



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 02:33 AM UTC

PDB ID : 3VA7 / pdb_00003va7
Title : Crystal structure of the Kluyveromyces lactis Urea Carboxylase
Authors : Fan, C.; Xiang, S.
Deposited on : 2011-12-29
Resolution : 2.60 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

<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

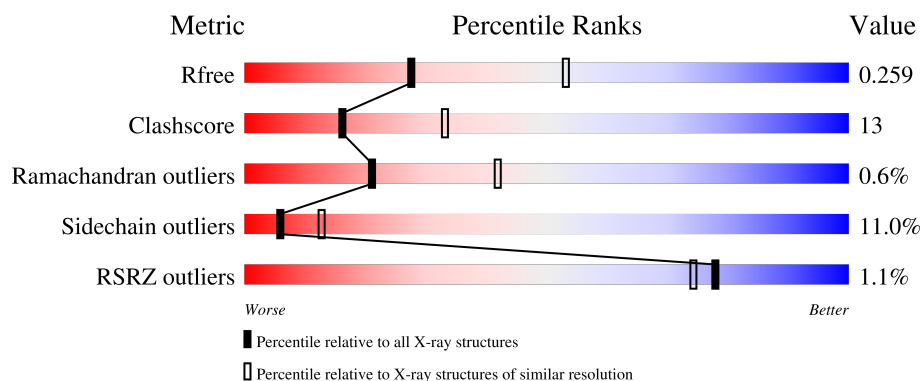
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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 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	1236	

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	URE	A	1902	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	A	1905	-	-	X	-
4	GOL	A	1906	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9268 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.

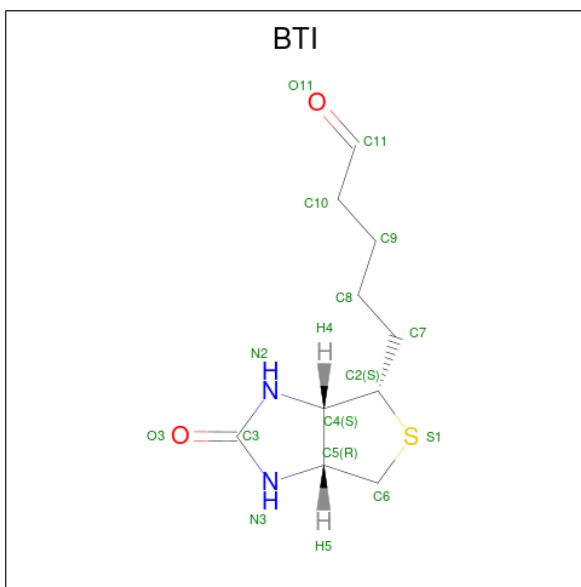
- Molecule 1 is a protein called KLLA0E08119p.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1130	8829	5608	1499	1686	36	0	0	0

There are 23 discrepancies between the modelled and reference sequences:

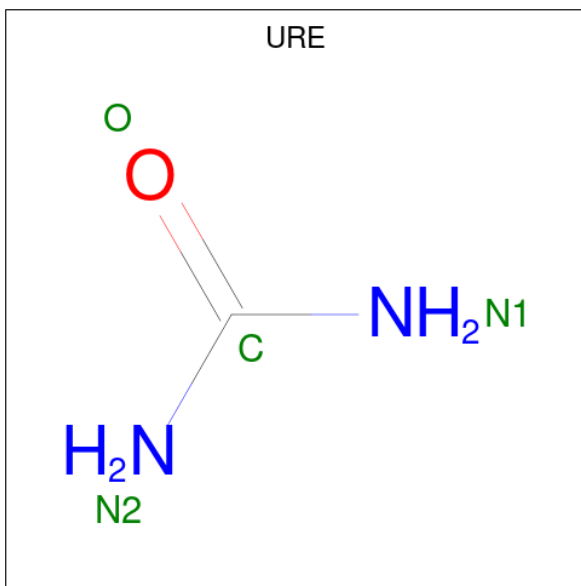
Chain	Residue	Modelled	Actual	Comment	Reference
A	594	MET	-	expression tag	UNP Q6CP22
A	595	GLY	-	expression tag	UNP Q6CP22
A	596	SER	-	expression tag	UNP Q6CP22
A	597	SER	-	expression tag	UNP Q6CP22
A	598	HIS	-	expression tag	UNP Q6CP22
A	599	HIS	-	expression tag	UNP Q6CP22
A	600	HIS	-	expression tag	UNP Q6CP22
A	601	HIS	-	expression tag	UNP Q6CP22
A	602	HIS	-	expression tag	UNP Q6CP22
A	603	HIS	-	expression tag	UNP Q6CP22
A	604	SER	-	expression tag	UNP Q6CP22
A	605	SER	-	expression tag	UNP Q6CP22
A	606	GLY	-	expression tag	UNP Q6CP22
A	607	LEU	-	expression tag	UNP Q6CP22
A	608	VAL	-	expression tag	UNP Q6CP22
A	609	PRO	-	expression tag	UNP Q6CP22
A	610	ARG	-	expression tag	UNP Q6CP22
A	611	GLY	-	expression tag	UNP Q6CP22
A	612	SER	-	expression tag	UNP Q6CP22
A	613	HIS	-	expression tag	UNP Q6CP22
A	614	MET	-	expression tag	UNP Q6CP22
A	615	ALA	-	expression tag	UNP Q6CP22
A	616	SER	-	expression tag	UNP Q6CP22

- Molecule 2 is 5-(HEXAHYDRO-2-OXO-1H-THIENO[3,4-D]IMIDAZOL-6-YL)PENTANAL (CCD ID: BTI) (formula: C₁₀H₁₆N₂O₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			15	10	2	2	1		

- Molecule 3 is UREA (CCD ID: URE) (formula: $\text{CH}_4\text{N}_2\text{O}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			4	1	2	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).



