



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:51 PM GMT

PDB ID : 3VA7
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

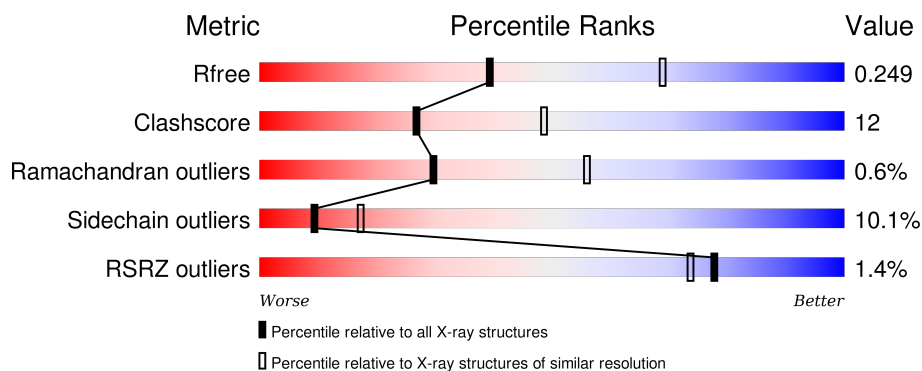
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

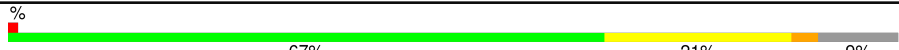
The reported resolution of this entry is 2.60 Å.

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}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	1903	-	-	-	X
4	GOL	A	1904	-	-	-	X
4	GOL	A	1905	-	-	X	X
4	GOL	A	1906	-	-	X	-
4	GOL	A	1908	-	-	-	X
4	GOL	A	1909	-	-	-	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.

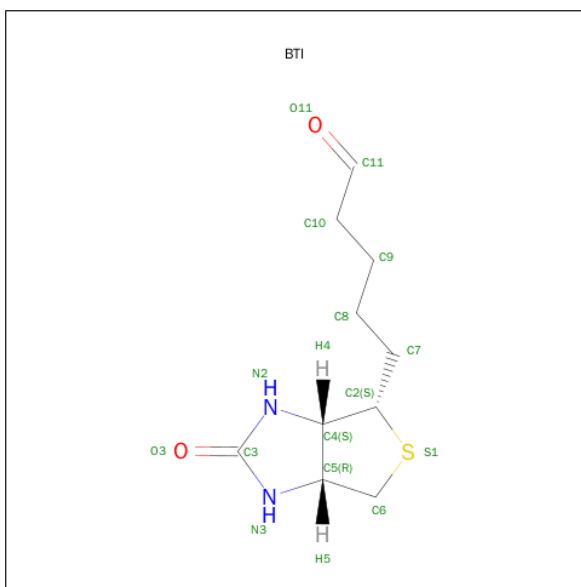
- Molecule 1 is a protein called KLLA0E08119p.

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:

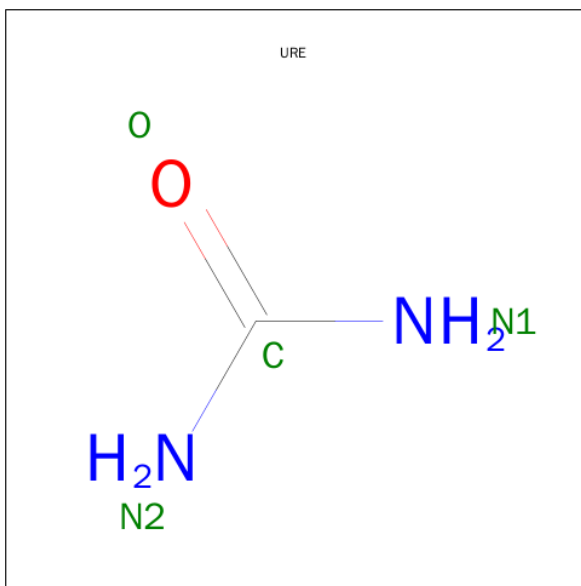
Chain	Residue	Modelled	Actual	Comment	Reference
A	594	MET	-	EXPRESSION TAG	UNP Q6CP22
A	595	GLY	-	EXPRESSION TAG	UNP Q6CP22
A	596	SER	-	EXPRESSION TAG	UNP Q6CP22
A	597	SER	-	EXPRESSION TAG	UNP Q6CP22
A	598	HIS	-	EXPRESSION TAG	UNP Q6CP22
A	599	HIS	-	EXPRESSION TAG	UNP Q6CP22
A	600	HIS	-	EXPRESSION TAG	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 (three-letter code: 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 (three-letter code: 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 (three-letter code: 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 (three-letter code: NA) (formula: Na).

