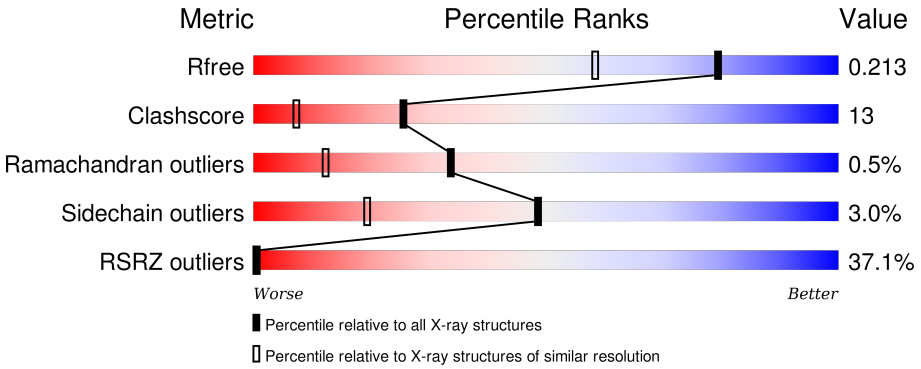
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 1.60 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}	91344	2475 (1.60-1.60)
Clashscore	102246	2732 (1.60-1.60)
Ramachandran outliers	100387	2654 (1.60-1.60)
Sidechain outliers	100360	2653 (1.60-1.60)
RSRZ outliers	91569	2479 (1.60-1.60)

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. 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	339	17% 79% 13% • 7%
1	B	339	52% 78% 13% •• 7%

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	GOL	A	1268	-	-	-	X
3	GOL	A	1271	-	-	-	X
3	GOL	A	1272	-	-	-	X
3	GOL	A	1274	-	-	-	X
3	GOL	B	1269	-	-	-	X
3	GOL	B	1270	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5465 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 INOSINE-ADENOSINE-GUANOSINE-PREFERRING NUCLEOSIDE HYDROLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	316	Total	C	N	O	S	0	20	0
			2498	1595	403	475	25			
1	B	315	Total	C	N	O	S	0	18	0
			2493	1592	405	471	25			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	MET	-	EXPRESSION TAG	UNP Q9GPQ4
A	-11	ARG	-	EXPRESSION TAG	UNP Q9GPQ4
A	-10	GLY	-	EXPRESSION TAG	UNP Q9GPQ4
A	-9	SER	-	EXPRESSION TAG	UNP Q9GPQ4
A	-8	PRO	-	EXPRESSION TAG	UNP Q9GPQ4
A	-7	HIS	-	EXPRESSION TAG	UNP Q9GPQ4
A	-6	HIS	-	EXPRESSION TAG	UNP Q9GPQ4
A	-5	HIS	-	EXPRESSION TAG	UNP Q9GPQ4
A	-4	HIS	-	EXPRESSION TAG	UNP Q9GPQ4
A	-3	HIS	-	EXPRESSION TAG	UNP Q9GPQ4
A	-2	HIS	-	EXPRESSION TAG	UNP Q9GPQ4
A	-1	GLY	-	EXPRESSION TAG	UNP Q9GPQ4
A	0	SER	-	EXPRESSION TAG	UNP Q9GPQ4
A	301	ASN	LYS	SEE REMARK 999	UNP Q9GPQ4
B	-12	MET	-	EXPRESSION TAG	UNP Q9GPQ4
B	-11	ARG	-	EXPRESSION TAG	UNP Q9GPQ4
B	-10	GLY	-	EXPRESSION TAG	UNP Q9GPQ4
B	-9	SER	-	EXPRESSION TAG	UNP Q9GPQ4
B	-8	PRO	-	EXPRESSION TAG	UNP Q9GPQ4
B	-7	HIS	-	EXPRESSION TAG	UNP Q9GPQ4
B	-6	HIS	-	EXPRESSION TAG	UNP Q9GPQ4
B	-5	HIS	-	EXPRESSION TAG	UNP Q9GPQ4
B	-4	HIS	-	EXPRESSION TAG	UNP Q9GPQ4
B	-3	HIS	-	EXPRESSION TAG	UNP Q9GPQ4