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

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Na	0	0
			1	1		

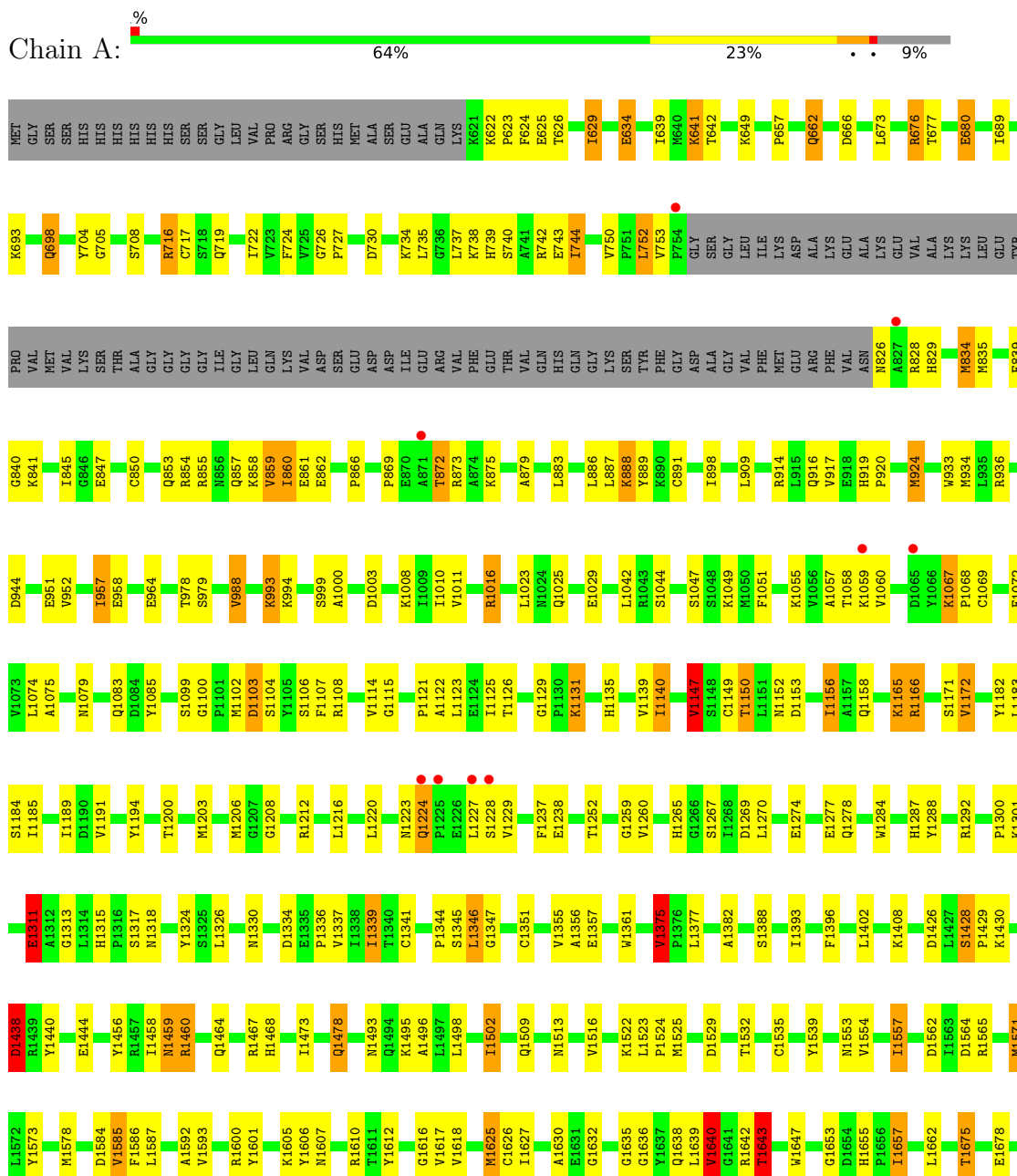
- Molecule 6 is water.

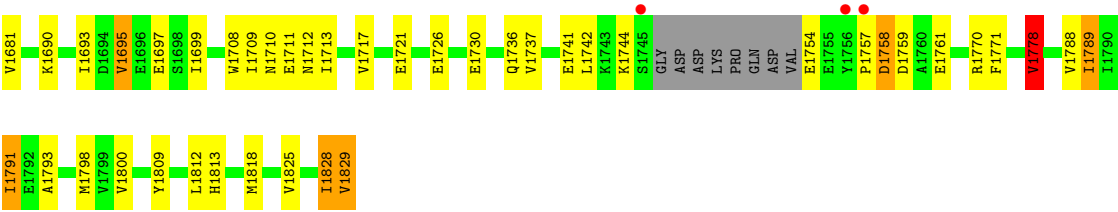
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	377	Total	O	0	0
			377	377		

3 Residue-property plots

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: KLLA0E08119p





4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	126.66Å 126.66Å 217.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.60 50.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.1 (50.00-2.60) 99.1 (50.00-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.75 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.187 , 0.255 (Not available) , 0.259	Depositor DCC
R_{free} test set	2790 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	40.0	Xtriage
Anisotropy	0.512	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9268	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% 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

