



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:27 PM UTC

PDB ID : 2X8T / pdb_00002x8t
Title : Crystal Structure of the Abn2 H318A mutant
Authors : deSanctis, D.; Inacio, J.M.; Lindley, P.F.; de Sa-Nogueira, I.; Bento, I.
Deposited on : 2010-03-11
Resolution : 1.79 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

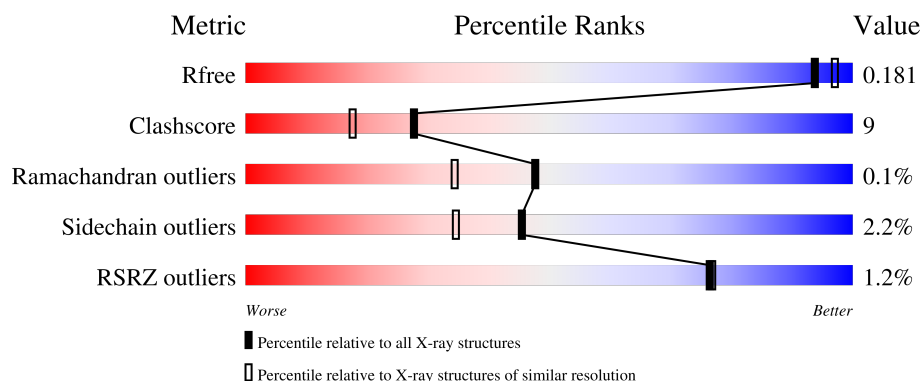
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.79 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}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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 $\leq 5\%$. 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	471	% 77% 13% • 6%
1	B	471	% 75% 16% • 6%

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
5	GOL	B	1474	-	X	X	-
5	GOL	B	1475	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 7685 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 ENDO-ALPHA-1,5-ARABINANASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	443	Total	C	N	O	S	7	5	0
			3535	2247	594	681	13			
1	B	444	Total	C	N	O	S	10	15	0
			3622	2301	612	697	12			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	318	ALA	HIS	engineered mutation	UNP ?
A	470	LEU	-	expression tag	UNP B3FRL6
A	471	ALA	-	expression tag	UNP B3FRL6
B	318	ALA	HIS	engineered mutation	UNP ?
B	470	LEU	-	expression tag	UNP B3FRL6
B	471	ALA	-	expression tag	UNP B3FRL6

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		
3	B	1	Total	Cl	0	0
			1	1		

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			8	6	2		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).

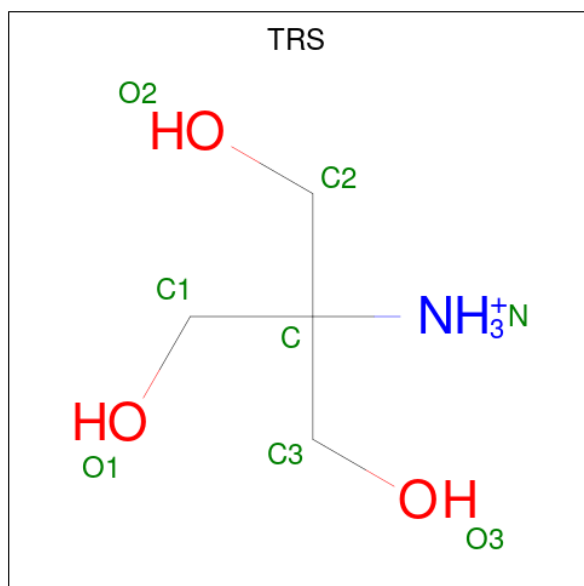


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Na	0	0
			1	1		

- Molecule 7 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	N	O	0	0
			8	4	1	3		