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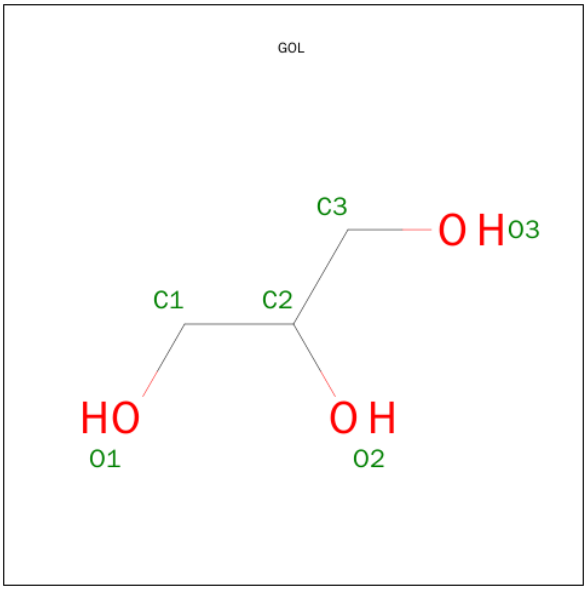
Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	HIS	-	EXPRESSION TAG	UNP Q9GPQ4
B	-1	GLY	-	EXPRESSION TAG	UNP Q9GPQ4
B	0	SER	-	EXPRESSION TAG	UNP Q9GPQ4
B	301	ASN	LYS	SEE REMARK 999	UNP Q9GPQ4

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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

- Molecule 4 is water.

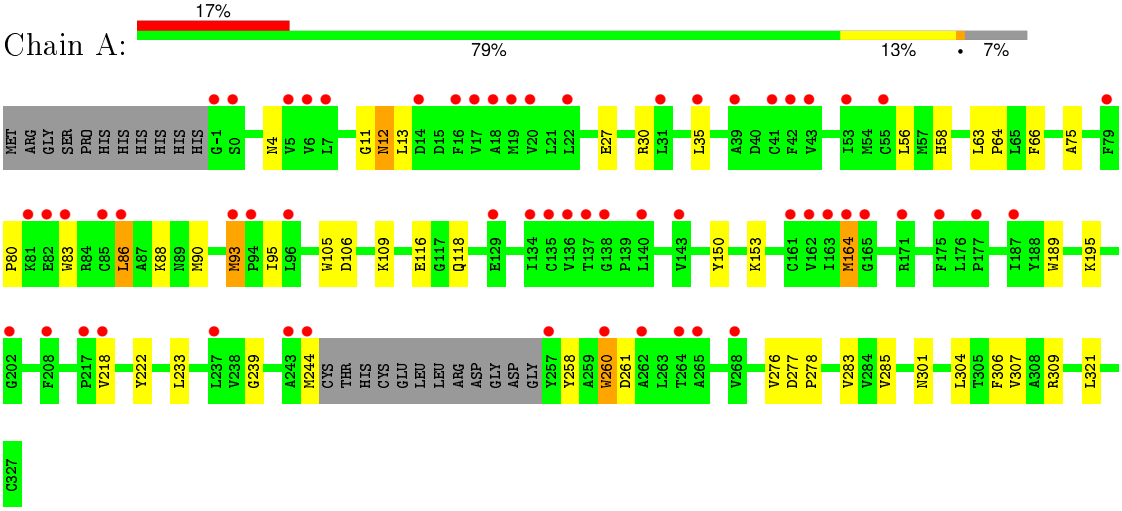
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	214	Total O 214 214	0	0
4	B	210	Total O 210 210	0	0

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 errors 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.