5.1 Standard geometry

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

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	1.13	9/9017 (0.1%)	1.21	43/12220 (0.4%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1099	SER	C-O	-6.57	1.18	1.24
1	A	1778	VAL	CA-CB	6.35	1.61	1.54
1	A	1339	ILE	CA-CB	6.06	1.61	1.53
1	A	1182	TYR	CA-C	-5.96	1.45	1.52
1	A	1438	ASP	CA-C	5.85	1.60	1.52
1	A	988	VAL	CA-CB	5.65	1.61	1.54
1	A	1699	ILE	CA-CB	5.57	1.61	1.54
1	A	1737	VAL	CA-CB	5.38	1.60	1.54
1	A	839	PHE	CA-C	-5.16	1.46	1.53

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1643	THR	CB-CA-C	-9.49	98.09	113.37
1	A	673	LEU	N-CA-C	-7.38	98.59	110.32
1	A	1557	ILE	CB-CA-C	-6.91	103.04	111.88
1	A	1593	VAL	CA-C-N	-6.81	112.95	119.76
1	A	1593	VAL	C-N-CA	-6.81	112.95	119.76
1	A	629	ILE	CB-CA-C	-6.78	101.82	111.31
1	A	1238	GLU	CA-C-N	-6.70	112.76	119.92
1	A	1238	GLU	C-N-CA	-6.70	112.76	119.92
1	A	1502	ILE	CB-CA-C	-6.61	102.41	112.05
1	A	673	LEU	CA-C-N	-6.46	114.08	123.00
1	A	673	LEU	C-N-CA	-6.46	114.08	123.00
1	A	1438	ASP	N-CA-CB	-6.44	99.60	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1557	ILE	N-CA-CB	6.33	117.53	110.51
1	A	1788	VAL	CB-CA-C	-6.25	105.48	111.05
1	A	1049	LYS	N-CA-C	-6.18	104.63	111.36
1	A	924	MET	N-CA-C	-6.12	103.93	111.40
1	A	1812	LEU	N-CA-C	6.11	118.02	111.36
1	A	1695	VAL	CB-CA-C	-5.92	101.69	110.33
1	A	1060	VAL	N-CA-C	5.84	116.31	110.23
1	A	1228	SER	N-CA-C	5.76	118.86	109.06
1	A	1147	VAL	CB-CA-C	-5.70	100.84	110.71
1	A	988	VAL	CB-CA-C	5.67	118.08	110.42
1	A	1375	VAL	CB-CA-C	5.50	116.63	110.52
1	A	1513	ASN	N-CA-C	5.46	119.05	112.93
1	A	1655	HIS	CA-C-N	-5.45	113.02	119.84
1	A	1655	HIS	C-N-CA	-5.45	113.02	119.84
1	A	1440	TYR	CB-CA-C	-5.40	100.58	110.62
1	A	1341	CYS	N-CA-C	5.40	118.96	112.38
1	A	1375	VAL	N-CA-CB	-5.39	104.20	111.86
1	A	1758	ASP	N-CA-C	5.39	118.08	111.82
1	A	1010	ILE	N-CA-C	5.38	115.64	108.11
1	A	639	ILE	N-CA-C	-5.36	105.31	110.72
1	A	1067	LYS	CA-C-N	5.32	125.58	119.83
1	A	1067	LYS	C-N-CA	5.32	125.58	119.83
1	A	1640	VAL	N-CA-CB	-5.25	102.56	111.23
1	A	1535	CYS	N-CA-C	-5.23	105.66	111.36
1	A	1681	VAL	N-CA-C	-5.19	105.65	110.53
1	A	994	LYS	N-CA-C	-5.18	102.62	110.24
1	A	642	THR	N-CA-C	-5.17	105.56	111.14
1	A	1311	GLU	N-CA-C	5.09	118.27	111.75
1	A	1029	GLU	N-CA-C	-5.06	106.80	113.17
1	A	1129	GLY	CA-C-N	5.01	126.13	120.66
1	A	1129	GLY	C-N-CA	5.01	126.13	120.66

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	8829	0	8753	230	0
2	A	15	0	15	0	0
3	A	4	0	4	3	0
4	A	42	0	56	22	0
5	A	1	0	0	0	0
6	A	377	0	0	17	0
All	All	9268	0	8828	232	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 13.

