

Full wwPDB X-ray Structure Validation Report (i)

Jan 29, 2024 - 01:38 PM EST

PDB ID	:	8TC7
Title	:	Human asparaginyl-tRNA synthetase, apo form
Authors	:	Dogovski, C.; Metcalfe, R.D.; Xie, S.C.; Morton, C.J.; Tilley, L.; Griffin,
		M.D.W.
Deposited on	:	2023-06-30
Resolution	:	1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) 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 (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 1.90 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.



Motric	Whole archive	Similar resolution
IVIETIC	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	А	453	87%	7%	6%
1	В	453	87%	8%	5%
1	С	453	8%	8%	6%
1	D	453	8%	8%	6%



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 15123 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.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	Λ	496	Total	С	Ν	0	\mathbf{S}	0	2	0
	A	420	3471	2215	593	637	26	0		
1	Р	420	Total	С	Ν	0	S	0	0 2	0
1		429	3488	2224	597	641	26	0		
1	C	C 499	Total	С	Ν	0	S	0	0	0
	420	3464	2210	590	638	26	0	0	U	
1 D	428	Total	С	Ν	0	S	0	0	0	
		3461	2207	591	637	26			0	

• Molecule 1 is a protein called Asparagine–tRNA ligase, cytoplasmic.

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	96	GLY	-	expression tag	UNP O43776
А	97	MET	-	expression tag	UNP O43776
В	96	GLY	-	expression tag	UNP O43776
В	97	MET	-	expression tag	UNP O43776
С	96	GLY	-	expression tag	UNP O43776
С	97	MET	-	expression tag	UNP O43776
D	96	GLY	-	expression tag	UNP O43776
D	97	MET	-	expression tag	UNP 043776

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





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
2	В	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
2	В	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
2	В	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
2	В	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
2	В	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
2	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
2	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0



Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
2	В	1	Total C O 6 3 3	0	0
2	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
2	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
2	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
2	D	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
2	D	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
2	D	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0

• Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	В	1	Total Cl 1 1	0	0
3	С	1	Total Cl 1 1	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	288	Total O 288 288	0	0
4	В	329	Total O 329 329	0	0
4	С	229	Total O 229 229	0	0
4	D	259	Total O 259 259	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: Asparagine–tRNA ligase, cytoplasmic









4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	113.49Å 127.19Å 163.16Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Bosolution(A)	46.58 - 1.90	Depositor
Resolution (A)	46.58 - 1.90	EDS
% Data completeness	99.7 (46.58-1.90)	Depositor
(in resolution range)	99.8 (46.58-1.90)	EDS
R_{merge}	0.10	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.34 (at 1.90 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
P. P.	0.180 , 0.217	Depositor
n, n_{free}	0.187 , 0.221	DCC
R_{free} test set	9081 reflections (4.90%)	wwPDB-VP
Wilson B-factor $(Å^2)$	28.9	Xtriage
Anisotropy	0.660	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.35 , 49.9	EDS
L-test for $twinning^2$	$ < L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	15123	wwPDB-VP
Average B, all atoms $(Å^2)$	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 40.40 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.7501e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, 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	Bo	nd lengths	Bond angles		
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.64	4/3555~(0.1%)	0.74	0/4810	
1	В	0.63	0/3572	0.76	0/4832	
1	С	0.57	1/3547~(0.0%)	0.71	0/4800	
1	D	0.61	0/3544	0.72	0/4795	
All	All	0.61	5/14218~(0.0%)	0.73	0/19237	

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms		Observed(Å)	Ideal(Å)
1	А	452	CYS	CB-SG	-5.71	1.72	1.81
1	А	483	GLU	CD-OE2	5.29	1.31	1.25
1	С	165	CYS	CB-SG	-5.28	1.73	1.81
1	А	483	GLU	CG-CD	5.22	1.59	1.51
1	А	165	CYS	CB-SG	-5.09	1.73	1.81

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	3471	0	3399	21	0
1	В	3488	0	3413	22	0



001000	iraca jien	r precedue	pagem			
Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	С	3464	0	3394	19	0
1	D	3461	0	3390	18	1
2	А	42	0	54	5	1
2	В	54	0	70	2	0
2	С	18	0	23	1	0
2	D	18	0	24	1	0
3	В	1	0	0	1	0
3	С	1	0	0	0	0
4	А	288	0	0	6	0
4	В	329	0	0	10	0
4	С	229	0	0	7	0
4	D	259	0	0	1	0
All	All	15123	0	13767	78	1

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 3.