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

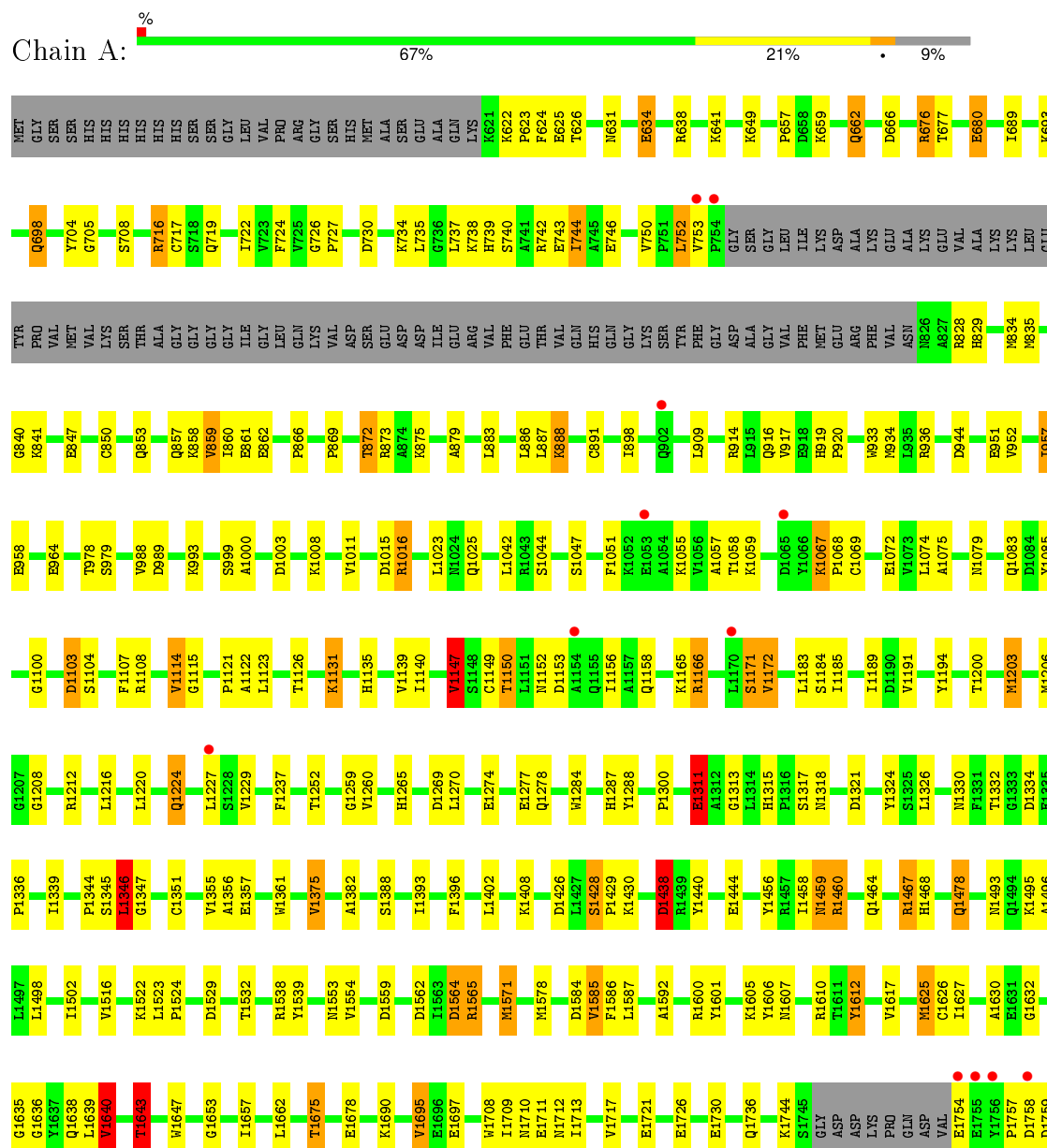
- Molecule 6 is water.