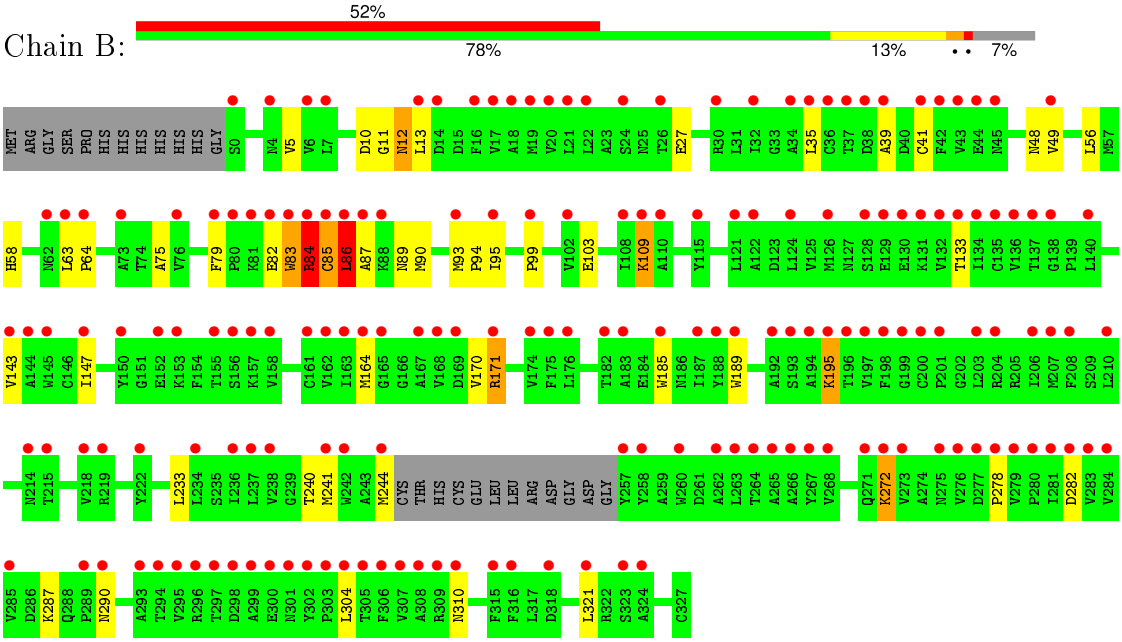
• Molecule 1: INOSINE-ADENOSINE-GUANOSINE-PREFERRING NUCLEOSIDE HYDROLASE

Chain A:



• Molecule 1: INOSINE-ADENOSINE-GUANOSINE-PREFERRING NUCLEOSIDE HYDROLASE

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	52.09Å 74.00Å 82.00Å 90.00° 104.56° 90.00°	Depositor
Resolution (Å)	30.00 – 1.60 29.83 – 1.60	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-1.60) 99.8 (29.83-1.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.44 (at 1.60Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.186 , 0.210 0.195 , 0.213	Depositor DCC
R_{free} test set	3988 reflections (5.03%)	DCC
Wilson B-factor (Å^2)	33.4	Xtriage
Anisotropy	0.293	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 47.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Outliers	0 of 79329 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	5465	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.67% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, CA

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	0.48	0/2635	0.73	1/3590 (0.0%)
1	B	0.53	1/2620 (0.0%)	0.76	3/3568 (0.1%)
All	All	0.50	1/5255 (0.0%)	0.75	4/7158 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	85	CYS	CB-SG	-13.13	1.59	1.82

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	84	ARG	NE-CZ-NH2	-10.55	115.03	120.30
1	B	84	ARG	NE-CZ-NH1	6.41	123.51	120.30
1	B	84	ARG	N-CA-C	6.32	128.05	111.00
1	A	11	GLY	N-CA-C	5.23	126.17	113.10

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	2498	0	2441	59	3

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2493	0	2440	70	2
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	36	0	48	3	0
3	B	12	0	16	0	0
4	A	214	0	0	2	3
4	B	210	0	0	10	4
All	All	5465	0	4945	126	6

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 13.

