



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:02 AM UTC

PDB ID : 1J04 / pdb_00001j04
Title : Structural mechanism of enzyme mistargeting in hereditary kidney stone disease in vitro
Authors : Zhang, X.; Djordjevic, S.; Bartlam, M.; Ye, S.; Rao, Z.; Danpure, C.J.
Deposited on : 2002-10-30
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

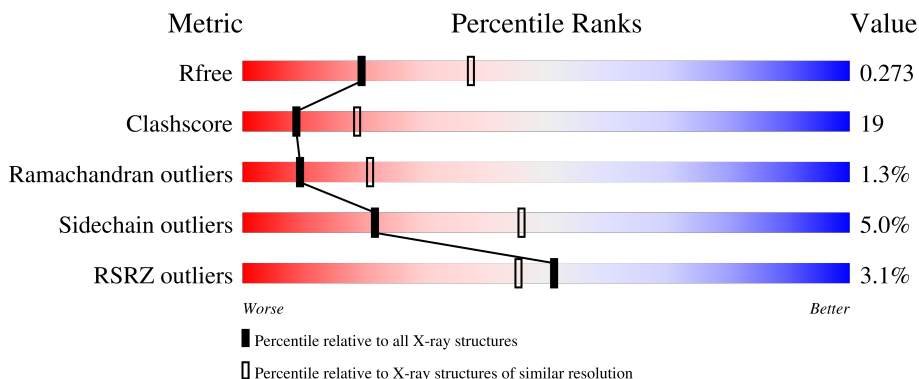
1 Overall quality at a glance

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	392	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3148 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.

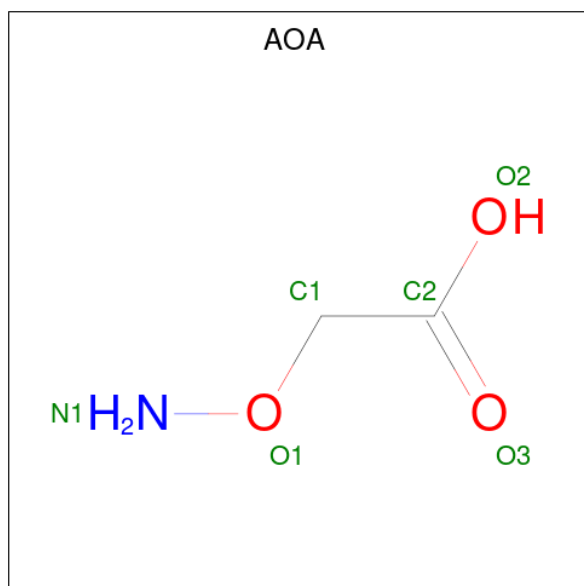
- Molecule 1 is a protein called alanine-glyoxylate aminotransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	387	2987	1907	519	544	1	16	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	170	ARG	GLY	engineered mutation	UNP P21549

- Molecule 2 is (AMINOXY)ACETIC ACID (CCD ID: AOA) (formula: $C_2H_5NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	6	2	1	3	0	0