All (232) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:914:ARG:HA	4:A:1905:GOL:H32	1.27	1.12
1:A:1625:MET:HE1	1:A:1627:ILE:HG13	1.34	1.05
1:A:1025:GLN:HG3	6:A:2003:HOH:O	1.52	1.04
1:A:1625:MET:HE2	1:A:1626:CYS:C	1.89	0.96
1:A:1565:ARG:HD3	6:A:2069:HOH:O	1.68	0.94
1:A:1459:ASN:HD21	1:A:1460:ARG:HH11	1.15	0.93
1:A:1553:ASN:HD22	1:A:1639:LEU:H	1.22	0.88
1:A:1311:GLU:HG3	6:A:2196:HOH:O	1.73	0.87
1:A:914:ARG:CA	4:A:1905:GOL:H32	2.06	0.85
1:A:1108:ARG:HD2	6:A:2024:HOH:O	1.74	0.85
1:A:934:MET:HE3	4:A:1905:GOL:H11	1.58	0.84
1:A:860:ILE:HG23	1:A:957:ILE:CD1	2.08	0.84
1:A:860:ILE:HG23	1:A:957:ILE:HD11	1.60	0.84
1:A:726:GLY:HA2	4:A:1905:GOL:H2	1.63	0.79
1:A:1126:THR:HG21	4:A:1908:GOL:H32	1.66	0.78
1:A:1636:GLY:H	3:A:1902:URE:HN12	1.28	0.77
1:A:859:VAL:HG23	1:A:860:ILE:HD12	1.66	0.76
1:A:1313:GLY:HA3	1:A:1318:ASN:HD22	1.49	0.75
1:A:1259:GLY:HA2	1:A:1375:VAL:HG12	1.69	0.74
1:A:1789:ILE:HG13	1:A:1800:VAL:CG1	2.17	0.74
1:A:1625:MET:HE2	1:A:1626:CYS:O	1.88	0.74
1:A:934:MET:CE	4:A:1905:GOL:H11	2.19	0.72
1:A:726:GLY:CA	4:A:1905:GOL:H2	2.20	0.72
1:A:861:GLU:O	1:A:957:ILE:HD12	1.89	0.72
1:A:1458:ILE:HG21	1:A:1478:GLN:HG2	1.73	0.71
1:A:1708:TRP:HE3	1:A:1709:ILE:HD12	1.55	0.71
1:A:834:MET:HE1	1:A:889:TYR:CD2	2.27	0.70
1:A:1625:MET:CE	1:A:1626:CYS:C	2.64	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1585:VAL:HG13	1:A:1586:PHE:CD1	2.28	0.69
1:A:857:GLN:HB2	4:A:1906:GOL:H32	1.75	0.68
1:A:1165:LYS:O	1:A:1166:ARG:CB	2.41	0.68
1:A:705:GLY:O	1:A:708:SER:HB2	1.94	0.68
1:A:634:GLU:CD	1:A:1008:LYS:HE2	2.20	0.67
1:A:1459:ASN:ND2	1:A:1460:ARG:HD2	2.10	0.67
1:A:1564:ASP:HB2	6:A:2219:HOH:O	1.96	0.66
1:A:857:GLN:CB	4:A:1906:GOL:H32	2.26	0.66
1:A:1789:ILE:HD11	1:A:1825:VAL:HG21	1.77	0.66
1:A:1114:VAL:HG12	1:A:1114:VAL:O	1.97	0.65
1:A:964:GLU:OE1	4:A:1906:GOL:H12	1.96	0.65
1:A:1075:ALA:HB3	1:A:1131:LYS:HG2	1.79	0.65
1:A:1203:MET:CE	1:A:1630:ALA:CB	2.74	0.65
1:A:742:ARG:HH22	1:A:753:VAL:HB	1.62	0.64
1:A:1318:ASN:HD21	1:A:1605:LYS:H	1.45	0.64
1:A:1625:MET:HE2	1:A:1626:CYS:CA	2.27	0.64
1:A:626:THR:HG22	1:A:649:LYS:HB2	1.78	0.64
1:A:1636:GLY:N	3:A:1902:URE:HN12	1.96	0.63
1:A:1524:PRO:O	1:A:1643:THR:HG23	2.00	0.62
1:A:1571:MET:HG2	1:A:1601:TYR:CE2	2.34	0.62
1:A:916:GLN:HB2	6:A:2075:HOH:O	1.99	0.60
1:A:1150:THR:HG23	1:A:1153:ASP:H	1.66	0.60
1:A:744:ILE:CG2	1:A:886:LEU:HD23	2.30	0.60
1:A:752:LEU:HD12	1:A:752:LEU:H	1.66	0.60
1:A:883:LEU:HD23	1:A:887:LEU:HD12	1.84	0.59
1:A:1553:ASN:HB3	1:A:1638:GLN:HE21	1.67	0.59
1:A:1464:GLN:HE22	1:A:1467:ARG:HH11	1.48	0.59
1:A:634:GLU:OE1	1:A:1008:LYS:HE2	2.02	0.59
1:A:1121:PRO:HG2	1:A:1189:ILE:H	1.66	0.59
1:A:1016:ARG:NH2	1:A:1051:PHE:O	2.36	0.59
1:A:1675:THR:HG21	6:A:2192:HOH:O	2.02	0.59
1:A:1184:SER:C	1:A:1185:ILE:HD13	2.28	0.58
1:A:1189:ILE:HG21	1:A:1220:LEU:HD23	1.85	0.58
1:A:1194:TYR:HE2	1:A:1206:MET:HE3	1.67	0.58
1:A:1789:ILE:HG13	1:A:1800:VAL:HG12	1.84	0.58
1:A:1587:LEU:HB3	1:A:1647:TRP:CD2	2.39	0.58
1:A:914:ARG:HA	4:A:1905:GOL:H12	1.84	0.58
1:A:1203:MET:CE	1:A:1630:ALA:HB3	2.34	0.57
1:A:1107:PHE:CE1	1:A:1122:ALA:HB3	2.39	0.57
1:A:1265:HIS:HD2	1:A:1351:CYS:H	1.51	0.57
1:A:1625:MET:CE	1:A:1626:CYS:O	2.53	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1203:MET:HE3	1:A:1630:ALA:CB	2.35	0.57
1:A:1000:ALA:HB1	6:A:2231:HOH:O	2.05	0.57
1:A:869:PRO:HD2	1:A:872:THR:CG2	2.35	0.57
1:A:1339:ILE:HG23	1:A:1344:PRO:HD2	1.85	0.57
1:A:1708:TRP:CE3	1:A:1709:ILE:HD12	2.38	0.56
1:A:1625:MET:HE2	1:A:1626:CYS:N	2.20	0.56
1:A:964:GLU:CD	4:A:1906:GOL:H12	2.30	0.56