All (78) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	$distance ({ m \AA})$	overlap (Å)
3:B:610:CL:CL	4:B:968:HOH:O	2.32	0.84
1:C:483:GLU:OE2	4:C:701:HOH:O	2.00	0.77
1:B:375:HIS:ND1	4:B:705:HOH:O	2.18	0.75
1:B:231:ASN:HB3	2:B:603:GOL:H32	1.70	0.72
1:D:219:LEU:HD13	1:D:221:ASN:HD22	1.58	0.67
1:B:192:LYS:O	4:B:701:HOH:O	2.14	0.66
1:D:143:ASN:ND2	1:D:166:GLN:OE1	2.29	0.65
1:C:143:ASN:OD1	1:C:166:GLN:NE2	2.30	0.65
1:B:298:GLN:OE1	4:B:702:HOH:O	2.16	0.62
1:D:138:ARG:NH2	1:D:140:GLN:OE1	2.34	0.61
2:D:603:GOL:O1	4:D:702:HOH:O	2.16	0.60
1:B:451[A]:ARG:NH2	4:B:714:HOH:O	2.37	0.57
1:A:501:TRP:CD1	1:D:548:PRO:HB3	2.40	0.57
1:B:539:TYR:CD1	1:B:548:PRO:HG2	2.41	0.55
1:A:109:LEU:N	4:A:714:HOH:O	2.40	0.55
1:C:433:GLU:HG2	4:C:770:HOH:O	2.05	0.55
1:B:298:GLN:HG2	1:B:321:TYR:O	2.08	0.54
1:A:455:ASP:HA	2:A:601:GOL:H2	1.90	0.53
1:A:456:SER:OG	4:A:703:HOH:O	2.19	0.53
1:B:116:LYS:NZ	4:B:720:HOH:O	2.41	0.53
2:A:602:GOL:H11	4:A:942:HOH:O	2.09	0.52



		Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:A:231:ASN:HB3	2:A:607:GOL:H12	1.91	0.52	
1:A:143:ASN:OD1	1:A:166:GLN:NE2	2.43	0.52	
1:C:439:ARG:HA	1:C:459:THR:O	2.10	0.52	
1:C:330:ARG:NH1	4:C:710:HOH:O	2.43	0.51	
1:C:375:HIS:HB2	4:C:884:HOH:O	2.10	0.51	
1:C:447:PHE:HB3	1:C:492:GLU:HG3	1.91	0.51	
1:B:143:ASN:OD1	1:B:166:GLN:NE2	2.44	0.50	
1:C:167:CYS:SG	4:C:910:HOH:O	2.57	0.50	
1:C:521:GLU:OE2	2:C:603:GOL:H31	2.10	0.50	
1:B:414:GLU:O	1:B:417:GLU:HG2	2.11	0.50	
1:A:539:TYR:CD1	1:A:548:PRO:HG2	2.47	0.50	
1:C:286:LYS:HE3	1:C:293:GLU:HG3	1.94	0.49	
1:C:425:ARG:NH1	4:C:707:HOH:O	2.37	0.49	
1:A:414:GLU:O	1:A:417:GLU:HG2	2.13	0.49	
1:A:290:PHE:CE1	1:D:543:VAL:HG22	2.47	0.49	
1:D:414:GLU:O	1:D:417:GLU:HG2	2.13	0.49	
1:D:439:ARG:HA	1:D:459:THR:O	2.12	0.49	
1:B:439:ARG:HA	1:B:459:THR:O	2.13	0.49	
1:D:113:LYS:HD3	1:D:123:TYR:HE2	1.78	0.48	
1:D:298:GLN:HG2	1:D:321:TYR:O	2.14	0.48	
1:A:439:ARG:HA	1:A:459:THR:O	2.13	0.48	
1:A:516:TYR:OH	4:A:701:HOH:O	2.13	0.47	
1:C:138:ARG:NH2	1:C:140:GLN:OE1	2.47	0.47	
1:A:433:GLU:HG2	4:A:795:HOH:O	2.15	0.46	
1:D:447:PHE:HA	1:D:491:ARG:HH21	1.80	0.45	
1:C:225:ASP:OD2	1:C:227:ASP:HB2	2.16	0.45	
1:D:349:ASP:O	1:D:353:ARG:HG3	2.17	0.45	
1:C:414:GLU:O	1:C:417:GLU:HG2	2.16	0.45	
1:B:543:VAL:HG23	4:B:767:HOH:O	2.16	0.45	
1:A:403:HIS:HB3	2:A:605:GOL:H12	1.99	0.44	
1:A:276:THR:HB	1:A:499:TYR:CZ	2.53	0.43	
1:A:168:TYR:CE2	2:A:602:GOL:H12	2.53	0.43	
1:B:270:PRO:HG3	1:B:300:SER:HB3	2.01	0.43	
1:C:434:PRO:HB3	1:C:466:MET:CE	2.48	0.43	
1:B:225:ASP:HB3	1:B:228:VAL:HG23	2.01	0.43	
1:A:548:PRO:HB3	1:D:501:TRP:CD1	2.53	0.42	
1:B:276:THR:HB	1:B:499:TYR:CZ	2.55	0.42	
1:B:548:PRO:HB3	1:C:501:TRP:CD1	2.54	0.42	
1:C:302:LEU:HD22	1:C:502:TYR:CE1	2.55	0.42	
1:D:539:TYR:CD1	1:D:548:PRO:HG2	2.55	0.41	
1:A:302:LEU:HD22	1:A:502:TYR:CE1	2.55	0.41	



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:332:LEU:HD23	1:B:542:PHE:CE1	2.55	0.41
1:B:345:LEU:H	1:B:345:LEU:HD23	1.85	0.41
1:B:192:LYS:HB3	4:B:701:HOH:O	2.20	0.41
1:B:195:PRO:HG3	2:B:605:GOL:H32	2.02	0.41
1:A:168:TYR:CZ	1:A:172:LEU:HD11	2.54	0.41
1:C:543:VAL:HG23	4:C:779:HOH:O	2.21	0.41
1:D:168:TYR:CZ	1:D:172:LEU:HD11	2.56	0.41
1:B:355:GLU:OE1	4:B:708:HOH:O	2.22	0.41
1:A:543:VAL:HG22	1:D:290:PHE:CZ	2.56	0.40
1:D:157:GLN:HG3	1:D:195:PRO:HD2	2.03	0.40
1:B:189:PRO:HD3	4:B:972:HOH:O	2.20	0.40
1:C:503:THR:HG22	1:C:507:LYS:HE3	2.03	0.40
1:A:409:ASP:O	4:A:704:HOH:O	2.22	0.40
1:A:276:THR:HB	1:A:499:TYR:OH	2.21	0.40
1:D:283:THR:O	1:D:323:ALA:HB3	2.22	0.40
1:D:383:PRO:HA	1:D:384:PRO:HD3	1.94	0.40

All (1) 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:D:142:LYS:NZ	2:A:607:GOL:O1[2_455]	2.13	0.07

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	Perce	ntiles
1	А	420/453~(93%)	410 (98%)	9 (2%)	1 (0%)	47	38
1	В	423/453~(93%)	414 (98%)	7 (2%)	2 (0%)	29	18
1	С	420/453~(93%)	414 (99%)	5 (1%)	1 (0%)	47	38
1	D	420/453~(93%)	410 (98%)	9 (2%)	1 (0%)	47	38



Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1683/1812~(93%)	1648 (98%)	30~(2%)	5~(0%)	41 31

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	324	GLU
1	А	469	VAL
1	С	469	VAL
1	D	469	VAL
1	В	469	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	А	380/398~(96%)	378~(100%)	2(0%)	88 89
1	В	381/398~(96%)	375~(98%)	6(2%)	62 60
1	С	380/398~(96%)	377~(99%)	3~(1%)	81 82
1	D	379/398~(95%)	373~(98%)	6(2%)	62 60
All	All	1520/1592~(96%)	1503~(99%)	17 (1%)	73 73

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	287	LEU
1	А	404	ASP
1	В	147	LEU
1	В	198	HIS
1	В	287	LEU
1	В	325	GLN
1	В	404	ASP
1	В	424	GLU
1	С	198	HIS
1	С	287	LEU



Continued from previous page...

Mol	Chain	Res	Type
1	С	404	ASP
1	D	138	ARG
1	D	182	TYR
1	D	219	LEU
1	D	287	LEU
1	D	330	ARG
1	D	404	ASP

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such side chains are listed below:

Mol	Chain	Res	Type
1	D	143	ASN
1	D	166	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 24 ligands modelled in this entry, 2 are monoatomic - leaving 22 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).



Mal	Turne	Chain	Dec	Tink	Bond lengths			E	Bond ang	gles
	Type	Ullalli	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
2	GOL	В	604	-	$5,\!5,\!5$	1.29	0	$5,\!5,\!5$	1.01	0
2	GOL	С	601	-	$5,\!5,\!5$	0.98	0	$5,\!5,\!5$	0.77	0
2	GOL	В	605	-	$5,\!5,\!5$	0.97	0	$5,\!5,\!5$	0.97	0
2	GOL	А	604	-	$5,\!5,\!5$	0.73	0	5,5,5	1.11	0
2	GOL	В	601	-	$5,\!5,\!5$	1.05	0	$5,\!5,\!5$	1.56	1 (20%)
2	GOL	С	602	-	$5,\!5,\!5$	0.81	0	$5,\!5,\!5$	1.01	0
2	GOL	А	601	-	$5,\!5,\!5$	0.65	0	$5,\!5,\!5$	1.40	1 (20%)
2	GOL	D	601	-	$5,\!5,\!5$	0.85	0	$5,\!5,\!5$	1.56	1 (20%)
2	GOL	А	603	-	5,5,5	1.40	1 (20%)	$5,\!5,\!5$	0.82	0
2	GOL	D	602	-	5,5,5	1.29	1 (20%)	$5,\!5,\!5$	1.32	1 (20%)
2	GOL	D	603	-	$5,\!5,\!5$	1.20	0	$5,\!5,\!5$	0.78	0
2	GOL	В	608	-	$5,\!5,\!5$	1.15	0	$5,\!5,\!5$	0.75	0
2	GOL	В	609	-	$5,\!5,\!5$	1.25	1 (20%)	$5,\!5,\!5$	1.05	0
2	GOL	В	606	-	$5,\!5,\!5$	1.58	1 (20%)	$5,\!5,\!5$	0.94	0
2	GOL	В	607	-	$5,\!5,\!5$	0.64	0	$5,\!5,\!5$	1.09	1 (20%)
2	GOL	А	606	-	$5,\!5,\!5$	2.53	2 (40%)	$5,\!5,\!5$	1.14	0
2	GOL	А	607	-	$5,\!5,\!5$	1.04	0	$5,\!5,\!5$	1.24	0
2	GOL	А	602	-	$5,\!5,\!5$	1.42	1 (20%)	$5,\!5,\!5$	0.83	0
2	GOL	А	605	-	$5,\!5,\!5$	0.99	0	$5,\!5,\!5$	1.01	0
2	GOL	С	603	-	$5,\!5,\!5$	1.79	2(40%)	$5,\!5,\!5$	2.02	2(40%)
2	GOL	В	602	-	$5,\!5,\!5$	1.17	1 (20%)	$5,\!5,\!5$	1.46	1 (20%)
2	GOL	В	603	-	5,5,5	1.13	0	5,5,5	1.13	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
2	GOL	В	604	-	-	1/4/4/4	-
2	GOL	С	601	-	-	0/4/4/4	-
2	GOL	В	605	-	-	2/4/4/4	-
2	GOL	А	604	-	-	0/4/4/4	-
2	GOL	В	601	-	-	2/4/4/4	-
2	GOL	С	602	-	-	0/4/4/4	-
2	GOL	А	601	-	-	3/4/4/4	-
2	GOL	D	601	-	-	0/4/4/4	-
2	GOL	А	603	-	-	2/4/4/4	-
2	GOL	D	602	-	-	2/4/4/4	-