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

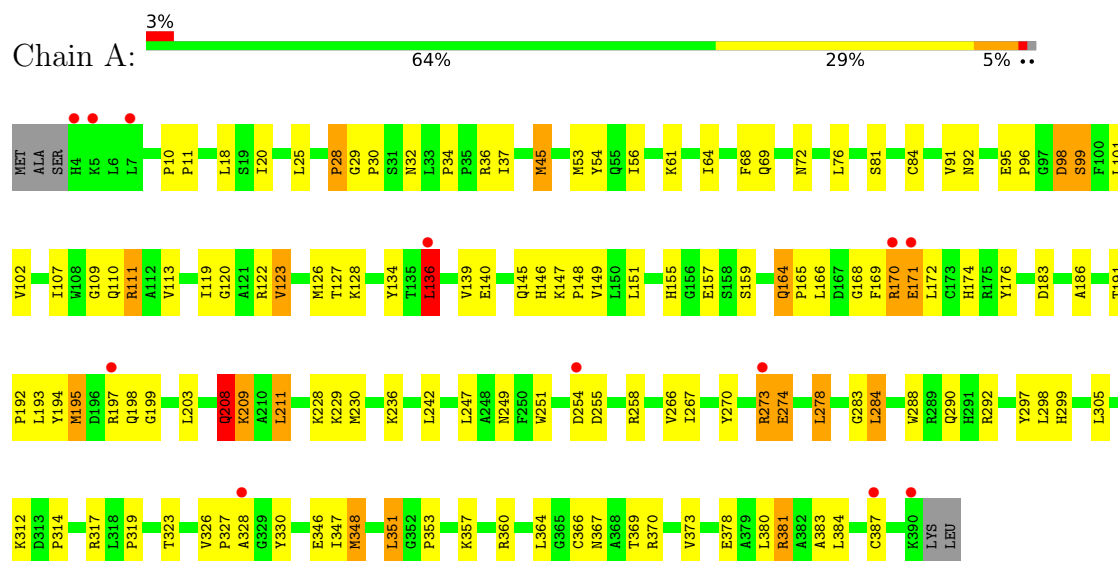
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	113	Total	O	0	0
			113	113		

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: alanine-glyoxylate aminotransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	89.49Å 89.49Å 142.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.40 – 2.60 47.40 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.2 (47.40-2.60) 97.3 (47.40-2.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.32 (at 2.61Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.223 , 0.273 0.223 , 0.273	Depositor DCC
R_{free} test set	1763 reflections (9.54%)	wwPDB-VP
Wilson B-factor (Å ²)	42.2	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 37.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3148	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.08% 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: AOA, GOL, LLP

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	0.50	1/3032 (0.0%)	1.07	14/4118 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	45	MET	SD-CE	-5.04	1.67	1.79

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	208	GLN	OE1-CD-NE2	-10.18	112.42	122.60
1	A	255	ASP	N-CA-C	-8.12	103.17	113.72
1	A	98	ASP	N-CA-C	7.58	122.16	113.15
1	A	208	GLN	CG-CD-NE2	7.12	127.08	116.40
1	A	165	PRO	N-CA-C	-6.13	100.84	111.32
1	A	136	LEU	N-CA-C	-5.91	104.97	111.82
1	A	347	ILE	N-CA-C	-5.77	100.74	108.35
1	A	95	GLU	N-CA-C	-5.60	102.56	110.29
1	A	111	ARG	N-CA-C	-5.43	105.44	111.36
1	A	283	GLY	N-CA-C	-5.24	100.75	113.18
1	A	123	VAL	N-CA-C	5.20	116.07	108.58
1	A	364	LEU	N-CA-C	5.14	116.79	108.41
1	A	102	VAL	N-CA-C	5.13	115.86	108.48
1	A	170	ARG	N-CA-C	-5.10	99.94	110.80

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	2987	0	2998	113	0
2	A	6	0	4	1	0
3	A	42	0	56	2	0
4	A	113	0	0	4	0
All	All	3148	0	3058	113	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 19.