1:A:1789:ILE:CG1	1:A:1800:VAL:CG1	2.82	0.56
1:A:1713:ILE:O	1:A:1717:VAL:HG23	2.05	0.56
1:A:862:GLU:OE1	1:A:1016:ARG:NH1	2.39	0.56
1:A:1771:PHE:HA	1:A:1791:ILE:CD1	2.36	0.56
1:A:957:ILE:HG12	1:A:1023:LEU:HD22	1.86	0.56
1:A:1315:HIS:HD2	1:A:1317:SER:H	1.52	0.56
1:A:1057:ALA:C	1:A:1059:LYS:H	2.13	0.55
1:A:1200:THR:OG1	1:A:1208:GLY:HA3	2.07	0.55
1:A:853:GLN:HG2	1:A:858:LYS:HG2	1.87	0.55
1:A:1778:VAL:HG13	6:A:2172:HOH:O	2.06	0.55
1:A:1553:ASN:ND2	1:A:1606:TYR:OH	2.25	0.55
1:A:1618:VAL:HG13	1:A:1625:MET:HE3	1.89	0.54
1:A:829:HIS:CD2	1:A:850:CYS:HB2	2.42	0.54
1:A:1498:LEU:O	1:A:1502:ILE:HG12	2.07	0.54
1:A:1131:LYS:HB3	1:A:1171:SER:HB2	1.90	0.54
1:A:1356:ALA:O	1:A:1357:GLU:C	2.48	0.53
1:A:914:ARG:HA	4:A:1905:GOL:C3	2.19	0.53
1:A:1267:SER:OG	1:A:1269:ASP:OD2	2.19	0.53
1:A:1771:PHE:CD1	1:A:1813:HIS:HB2	2.44	0.53
1:A:704:TYR:CE1	1:A:917:VAL:HG22	2.45	0.52
1:A:1793:ALA:HB3	1:A:1798:MET:HG3	1.90	0.52
1:A:1459:ASN:HD22	1:A:1460:ARG:HD2	1.74	0.52
1:A:1147:VAL:H	1:A:1158:GLN:HE22	1.58	0.52
1:A:1203:MET:CE	1:A:1630:ALA:HB1	2.40	0.52
1:A:1809:TYR:HB2	1:A:1829:VAL:HB	1.92	0.52
1:A:1139:VAL:O	1:A:1140:ILE:HD12	2.10	0.52
1:A:1493:ASN:ND2	1:A:1496:ALA:H	2.08	0.52
1:A:1459:ASN:ND2	1:A:1460:ARG:HH11	1.96	0.51
1:A:1229:VAL:O	1:A:1229:VAL:HG13	2.10	0.51
1:A:1710:ASN:C	1:A:1712:ASN:H	2.19	0.51
1:A:677:THR:OG1	1:A:680:GLU:HB2	2.10	0.51
1:A:1456:TYR:CZ	1:A:1460:ARG:HD3	2.46	0.51
1:A:859:VAL:CG2	1:A:860:ILE:HD12	2.39	0.51
1:A:1771:PHE:HA	1:A:1791:ILE:HD13	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:847:GLU:OE2	1:A:873:ARG:NH1	2.43	0.50
1:A:1149:CYS:HB2	1:A:1156:ILE:HG22	1.92	0.50
1:A:1069:CYS:SG	1:A:1224:GLN:HB2	2.51	0.50
1:A:662:GLN:OE1	1:A:666:ASP:OD1	2.29	0.50
1:A:1742:LEU:HB3	1:A:1818:MET:HE3	1.93	0.50
1:A:1203:MET:HE3	1:A:1630:ALA:HB1	1.94	0.50
1:A:860:ILE:CG2	1:A:957:ILE:HD11	2.39	0.49
1:A:1334:ASP:H	1:A:1607:ASN:ND2	2.10	0.49
1:A:744:ILE:HG22	1:A:886:LEU:HD23	1.93	0.49
1:A:1085:TYR:CD2	1:A:1108:ARG:HD3	2.48	0.49
1:A:625:GLU:H	1:A:698:GLN:NE2	2.11	0.49
1:A:1761:GLU:HB2	1:A:1828:ILE:HG13	1.94	0.49
1:A:1657:ILE:N	1:A:1657:ILE:HD13	2.28	0.49
1:A:860:ILE:CG2	1:A:957:ILE:CD1	2.88	0.49
1:A:936:ARG:HD2	6:A:2326:HOH:O	2.13	0.49
1:A:716:ARG:HG3	1:A:716:ARG:HH11	1.77	0.49
1:A:1524:PRO:O	1:A:1643:THR:CG2	2.61	0.49
1:A:1165:LYS:O	1:A:1166:ARG:HB3	2.12	0.48
1:A:1265:HIS:HB3	1:A:1270:LEU:HD13	1.95	0.48
1:A:724:PHE:CE2	1:A:726:GLY:HA3	2.47	0.48
1:A:919:HIS:ND1	1:A:920:PRO:HD3	2.28	0.48
1:A:1464:GLN:O	1:A:1468:HIS:HD2	1.97	0.48
1:A:1529:ASP:OD1	1:A:1532:THR:OG1	2.28	0.48
1:A:1115:GLY:HA2	1:A:1237:PHE:HB2	1.93	0.48
1:A:717:CYS:HB3	1:A:722:ILE:O	2.13	0.48
1:A:1269:ASP:OD2	1:A:1269:ASP:N	2.46	0.48
1:A:1104:SER:O	1:A:1108:ARG:HG3	2.14	0.47
1:A:1625:MET:CE	1:A:1627:ILE:HG13	2.25	0.47
1:A:1072:GLU:OE2	1:A:1135:HIS:HE1	1.97	0.47
1:A:1301:LYS:NZ	1:A:1741:GLU:OE2	2.36	0.47
1:A:1194:TYR:CE2	1:A:1206:MET:HE3	2.49	0.47
1:A:750:VAL:HG22	1:A:879:ALA:HB1	1.95	0.47
1:A:1523:LEU:HB3	1:A:1643:THR:HG21	1.96	0.47
1:A:1315:HIS:CD2	1:A:1317:SER:H	2.31	0.47
1:A:1057:ALA:C	1:A:1059:LYS:N	2.72	0.47
1:A:1274:GLU:O	1:A:1278:GLN:HG3	2.15	0.47
1:A:1789:ILE:HG13	1:A:1800:VAL:HG13	1.96	0.46
1:A:1284:TRP:CH2	1:A:1300:PRO:HD2	2.50	0.46
1:A:898:ILE:HD11	1:A:909:LEU:HD13	1.97	0.46
1:A:1147:VAL:HG11	1:A:1172:VAL:HG23	1.97	0.46
1:A:1212:ARG:HE	4:A:1909:GOL:H2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1789:ILE:CD1	1:A:1825:VAL:HG21	2.42	0.46
1:A:641:LYS:HB3	1:A:641:LYS:HE3	1.67	0.46
1:A:919:HIS:N	1:A:920:PRO:CD	2.79	0.46
1:A:1274:GLU:HA	1:A:1277:GLU:HG3	1.98	0.46