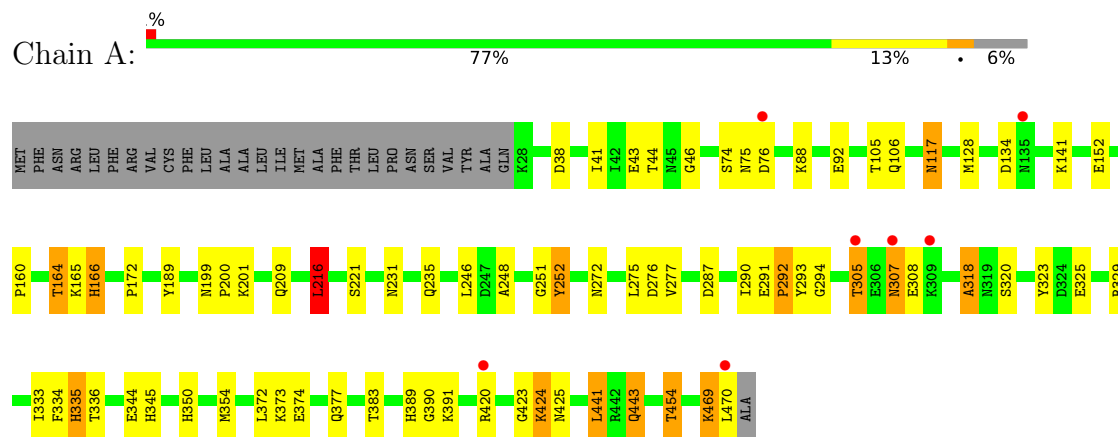
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	225	Total	O	0	0
			225	225		
8	B	264	Total	O	0	0
			264	264		

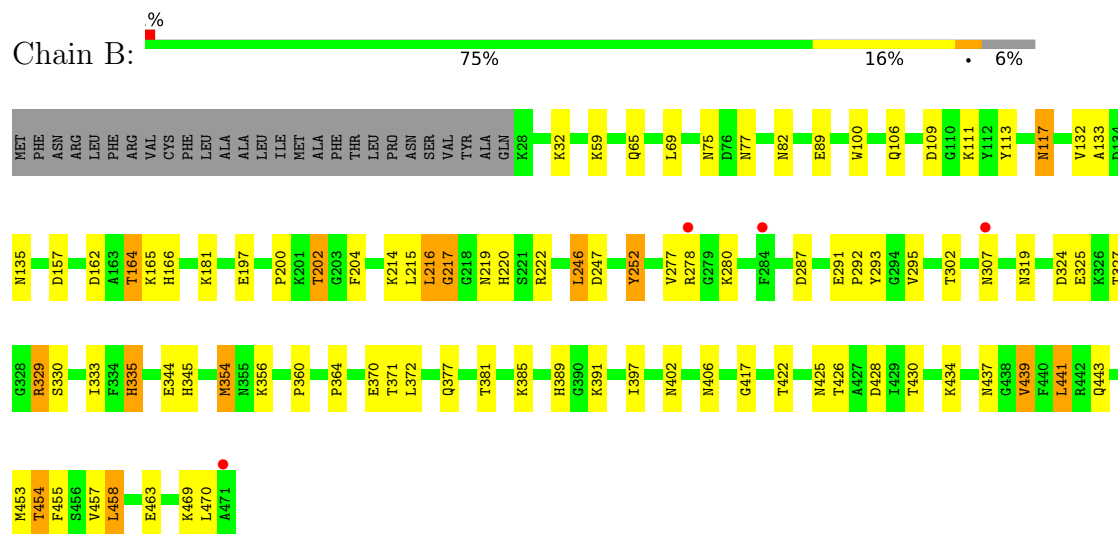
3 Residue-property plots [i](#)

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: ENDO-ALPHA-1,5-ARABINANASE



• Molecule 1: ENDO-ALPHA-1,5-ARABINANASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	51.80Å 57.37Å 85.48Å 82.10° 88.21° 63.61°	Depositor
Resolution (Å)	31.79 – 1.79 31.79 – 1.79	Depositor EDS
% Data completeness (in resolution range)	92.4 (31.79-1.79) 88.2 (31.79-1.79)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 1.79Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.158 , 0.189 0.153 , 0.181	Depositor DCC
R_{free} test set	3648 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	14.0	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 55.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.026 for h,h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7685	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.91% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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.