All (113) 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:45:MET:HE1	1:A:266:VAL:HB	1.44	0.99
1:A:273:ARG:NH1	1:A:273:ARG:HB3	1.79	0.98
1:A:170:ARG:HG2	1:A:199:GLY:HA3	1.52	0.92
1:A:273:ARG:HB3	1:A:273:ARG:HH11	1.29	0.92
1:A:136:LEU:HD12	1:A:136:LEU:H	1.39	0.86
1:A:208:GLN:H	1:A:208:GLN:HE21	1.21	0.85
1:A:140:GLU:CG	1:A:172:LEU:HD11	2.08	0.83
1:A:25:LEU:H	1:A:32:ASN:HD21	1.30	0.79
1:A:101:LEU:HG	1:A:126:MET:HE2	1.66	0.76
1:A:107:ILE:HG21	1:A:351:LEU:HD13	1.68	0.75
1:A:136:LEU:HD12	1:A:136:LEU:N	2.03	0.72
1:A:378:GLU:HG2	1:A:381:ARG:HH12	1.54	0.72
1:A:136:LEU:H	1:A:136:LEU:CD1	2.03	0.72
1:A:28:PRO:O	1:A:209:LLP:HE3	1.92	0.69
1:A:140:GLU:HG3	1:A:172:LEU:HD11	1.73	0.68
1:A:168:GLY:O	1:A:171:GLU:HB2	1.94	0.67
1:A:273:ARG:HH11	1:A:273:ARG:CB	2.07	0.66
1:A:157:GLU:OE2	1:A:159:SER:HB3	1.96	0.66
1:A:98:ASP:HB3	1:A:149:VAL:HG11	1.78	0.65
1:A:140:GLU:HG2	1:A:172:LEU:HD11	1.77	0.65
1:A:380:LEU:O	1:A:384:LEU:HD13	1.97	0.65
1:A:370:ARG:HB2	3:A:1003:GOL:O1	1.97	0.64
1:A:147:LYS:N	1:A:148:PRO:HD3	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:MET:HE3	1:A:267:ILE:HG12	1.81	0.63
1:A:61:LYS:HE3	1:A:251:TRP:O	1.98	0.62
1:A:91:VAL:HG22	1:A:119:ILE:HG21	1.82	0.61
1:A:99:SER:HA	1:A:122:ARG:O	2.00	0.61
1:A:45:MET:HE1	1:A:266:VAL:CB	2.27	0.60
1:A:101:LEU:HB2	1:A:148:PRO:HG2	1.83	0.60
1:A:369:THR:O	1:A:373:VAL:HG23	2.02	0.60
1:A:68:PHE:O	1:A:69:GLN:HB2	2.00	0.59
1:A:113:VAL:HG13	1:A:123:VAL:HG11	1.83	0.59
1:A:170:ARG:CG	1:A:199:GLY:HA3	2.31	0.59
1:A:274:GLU:HA	1:A:274:GLU:OE2	2.03	0.58
1:A:34:PRO:HG3	1:A:366:CYS:SG	2.43	0.58
1:A:290:GLN:HE21	3:A:1003:GOL:H32	1.68	0.57
1:A:191:THR:HG22	1:A:319:PRO:HG2	1.87	0.57
1:A:127:THR:HG22	1:A:128:LYS:N	2.20	0.57
1:A:56:ILE:HG23	1:A:273:ARG:HG3	1.87	0.56
1:A:149:VAL:HG21	1:A:229:LYS:CE	2.36	0.56
1:A:186:ALA:HB2	1:A:209:LLP:O3	2.05	0.56
1:A:36:ARG:HH21	1:A:274:GLU:CD	2.15	0.55
1:A:192:PRO:HA	1:A:288:TRP:CZ2	2.41	0.55
1:A:32:ASN:HD22	1:A:367:ASN:HD21	1.55	0.55
1:A:155:HIS:CD2	1:A:193:LEU:HD13	2.43	0.54
1:A:164:GLN:HG3	4:A:1050:HOH:O	2.08	0.53
1:A:28:PRO:HG3	1:A:360:ARG:CZ	2.39	0.53
1:A:98:ASP:O	1:A:149:VAL:HG12	2.08	0.53
1:A:127:THR:HG22	1:A:128:LYS:H	1.74	0.52
1:A:25:LEU:N	1:A:32:ASN:HD21	2.02	0.52
1:A:109:GLY:O	1:A:113:VAL:HG23	2.10	0.52
1:A:249:ASN:HB2	1:A:254:ASP:OD2	2.10	0.52