1:A:1675:THR:HG22	1:A:1678:GLU:H	1.81	0.46
1:A:993:LYS:HE2	6:A:2039:HOH:O	2.16	0.46
1:A:1382:ALA:HB1	1:A:1438:ASP:OD1	2.15	0.46
1:A:1600:ARG:HA	6:A:2138:HOH:O	2.16	0.45
1:A:622:LYS:HE3	1:A:622:LYS:HB2	1.61	0.45
1:A:657:PRO:HG3	1:A:676:ARG:HG3	1.98	0.45
1:A:1152:ASN:O	1:A:1153:ASP:HB2	2.17	0.45
1:A:1612:TYR:CD1	1:A:1632:GLY:HA2	2.51	0.45
1:A:1265:HIS:HB3	1:A:1270:LEU:CD1	2.46	0.45
1:A:1287:HIS:CE1	1:A:1288:TYR:CE2	3.04	0.45
1:A:624:PHE:HD1	1:A:698:GLN:HG3	1.82	0.45
1:A:1315:HIS:HE1	1:A:1334:ASP:OD2	2.00	0.44
1:A:1083:GLN:HE21	1:A:1100:GLY:HA2	1.83	0.44
1:A:1730:GLU:OE2	1:A:1730:GLU:HA	2.16	0.44
1:A:1123:LEU:HD12	1:A:1183:LEU:HD23	1.98	0.44
1:A:1616:GLY:C	1:A:1642:ARG:HG3	2.42	0.44
1:A:1330:ASN:O	1:A:1336:PRO:HA	2.17	0.44
1:A:914:ARG:CB	4:A:1905:GOL:H32	2.48	0.44
1:A:957:ILE:HG13	1:A:958:GLU:N	2.27	0.44
1:A:1653:GLY:HA3	6:A:2025:HOH:O	2.18	0.44
1:A:840:GLY:N	1:A:888:LYS:HG3	2.33	0.44
1:A:1525:MET:HE2	1:A:1573:TYR:OH	2.18	0.44
4:A:1908:GOL:H31	6:A:2082:HOH:O	2.17	0.44
1:A:1260:VAL:HG12	1:A:1355:VAL:HA	2.00	0.43
1:A:1554:VAL:HG22	1:A:1640:VAL:HG22	2.00	0.43
1:A:693:LYS:HD3	1:A:693:LYS:HA	1.83	0.43
1:A:1067:LYS:HA	1:A:1068:PRO:HD2	1.76	0.43
1:A:677:THR:HG1	1:A:680:GLU:HB2	1.83	0.43
4:A:1904:GOL:H31	6:A:2261:HOH:O	2.18	0.43
1:A:964:GLU:OE2	4:A:1906:GOL:H12	2.19	0.43
1:A:1114:VAL:O	1:A:1114:VAL:CG1	2.65	0.43
1:A:1690:LYS:HA	1:A:1690:LYS:HD3	1.77	0.43
1:A:1165:LYS:O	1:A:1166:ARG:HB2	2.16	0.43
1:A:1585:VAL:HG13	1:A:1586:PHE:HD1	1.80	0.43
1:A:1522:LYS:HG2	6:A:2285:HOH:O	2.19	0.43
1:A:1539:TYR:CD1	1:A:1610:ARG:HG2	2.53	0.43
1:A:1770:ARG:HG2	1:A:1770:ARG:HH11	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:857:GLN:HB3	4:A:1906:GOL:H32	1.97	0.43
1:A:716:ARG:HG3	1:A:716:ARG:NH1	2.34	0.42
1:A:744:ILE:HG23	1:A:886:LEU:HD23	1.99	0.42
1:A:835:MET:HG2	1:A:933:TRP:HE3	1.83	0.42
1:A:1710:ASN:O	1:A:1712:ASN:N	2.51	0.42
1:A:1324:TYR:CZ	1:A:1347:GLY:HA3	2.54	0.42
1:A:917:VAL:CG1	1:A:1008:LYS:HD3	2.48	0.42
1:A:1612:TYR:CD2	1:A:1612:TYR:C	2.97	0.42
1:A:924:MET:HE2	1:A:924:MET:HA	2.00	0.42
1:A:1553:ASN:CB	1:A:1638:GLN:HE21	2.32	0.42
1:A:1438:ASP:HB3	6:A:2092:HOH:O	2.18	0.42
1:A:1346:LEU:HD13	1:A:1584:ASP:HB2	2.01	0.42
1:A:1617:VAL:HG11	1:A:1639:LEU:HD22	2.02	0.42
1:A:727:PRO:HD2	4:A:1905:GOL:O3	2.19	0.42
1:A:1203:MET:HE3	1:A:1630:ALA:HB3	1.97	0.41
1:A:1464:GLN:HA	1:A:1464:GLN:NE2	2.34	0.41
1:A:883:LEU:HD23	1:A:883:LEU:C	2.45	0.41
1:A:1184:SER:O	1:A:1185:ILE:HD13	2.20	0.41
1:A:1265:HIS:HE1	1:A:1444:GLU:OE2	2.03	0.41
1:A:1635:GLY:HA2	3:A:1902:URE:N1	2.36	0.41
1:A:1057:ALA:O	1:A:1059:LYS:N	2.53	0.41
1:A:1147:VAL:H	1:A:1158:GLN:NE2	2.17	0.41
1:A:726:GLY:HA3	4:A:1905:GOL:H2	1.99	0.41
1:A:740:SER:O	1:A:744:ILE:HG12	2.21	0.41
1:A:934:MET:HE3	4:A:1905:GOL:C1	2.40	0.41
1:A:1456:TYR:CE2	1:A:1460:ARG:HD3	2.56	0.41
1:A:705:GLY:O	1:A:708:SER:CB	2.66	0.40
1:A:1102:MET:HE1	1:A:1292:ARG:HA	2.02	0.40
1:A:1103:ASP:HA	1:A:1361:TRP:HA	2.02	0.40
1:A:622:LYS:HA	1:A:623:PRO:HD2	1.97	0.40
1:A:1578:MET:O	1:A:1592:ALA:HA	2.21	0.40
1:A:1789:ILE:CD1	1:A:1825:VAL:CG2	2.99	0.40
1:A:744:ILE:HG12	1:A:744:ILE:H	1.64	0.40
1:A:854:ARG:O	1:A:855:ARG:C	2.64	0.40
1:A:1223:ASN:O	1:A:1223:ASN:CG	2.65	0.40
1:A:1428:SER:HA	1:A:1429:PRO:HD2	1.93	0.40
1:A:1493:ASN:HD22	1:A:1495:LYS:H	1.69	0.40
1:A:1103:ASP:OD1	1:A:1106:SER:OG	2.38	0.40
1:A:1194:TYR:CE2	1:A:1206:MET:HG2	2.56	0.40
1:A:828:ARG:NH2	1:A:866:PRO:O	2.45	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	1124/1236 (91%)	1046 (93%)	71 (6%)	7 (1%)	21 42