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	D	603	-	-	0/4/4/4	-
2	GOL	В	608	-	-	2/4/4/4	-
2	GOL	В	609	-	-	4/4/4/4	-
2	GOL	В	606	-	-	2/4/4/4	-
2	GOL	В	607	-	-	2/4/4/4	-
2	GOL	А	606	-	-	2/4/4/4	-
2	GOL	А	607	-	-	0/4/4/4	-
2	GOL	А	602	-	-	2/4/4/4	-
2	GOL	А	605	-	-	0/4/4/4	-
2	GOL	С	603	-	-	0/4/4/4	-
2	GOL	В	602	-	-	0/4/4/4	-
2	GOL	В	603	-	-	2/4/4/4	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	А	606	GOL	O3-C3	4.43	1.61	1.42
2	А	606	GOL	C3-C2	3.19	1.64	1.51
2	В	606	GOL	C1-C2	3.15	1.64	1.51
2	С	603	GOL	O3-C3	-2.80	1.30	1.42
2	А	602	GOL	O2-C2	-2.70	1.35	1.43
2	А	603	GOL	O2-C2	-2.65	1.35	1.43
2	С	603	GOL	C3-C2	2.54	1.62	1.51
2	В	609	GOL	C1-C2	2.26	1.61	1.51
2	В	602	GOL	O3-C3	-2.15	1.33	1.42
2	D	602	GOL	O2-C2	-2.09	1.37	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
2	С	603	GOL	C3-C2-C1	-3.74	97.14	111.70
2	В	602	GOL	C3-C2-C1	-2.51	101.93	111.70
2	D	602	GOL	C3-C2-C1	-2.41	102.33	111.70
2	А	601	GOL	O2-C2-C3	2.27	119.14	109.12
2	В	601	GOL	O1-C1-C2	-2.24	99.47	110.20
2	D	601	GOL	O3-C3-C2	-2.20	99.67	110.20
2	В	607	GOL	C3-C2-C1	-2.11	103.48	111.70
2	С	603	GOL	O1-C1-C2	2.00	119.80	110.20

There are no chirality outliers.



Mol	Chain	Res	Type	Atoms
2	А	601	GOL	O1-C1-C2-O2
2	А	603	GOL	C1-C2-C3-O3
2	В	601	GOL	O1-C1-C2-O2
2	В	601	GOL	O1-C1-C2-C3
2	В	605	GOL	C1-C2-C3-O3
2	В	608	GOL	C1-C2-C3-O3
2	В	609	GOL	O1-C1-C2-C3
2	В	609	GOL	C1-C2-C3-O3
2	D	602	GOL	C1-C2-C3-O3
2	В	606	GOL	O2-C2-C3-O3
2	В	609	GOL	O2-C2-C3-O3
2	D	602	GOL	O2-C2-C3-O3
2	А	601	GOL	O1-C1-C2-C3
2	А	602	GOL	O1-C1-C2-C3
2	А	606	GOL	O1-C1-C2-C3
2	В	603	GOL	C1-C2-C3-O3
2	В	606	GOL	C1-C2-C3-O3
2	А	601	GOL	O2-C2-C3-O3
2	А	603	GOL	O2-C2-C3-O3
2	В	608	GOL	O2-C2-C3-O3
2	А	602	GOL	O1-C1-C2-O2
2	В	605	GOL	O2-C2-C3-O3
2	В	603	GOL	O2-C2-C3-O3
2	В	609	GOL	O1-C1-C2-O2
2	А	606	GOL	O2-C2-C3-O3
2	В	604	GOL	C1-C2-C3-O3
2	В	607	GOL	O2-C2-C3-O3
2	В	607	GOL	C1-C2-C3-O3