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: NA, CA, CL, MPD, TRS, 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	1.07	41/3630 (1.1%)	0.87	10/4918 (0.2%)
1	B	1.01	40/3718 (1.1%)	0.84	10/5038 (0.2%)
All	All	1.04	81/7348 (1.1%)	0.86	20/9956 (0.2%)

All (81) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	457	VAL	C-O	-9.00	1.14	1.23
1	A	252	TYR	C-O	-8.92	1.12	1.23
1	B	458[A]	LEU	C-O	-8.56	1.13	1.23
1	B	458[B]	LEU	C-O	-8.56	1.13	1.23
1	A	425	ASN	C-O	-8.17	1.17	1.23
1	B	333	ILE	C-O	-8.05	1.15	1.24
1	A	290	ILE	C-O	-7.90	1.16	1.24
1	A	231	ASN	C-O	-7.85	1.17	1.25
1	A	292	PRO	C-O	-7.61	1.13	1.24
1	B	117	ASN	CG-ND2	-7.31	1.17	1.33
1	A	334	PHE	C-O	-7.11	1.15	1.23
1	A	134	ASP	C-O	-6.98	1.15	1.24
1	B	344	GLU	C-O	-6.94	1.15	1.23
1	A	350	HIS	C-O	-6.92	1.16	1.24
1	B	135	ASN	C-O	-6.66	1.15	1.24
1	B	133	ALA	C-O	-6.60	1.15	1.23
1	A	246	LEU	C-O	-6.58	1.15	1.24
1	A	209	GLN	CD-NE2	-6.51	1.19	1.33
1	A	423	GLY	C-O	-6.35	1.15	1.24
1	B	324	ASP	C-O	-6.29	1.16	1.24
1	B	370	GLU	C-N	-6.29	1.25	1.33
1	A	441	LEU	C-O	-6.25	1.16	1.23
1	B	106	GLN	C-O	-6.21	1.16	1.24
1	B	75	ASN	CG-ND2	-6.10	1.20	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	105	THR	C-O	-6.09	1.17	1.24
1	A	106	GLN	C-O	-5.99	1.16	1.24
1	B	443	GLN	C-O	-5.97	1.17	1.23
1	A	344	GLU	C-O	-5.94	1.16	1.23
1	B	216	LEU	C-O	-5.92	1.17	1.23
1	B	77	ASN	C-O	-5.90	1.16	1.24
1	A	117	ASN	C-O	-5.90	1.16	1.23
1	A	329	ARG	C-O	-5.88	1.16	1.23
1	A	390	GLY	C-O	-5.82	1.15	1.23
1	B	220	HIS	ND1-CE1	5.76	1.38	1.32
1	B	441	LEU	C-O	-5.69	1.17	1.23
1	A	336	THR	C-O	-5.67	1.17	1.23
1	A	424	LYS	C-O	-5.63	1.17	1.24
1	A	345	HIS	CD2-NE2	-5.60	1.31	1.37
1	B	428	ASP	C-O	-5.58	1.17	1.24
1	A	276	ASP	C-O	-5.56	1.16	1.24
1	A	389	HIS	ND1-CE1	5.53	1.38	1.32
1	A	377	GLN	C-O	-5.51	1.17	1.24
1	B	329[A]	ARG	C-O	-5.49	1.17	1.23
1	B	329[B]	ARG	C-O	-5.49	1.17	1.23
1	B	166	HIS	ND1-CE1	5.47	1.38	1.32
1	A	75	ASN	CG-OD1	5.46	1.33	1.23
1	B	214	LYS	C-O	-5.46	1.17	1.23
1	B	377	GLN	C-O	-5.45	1.17	1.24
1	A	166	HIS	ND1-CE1	5.45	1.38	1.32
1	A	335	HIS	CD2-NE2	-5.44	1.31	1.37
1	A	248	ALA	CA-CB	-5.43	1.44	1.53
1	A	216	LEU	C-O	-5.40	1.18	1.23
1	B	389	HIS	ND1-CE1	5.38	1.38	1.32
1	A	345	HIS	C-O	-5.36	1.17	1.23
1	B	330	SER	C-O	-5.33	1.17	1.23
1	A	307	ASN	CG-OD1	5.27	1.33	1.23
1	B	82	ASN	CG-OD1	5.26	1.33	1.23
1	B	345	HIS	C-O	-5.22	1.17	1.23
1	B	307	ASN	CG-ND2	-5.22	1.22	1.33
1	A	152	GLU	C-O	-5.22	1.17	1.24
1	A	272	ASN	CG-OD1	5.20	1.33	1.23
1	B	133	ALA	CA-CB	-5.20	1.43	1.54
1	A	424	LYS	CB-CG	-5.17	1.36	1.52
1	B	327	THR	CA-CB	-5.17	1.46	1.54
1	B	402	ASN	C-O	-5.16	1.17	1.24
1	B	219	ASN	CG-OD1	5.15	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	381	THR	C-O	-5.15	1.17	1.23
1	A	345	HIS	ND1-CE1	5.13	1.37	1.32
1	A	335	HIS	C-O	-5.13	1.17	1.23
1	B	335	HIS	ND1-CE1	5.13	1.37	1.32
1	B	117	ASN	C-O	-5.11	1.17	1.23
1	A	251	GLY	C-O	-5.11	1.17	1.23
1	B	443	GLN	CD-NE2	-5.09	1.22	1.33
1	B	217	GLY	C-O	-5.07	1.18	1.23
1	A	235	GLN	C-O	-5.04	1.16	1.23
1	B	319	ASN	CG-OD1	5.04	1.33	1.23
1	A	372	LEU	C-O	-5.03	1.17	1.23
1	B	406	ASN	CG-OD1	5.02	1.33	1.23
1	A	318	ALA	C-O	-5.01	1.17	1.23
1	B	215	LEU	C-O	-5.01	1.17	1.24
1	A	199	ASN	CG-OD1	5.00	1.33	1.23