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1166	ARG
1	A	1438	ASP
1	A	1711	GLU
1	A	891	CYS
1	A	1003	ASP
1	A	1058	THR
1	A	1757	PRO

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	955/1040 (92%)	850 (89%)	105 (11%)	6 13

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	629	ILE
1	A	634	GLU
1	A	641	LYS
1	A	662	GLN

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Mol	Chain	Res	Type
1	A	676	ARG
1	A	680	GLU
1	A	689	ILE
1	A	698	GLN
1	A	716	ARG
1	A	719	GLN
1	A	730	ASP
1	A	734	LYS
1	A	735	LEU
1	A	737	LEU
1	A	738	LYS
1	A	739	HIS
1	A	743	GLU
1	A	744	ILE
1	A	752	LEU
1	A	826	ASN
1	A	834	MET
1	A	841	LYS
1	A	845	ILE
1	A	859	VAL
1	A	860	ILE
1	A	872	THR
1	A	875	LYS
1	A	888	LYS
1	A	944	ASP
1	A	951	GLU
1	A	952	VAL
1	A	957	ILE
1	A	978	THR
1	A	979	SER
1	A	988	VAL
1	A	993	LYS
1	A	999	SER
1	A	1011	VAL
1	A	1016	ARG
1	A	1042	LEU
1	A	1044	SER
1	A	1047	SER
1	A	1055	LYS
1	A	1074	LEU
1	A	1079	ASN
1	A	1103	ASP

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Mol	Chain	Res	Type
1	A	1125	ILE
1	A	1131	LYS
1	A	1140	ILE
1	A	1147	VAL
1	A	1150	THR
1	A	1156	ILE
1	A	1165	LYS
1	A	1172	VAL
1	A	1191	VAL
1	A	1216	LEU
1	A	1224	GLN
1	A	1227	LEU
1	A	1252	THR
1	A	1311	GLU
1	A	1326	LEU
1	A	1337	VAL
1	A	1345	SER
1	A	1346	LEU
1	A	1375	VAL
1	A	1377	LEU
1	A	1388	SER
1	A	1393	ILE
1	A	1396	PHE
1	A	1402	LEU
1	A	1408	LYS
1	A	1426	ASP
1	A	1428	SER
1	A	1430	LYS
1	A	1459	ASN
1	A	1460	ARG
1	A	1473	ILE
1	A	1478	GLN
1	A	1509	GLN
1	A	1516	VAL
1	A	1557	ILE
1	A	1562	ASP
1	A	1571	MET
1	A	1585	VAL
1	A	1625	MET
1	A	1640	VAL
1	A	1643	THR
1	A	1657	ILE

