



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 07:47 PM GMT

PDB ID : 4ISS
Title : SeMet-substituted Kluyveromyces lactis Allophanate Hydrolase
Authors : Fan, C.; Xiang, S.
Deposited on : 2013-01-17
Resolution : 2.50 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

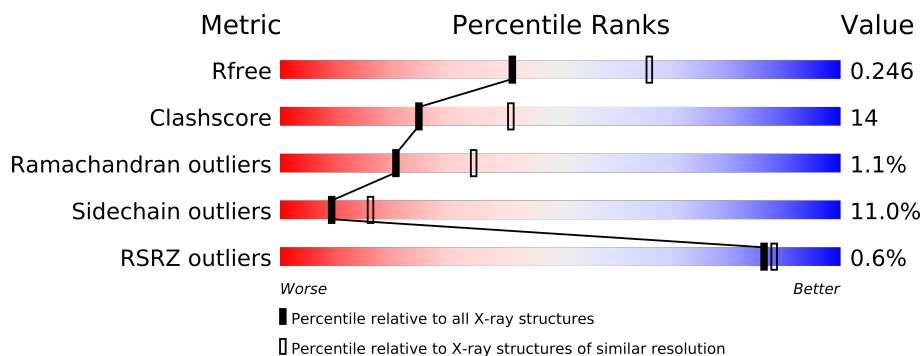
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.50 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}	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	644	
1	B	644	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	GOL	B	701	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9768 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Allophanate Hydrolase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	614	Total	C	N	O	S	Se	0	0	0
			4748	3051	786	897	11	3			
1	B	612	Total	C	N	O	S	Se	0	0	0
			4731	3041	784	893	11	2			

There are 46 discrepancies between the modelled and reference sequences:

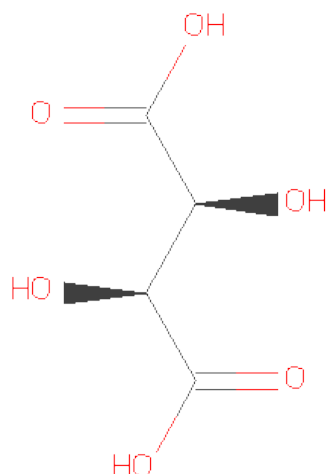
Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MSE	-	EXPRESSION TAG	UNP Q6CP22
A	-21	GLY	-	EXPRESSION TAG	UNP Q6CP22
A	-20	SER	-	EXPRESSION TAG	UNP Q6CP22
A	-19	SER	-	EXPRESSION TAG	UNP Q6CP22
A	-18	HIS	-	EXPRESSION TAG	UNP Q6CP22
A	-17	HIS	-	EXPRESSION TAG	UNP Q6CP22
A	-16	HIS	-	EXPRESSION TAG	UNP Q6CP22
A	-15	HIS	-	EXPRESSION TAG	UNP Q6CP22
A	-14	HIS	-	EXPRESSION TAG	UNP Q6CP22
A	-13	HIS	-	EXPRESSION TAG	UNP Q6CP22
A	-12	SER	-	EXPRESSION TAG	UNP Q6CP22
A	-11	SER	-	EXPRESSION TAG	UNP Q6CP22
A	-10	GLY	-	EXPRESSION TAG	UNP Q6CP22
A	-9	LEU	-	EXPRESSION TAG	UNP Q6CP22
A	-8	VAL	-	EXPRESSION TAG	UNP Q6CP22
A	-7	PRO	-	EXPRESSION TAG	UNP Q6CP22
A	-6	ARG	-	EXPRESSION TAG	UNP Q6CP22
A	-5	GLY	-	EXPRESSION TAG	UNP Q6CP22
A	-4	SER	-	EXPRESSION TAG	UNP Q6CP22
A	-3	HIS	-	EXPRESSION TAG	UNP Q6CP22
A	-2	MSE	-	EXPRESSION TAG	UNP Q6CP22
A	-1	ALA	-	EXPRESSION TAG	UNP Q6CP22
A	0	SER	-	EXPRESSION TAG	UNP Q6CP22
B	-22	MSE	-	EXPRESSION TAG	UNP Q6CP22
B	-21	GLY	-	EXPRESSION TAG	UNP Q6CP22

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	SER	-	EXPRESSION TAG	UNP Q6CP22
B	-19	SER	-	EXPRESSION TAG	UNP Q6CP22
B	-18	HIS	-	EXPRESSION TAG	UNP Q6CP22
B	-17	HIS	-	EXPRESSION TAG	UNP Q6CP22
B	-16	HIS	-	EXPRESSION TAG	UNP Q6CP22
B	-15	HIS	-	EXPRESSION TAG	UNP Q6CP22
B	-14	HIS	-	EXPRESSION TAG	UNP Q6CP22
B	-13	HIS	-	EXPRESSION TAG	UNP Q6CP22
B	-12	SER	-	EXPRESSION TAG	UNP Q6CP22
B	-11	SER	-	EXPRESSION TAG	UNP Q6CP22
B	-10	GLY	-	EXPRESSION TAG	UNP Q6CP22
B	-9	LEU	-	EXPRESSION TAG	UNP Q6CP22
B	-8	VAL	-	EXPRESSION TAG	UNP Q6CP22
B	-7	PRO	-	EXPRESSION TAG	UNP Q6CP22
B	-6	ARG	-	EXPRESSION TAG	UNP Q6CP22
B	-5	GLY	-	EXPRESSION TAG	UNP Q6CP22
B	-4	SER	-	EXPRESSION TAG	UNP Q6CP22
B	-3	HIS	-	EXPRESSION TAG	UNP Q6CP22
B	-2	MSE	-	EXPRESSION TAG	UNP Q6CP22
B	-1	ALA	-	EXPRESSION TAG	UNP Q6CP22
B	0	SER	-	EXPRESSION TAG	UNP Q6CP22

- Molecule 2 is D(-)-TARTARIC ACID (three-letter code: TAR) (formula: C₄H₆O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	4	6		

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



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

- Molecule 4 is water.