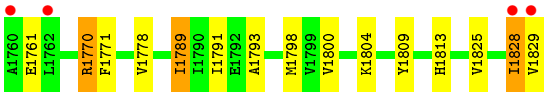
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	377	Total	O	0	0
			377	377		

3 Residue-property plots

These plots are drawn for all protein, RNA 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: KLLA0E08119p





4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	126.66 Å 126.66 Å 217.87 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.60 47.73 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.1 (50.00-2.60) 99.1 (47.73-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.75 (at 2.61 Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.187 , 0.255 0.184 , 0.249	Depositor DCC
R_{free} test set	2790 reflections (5.37%)	DCC
Wilson B-factor (Å ²)	40.0	Xtriage
Anisotropy	0.512	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 54739 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, BTI, URE, 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	0.94	4/9017 (0.0%)	0.94	13/12220 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1311	GLU	CG-CD	5.92	1.60	1.51
1	A	1114	VAL	CB-CG1	-5.78	1.40	1.52
1	A	1612	TYR	CG-CD2	5.55	1.46	1.39
1	A	1564	ASP	CB-CG	5.07	1.62	1.51

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1467	ARG	NE-CZ-NH2	-8.00	116.30	120.30
1	A	1467	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	A	989	ASP	CB-CG-OD1	6.31	123.98	118.30
1	A	1438	ASP	N-CA-CB	-6.11	99.60	110.60
1	A	1203	MET	CG-SD-CE	-5.97	90.64	100.20
1	A	1770	ARG	NE-CZ-NH2	-5.93	117.34	120.30
1	A	1538	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	A	1147	VAL	CB-CA-C	-5.56	100.84	111.40
1	A	1559	ASP	CB-CG-OD2	5.23	123.01	118.30
1	A	1346	LEU	CB-CG-CD2	5.16	119.78	111.00
1	A	1695	VAL	CB-CA-C	-5.11	101.69	111.40
1	A	1640	VAL	CG1-CB-CG2	5.11	119.07	110.90
1	A	1643	THR	CB-CA-C	-5.00	98.09	111.60

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	213	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	215	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 12.