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	469	LYS	O-C-N	9.72	134.42	123.04
1	B	220	HIS	CB-CG-CD2	-6.64	122.57	131.20
1	B	166	HIS	CB-CG-CD2	-6.56	122.67	131.20
1	B	443	GLN	N-CA-C	6.45	116.58	108.45
1	A	345	HIS	CB-CG-CD2	-6.40	122.88	131.20
1	A	335	HIS	CB-CG-CD2	-6.37	122.92	131.20
1	B	389	HIS	CB-CG-CD2	-6.34	122.95	131.20
1	A	166	HIS	CB-CG-CD2	-6.28	123.03	131.20
1	A	389	HIS	CB-CG-CD2	-6.22	123.11	131.20
1	B	354	MET	CG-SD-CE	-6.19	87.28	100.90
1	B	335	HIS	CB-CG-CD2	-6.12	123.24	131.20
1	A	345	HIS	CB-CG-ND1	5.70	131.26	122.70
1	A	335	HIS	CB-CG-ND1	5.66	131.19	122.70
1	B	166	HIS	CB-CG-ND1	5.63	131.15	122.70
1	B	220	HIS	CB-CG-ND1	5.51	130.97	122.70
1	B	389	HIS	CB-CG-ND1	5.50	130.95	122.70
1	A	389	HIS	CB-CG-ND1	5.43	130.85	122.70
1	A	166	HIS	CB-CG-ND1	5.38	130.78	122.70
1	B	335	HIS	CB-CG-ND1	5.28	130.61	122.70
1	A	443	GLN	N-CA-C	5.24	115.05	108.45

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	3535	0	3389	52	0
1	B	3622	0	3487	66	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	8	0	14	2	0
5	A	6	0	8	3	0
5	B	12	0	13	11	0
6	B	1	0	0	0	0
7	B	8	0	12	1	0
8	A	225	0	0	9	0
8	B	264	0	0	20	0
All	All	7685	0	6923	127	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 9.