All (28) torsion outliers are listed below:

There are no ring outliers.

8 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	В	605	GOL	1	0
2	А	601	GOL	1	0
2	D	603	GOL	1	0
2	А	607	GOL	1	1
2	А	602	GOL	2	0
2	А	605	GOL	1	0
2	С	603	GOL	1	0
2	В	603	GOL	1	0



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	А	426/453~(94%)	0.14	23 (5%) 25 29	22, 38, 72, 105	0
1	В	429/453~(94%)	-0.04	12 (2%) 53 56	23, 37, 77, 118	0
1	С	428/453~(94%)	0.26	34 (7%) 12 14	24, 43, 89, 117	0
1	D	428/453~(94%)	0.23	35 (8%) 11 13	25, 41, 89, 128	0
All	All	1711/1812 (94%)	0.15	104 (6%) 21 24	22, 39, 81, 128	0

All (104) RSRZ outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	RSRZ
1	В	109	LEU	9.5
1	А	109	LEU	8.6
1	А	110	PRO	7.3
1	D	193	GLN	6.5
1	D	191	GLY	6.3
1	В	110	PRO	6.3
1	С	109	LEU	6.1
1	D	325	GLN	6.0
1	D	223	GLU	5.4
1	D	219	LEU	5.1
1	С	408	GLU	5.0
1	D	408	GLU	4.9
1	D	412	PHE	4.8
1	С	411	THR	4.7
1	С	219	LEU	4.7
1	С	410	GLY	4.6
1	С	190	LYS	4.6
1	D	190	LYS	4.5
1	С	193	GLN	4.5
1	D	110	PRO	4.5
1	С	191	GLY	4.4



8TC7	
------	--

Mol	Chain	Res	Type	RSRZ	
1	С	412	PHE	4.3	
1	В	219	LEU	4.1	
1	А	490	LYS	3.8	
1	А	317	ILE	3.8	
1	С	223	GLU	3.7	
1	D	411	THR	3.7	
1	D	531	TYR	3.7	
1	D	324	GLU	3.7	
1	С	110	PRO	3.7	
1	С	111	GLU	3.6	
1	С	413	TYR	3.6	
1	С	409	ASP	3.5	
1	С	278	VAL	3.5	
1	D	222	GLU	3.5	
1	D	317	ILE	3.4	
1	В	281	GLY	3.4	
1	С	531	TYR	3.4	
1	D	189	PRO	3.4	
1	С	189	PRO	3.3	
1	D	410	GLY	3.3	
1	D	192	LYS	3.3	
1	D	109	LEU	3.3	
1	D	385	LYS	3.1	
1	D	281	GLY	3.1	
1	С	414	GLU	3.0	
1	А	111	GLU	3.0	
1	D	220	ILE	2.9	
1	A	187	LEU	2.9	
1	A	316	CYS	2.9	
1	D	330	ARG	2.9	
1	С	194	ALA	2.9	
1	А	447	PHE	2.8	
1	С	192	LYS	2.8	
1	С	188	THR	2.8	
1	В	493	GLY	2.8	
1	А	493	GLY	2.7	
1	С	324	GLU	2.7	
1	В	317	ILE	2.7	
1	С	385	LYS	2.7	
1	A	318	ALA	2.6	
1	В	222	GLU	2.6	
1	D	382	GLN	2.6	