All (215) 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:1025:GLN:HG3	6:A:2003:HOH:O	1.52	1.04
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1708:TRP:HE3	1:A:1709:ILE:HD12	1.55	0.71
1:A:1625:MET:HE1	1:A:1626:CYS:C	2.11	0.70
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:1625:MET:HE2	1:A:1626:CYS:O	1.95	0.67
1:A:1459:ASN:ND2	1:A:1460:ARG:HD2	2.10	0.67
1:A:1625:MET:CE	1:A:1626:CYS:C	2.64	0.66
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:1625:MET:CE	1:A:1627:ILE:HG13	2.25	0.66
1:A:1789:ILE:HD11	1:A:1825:VAL:HG21	1.77	0.66
1:A:934:MET:HE1	4:A:1905:GOL:H11	1.78	0.66
1:A:1625:MET:HE1	1:A:1627:ILE:HG13	1.78	0.65
1:A:1114:VAL:O	1:A:1114:VAL:HG12	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:1318:ASN:HD21	1:A:1605:LYS:H	1.45	0.64
1:A:742:ARG:HH22	1:A:753:VAL:HB	1.62	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:634:GLU:CD	1:A:1008:LYS:HE2	2.20	0.62
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:1150:THR:HG23	1:A:1153:ASP:H	1.66	0.60
1:A:916:GLN:HB2	6:A:2075:HOH:O	1.99	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:1553:ASN:HB3	1:A:1638:GLN:HE21	1.67	0.59
1:A:883:LEU:HD23	1:A:887:LEU:HD12	1.84	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:1675:THR:HG21	6:A:2192:HOH:O	2.02	0.59
1:A:1016:ARG:NH2	1:A:1051:PHE:O	2.36	0.59
1:A:1189:ILE:HG21	1:A:1220:LEU:HD23	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1203:MET:HE3	1:A:1630:ALA:CB	2.35	0.57
1:A:1625:MET:CE	1:A:1626:CYS:O	2.53	0.57
1:A:1265:HIS:HD2	1:A:1351:CYS:H	1.51	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: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:1200:THR:OG1	1:A:1208:GLY:HA3	2.07	0.55
1:A:1778:VAL:HG13	6:A:2172:HOH:O	2.06	0.55
1:A:853:GLN:HG2	1:A:858:LYS:HG2	1.87	0.55
1:A:1553:ASN:ND2	1:A:1606:TYR:OH	2.25	0.55
1:A:934:MET:HE3	4:A:1905:GOL:H11	1.89	0.55
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:1184:SER:C	1:A:1185:ILE:HD13	2.28	0.54
1:A:1131:LYS:HB3	1:A:1171:SER:HB2	1.90	0.54
1:A:914:ARG:HA	4:A:1905:GOL:C3	2.19	0.53
1:A:1771:PHE:CD1	1:A:1813:HIS:HB2	2.44	0.53
1:A:964:GLU:CD	4:A:1906:GOL:H12	2.30	0.52
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:1203:MET:CE	1:A:1630:ALA:HB1	2.40	0.52
1:A:1147:VAL:H	1:A:1158:GLN:HE22	1.58	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:1203:MET:HE3	1:A:1630:ALA:HB1	1.92	0.51
1:A:1459:ASN:ND2	1:A:1460:ARG:HH11	1.96	0.51
1:A:1229:VAL:HG13	1:A:1229:VAL:O	2.10	0.51
1:A:1057:ALA:C	1:A:1059:LYS:H	2.13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:HD13	1:A:1657:ILE:N	2.28	0.49
1:A:860:ILE:CG2	1:A:957:ILE:CD1	2.88	0.49
1:A:1356:ALA:O	1:A:1357:GLU:C	2.48	0.49
1:A:936:ARG:HD2	6:A:2326:HOH:O	2.13	0.49
1:A:1524:PRO:O	1:A:1643:THR:CG2	2.61	0.49
1:A:716:ARG:HG3	1:A:716:ARG:HH11	1.77	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: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:919:HIS:ND1	1:A:920:PRO:HD3	2.28	0.48