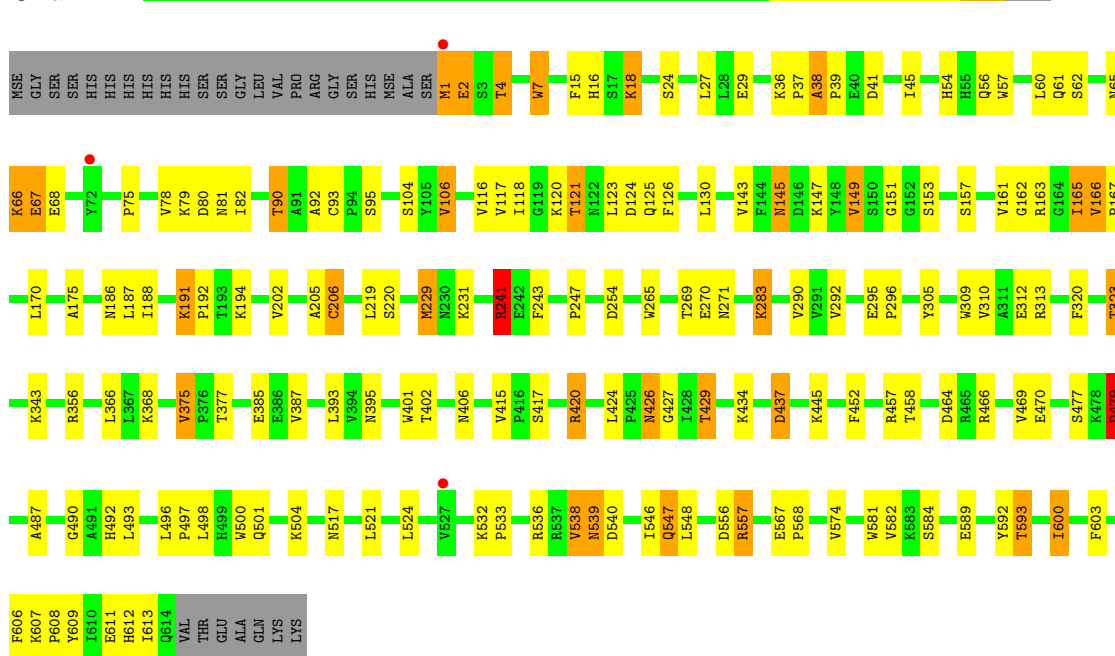
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	124	Total	O	0	0
			124	124		
4	B	149	Total	O	0	0
			149	149		

3 Residue-property plots

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.

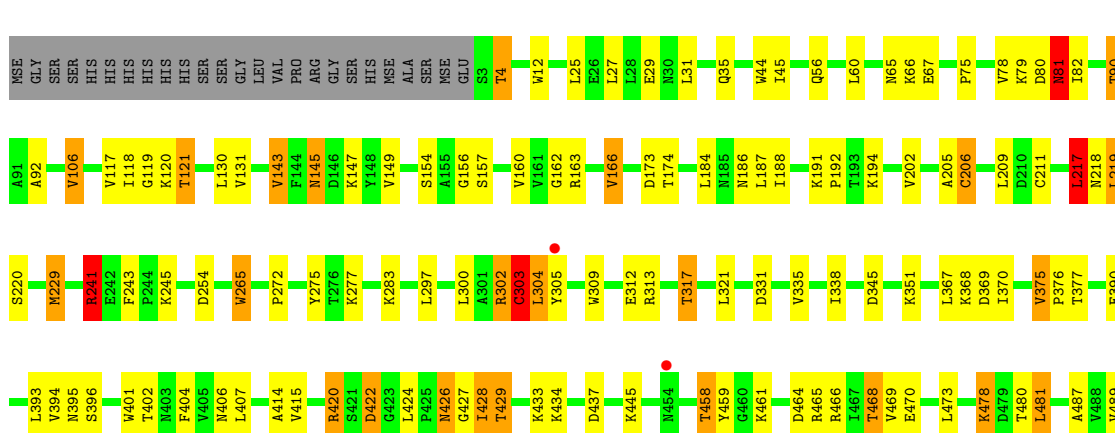
• Molecule 1: Allophanate Hydrolase

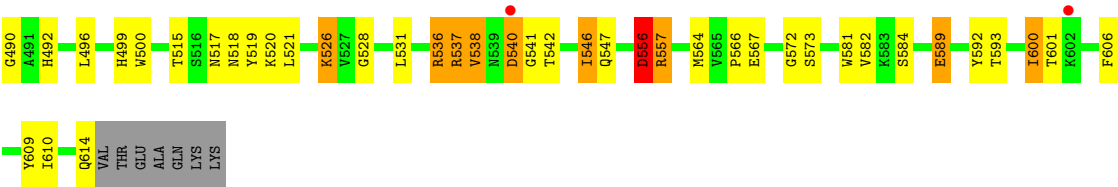
Chain A:



• Molecule 1: Allophanate Hydrolase

Chain B:





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	93.05Å 107.72Å 150.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.53 – 2.50 46.53 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.53-2.50) 99.9 (46.53-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.18 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.176 , 0.247 0.176 , 0.246	Depositor DCC
R_{free} test set	2715 reflections (5.39%)	DCC
Wilson B-factor (Å ²)	37.2	Xtriage
Anisotropy	0.187	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 17.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 53047 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9768	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, TAR

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	0.77	5/4860 (0.1%)	0.93	9/6612 (0.1%)
1	B	0.83	6/4843 (0.1%)	0.96	15/6590 (0.2%)
All	All	0.80	11/9703 (0.1%)	0.95	24/13202 (0.2%)

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	0	1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	254	ASP	CB-CG	-6.13	1.38	1.51
1	A	265	TRP	CD2-CE2	5.77	1.48	1.41
1	A	309	TRP	CD2-CE2	5.69	1.48	1.41
1	A	581	TRP	CD2-CE2	5.68	1.48	1.41
1	A	500	TRP	CD2-CE2	5.64	1.48	1.41
1	B	265	TRP	CD2-CE2	5.45	1.47	1.41
1	B	500	TRP	CD2-CE2	5.21	1.47	1.41
1	B	401	TRP	CD2-CE2	5.14	1.47	1.41
1	B	581	TRP	CD2-CE2	5.13	1.47	1.41
1	A	7	TRP	CD2-CE2	5.11	1.47	1.41
1	B	309	TRP	CD2-CE2	5.01	1.47	1.41

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	241	ARG	NE-CZ-NH1	8.53	124.56	120.30
1	A	188	ILE	CG1-CB-CG2	-7.83	94.18	111.40
1	B	241	ARG	NE-CZ-NH1	7.27	123.93	120.30
1	A	313	ARG	NE-CZ-NH2	-7.23	116.68	120.30
1	A	254	ASP	CB-CA-C	-6.95	96.50	110.40
1	B	229	MSE	CG-SE-CE	-6.75	84.05	98.90
1	B	481	LEU	CB-CG-CD1	-6.58	99.82	111.00
1	B	254	ASP	CB-CA-C	-6.24	97.92	110.40
1	B	254	ASP	N-CA-CB	-6.09	99.64	110.60
1	B	217	LEU	CA-CB-CG	6.03	129.18	115.30
1	A	229	MSE	CG-SE-CE	-5.94	85.82	98.90
1	B	557	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	B	546	ILE	CG1-CB-CG2	-5.74	98.77	111.40
1	A	556	ASP	CB-CG-OD2	5.68	123.42	118.30
1	B	254	ASP	N-CA-C	5.65	126.25	111.00
1	B	557	ARG	CG-CD-NE	-5.54	100.16	111.80
1	B	254	ASP	CB-CG-OD1	-5.54	113.31	118.30
1	A	241	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	B	556	ASP	N-CA-CB	-5.43	100.83	110.60
1	B	557	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	A	479	ASP	CB-CA-C	-5.28	99.84	110.40
1	B	367	LEU	CA-CB-CG	5.21	127.27	115.30
1	A	557	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	B	81	ASN	N-CA-CB	-5.02	101.57	110.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	539	ASN	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4748	0	4774	123	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4731	0	4756	144	0
2	A	10	0	4	1	0
3	B	6	0	8	5	0
4	A	124	0	0	6	0
4	B	149	0	0	13	0
All	All	9768	0	9542	264	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 14.

All (264) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:106:VAL:HG22	1:A:229:MSE:HE2	1.29	1.14
1:B:600:ILE:HD11	1:B:609:TYR:CE1	1.82	1.14
1:B:90:THR:HG22	1:B:92:ALA:H	1.15	1.10
1:A:38:ALA:HB1	1:A:39:PRO:HD3	1.36	1.07
1:B:186:ASN:HD21	1:B:458:THR:HG22	1.13	1.06
1:A:79:LYS:HA	1:A:121:THR:HG22	1.34	1.05
1:B:540:ASP:HB3	1:B:541:GLY:HA2	1.40	1.00
1:A:90:THR:HG22	1:A:92:ALA:H	1.24	1.00
1:B:540:ASP:CB	1:B:541:GLY:HA2	1.91	0.98
1:A:130:LEU:H	1:A:395:ASN:HD21	1.04	0.97
1:A:106:VAL:HG22	1:A:229:MSE:CE	1.95	0.97
1:B:205:ALA:O	1:B:206:CYS:HB2	1.65	0.96
1:A:426:ASN:HD22	1:A:427:GLY:H	1.08	0.96
1:B:283:LYS:HE2	4:B:905:HOH:O	1.68	0.94
1:B:426:ASN:HD22	1:B:427:GLY:H	1.16	0.94
1:A:38:ALA:HB1	1:A:39:PRO:CD	1.98	0.93
1:B:130:LEU:H	1:B:395:ASN:HD21	1.10	0.93
1:A:493:LEU:HB2	1:A:496:LEU:HD12	1.51	0.90
1:A:205:ALA:O	1:A:206:CYS:HB2	1.71	0.90
1:B:106:VAL:HG22	1:B:229:MSE:HE2	1.54	0.90
1:A:38:ALA:CB	1:A:39:PRO:CD	2.50	0.90
1:A:592:TYR:OH	1:B:589:GLU:HG3	1.70	0.90
1:A:106:VAL:CG2	1:A:229:MSE:HE2	2.03	0.88
1:B:186:ASN:HD21	1:B:458:THR:CG2	1.87	0.87
1:B:145:ASN:HD22	1:B:147:LYS:H	1.21	0.85
1:B:145:ASN:ND2	1:B:147:LYS:H	1.77	0.81
1:A:186:ASN:HD21	1:A:458:THR:HG22	1.45	0.80
1:B:600:ILE:HD11	1:B:609:TYR:CD1	2.17	0.80
1:B:90:THR:CG2	1:B:92:ALA:H	1.93	0.80
1:B:600:ILE:HD11	1:B:609:TYR:CZ	2.17	0.80