All (127) 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)
5:B:1475:GOL:H12	8:B:2013:HOH:O	1.57	1.04
1:A:141:LYS:NZ	8:A:2058:HOH:O	1.94	0.99
1:B:422:THR:HB	1:B:426[A]:THR:OG1	1.65	0.95
5:B:1474:GOL:H2	8:B:2176:HOH:O	1.68	0.94
1:B:217:GLY:O	1:B:278:ARG:HG2	1.68	0.92
1:A:469:LYS:HG2	1:A:470:LEU:HD22	1.50	0.91
1:B:302:THR:HB	1:B:397[B]:ILE:HD11	1.58	0.86
1:A:469:LYS:O	1:A:470:LEU:HB2	1.75	0.86
1:B:372:LEU:HD11	1:B:439[A]:VAL:HG11	1.61	0.82
1:A:374:GLU:HA	1:A:424:LYS:HG2	1.61	0.81
1:A:88:LYS:HE2	1:A:92:GLU:OE2	1.80	0.80
1:A:164[A]:THR:HG23	1:B:278:ARG:NH1	1.95	0.80
1:A:128[B]:MET:HE1	1:A:172:PRO:HB3	1.64	0.80
1:B:181:LYS:HZ1	1:B:197:GLU:HG2	1.46	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:277:VAL:O	1:B:278:ARG:HG3	1.81	0.79
4:A:1472:MPD:H11	8:A:2083:HOH:O	1.84	0.77
1:B:426[A]:THR:HG23	8:B:2234:HOH:O	1.85	0.76
1:B:329[A]:ARG:HG2	1:B:329[A]:ARG:HH11	1.49	0.76
4:A:1472:MPD:H13	8:A:2081:HOH:O	1.89	0.72
1:A:325:GLU:OE2	5:A:1473:GOL:H31	1.90	0.71
1:A:305:THR:HG23	1:A:307:ASN:H	1.56	0.71
1:A:469:LYS:CG	1:A:470:LEU:HD22	2.20	0.70
1:B:397[B]:ILE:HG22	8:B:2220:HOH:O	1.91	0.70
1:A:277[B]:VAL:HG12	1:A:293:TYR:CD2	2.26	0.70
1:A:323:TYR:O	5:A:1473:GOL:H32	1.94	0.68
5:B:1475:GOL:H11	8:B:2059:HOH:O	1.93	0.68
1:B:89:GLU:OE1	8:B:2043:HOH:O	2.11	0.68
1:B:426[B]:THR:HG22	8:B:2234:HOH:O	1.94	0.67
1:B:202[A]:THR:CG2	1:B:204:PHE:HD1	2.07	0.67
5:B:1475:GOL:H32	8:B:2092:HOH:O	1.93	0.67
1:B:181:LYS:HE2	8:B:2103:HOH:O	1.94	0.67
1:B:202[A]:THR:HG22	1:B:204:PHE:H	1.62	0.65
1:B:222[A]:ARG:HD3	1:B:287:ASP:OD1	1.97	0.64
5:B:1474:GOL:C2	8:B:2176:HOH:O	2.37	0.63
1:B:202[A]:THR:HG21	8:B:2110:HOH:O	1.99	0.62
1:B:372:LEU:HD11	1:B:439[A]:VAL:CG1	2.29	0.62
1:A:305:THR:HG22	1:A:308:GLU:H	1.64	0.62
1:B:329[A]:ARG:HG2	1:B:329[A]:ARG:NH1	2.15	0.61
1:B:278:ARG:HD3	8:B:2157:HOH:O	2.01	0.61
1:B:364:PRO:HD2	1:B:454[A]:THR:HG21	1.83	0.60
1:B:109:ASP:OD2	1:B:111:LYS:HE3	2.03	0.59
5:B:1475:GOL:H11	8:B:2129:HOH:O	2.02	0.58