1:A:1625:MET:HE3	1:A:1627:ILE:HG13	1.95	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:1072:GLU:OE2	1:A:1135:HIS:HE1	1.97	0.47
1:A:1523:LEU:HB3	1:A:1643:THR:HG21	1.96	0.47
1:A:750:VAL:HG22	1:A:879:ALA:HB1	1.95	0.47
1:A:1315:HIS:CD2	1:A:1317:SER:H	2.31	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:1710:ASN:C	1:A:1712:ASN:H	2.19	0.46
1:A:1789:ILE:CD1	1:A:1825:VAL:HG21	2.42	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
1:A:898:ILE:HD11	1:A:909:LEU:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:641:LYS:HE3	1:A:641:LYS:HB3	1.67	0.46
1:A:1675:THR:HG22	1:A:1678:GLU:H	1.81	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:1382:ALA:HB1	1:A:1438:ASP:OD1	2.15	0.46
1:A:993:LYS:HE2	6:A:2039:HOH:O	2.16	0.46
1:A:1600:ARG:HA	6:A:2138:HOH:O	2.16	0.45
1:A:622:LYS:HB2	1:A:622:LYS:HE3	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:1730:GLU:OE2	1:A:1730:GLU:HA	2.16	0.44
1:A:1083:GLN:HE21	1:A:1100:GLY:HA2	1.83	0.44
1:A:1123:LEU:HD12	1:A:1183:LEU:HD23	1.98	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
4:A:1908:GOL:H31	6:A:2082:HOH:O	2.17	0.44
1:A:840:GLY:N	1:A:888:LYS:HG3	2.33	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:HA	1:A:693:LYS:HD3	1.83	0.43
1:A:1067:LYS:HA	1:A:1068:PRO:HD2	1.76	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:1625:MET:HE2	1:A:1626:CYS:C	2.36	0.43
1:A:1690:LYS:HD3	1:A:1690:LYS:HA	1.77	0.43
1:A:1585:VAL:HG13	1:A:1586:PHE:HD1	1.80	0.43
1:A:1165:LYS:O	1:A:1166:ARG:HB2	2.16	0.43
1:A:1770:ARG:HH11	1:A:1770:ARG:HG2	1.84	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:857:GLN:HB3	4:A:1906:GOL:H32	1.97	0.43
1:A:744:ILE:HG23	1:A:886:LEU:HD23	1.99	0.42
1:A:716:ARG:HG3	1:A:716:ARG:NH1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1710:ASN:O	1:A:1712:ASN:N	2.51	0.42
1:A:835:MET:HG2	1:A:933:TRP:HE3	1.83	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: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:1332:THR:OG1	1:A:1332:THR:O	2.38	0.42
1:A:1346:LEU:HD13	1:A:1584:ASP:HB2	2.01	0.42
1:A:1057:ALA:C	1:A:1059:LYS:N	2.72	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:1464:GLN:HA	1:A:1464:GLN:NE2	2.34	0.41
1:A:1265:HIS:HE1	1:A:1444:GLU:OE2	2.03	0.41
1:A:1184:SER:O	1:A:1185:ILE:HD13	2.20	0.41
1:A:1635:GLY:HA2	3:A:1902:URE:N1	2.36	0.41
1:A:1147:VAL:H	1:A:1158:GLN:NE2	2.17	0.41
1:A:1057:ALA:O	1:A:1059:LYS:N	2.53	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: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:1103:ASP:HA	1:A:1361:TRP:HA	2.02	0.40
1:A:1789:ILE:CD1	1:A:1825:VAL:CG2	2.99	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:744:ILE:HG12	1:A:744:ILE:H	1.64	0.40
1:A:1493:ASN:HD22	1:A:1495:LYS:H	1.69	0.40
1:A:1428:SER:HA	1:A:1429:PRO:HD2	1.93	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 ⓘ