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:4:THR:HG23	4:B:932:HOH:O	1.81	0.80
1:B:90:THR:HG22	1:B:92:ALA:N	1.95	0.79
1:B:174:THR:HB	3:B:701:GOL:H31	1.64	0.79
1:B:130:LEU:H	1:B:395:ASN:ND2	1.82	0.77
1:A:79:LYS:HG2	1:A:81:ASN:HB2	1.67	0.77
1:A:90:THR:HG22	1:A:92:ALA:N	1.98	0.77
1:B:317:THR:HG21	1:B:338:ILE:HG21	1.67	0.77
1:A:130:LEU:H	1:A:395:ASN:ND2	1.80	0.76
1:B:458:THR:HB	4:B:923:HOH:O	1.85	0.76
1:A:121:THR:HG21	1:A:157:SER:OG	1.85	0.75
1:B:106:VAL:CG2	1:B:229:MSE:HE2	2.17	0.75
1:A:4:THR:HG23	4:A:924:HOH:O	1.85	0.75
1:B:429:THR:HG21	4:B:823:HOH:O	1.85	0.75
1:A:429:THR:HG21	4:A:812:HOH:O	1.86	0.75
1:B:556:ASP:HB3	1:B:557:ARG:HG2	1.69	0.75
1:B:186:ASN:ND2	1:B:458:THR:HG22	1.97	0.74
1:B:426:ASN:ND2	1:B:427:GLY:H	1.84	0.74
1:A:79:LYS:CA	1:A:121:THR:HG22	2.16	0.73
1:B:35:GLN:HE21	1:B:44:TRP:HE1	1.37	0.72
1:B:540:ASP:HB3	1:B:541:GLY:CA	2.18	0.72
1:A:80:ASP:OD1	1:A:90:THR:HB	1.91	0.70
1:A:145:ASN:HD22	1:A:147:LYS:H	1.38	0.70
1:A:426:ASN:ND2	1:A:427:GLY:H	1.87	0.69
1:B:300:LEU:O	1:B:303:CYS:HB2	1.93	0.68
1:B:131:VAL:O	1:B:149:VAL:HG13	1.93	0.67
1:B:540:ASP:CB	1:B:541:GLY:CA	2.72	0.67
1:B:90:THR:CG2	1:B:92:ALA:N	2.57	0.64
1:A:607:LYS:HB2	1:A:608:PRO:CD	2.28	0.64
1:B:130:LEU:N	1:B:395:ASN:HD21	1.90	0.64
1:B:490:GLY:O	1:B:496:LEU:HD12	1.98	0.64
1:B:536:ARG:HG3	1:B:592:TYR:CZ	2.33	0.64
1:B:481:LEU:C	1:B:481:LEU:HD12	2.18	0.64
1:A:79:LYS:HA	1:A:121:THR:CG2	2.22	0.63
1:A:603:PHE:HB3	1:A:608:PRO:HB2	1.80	0.63
1:A:145:ASN:ND2	1:A:147:LYS:H	1.95	0.63
1:A:106:VAL:CG2	1:A:229:MSE:CE	2.69	0.63
1:A:130:LEU:N	1:A:395:ASN:HD21	1.87	0.62
1:A:464:ASP:HA	1:A:466:ARG:HH21	1.64	0.62
1:A:145:ASN:HD22	1:A:145:ASN:C	2.02	0.62
1:A:504:LYS:O	1:A:557:ARG:NH2	2.33	0.61
1:B:377:THR:OG1	1:B:429:THR:HG22	2.00	0.61
1:A:607:LYS:HB2	1:A:608:PRO:HD3	1.83	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:468:THR:CG2	1:B:469:VAL:N	2.63	0.61
1:B:80:ASP:OD1	1:B:90:THR:HB	2.01	0.61
1:B:275:TYR:HD1	1:B:428:ILE:HD11	1.65	0.61
1:B:468:THR:HG22	1:B:469:VAL:H	1.65	0.60
1:B:275:TYR:CD1	1:B:428:ILE:HD11	2.36	0.60
1:A:81:ASN:HB3	1:A:82:ILE:HG13	1.82	0.60
1:B:56:GLN:HE22	1:B:117:VAL:H	1.49	0.60
1:A:16:HIS:CE1	1:A:24:SER:HB2	2.37	0.60
1:B:35:GLN:NE2	1:B:44:TRP:HE1	2.00	0.59
1:B:186:ASN:ND2	1:B:458:THR:CG2	2.59	0.59
1:B:145:ASN:HD22	1:B:145:ASN:C	2.05	0.59
1:B:396:SER:HB3	4:B:938:HOH:O	2.03	0.59
1:B:79:LYS:HA	1:B:121:THR:HG22	1.85	0.59
1:B:487:ALA:HB3	1:B:584:SER:HB2	1.85	0.59
1:A:161:VAL:HG12	1:A:187:LEU:HD22	1.83	0.58
1:A:320:PHE:O	1:A:323:THR:HB	2.02	0.58
1:B:313:ARG:HH22	3:B:701:GOL:H11	1.69	0.58