1:A:294:GLY:O	1:A:391:LYS:HE3	2.04	0.58
1:A:160:PRO:HB3	1:B:280:LYS:HE3	1.86	0.58
1:A:164[A]:THR:CG2	1:B:278:ARG:NH1	2.65	0.57
1:A:128[B]:MET:HE1	1:A:172:PRO:CB	2.34	0.57
1:A:43:GLU:OE1	1:A:46:GLY:N	2.32	0.56
1:A:165:LYS:HE3	1:A:166:HIS:CE1	2.40	0.56
5:A:1473:GOL:H2	8:A:2152:HOH:O	2.05	0.56
1:B:217:GLY:C	1:B:278:ARG:HG2	2.28	0.56
1:A:277[A]:VAL:HG22	1:A:293:TYR:CG	2.40	0.55
1:A:277[B]:VAL:HG12	1:A:293:TYR:CG	2.42	0.54
1:A:200:PRO:HG3	8:A:2080:HOH:O	2.07	0.54
1:B:329[A]:ARG:HH11	1:B:329[A]:ARG:CG	2.19	0.54
1:A:128[B]:MET:HE2	1:A:172:PRO:HG3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:LYS:CD	1:A:470:LEU:CD2	2.86	0.54
1:B:422:THR:HB	1:B:426[B]:THR:HG23	1.90	0.54
1:A:277[A]:VAL:HG22	1:A:293:TYR:CD2	2.43	0.53
1:A:383:THR:O	1:A:470:LEU:N	2.33	0.53
1:B:277:VAL:O	1:B:278:ARG:CG	2.54	0.53
1:B:277:VAL:C	1:B:278:ARG:HG3	2.33	0.53
1:B:202[A]:THR:CG2	1:B:204:PHE:CD1	2.90	0.53
5:B:1475:GOL:C1	8:B:2059:HOH:O	2.55	0.52
1:A:287:ASP:O	1:A:291:GLU:HG3	2.10	0.52
1:B:372:LEU:CD1	1:B:439[A]:VAL:HG11	2.38	0.52
1:B:422:THR:O	1:B:426[B]:THR:HG23	2.10	0.51
1:A:216:LEU:HB2	1:A:277[B]:VAL:HG22	1.93	0.51
1:B:422:THR:CB	1:B:426[A]:THR:OG1	2.50	0.51
1:A:441:LEU:O	1:A:454[A]:THR:HB	2.10	0.50
1:A:354:MET:HE2	8:A:2155:HOH:O	2.10	0.50
1:A:469:LYS:CD	1:A:470:LEU:HD22	2.41	0.50
1:B:329[A]:ARG:NH1	1:B:329[A]:ARG:CG	2.71	0.50
1:A:335:HIS:C	1:A:335:HIS:CD2	2.90	0.50
1:A:128[B]:MET:CE	1:A:172:PRO:HG3	2.43	0.49
1:A:160:PRO:CB	1:B:280:LYS:HE3	2.41	0.49
1:B:59:LYS:HE2	1:B:69:LEU:HD21	1.93	0.49
1:A:469:LYS:HG2	1:A:470:LEU:N	2.26	0.49
5:B:1474:GOL:H11	8:B:2176:HOH:O	2.13	0.49
1:A:88:LYS:CE	1:A:92:GLU:OE2	2.56	0.47
1:B:200:PRO:HG3	8:B:2097:HOH:O	2.13	0.47
1:B:295:VAL:HG11	1:B:458[B]:LEU:HD21	1.96	0.47
1:B:356:LYS:HD3	1:B:437:ASN:ND2	2.29	0.47
1:B:354:MET:HE1	1:B:360:PRO:HB3	1.96	0.47
1:A:373:LYS:HE2	8:A:2180:HOH:O	2.15	0.47
1:B:385:LYS:HG3	1:B:470:LEU:HD21	1.96	0.47
1:B:441:LEU:O	1:B:454[A]:THR:HB	2.15	0.47