All (126) 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:12[A]:ASN:ND2	1:B:86:LEU:HD13	1.68	1.07
1:A:13:LEU:HD21	1:A:86:LEU:HG	1.30	1.07
1:B:12[A]:ASN:HD21	1:B:86:LEU:HD13	1.13	1.06
1:A:276[A]:VAL:HG11	1:A:306:PHE:HB3	1.42	1.00
1:A:93[A]:MET:HE2	1:A:95:ILE:H	1.29	0.98
1:B:171:ARG:H	1:B:171:ARG:HD2	1.27	0.95
1:A:13:LEU:HD21	1:A:86:LEU:CG	2.03	0.88
1:B:93[B]:MET:SD	1:B:95:ILE:HG22	2.17	0.85
1:A:93[A]:MET:SD	1:A:95:ILE:HG22	2.18	0.83
1:A:276[A]:VAL:CG1	1:A:306:PHE:HB3	2.10	0.81
1:A:276[A]:VAL:HG11	1:A:306:PHE:CB	2.11	0.80
1:A:56[A]:LEU:HD11	1:A:233:LEU:HD13	1.66	0.77
1:B:133[A]:THR:HG21	4:B:1305:HOH:O	1.85	0.74
1:B:5:VAL:HG22	1:B:133[A]:THR:OG1	1.90	0.72
1:B:171:ARG:H	1:B:171:ARG:CD	1.98	0.71
1:A:12:ASN:HD22	1:A:13:LEU:H	1.36	0.70
1:B:195[A]:LYS:HE3	1:B:282:ASP:OD1	1.92	0.70
1:B:143:VAL:O	1:B:147[B]:ILE:HG12	1.93	0.68
1:B:12[A]:ASN:ND2	1:B:13:LEU:H	1.92	0.67
1:B:83:TRP:O	1:B:86:LEU:HD12	1.95	0.67
1:B:99[A]:PRO:HG2	4:B:1294:HOH:O	1.94	0.66
1:B:272:LYS:O	1:B:272:LYS:HD3	1.96	0.66
1:B:287:LYS:HE3	4:B:1416:HOH:O	1.94	0.66
1:B:12[B]:ASN:ND2	1:B:86:LEU:HD13	2.11	0.64
1:A:195[A]:LYS:NZ	1:A:285:VAL:HG13	2.14	0.63
1:B:12[B]:ASN:HD21	1:B:86:LEU:HD13	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:GLU:H	1:B:82:GLU:CD	2.01	0.62
1:A:12:ASN:ND2	1:A:13:LEU:HD23	2.14	0.62
1:A:13:LEU:H	1:A:13:LEU:HD22	1.65	0.62
1:A:276[A]:VAL:CG1	1:A:306:PHE:C	2.68	0.61
1:A:13:LEU:HD22	1:A:13:LEU:N	2.14	0.61
1:B:170:VAL:HA	1:B:171:ARG:NH1	2.15	0.61
1:A:13:LEU:HD13	1:A:90[B]:MET:SD	2.40	0.61
1:A:58:HIS:HD2	1:A:63:LEU:O	1.84	0.61
1:A:164[B]:MET:SD	1:A:260:TRP:HB3	2.41	0.60
1:B:171:ARG:N	1:B:171:ARG:HD2	2.08	0.59
1:A:13:LEU:CD2	1:A:86:LEU:HG	2.21	0.59
1:A:12:ASN:ND2	1:A:13:LEU:H	2.01	0.58
1:A:164[B]:MET:HG2	1:A:261:ASP:OD1	2.03	0.58
1:B:321[B]:LEU:HD23	4:B:1441:HOH:O	2.02	0.58
1:B:241:MET:HA	1:B:244:MET:HE2	1.84	0.58
1:B:64[B]:PRO:HG2	4:B:1293:HOH:O	2.02	0.58
1:B:84:ARG:NH1	4:B:1396:HOH:O	2.27	0.58
1:B:240:THR:HG22	1:B:244:MET:HE1	1.87	0.56
1:A:88:LYS:O	1:A:88:LYS:HD3	2.05	0.56
1:B:49:VAL:HG11	1:B:90[A]:MET:HE2	1.88	0.56
1:B:48:ASN:OD1	1:B:109:LYS:HE3	2.05	0.55
1:A:75:ALA:HB2	1:A:189:TRP:CZ2	2.42	0.55
1:B:75:ALA:HB2	1:B:189:TRP:CE2	2.43	0.54
1:A:13:LEU:CD2	1:A:13:LEU:H	2.21	0.54
1:A:222:TYR:CZ	1:A:321:LEU:CD2	2.91	0.54
1:B:12[A]:ASN:HD22	1:B:13:LEU:H	1.53	0.54
1:A:222:TYR:OH	1:A:321:LEU:HD23	2.08	0.54
1:A:239:GLY:HA3	1:B:94[A]:PRO:HG3	1.89	0.53
1:B:240:THR:O	1:B:244:MET:HE2	2.08	0.53
1:B:133[A]:THR:HG23	4:B:1300:HOH:O	2.07	0.53
1:A:13:LEU:HD13	1:A:90[B]:MET:CE	2.40	0.52
1:B:41:CYS:HB2	4:B:1421:HOH:O	2.09	0.52
1:A:218:VAL:HG23	1:A:218:VAL:O	2.10	0.52