Mol	Chain	Res	Type	RSRZ	
1	С	318	ALA	2.6	
1	D	409	ASP	2.6	
1	А	268	VAL	2.6	
1	D	269	THR	2.5	
1	С	317	ILE	2.5	
1	А	219	LEU	2.5	
1	А	185	LEU	2.5	
1	D	426	LEU	2.5	
1	А	382	GLN	2.5	
1	D	268	VAL	2.4	
1	С	221	ASN	2.4	
1	D	318	ALA	2.4	
1	D	225	ASP	2.4	
1	В	385	LYS	2.4	
1	С	187	LEU	2.3	
1	С	407	LYS	2.3	
1	С	269	THR	2.3	
1	С	268	VAL	2.3	
1	В	490	LYS	2.3	
1	С	220	ILE	2.3	
1	В	325	GLN	2.3	
1	С	222	GLU	2.2	
1	А	113	LYS	2.2	
1	С	270	PRO	2.2	
1	А	222	GLU	2.2	
1	А	144	LEU	2.2	
1	В	111	GLU	2.2	
1	D	406	LYS	2.2	
1	D	338	VAL	2.2	
1	А	128	VAL	2.2	
1	D	143	ASN	2.1	
1	А	184	MET	2.1	
1	А	190	LYS	2.1	
1	А	123	TYR	2.1	
1	В	269	THR	2.1	
1	D	224	SER	2.1	
1	D	414	GLU	2.1	
1	D	292	GLU	2.0	
1	A	269	THR	2.0	
1	С	375	HIS	2.0	
1	A	246	LEU	2.0	

Continued from previous page...



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
2	GOL	В	606	6/6	0.55	0.28	60,67,73,74	0
3	CL	С	604	1/1	0.81	0.15	83,83,83,83	0
2	GOL	А	607	6/6	0.82	0.36	65,67,71,73	0
2	GOL	А	606	6/6	0.86	0.18	$36,\!37,\!46,\!52$	0
2	GOL	А	605	6/6	0.87	0.30	47,65,67,81	0
2	GOL	В	603	6/6	0.87	0.25	$63,\!68,\!74,\!78$	0
2	GOL	D	601	6/6	0.88	0.24	43,54,57,62	0
2	GOL	С	601	6/6	0.88	0.17	$48,\!53,\!54,\!74$	0
2	GOL	В	605	6/6	0.90	0.18	$59,\!65,\!66,\!74$	0
2	GOL	D	602	6/6	0.90	0.12	$41,\!51,\!61,\!67$	0
2	GOL	С	603	6/6	0.90	0.19	38,41,45,54	0
2	GOL	В	609	6/6	0.91	0.16	35,44,50,60	0
2	GOL	А	601	6/6	0.91	0.12	35,42,44,48	0
2	GOL	В	607	6/6	0.91	0.16	$47,\!54,\!58,\!73$	0
2	GOL	А	604	6/6	0.93	0.10	47,49,61,64	0
2	GOL	D	603	6/6	0.93	0.13	35,44,51,52	0
2	GOL	В	601	6/6	0.93	0.19	44,52,58,60	0
2	GOL	А	602	6/6	0.94	0.11	45,48,61,62	0
2	GOL	В	608	6/6	0.94	0.22	$40,\!61,\!65,\!72$	0
2	GOL	В	604	6/6	0.94	0.12	50,58,62,73	0
2	GOL	С	602	6/6	0.95	0.13	47,51,55,57	0
2	GOL	В	602	6/6	0.95	0.10	36,40,45,45	0
2	GOL	А	603	6/6	0.96	0.14	43,49,52,53	0
3	CL	В	610	1/1	0.97	0.21	70,70,70,70	0



6.5 Other polymers (i)

There are no such residues in this entry.