1:B:191:LYS:HE2	1:B:192:PRO:O	2.04	0.58
1:A:205:ALA:O	1:A:206:CYS:CB	2.48	0.57
1:A:16:HIS:ND1	1:A:24:SER:HB2	2.19	0.57
1:A:175:ALA:HB3	2:A:701:TAR:H3	1.85	0.57
1:B:492:HIS:O	1:B:499:HIS:HD2	1.87	0.57
1:B:487:ALA:HB3	1:B:584:SER:CB	2.35	0.57
1:A:600:ILE:HD11	1:A:609:TYR:CZ	2.40	0.57
1:B:145:ASN:HD22	1:B:147:LYS:N	1.98	0.57
1:A:162:GLY:HA2	1:A:187:LEU:HD21	1.87	0.57
1:A:241:ARG:HG3	4:A:820:HOH:O	2.04	0.56
1:A:547:GLN:HE21	1:A:547:GLN:HA	1.70	0.56
1:B:143:VAL:HG22	1:B:163:ARG:HG3	1.88	0.56
1:B:106:VAL:HG22	1:B:229:MSE:CE	2.31	0.55
1:B:79:LYS:C	1:B:81:ASN:H	2.09	0.55
1:B:465:ARG:O	1:B:466:ARG:HD3	2.06	0.55
1:B:540:ASP:CG	1:B:541:GLY:HA2	2.27	0.55
1:A:600:ILE:HD11	1:A:609:TYR:CE1	2.42	0.55
1:B:143:VAL:HG13	1:B:461:LYS:HB3	1.87	0.55
1:A:75:PRO:HB2	1:A:118:ILE:CD1	2.36	0.55
1:A:295:GLU:HB3	1:A:296:PRO:HD3	1.88	0.55
1:A:66:LYS:O	1:A:67:GLU:HB2	2.06	0.55
1:A:38:ALA:CB	1:A:39:PRO:HD2	2.36	0.54
1:B:121:THR:HG21	1:B:157:SER:OG	2.06	0.54
1:B:468:THR:HG22	1:B:469:VAL:N	2.22	0.54
1:B:420:ARG:HH11	1:B:424:LEU:HB2	1.73	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:90:THR:CG2	1:A:92:ALA:N	2.68	0.54
1:A:191:LYS:HE2	1:A:192:PRO:O	2.06	0.54
1:A:121:THR:HG23	4:A:811:HOH:O	2.07	0.54
1:A:65:ASN:O	1:A:68:GLU:HB2	2.08	0.54
1:B:377:THR:HA	1:B:429:THR:CG2	2.38	0.54
1:A:375:VAL:HG13	1:A:401:TRP:HB3	1.90	0.54
1:B:317:THR:HG23	1:B:321:LEU:CD1	2.39	0.53
1:A:296:PRO:HG2	1:A:366:LEU:HD22	1.91	0.53
1:B:241:ARG:HD2	4:B:801:HOH:O	2.08	0.53
1:B:420:ARG:HG2	1:B:424:LEU:O	2.09	0.53
1:A:38:ALA:HB3	1:A:39:PRO:HD2	1.90	0.53
1:B:191:LYS:NZ	1:B:406:ASN:HD21	2.06	0.53
1:A:36:LYS:O	1:A:41:ASP:HB3	2.08	0.53
1:A:191:LYS:NZ	1:A:406:ASN:HD21	2.06	0.53
1:A:377:THR:OG1	1:A:429:THR:HG22	2.09	0.53
1:B:519:TYR:CZ	1:B:537:ARG:HG3	2.44	0.53
1:B:489:VAL:O	1:B:489:VAL:HG22	2.09	0.53
1:A:611:GLU:C	1:A:613:ILE:H	2.12	0.52
1:A:38:ALA:HB3	1:A:39:PRO:CD	2.39	0.52
1:A:490:GLY:HA2	1:A:533:PRO:HG3	1.90	0.51
1:B:79:LYS:HE3	1:B:154:SER:HA	1.92	0.51
1:A:75:PRO:O	1:A:166:VAL:HG22	2.09	0.51
1:B:302:ARG:O	1:B:304:LEU:N	2.43	0.51
1:A:186:ASN:ND2	1:A:458:THR:HG22	2.19	0.51
1:A:492:HIS:NE2	1:A:501:GLN:OE1	2.36	0.51
1:B:600:ILE:CD1	1:B:609:TYR:CZ	2.91	0.51
1:A:490:GLY:HA3	1:A:533:PRO:CG	2.41	0.51
1:A:487:ALA:HB3	1:A:584:SER:HB2	1.93	0.51
1:A:75:PRO:O	1:A:167:PRO:HD2	2.11	0.50
1:A:66:LYS:O	1:A:67:GLU:CB	2.58	0.50
1:A:149:VAL:HG13	1:A:151:GLY:H	1.74	0.50
1:A:536:ARG:HD3	1:A:538:VAL:HG23	1.92	0.50
1:B:317:THR:CG2	1:B:338:ILE:HG21	2.40	0.49
1:B:121:THR:CG2	4:B:822:HOH:O	2.60	0.49
1:B:402:THR:HG22	4:B:823:HOH:O	2.12	0.49