4:A:1298:HOH:O	1:B:94[A]:PRO:HG3	2.10	0.51
1:A:222:TYR:CE1	1:A:321:LEU:HD23	2.45	0.51
1:B:58:HIS:HD2	1:B:63:LEU:O	1.94	0.51
1:B:278:PRO:HB2	1:B:304:LEU:HD13	1.92	0.51
1:B:85:CYS:O	1:B:87:ALA:N	2.43	0.51
1:A:195[A]:LYS:NZ	1:A:283:VAL:O	2.43	0.51
1:A:239:GLY:HA3	1:B:94[A]:PRO:CG	2.41	0.51
1:B:79:PHE:CE2	1:B:185:TRP:HB3	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:ILE:HD11	1:B:233:LEU:CD2	2.40	0.51
1:A:222:TYR:CE1	1:A:321:LEU:CD2	2.93	0.51
1:A:13:LEU:HD21	1:A:86:LEU:CB	2.40	0.50
1:B:171:ARG:HH11	1:B:171:ARG:N	2.08	0.50
1:A:64[A]:PRO:HB2	3:A:1271:GOL:H2	1.94	0.50
1:A:195[A]:LYS:HZ2	1:A:285:VAL:HG13	1.76	0.50
1:A:80:PRO:HD2	1:A:83:TRP:CE3	2.47	0.50
1:B:241:MET:HA	1:B:244:MET:CE	2.41	0.49
1:A:276[A]:VAL:HG13	1:A:307:VAL:C	2.33	0.49
1:A:12:ASN:ND2	1:A:13:LEU:CD2	2.76	0.49
1:B:310:ASN:N	1:B:310:ASN:ND2	2.61	0.49
1:A:222:TYR:OH	1:A:321:LEU:CD2	2.61	0.48
1:B:13:LEU:HG	1:B:86:LEU:HD22	1.96	0.48
1:A:276[A]:VAL:HG11	1:A:306:PHE:C	2.33	0.48
1:A:276[A]:VAL:HG12	1:A:277:ASP:N	2.29	0.48
1:B:310:ASN:HD22	1:B:310:ASN:N	2.11	0.48
1:B:95:ILE:HD11	1:B:233:LEU:HD22	1.96	0.47
1:B:75:ALA:HB2	1:B:189:TRP:CZ2	2.50	0.47
1:B:12[B]:ASN:HD22	1:B:13:LEU:H	1.62	0.46
1:B:310:ASN:HD22	1:B:310:ASN:H	1.63	0.46
1:B:27:GLU:HG3	4:B:1436:HOH:O	2.15	0.46
1:A:75:ALA:HB2	1:A:189:TRP:CE2	2.51	0.46
1:B:83:TRP:O	1:B:86:LEU:CD1	2.63	0.46
1:A:64[B]:PRO:HG2	4:A:1316:HOH:O	2.16	0.46
1:B:12[B]:ASN:ND2	1:B:13:LEU:H	2.13	0.45
1:A:258:TYR:CD1	1:A:258:TYR:N	2.84	0.45
1:A:150:TYR:O	1:A:153:LYS:HE3	2.17	0.45
1:A:195[A]:LYS:HZ3	1:A:285:VAL:HG13	1.81	0.45
1:B:10:ASP:O	1:B:41:CYS:HB3	2.16	0.45
1:B:11:GLY:O	1:B:87:ALA:HB2	2.16	0.45
1:B:12[A]:ASN:HD21	1:B:86:LEU:CD1	2.04	0.45
1:A:222:TYR:CZ	1:A:321:LEU:HD23	2.51	0.45
1:B:39:ALA:HB1	1:B:79:PHE:CE1	2.52	0.45
1:A:93[A]:MET:CE	1:A:95:ILE:H	2.13	0.44
1:B:13:LEU:HD23	1:B:90[A]:MET:SD	2.57	0.44
1:B:56:LEU:HD23	1:B:56:LEU:C	2.39	0.44
1:A:13:LEU:CD2	1:A:13:LEU:N	2.80	0.43
1:B:84:ARG:NH1	4:B:1307:HOH:O	2.50	0.43
1:A:66:PHE:HB3	3:A:1271:GOL:H31	2.01	0.43
1:A:88:LYS:C	1:A:88:LYS:HD3	2.39	0.42
1:B:41:CYS:HA	1:B:84:ARG:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12[A]:ASN:HD22	1:B:13:LEU:N	2.16	0.42
1:B:171:ARG:HH11	1:B:171:ARG:H	1.67	0.41
1:A:244:MET:CB	1:B:89:ASN:HB3	2.49	0.41
1:A:27:GLU:HG3	3:A:1272:GOL:H11	2.01	0.41
1:B:49:VAL:CG1	1:B:90[A]:MET:HE2	2.51	0.41
1:A:222:TYR:CE1	1:A:321:LEU:HD21	2.55	0.41
1:A:4:ASN:OD1	1:A:30:ARG:HD2	2.20	0.41
1:A:116[B]:GLU:OE2	1:A:118:GLN:HB2	2.21	0.40
1:A:86:LEU:HA	1:A:86:LEU:HD13	1.85	0.40
1:B:12[A]:ASN:ND2	1:B:13:LEU:N	2.65	0.40
1:A:278:PRO:HB2	1:A:304:LEU:HD13	2.03	0.40
1:B:90[A]:MET:CE	1:B:241:MET:SD	3.09	0.40