1:A:74:SER:C	1:A:76:ASP:H	2.22	0.46
1:B:453:MET:HB3	1:B:469:LYS:HD3	1.97	0.46
1:B:181:LYS:NZ	1:B:197:GLU:HG2	2.23	0.46
1:A:443:GLN:HB2	8:A:2179:HOH:O	2.16	0.45
1:B:181:LYS:CE	8:B:2103:HOH:O	2.60	0.45
1:B:434:LYS:HE3	1:B:434:LYS:HB2	1.77	0.45
1:A:44:THR:O	1:A:44:THR:HG23	2.17	0.45
1:B:335:HIS:CD2	1:B:335:HIS:C	2.95	0.44
1:B:100:TRP:CE3	7:B:1472:TRS:H31	2.53	0.43
1:B:277:VAL:HG22	1:B:293:TYR:CG	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:THR:HG23	1:A:307:ASN:N	2.29	0.43
1:B:162:ASP:OD1	1:B:164[A]:THR:HB	2.19	0.43
1:A:333:ILE:HD12	1:A:333:ILE:N	2.34	0.43
1:A:291:GLU:HB2	1:A:292:PRO:HD3	2.01	0.42
1:B:246[A]:LEU:HD22	1:B:247:ASP:N	2.34	0.42
1:B:325:GLU:OE2	5:B:1474:GOL:O1	2.38	0.42
1:A:128[B]:MET:CE	1:A:172:PRO:HB3	2.43	0.42
1:B:454[A]:THR:CG2	1:B:455:PHE:N	2.81	0.42
1:A:38:ASP:HA	1:A:318:ALA:HB1	2.01	0.42
1:B:417:GLY:HA3	1:B:430[B]:THR:O	2.20	0.41
1:A:420:ARG:NH2	8:A:2203:HOH:O	0.57	0.41
1:B:162:ASP:HB3	1:B:165:LYS:HE2	2.02	0.41
5:B:1474:GOL:C1	8:B:2131:HOH:O	2.68	0.41
1:B:109:ASP:CG	1:B:111:LYS:HE3	2.45	0.41
1:B:391:LYS:HG2	1:B:463:GLU:HG2	2.02	0.41
1:A:469:LYS:CG	1:A:470:LEU:CD2	2.96	0.41
1:B:113:TYR:CD2	1:B:132[A]:VAL:HG12	2.56	0.41
1:B:385:LYS:NZ	8:B:2214:HOH:O	2.53	0.41
1:A:41:ILE:HG22	1:A:320:SER:HB2	2.03	0.41
1:B:246[B]:LEU:HD12	1:B:246[B]:LEU:C	2.46	0.41
1:A:74:SER:C	1:A:76:ASP:N	2.80	0.40
1:A:128[B]:MET:CE	1:A:172:PRO:CG	3.00	0.40
1:B:157:ASP:OD1	1:B:157:ASP:C	2.64	0.40
1:B:371[A]:THR:CG2	1:B:372:LEU:N	2.83	0.40
1:A:189:TYR:HA	1:A:221:SER:O	2.21	0.40
1:B:32:LYS:HE2	1:B:65:GLN:OE1	2.21	0.40
1:B:246[A]:LEU:HA	1:B:252:TYR:CG	2.55	0.40
1:B:291:GLU:N	1:B:292:PRO:CD	2.85	0.40
1:B:417:GLY:HA3	1:B:430[A]:THR:O	2.21	0.40
5:B:1474:GOL:C1	8:B:2176:HOH:O	2.63	0.40
1:A:470:LEU:HD13	1:A:470:LEU:HA	1.92	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	446/471 (95%)	438 (98%)	8 (2%)	0	100	100
1	B	457/471 (97%)	449 (98%)	7 (2%)	1 (0%)	43	31
All	All	903/942 (96%)	887 (98%)	15 (2%)	1 (0%)	48	34