1:B:206:CYS:HA	1:B:312:GLU:CB	2.43	0.49
1:A:589:GLU:O	1:A:593:THR:HB	2.13	0.49
1:B:302:ARG:O	1:B:303:CYS:C	2.50	0.49
1:A:477:SER:OG	1:A:479:ASP:HB2	2.13	0.48
1:A:90:THR:HG23	1:A:93:CYS:H	1.76	0.48
1:A:78:VAL:O	1:A:120:LYS:HA	2.13	0.48
1:B:331:ASP:O	1:B:335:VAL:HG23	2.13	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:271:ASN:OD1	1:A:420:ARG:HD2	2.13	0.48
1:B:188:ILE:HD12	1:B:219:LEU:CD1	2.42	0.48
1:B:434:LYS:HG2	4:B:840:HOH:O	2.12	0.48
1:A:75:PRO:HB2	1:A:118:ILE:HD11	1.95	0.48
1:A:290:VAL:HG12	1:A:292:VAL:HG23	1.95	0.48
1:A:490:GLY:CA	1:A:533:PRO:HG3	2.43	0.47
1:B:219:LEU:HB3	1:B:473:LEU:HD21	1.96	0.47
1:A:220:SER:HB2	1:A:470:GLU:O	2.14	0.47
1:B:606:PHE:CZ	1:B:610:ILE:HD11	2.49	0.47
1:B:521:LEU:O	1:B:600:ILE:HG22	2.14	0.47
1:A:521:LEU:HB2	1:A:546:ILE:HG12	1.97	0.47
1:B:131:VAL:HG13	1:B:395:ASN:HD22	1.80	0.47
1:B:317:THR:HG23	1:B:321:LEU:HD12	1.97	0.47
1:A:567:GLU:HG2	1:A:568:PRO:HA	1.97	0.47
1:B:515:THR:HB	1:B:519:TYR:CD1	2.49	0.47
1:A:56:GLN:HE22	1:A:117:VAL:H	1.63	0.47
1:B:313:ARG:NH2	3:B:701:GOL:C1	2.77	0.46
1:A:417:SER:OG	1:A:427:GLY:HA2	2.15	0.46
1:A:125:GLN:HG2	1:A:126:PHE:CD1	2.50	0.46
1:A:420:ARG:HG3	1:A:424:LEU:O	2.14	0.46
1:B:191:LYS:CE	1:B:192:PRO:O	2.63	0.46
1:A:163:ARG:HG3	1:A:165:ILE:CD1	2.45	0.46
1:B:45:ILE:HD13	1:B:90:THR:HG21	1.97	0.46
1:B:56:GLN:HE22	1:B:117:VAL:N	2.14	0.46
1:A:567:GLU:CG	1:B:537:ARG:HH22	2.29	0.46
1:B:297:LEU:HD22	1:B:404:PHE:CD1	2.49	0.45
1:B:519:TYR:CE2	1:B:537:ARG:HG3	2.50	0.45
1:B:520:LYS:HG2	1:B:601:THR:OG1	2.16	0.45
1:B:313:ARG:NH2	3:B:701:GOL:H11	2.31	0.45
1:B:464:ASP:HB2	4:B:936:HOH:O	2.15	0.45
1:A:592:TYR:OH	1:B:589:GLU:CG	2.55	0.45
1:B:556:ASP:HB2	4:B:838:HOH:O	2.16	0.45
1:B:205:ALA:HB2	4:B:843:HOH:O	2.17	0.45
1:A:206:CYS:HA	1:A:312:GLU:CB	2.47	0.45
1:A:547:GLN:NE2	1:A:548:LEU:H	2.14	0.45
1:B:420:ARG:NH1	1:B:422:ASP:OD2	2.49	0.45
1:A:93:CYS:HA	1:A:125:GLN:HE21	1.82	0.44
1:A:547:GLN:NE2	1:A:547:GLN:HA	2.31	0.44
1:A:57:TRP:O	1:A:61:GLN:HG2	2.17	0.44
1:A:45:ILE:HD13	1:A:90:THR:HG21	2.00	0.44
1:A:589:GLU:HA	1:A:592:TYR:CZ	2.53	0.44
1:B:600:ILE:HG12	1:B:609:TYR:CG	2.53	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:81:ASN:HB3	1:B:82:ILE:HG13	1.98	0.44
1:B:191:LYS:HE3	1:B:211:CYS:SG	2.58	0.44
1:A:191:LYS:NZ	1:A:406:ASN:ND2	2.66	0.44
1:B:75:PRO:HB2	1:B:166:VAL:HG22	2.00	0.44
1:B:245:LYS:HD2	1:B:480:THR:O	2.17	0.44
1:B:173:ASP:C	1:B:173:ASP:OD1	2.56	0.44
1:B:162:GLY:HA2	1:B:187:LEU:HD21	1.99	0.44
1:B:78:VAL:HG22	1:B:120:LYS:HE3	1.99	0.44
1:B:377:THR:HA	1:B:429:THR:HG23	2.00	0.44
1:A:452:PHE:CD1	1:A:457:ARG:HG3	2.52	0.44