All (6) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:ASN:OD1	4:B:1375:HOH:O[1_454]	1.55	0.65
4:A:1482:HOH:O	4:B:1478:HOH:O[1_454]	1.96	0.24
1:B:195[A]:LYS:NZ	4:A:1393:HOH:O[1_656]	1.97	0.23
1:A:106:ASP:OD2	1:B:290:ASN:ND2[2_656]	2.02	0.18
1:A:105:TRP:CD1	4:B:1364:HOH:O[2_656]	2.12	0.08
4:A:1321:HOH:O	4:B:1286:HOH:O[2_656]	2.14	0.06

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	332/339 (98%)	325 (98%)	6 (2%)	1 (0%)	46 23
1	B	329/339 (97%)	316 (96%)	11 (3%)	2 (1%)	30 9
All	All	661/678 (98%)	641 (97%)	17 (3%)	3 (0%)	34 12

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	84	ARG
1	B	86	LEU
1	A	260	TRP

5.3.2 Protein sidechains

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	283/290 (98%)	274 (97%)	9 (3%)	46 18
1	B	280/290 (97%)	269 (96%)	11 (4%)	39 13
All	All	563/580 (97%)	543 (96%)	20 (4%)	48 15

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	35	LEU
1	A	86	LEU
1	A	93[A]	MET
1	A	93[B]	MET
1	A	109	LYS
1	A	164[A]	MET
1	A	164[B]	MET
1	A	309	ARG
1	B	12[A]	ASN
1	B	12[B]	ASN
1	B	35	LEU
1	B	83	TRP
1	B	86	LEU
1	B	109	LYS
1	B	164	MET
1	B	171	ARG
1	B	195[A]	LYS
1	B	195[B]	LYS
1	B	272	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	58	HIS
1	A	89	ASN
1	A	119	GLN
1	A	224	GLN
1	A	275	ASN
1	B	45	ASN
1	B	58	HIS
1	B	119	GLN
1	B	224	GLN
1	B	288	GLN
1	B	310	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 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	$\#\|Z\| > 2$
3	GOL	A	1267	2	5,5,5	0.57	0	5,5,5	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	GOL	A	1268	-	5,5,5	0.92	0	5,5,5	1.05	0
3	GOL	A	1271	-	5,5,5	0.93	0	5,5,5	0.86	0
3	GOL	A	1272	-	5,5,5	0.74	0	5,5,5	0.87	0
3	GOL	A	1273	-	5,5,5	0.60	0	5,5,5	0.63	0
3	GOL	A	1274	-	5,5,5	0.76	0	5,5,5	0.87	0
3	GOL	B	1269	-	5,5,5	0.74	0	5,5,5	0.93	0
3	GOL	B	1270	-	5,5,5	0.58	0	5,5,5	1.02	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
3	GOL	A	1267	2	-	0/4/4/4	0/0/0/0
3	GOL	A	1268	-	-	0/4/4/4	0/0/0/0
3	GOL	A	1271	-	-	0/4/4/4	0/0/0/0
3	GOL	A	1272	-	-	0/4/4/4	0/0/0/0
3	GOL	A	1273	-	-	0/4/4/4	0/0/0/0
3	GOL	A	1274	-	-	0/4/4/4	0/0/0/0
3	GOL	B	1269	-	-	0/4/4/4	0/0/0/0
3	GOL	B	1270	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1271	GOL	2	0
3	A	1272	GOL	1	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	316/339 (93%)	1.13	59 (18%)	2	1	28, 34, 49, 60	0
1	B	315/339 (92%)	2.36	175 (55%)	0	0	28, 34, 50, 71	0
All	All	631/678 (93%)	1.74	234 (37%)	0	0	28, 34, 49, 71	0