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	1124/1236 (91%)	1046 (93%)	71 (6%)	7 (1%)	30 56

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 ⓘ

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%)	859 (90%)	96 (10%)	9 17

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	631	ASN
1	A	634	GLU
1	A	638	ARG
1	A	659	LYS
1	A	662	GLN
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

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Mol	Chain	Res	Type
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	746	GLU
1	A	752	LEU
1	A	834	MET
1	A	841	LYS
1	A	859	VAL
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	999	SER
1	A	1011	VAL
1	A	1015	ASP
1	A	1016	ARG
1	A	1042	LEU
1	A	1044	SER
1	A	1047	SER
1	A	1055	LYS
1	A	1067	LYS
1	A	1074	LEU
1	A	1079	ASN
1	A	1103	ASP
1	A	1131	LYS
1	A	1147	VAL
1	A	1150	THR
1	A	1171	SER
1	A	1172	VAL
1	A	1191	VAL
1	A	1216	LEU
1	A	1224	GLN

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Mol	Chain	Res	Type
1	A	1227	LEU
1	A	1252	THR
1	A	1311	GLU
1	A	1321	ASP
1	A	1326	LEU
1	A	1345	SER
1	A	1346	LEU
1	A	1375	VAL
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	1440	TYR
1	A	1459	ASN
1	A	1460	ARG
1	A	1478	GLN
1	A	1516	VAL
1	A	1562	ASP
1	A	1565	ARG
1	A	1571	MET
1	A	1585	VAL
1	A	1625	MET
1	A	1640	VAL
1	A	1643	THR
1	A	1662	LEU
1	A	1675	THR
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	1789	ILE
1	A	1804	LYS
1	A	1828	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) 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	1224	GLN
1	A	1265	HIS
1	A	1278	GLN
1	A	1315	HIS
1	A	1318	ASN
1	A	1389	GLN
1	A	1459	ASN
1	A	1464	GLN
1	A	1493	ASN
1	A	1553	ASN
1	A	1607	ASN
1	A	1638	GLN
1	A	1659	HIS
1	A	1702	HIS
1	A	1815	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 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
2	BTI	A	1901	1	14,16,16	2.01	5 (35%)	13,21,21	1.84	3 (23%)
3	URE	A	1902	-	3,3,3	0.60	0	3,3,3	2.13	1 (33%)
4	GOL	A	1903	-	5,5,5	0.48	0	5,5,5	0.93	0
4	GOL	A	1904	-	5,5,5	0.53	0	5,5,5	0.87	0
4	GOL	A	1905	-	5,5,5	0.77	0	5,5,5	1.20	0
4	GOL	A	1906	-	5,5,5	0.35	0	5,5,5	0.96	0
4	GOL	A	1907	-	5,5,5	0.45	0	5,5,5	0.45	0
4	GOL	A	1908	-	5,5,5	0.96	0	5,5,5	1.05	0
4	GOL	A	1909	-	5,5,5	0.60	0	5,5,5	0.62	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	BTI	A	1901	1	-	0/5/27/27	0/2/2/2
3	URE	A	1902	-	-	0/0/0/0	0/0/0/0
4	GOL	A	1903	-	-	0/4/4/4	0/0/0/0
4	GOL	A	1904	-	-	0/4/4/4	0/0/0/0
4	GOL	A	1905	-	-	0/4/4/4	0/0/0/0
4	GOL	A	1906	-	-	0/4/4/4	0/0/0/0
4	GOL	A	1907	-	-	0/4/4/4	0/0/0/0
4	GOL	A	1908	-	-	0/4/4/4	0/0/0/0
4	GOL	A	1909	-	-	0/4/4/4	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1901	BTI	C2-S1	-3.33	1.77	1.82
2	A	1901	BTI	C3-N3	-2.95	1.31	1.35
2	A	1901	BTI	C3-N2	-2.23	1.32	1.35
2	A	1901	BTI	C10-C11	2.33	1.56	1.49
2	A	1901	BTI	O3-C3	4.34	1.32	1.23

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1902	URE	N2-C-N1	-3.10	111.44	117.76
2	A	1901	BTI	C4-N2-C3	-2.22	110.54	112.66
2	A	1901	BTI	O3-C3-N3	-2.14	123.42	125.90
2	A	1901	BTI	N2-C3-N3	4.83	112.22	108.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1902	URE	3	0
4	A	1904	GOL	1	0
4	A	1905	GOL	12	0
4	A	1906	GOL	6	0
4	A	1908	GOL	2	0
4	A	1909	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, 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%)	-0.39	16 (1%) 78 74	18, 37, 65, 105	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1227	LEU	4.3
1	A	1829	VAL	3.5
1	A	1065	ASP	3.3
1	A	1755	GLU	3.1
1	A	754	PRO	2.9
1	A	1758	ASP	2.8
1	A	753	VAL	2.7
1	A	1754	GLU	2.7
1	A	1756	TYR	2.6
1	A	902	GLN	2.6
1	A	1828	ILE	2.4
1	A	1760	ALA	2.2
1	A	1170	LEU	2.1
1	A	1053	GLU	2.1
1	A	1762	LEU	2.0
1	A	1154	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å ²)	Q<0.9
4	GOL	A	1905	6/6	0.90	0.33	12.57	48,50,51,52	0
4	GOL	A	1904	6/6	0.84	0.24	8.72	66,70,72,72	0
4	GOL	A	1908	6/6	0.85	0.29	4.45	46,53,54,55	0
4	GOL	A	1909	6/6	0.91	0.17	4.20	54,55,57,58	0
4	GOL	A	1903	6/6	0.96	0.17	2.23	43,48,50,54	0
4	GOL	A	1906	6/6	0.95	0.16	1.28	52,53,54,54	0
3	URE	A	1902	4/4	0.97	0.22	1.13	39,39,40,40	0
2	BTI	A	1901	15/15	0.99	0.20	0.52	18,24,26,28	0
4	GOL	A	1907	6/6	0.98	0.14	-1.24	34,37,40,43	0
5	NA	A	1910	1/1	0.98	0.14	-	62,62,62,62	0

6.5 Other polymers [i](#)

There are no such residues in this entry.