1:A:78:VAL:HG22	1:A:120:LYS:HE3	1.99	0.43
1:A:206:CYS:HA	1:A:312:GLU:HB3	1.99	0.43
1:A:7:TRP:O	1:A:167:PRO:HB3	2.18	0.43
1:B:143:VAL:HG22	1:B:163:ARG:CG	2.47	0.43
1:B:145:ASN:ND2	1:B:145:ASN:C	2.71	0.43
1:B:191:LYS:C	1:B:191:LYS:HE2	2.39	0.43
1:B:44:TRP:CZ3	1:B:119:GLY:HA3	2.54	0.43
1:B:458:THR:CG2	1:B:459:TYR:N	2.79	0.43
1:B:593:THR:CG2	1:B:593:THR:O	2.66	0.43
1:B:191:LYS:NZ	1:B:406:ASN:ND2	2.67	0.43
1:B:478:LYS:O	1:B:481:LEU:HG	2.19	0.43
1:A:15:PHE:HA	1:A:18:LYS:HE2	2.00	0.43
1:B:218:ASN:HB2	1:B:470:GLU:O	2.18	0.43
1:A:524:LEU:HB2	1:A:532:LYS:O	2.19	0.43
1:B:538:VAL:C	1:B:540:ASP:H	2.22	0.43
1:B:572:GLY:O	1:B:584:SER:N	2.44	0.43
1:A:283:LYS:HB2	1:A:283:LYS:HE2	1.74	0.43
1:A:29:GLU:OE2	1:A:54:HIS:CE1	2.72	0.43
1:B:526:LYS:HB2	1:B:531:LEU:HD13	2.00	0.42
1:A:1:MSE:HB2	1:A:2:GLU:H	1.66	0.42
1:A:402:THR:HG22	4:A:812:HOH:O	2.19	0.42
1:B:12:TRP:CZ2	1:B:75:PRO:HG3	2.53	0.42
1:B:209:LEU:HD21	1:B:407:LEU:HD23	2.01	0.42
1:B:145:ASN:HD21	1:B:147:LYS:HB2	1.85	0.42
1:B:156:GLY:O	1:B:160:VAL:HB	2.20	0.42
1:B:106:VAL:HB	4:B:805:HOH:O	2.20	0.42
1:A:247:PRO:HA	4:A:830:HOH:O	2.20	0.42
1:A:426:ASN:HD22	1:A:427:GLY:N	1.93	0.42
1:B:519:TYR:HB3	1:B:546:ILE:HD13	2.02	0.42
1:A:124:ASP:HB2	1:A:153:SER:HB2	2.01	0.42
1:A:270:GLU:HB3	1:A:420:ARG:HB3	2.02	0.42
1:A:165:ILE:N	1:A:165:ILE:CD1	2.83	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:490:GLY:HA3	1:A:533:PRO:HG2	2.01	0.42
1:A:533:PRO:HD3	1:A:606:PHE:CZ	2.55	0.42
1:A:437:ASP:N	1:A:437:ASP:OD1	2.52	0.42
1:B:375:VAL:HG22	1:B:376:PRO:HD2	2.02	0.42
1:A:497:PRO:O	1:A:498:LEU:HD23	2.20	0.41
1:B:481:LEU:O	1:B:481:LEU:HD12	2.19	0.41
1:B:487:ALA:HB3	1:B:584:SER:HB3	2.03	0.41
1:B:546:ILE:N	1:B:546:ILE:HD12	2.34	0.41
1:A:375:VAL:CG1	1:A:401:TRP:HB3	2.50	0.41
1:A:106:VAL:HG22	1:A:229:MSE:HE3	1.94	0.41
1:B:174:THR:CB	3:B:701:GOL:H31	2.43	0.41
1:B:121:THR:HG21	1:B:157:SER:N	2.35	0.41
1:A:377:THR:HA	1:A:429:THR:CG2	2.50	0.41
1:B:143:VAL:CG2	1:B:163:ARG:HG3	2.50	0.41
1:B:390:GLU:HB2	1:B:394:VAL:HG23	2.02	0.41
1:B:217:LEU:HG	1:B:459:TYR:HD1	1.85	0.41
1:B:265:TRP:CD2	1:B:272:PRO:HG3	2.55	0.41
1:B:65:ASN:O	1:B:67:GLU:N	2.54	0.41
1:A:15:PHE:CZ	1:A:27:LEU:HD22	2.55	0.41
1:B:564:MSE:O	1:B:566:PRO:HD3	2.20	0.40
1:A:66:LYS:HG3	1:A:66:LYS:H	1.50	0.40
1:A:464:ASP:HA	1:A:466:ARG:NH2	2.35	0.40
1:B:414:ALA:HA	1:B:429:THR:HB	2.02	0.40
1:B:60:LEU:HD12	1:B:60:LEU:HA	1.90	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	612/644 (95%)	563 (92%)	42 (7%)	7 (1%)	21	34
1	B	610/644 (95%)	580 (95%)	23 (4%)	7 (1%)	21	34
All	All	1222/1288 (95%)	1143 (94%)	65 (5%)	14 (1%)	21	34