All (234) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	85	CYS	13.9
1	A	85[A]	CYS	9.5
1	A	-1	GLY	9.2
1	B	84	ARG	7.8
1	B	83	TRP	7.6
1	B	80	PRO	7.5
1	B	86	LEU	7.4
1	B	88	LYS	6.6
1	B	0	SER	6.4
1	A	136	VAL	6.3
1	B	87	ALA	6.0
1	B	41	CYS	5.6
1	B	20	VAL	5.3
1	B	197	VAL	5.3
1	A	244	MET	5.2
1	B	275	ASN	5.1
1	A	257	TYR	5.0
1	B	203	LEU	5.0
1	B	79	PHE	4.9
1	A	163	ILE	4.8
1	A	41	CYS	4.8
1	B	136	VAL	4.8
1	B	135	CYS	4.7
1	B	218	VAL	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	83	TRP	4.7
1	B	81	LYS	4.6
1	B	258	TYR	4.6
1	B	162	VAL	4.6
1	A	7	LEU	4.6
1	B	168	VAL	4.5
1	B	42	PHE	4.5
1	B	283	VAL	4.5
1	A	134	ILE	4.4
1	B	198	PHE	4.4
1	B	110	ALA	4.4
1	A	137	THR	4.4
1	B	303[A]	PRO	4.4
1	A	177	PRO	4.3
1	B	278	PRO	4.3
1	B	307	VAL	4.3
1	B	17	VAL	4.3
1	B	161[A]	CYS	4.3
1	B	16	PHE	4.2
1	B	244	MET	4.1
1	A	86	LEU	4.1
1	B	208	PHE	4.1
1	B	145	TRP	4.1
1	A	17	VAL	4.1
1	A	164[A]	MET	4.0
1	B	306	PHE	4.0
1	B	315	PHE	4.0
1	B	130	GLU	3.9
1	A	161[A]	CYS	3.9
1	B	310	ASN	3.9
1	B	156	SER	3.9
1	B	134	ILE	3.8
1	A	22	LEU	3.8
1	A	175	PHE	3.8
1	B	39	ALA	3.7
1	B	201	PRO	3.7
1	A	217	PRO	3.7
1	B	304	LEU	3.6
1	B	206	ILE	3.6
1	B	265	ALA	3.6
1	A	135	CYS	3.6
1	B	18	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	279	VAL	3.6
1	B	185	TRP	3.6
1	B	140	LEU	3.6
1	B	268	VAL	3.6
1	B	284	VAL	3.6
1	B	200	CYS	3.6
1	B	260	TRP	3.6
1	B	272	LYS	3.5
1	B	301	ASN	3.5
1	B	276	VAL	3.5
1	B	158	VAL	3.4
1	A	82	GLU	3.4
1	B	7	LEU	3.4
1	A	18	ALA	3.4
1	A	20	VAL	3.3
1	B	35	LEU	3.3
1	B	163	ILE	3.3
1	A	42	PHE	3.3
1	A	79	PHE	3.3
1	B	164	MET	3.2
1	B	285	VAL	3.2
1	B	298	ASP	3.2
1	B	143	VAL	3.2
1	B	171	ARG	3.2
1	B	242	TRP	3.2
1	B	281	ILE	3.2
1	A	162	VAL	3.1
1	B	30[A]	ARG	3.1
1	B	305	THR	3.1
1	B	128[A]	SER	3.1
1	B	133[A]	THR	3.1
1	A	6	VAL	3.1
1	B	219	ARG	3.1
1	B	299	ALA	3.1
1	A	218	VAL	3.1
1	A	0	SER	3.0
1	B	43	VAL	3.0
1	B	62	ASN	3.0
1	A	138	GLY	2.9
1	B	277	ASP	2.9
1	B	267	TYR	2.9
1	B	115	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	43	VAL	2.9
1	B	308	ALA	2.9
1	B	126	MET	2.9
1	B	155	THR	2.9
1	A	165	GLY	2.9
1	A	262	ALA	2.9
1	B	147[A]	ILE	2.9
1	B	192	ALA	2.9
1	B	300	GLU	2.9
1	B	122	ALA	2.8
1	B	297	THR	2.8
1	B	257	TYR	2.8
1	B	63	LEU	2.8
1	B	73	ALA	2.8
1	B	264	THR	2.8
1	B	21	LEU	2.8
1	B	293	ALA	2.8
1	B	309	ARG	2.8
1	B	14[A]	ASP	2.8
1	A	93[A]	MET	2.8
1	B	36[A]	CYS	2.8
1	B	187	ILE	2.7
1	B	199	GLY	2.7
1	B	290	ASN	2.7
1	A	96	LEU	2.7
1	A	208	PHE	2.7
1	B	182	THR	2.7