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Mol	Chain	Res	Type
1	A	1662	LEU
1	A	1675	THR
1	A	1693	ILE
1	A	1695	VAL
1	A	1697	GLU
1	A	1721	GLU
1	A	1726	GLU
1	A	1736	GLN
1	A	1744	LYS
1	A	1754	GLU
1	A	1758	ASP
1	A	1759	ASP
1	A	1778	VAL
1	A	1789	ILE
1	A	1791	ILE
1	A	1828	ILE
1	A	1829	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	698	GLN
1	A	947	ASN
1	A	1083	GLN
1	A	1135	HIS
1	A	1158	GLN
1	A	1265	HIS
1	A	1278	GLN
1	A	1315	HIS
1	A	1318	ASN
1	A	1330	ASN
1	A	1389	GLN
1	A	1459	ASN
1	A	1464	GLN
1	A	1493	ASN
1	A	1509	GLN
1	A	1553	ASN
1	A	1607	ASN
1	A	1638	GLN
1	A	1659	HIS
1	A	1686	ASN
1	A	1688	ASN

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Mol	Chain	Res	Type
1	A	1702	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 1 is monoatomic - leaving 9 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	$\# Z > 2$
4	GOL	A	1904	-	5,5,5	0.60	0	5,5,5	0.96	0
4	GOL	A	1908	-	5,5,5	1.02	0	5,5,5	1.05	0
4	GOL	A	1909	-	5,5,5	0.60	0	5,5,5	0.66	0
3	URE	A	1902	-	3,3,3	0.61	0	3,3,3	2.45	2 (66%)
4	GOL	A	1906	-	5,5,5	0.36	0	5,5,5	1.07	0
4	GOL	A	1905	-	5,5,5	0.82	0	5,5,5	1.27	0
4	GOL	A	1903	-	5,5,5	0.56	0	5,5,5	0.97	0
4	GOL	A	1907	-	5,5,5	0.50	0	5,5,5	0.51	0
2	BTI	A	1901	1	15,16,16	1.72	3 (20%)	20,21,21	2.43	4 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	1904	-	-	1/4/4/4	-
4	GOL	A	1908	-	-	2/4/4/4	-
4	GOL	A	1909	-	-	0/4/4/4	-
4	GOL	A	1906	-	-	2/4/4/4	-
4	GOL	A	1905	-	-	4/4/4/4	-
4	GOL	A	1903	-	-	0/4/4/4	-
4	GOL	A	1907	-	-	1/4/4/4	-
2	BTI	A	1901	1	-	1/6/27/27	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1901	BTI	O3-C3	4.17	1.32	1.23
2	A	1901	BTI	C2-S1	-3.39	1.77	1.82
2	A	1901	BTI	C3-N3	-2.24	1.31	1.35

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1901	BTI	C6-C5-N3	-8.51	102.21	113.18
2	A	1901	BTI	C2-C4-N2	-4.42	108.66	113.34
3	A	1902	URE	N2-C-N1	-3.50	111.44	117.77
2	A	1901	BTI	N2-C3-N3	2.92	112.22	108.85
3	A	1902	URE	O-C-N2	2.31	126.11	121.04
2	A	1901	BTI	C6-S1-C2	2.01	94.16	89.98

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1905	GOL	O1-C1-C2-C3
4	A	1905	GOL	C1-C2-C3-O3
4	A	1906	GOL	C1-C2-C3-O3
4	A	1908	GOL	C1-C2-C3-O3
4	A	1908	GOL	O2-C2-C3-O3
4	A	1906	GOL	O2-C2-C3-O3
4	A	1905	GOL	O1-C1-C2-O2
4	A	1905	GOL	O2-C2-C3-O3
2	A	1901	BTI	C2-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
4	A	1907	GOL	O1-C1-C2-O2
4	A	1904	GOL	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1904	GOL	1	0
4	A	1908	GOL	2	0
4	A	1909	GOL	1	0
3	A	1902	URE	3	0
4	A	1906	GOL	6	0
4	A	1905	GOL	12	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	1130/1236 (91%)	-0.32	12 (1%) 78 74	18, 37, 65, 105	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1227	LEU	5.9
1	A	1745	SER	3.8
1	A	1756	TYR	3.1
1	A	1225	PRO	2.9
1	A	1757	PRO	2.8
1	A	1059	LYS	2.5
1	A	1228	SER	2.3
1	A	871	ALA	2.3
1	A	1224	GLN	2.2
1	A	754	PRO	2.2
1	A	827	ALA	2.0
1	A	1065	ASP	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 oligosaccharides 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, 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($\text{\AA}^2$)	Q<0.9
4	GOL	A	1908	6/6	0.80	0.20	46,53,54,55	0
4	GOL	A	1904	6/6	0.83	0.19	66,70,72,72	0
4	GOL	A	1909	6/6	0.86	0.17	54,55,57,58	0
4	GOL	A	1905	6/6	0.91	0.23	48,50,51,52	0
5	NA	A	1910	1/1	0.93	0.11	62,62,62,62	0
4	GOL	A	1906	6/6	0.94	0.08	52,53,54,54	0
3	URE	A	1902	4/4	0.94	0.10	39,39,40,40	0
4	GOL	A	1903	6/6	0.95	0.10	43,48,50,54	0
4	GOL	A	1907	6/6	0.96	0.08	34,37,40,43	0
2	BTI	A	1901	15/15	0.99	0.04	18,24,26,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.