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	38	ALA
1	B	66	LYS
1	B	303	CYS
1	A	206	CYS
1	A	479	ASP
1	B	206	CYS
1	B	422	ASP
1	B	528	GLY
1	B	556	ASP
1	A	104	SER
1	A	517	ASN
1	A	612	HIS
1	B	540	ASP
1	A	37	PRO

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	524/544 (96%)	469 (90%)	55 (10%)	10	18
1	B	522/544 (96%)	462 (88%)	60 (12%)	8	15
All	All	1046/1088 (96%)	931 (89%)	115 (11%)	9	16

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MSE
1	A	2	GLU
1	A	4	THR
1	A	18	LYS
1	A	60	LEU
1	A	62	SER
1	A	66	LYS
1	A	67	GLU
1	A	90	THR
1	A	95	SER

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Mol	Chain	Res	Type
1	A	106	VAL
1	A	116	VAL
1	A	121	THR
1	A	123	LEU
1	A	143	VAL
1	A	145	ASN
1	A	149	VAL
1	A	165	ILE
1	A	166	VAL
1	A	170	LEU
1	A	191	LYS
1	A	194	LYS
1	A	202	VAL
1	A	219	LEU
1	A	231	LYS
1	A	241	ARG
1	A	243	PHE
1	A	269	THR
1	A	283	LYS
1	A	305	TYR
1	A	310	VAL
1	A	323	THR
1	A	343	LYS
1	A	356	ARG
1	A	368	LYS
1	A	375	VAL
1	A	385	GLU
1	A	387	VAL
1	A	393	LEU
1	A	415	VAL
1	A	420	ARG
1	A	426	ASN
1	A	429	THR
1	A	434	LYS
1	A	437	ASP
1	A	445	LYS
1	A	469	VAL
1	A	538	VAL
1	A	539	ASN
1	A	540	ASP
1	A	547	GLN
1	A	574	VAL

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Mol	Chain	Res	Type
1	A	582	VAL
1	A	593	THR
1	A	600	ILE
1	B	4	THR
1	B	25	LEU
1	B	27	LEU
1	B	29	GLU
1	B	31	LEU
1	B	81	ASN
1	B	90	THR
1	B	106	VAL
1	B	118	ILE
1	B	121	THR
1	B	143	VAL
1	B	145	ASN
1	B	166	VAL
1	B	184	LEU
1	B	194	LYS
1	B	202	VAL
1	B	217	LEU
1	B	219	LEU
1	B	220	SER
1	B	241	ARG
1	B	243	PHE
1	B	277	LYS
1	B	302	ARG
1	B	303	CYS
1	B	304	LEU
1	B	305	TYR
1	B	317	THR
1	B	345	ASP
1	B	351	LYS
1	B	368	LYS
1	B	369	ASP
1	B	370	ILE
1	B	375	VAL
1	B	393	LEU
1	B	415	VAL
1	B	420	ARG
1	B	426	ASN
1	B	428	ILE
1	B	429	THR

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Mol	Chain	Res	Type
1	B	433	LYS
1	B	437	ASP
1	B	445	LYS
1	B	458	THR
1	B	468	THR
1	B	478	LYS
1	B	517	ASN
1	B	518	ASN
1	B	526	LYS
1	B	536	ARG
1	B	537	ARG
1	B	538	VAL
1	B	542	THR
1	B	547	GLN
1	B	556	ASP
1	B	567	GLU
1	B	573	SER
1	B	582	VAL
1	B	589	GLU
1	B	600	ILE
1	B	614	GLN

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

Mol	Chain	Res	Type
1	A	56	GLN
1	A	99	GLN
1	A	145	ASN
1	A	186	ASN
1	A	357	GLN
1	A	395	ASN
1	A	406	ASN
1	A	426	ASN
1	A	539	ASN
1	A	545	GLN
1	A	547	GLN
1	B	10	GLN
1	B	35	GLN
1	B	56	GLN
1	B	58	ASN
1	B	145	ASN
1	B	186	ASN

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Mol	Chain	Res	Type
1	B	357	GLN
1	B	395	ASN
1	B	406	ASN
1	B	426	ASN
1	B	499	HIS
1	B	547	GLN
1	B	614	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

2 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	$\# Z > 2$
2	TAR	A	701	-	9,9,9	1.22	0	12,12,12	1.58	2 (16%)
3	GOL	B	701	-	5,5,5	0.54	0	5,5,5	0.79	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	TAR	A	701	-	-	0/12/12/12	0/0/0/0
3	GOL	B	701	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	A	701	TAR	O2-C2-C3	-3.15	103.67	110.19
2	A	701	TAR	O11-C1-C2	2.77	121.96	113.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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, 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	614/644 (95%)	-0.11	3 (0%) 88 90	18, 36, 71, 134	0
1	B	612/644 (95%)	-0.25	4 (0%) 84 86	18, 33, 60, 103	0
All	All	1226/1288 (95%)	-0.18	7 (0%) 86 88	18, 34, 66, 134	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MSE	5.3
1	B	305	TYR	2.9
1	B	454	ASN	2.8
1	A	527	VAL	2.7
1	B	540	ASP	2.4
1	A	72	TYR	2.1
1	B	602	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates 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. 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, 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	GOL	B	701	6/6	0.22	2.00	43,44,52,55	0
2	TAR	A	701	10/10	0.18	1.00	52,61,80,81	0

6.5 Other polymers ⓘ

There are no such residues in this entry.