1	A	5	VAL	2.7
1	B	273	VAL	2.7
1	B	289	PRO	2.7
1	B	26	THR	2.7
1	B	196	THR	2.7
1	A	81	LYS	2.7
1	A	140	LEU	2.6
1	A	16	PHE	2.6
1	B	316	PHE	2.6
1	B	222	TYR	2.6
1	A	31	LEU	2.6
1	A	171	ARG	2.6
1	A	264	THR	2.6
1	B	137	THR	2.6
1	B	215	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	157	LYS	2.6
1	B	236	ILE	2.6
1	B	294	THR	2.5
1	A	143	VAL	2.5
1	A	187	ILE	2.5
1	B	32	ILE	2.5
1	B	22	LEU	2.5
1	B	296	ARG	2.5
1	B	99[A]	PRO	2.5
1	B	175	PHE	2.5
1	B	210	LEU	2.5
1	B	302	TYR	2.5
1	B	45	ASN	2.5
1	B	6	VAL	2.5
1	B	282	ASP	2.5
1	A	260	TRP	2.5
1	B	152[A]	GLU	2.5
1	B	13	LEU	2.5
1	A	265	ALA	2.5
1	B	44	GLU	2.5
1	B	237	LEU	2.5
1	B	188	TYR	2.4
1	B	194	ALA	2.5
1	A	19	MET	2.4
1	A	55	CYS	2.4
1	B	321[A]	LEU	2.4
1	B	280	PRO	2.4
1	A	268	VAL	2.4
1	B	4	ASN	2.4
1	B	176	LEU	2.4
1	B	204	ARG	2.4
1	A	243	ALA	2.4
1	B	102	VAL	2.4
1	B	195[A]	LYS	2.4
1	B	266	ALA	2.4
1	A	14	ASP	2.4
1	B	138	GLY	2.4
1	B	193	SER	2.4
1	B	318[A]	ASP	2.3
1	A	202	GLY	2.3
1	B	174	VAL	2.3
1	B	295	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	183	ALA	2.3
1	B	153	LYS	2.3
1	B	108	ILE	2.3
1	B	262	ALA	2.3
1	B	323	SER	2.3
1	A	39	ALA	2.3
1	B	129	GLU	2.3
1	B	150	TYR	2.3
1	B	238	VAL	2.3
1	B	271	GLN	2.3
1	B	214	ASN	2.2
1	B	64[A]	PRO	2.2
1	B	132	VAL	2.2
1	B	109	LYS	2.2
1	B	189	TRP	2.2
1	B	76	VAL	2.2
1	A	53	ILE	2.2
1	B	37	THR	2.1
1	B	19	MET	2.1
1	B	93[A]	MET	2.1
1	B	234	LEU	2.1
1	B	144	ALA	2.1
1	B	167	ALA	2.1
1	B	95	ILE	2.1
1	B	131	LYS	2.1
1	B	169	ASP	2.1
1	A	129	GLU	2.1
1	B	24	SER	2.1
1	B	165	GLY	2.1
1	B	49	VAL	2.1
1	B	121	LEU	2.1
1	B	124	LEU	2.1
1	B	34	ALA	2.0
1	B	38	ASP	2.0
1	B	207	MET	2.0
1	B	241	MET	2.0
1	B	324	ALA	2.0
1	B	82	GLU	2.0
1	A	35	LEU	2.0
1	A	94[A]	PRO	2.0
1	A	237	LEU	2.0
1	B	263	LEU	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 (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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
3	GOL	A	1268	6/6	0.60	0.24	6.40	44,56,59,60	0
3	GOL	A	1271	6/6	0.84	0.35	5.85	52,55,57,59	0
3	GOL	B	1270	6/6	0.65	0.36	5.82	49,55,56,61	0
3	GOL	A	1274	6/6	0.69	0.21	3.36	56,56,57,58	0
3	GOL	B	1269	6/6	0.39	0.43	3.23	45,54,56,57	0
3	GOL	A	1272	6/6	0.78	0.18	2.60	57,58,59,60	0
3	GOL	A	1273	6/6	0.62	0.21	0.38	44,53,55,56	0
3	GOL	A	1267	6/6	0.85	0.18	-0.16	38,46,47,49	0
2	CA	A	328	1/1	0.96	0.13	-1.55	29,29,29,29	0
2	CA	B	328	1/1	0.86	0.12	-3.49	29,29,29,29	0

6.5 Other polymers (i)

There are no such residues in this entry.