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	425	ASN

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	375/394 (95%)	365 (97%)	10 (3%)	39	27
1	B	386/394 (98%)	373 (97%)	13 (3%)	32	20
All	All	761/788 (97%)	738 (97%)	23 (3%)	45	24

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	117	ASN
1	A	164[A]	THR
1	A	164[B]	THR
1	A	201	LYS
1	A	216	LEU
1	A	252	TYR
1	A	275	LEU
1	A	305	THR
1	A	454[A]	THR
1	A	454[B]	THR
1	B	117	ASN
1	B	164[A]	THR

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Mol	Chain	Res	Type
1	B	164[B]	THR
1	B	202[A]	THR
1	B	202[B]	THR
1	B	216	LEU
1	B	246[A]	LEU
1	B	246[B]	LEU
1	B	252	TYR
1	B	439[A]	VAL
1	B	439[B]	VAL
1	B	454[A]	THR
1	B	454[B]	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	ASN
1	B	61	ASN
1	B	168	ASN
1	B	345	HIS
1	B	351	GLN
1	B	402	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 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
7	TRS	B	1472	-	7,7,7	0.39	0	9,9,9	0.59	0
5	GOL	B	1475	-	5,5,5	2.39	2 (40%)	5,5,5	1.30	1 (20%)
5	GOL	A	1473	-	5,5,5	0.38	0	5,5,5	0.44	0
5	GOL	B	1474	-	5,5,5	1.07	1 (20%)	5,5,5	2.05	2 (40%)
4	MPD	A	1472	-	7,7,7	0.29	0	9,10,10	0.27	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
7	TRS	B	1472	-	-	3/9/9/9	-
5	GOL	B	1475	-	-	2/4/4/4	-
5	GOL	A	1473	-	-	4/4/4/4	-
5	GOL	B	1474	-	-	4/4/4/4	-
4	MPD	A	1472	-	-	0/5/5/5	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1475	GOL	O2-C2	-4.77	1.29	1.43
5	B	1474	GOL	O1-C1	-2.36	1.32	1.42
5	B	1475	GOL	O1-C1	-2.32	1.32	1.42

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1474	GOL	C3-C2-C1	-3.23	99.93	111.80
5	B	1475	GOL	O2-C2-C1	-2.52	98.75	109.18
5	B	1474	GOL	O2-C2-C3	2.48	119.45	109.18

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1473	GOL	O1-C1-C2-C3
5	B	1474	GOL	O1-C1-C2-C3
5	B	1475	GOL	O1-C1-C2-O2
5	B	1475	GOL	O1-C1-C2-C3
5	A	1473	GOL	O1-C1-C2-O2
5	A	1473	GOL	C1-C2-C3-O3
5	B	1474	GOL	C1-C2-C3-O3
5	B	1474	GOL	O1-C1-C2-O2
5	B	1474	GOL	O2-C2-C3-O3
7	B	1472	TRS	C1-C-C3-O3
5	A	1473	GOL	O2-C2-C3-O3
7	B	1472	TRS	N-C-C3-O3
7	B	1472	TRS	C2-C-C3-O3

There are no ring outliers.

5 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	1472	TRS	1	0
5	B	1475	GOL	5	0
5	A	1473	GOL	3	0
5	B	1474	GOL	6	0
4	A	1472	MPD	2	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, 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	443/471 (94%)	-0.32	7 (1%) 70 71	6, 16, 34, 70	5 (1%)
1	B	444/471 (94%)	-0.46	4 (0%) 81 81	4, 13, 28, 57	15 (3%)
All	All	887/942 (94%)	-0.39	11 (1%) 76 77	4, 14, 32, 70	20 (2%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	284	PHE	3.9
1	B	278	ARG	3.5
1	A	470	LEU	3.4
1	A	76	ASP	2.5
1	B	471	ALA	2.5
1	A	420	ARG	2.4
1	A	135	ASN	2.4
1	A	305	THR	2.4
1	A	307	ASN	2.2
1	B	307	ASN	2.2
1	A	309	LYS	2.1

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 oligosaccharides 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
5	GOL	A	1473	6/6	0.69	0.18	39,47,50,58	0
5	GOL	B	1474	6/6	0.78	0.17	36,39,40,42	0
4	MPD	A	1472	8/8	0.86	0.12	16,29,40,42	0
6	NA	B	476	1/1	0.91	0.21	52,52,52,52	0
7	TRS	B	1472	8/8	0.91	0.10	16,18,33,39	0
5	GOL	B	1475	6/6	0.96	0.13	19,29,42,46	0
3	CL	A	1471	1/1	0.99	0.03	17,17,17,17	0
2	CA	B	474	1/1	1.00	0.02	9,9,9,9	0
2	CA	A	473	1/1	1.00	0.02	9,9,9,9	0
3	CL	B	1473	1/1	1.00	0.02	15,15,15,15	0

6.5 Other polymers

There are no such residues in this entry.