1:A:25:LEU:H	1:A:32:ASN:ND2	2.03	0.51
1:A:34:PRO:HD2	1:A:37:ILE:CG1	2.40	0.51
1:A:299:HIS:CE1	1:A:317:ARG:HD3	2.45	0.51
1:A:20:ILE:O	1:A:20:ILE:HG13	2.10	0.51
1:A:84:CYS:SG	1:A:242:LEU:HD21	2.51	0.51
1:A:139:VAL:HG21	1:A:169:PHE:HE2	1.75	0.51
1:A:110:GLN:HE22	1:A:353:PRO:HG3	1.75	0.50
1:A:149:VAL:CG2	1:A:229:LYS:HE3	2.41	0.50
1:A:28:PRO:HG2	1:A:348:MET:HE2	1.94	0.50
1:A:195:MET:HG3	1:A:203:LEU:HD22	1.93	0.49
1:A:149:VAL:HG21	1:A:229:LYS:NZ	2.28	0.49
1:A:378:GLU:HG2	1:A:381:ARG:NH1	2.24	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:ASN:HD22	1:A:367:ASN:ND2	2.10	0.48
1:A:101:LEU:HD23	1:A:151:LEU:HD13	1.94	0.48
1:A:326:VAL:HG23	1:A:357:LYS:C	2.39	0.48
1:A:211:LEU:HB2	4:A:1036:HOH:O	2.13	0.48
1:A:32:ASN:HB2	1:A:367:ASN:HD21	1.79	0.48
1:A:149:VAL:HG21	1:A:229:LYS:HZ1	1.80	0.47
1:A:284:LEU:HD22	1:A:288:TRP:CE2	2.49	0.47
1:A:327:PRO:HB2	1:A:330:TYR:CD1	2.49	0.47
1:A:28:PRO:HD2	1:A:348:MET:SD	2.54	0.47
1:A:270:TYR:O	1:A:273:ARG:HB2	2.15	0.47
1:A:134:TYR:N	1:A:164:GLN:OE1	2.42	0.47
1:A:64:ILE:O	1:A:68:PHE:HB2	2.15	0.47
1:A:228:LYS:O	1:A:229:LYS:C	2.55	0.47
1:A:98:ASP:O	1:A:99:SER:O	2.33	0.47
1:A:195:MET:CG	1:A:203:LEU:HD22	2.46	0.46
1:A:166:LEU:HB2	1:A:198:GLN:NE2	2.31	0.46
1:A:174:HIS:C	1:A:176:TYR:H	2.22	0.46
1:A:194:TYR:HB2	1:A:197:ARG:HB2	1.96	0.46
1:A:146:HIS:O	1:A:147:LYS:C	2.59	0.46
1:A:72:ASN:N	1:A:72:ASN:HD22	2.14	0.45
1:A:348:MET:HE3	2:A:1001:AOA:H1N1	1.81	0.45
1:A:54:TYR:CZ	1:A:258:ARG:HD2	2.51	0.45
1:A:76:LEU:HD12	1:A:76:LEU:C	2.41	0.45
1:A:34:PRO:HD2	1:A:37:ILE:HG12	1.98	0.45
1:A:92:ASN:HB3	1:A:230:MET:HG2	1.99	0.45
1:A:101:LEU:HB2	1:A:148:PRO:CG	2.45	0.45
1:A:195:MET:HG3	1:A:203:LEU:CD2	2.47	0.45
1:A:81:SER:HA	4:A:1018:HOH:O	2.17	0.45
1:A:174:HIS:C	1:A:176:TYR:N	2.74	0.45
1:A:36:ARG:HD3	1:A:278:LEU:CD1	2.47	0.45
1:A:81:SER:HB2	1:A:209:LLP:OP2	2.17	0.44
1:A:98:ASP:HB3	1:A:149:VAL:CG1	2.47	0.44
1:A:29:GLY:HA2	1:A:30:PRO:C	2.43	0.44
1:A:111:ARG:HA	1:A:111:ARG:HD3	1.85	0.44
1:A:208:GLN:H	1:A:208:GLN:NE2	2.00	0.44
1:A:96:PRO:HA	1:A:120:GLY:O	2.19	0.43
1:A:146:HIS:C	1:A:148:PRO:HD3	2.43	0.43
1:A:298:LEU:HA	1:A:373:VAL:CG1	2.49	0.42
1:A:383:ALA:O	1:A:387:CYS:HB3	2.19	0.42
1:A:236:LYS:NZ	4:A:1112:HOH:O	2.52	0.42
1:A:305:LEU:HD22	1:A:381:ARG:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:PHE:CG	1:A:203:LEU:HD23	2.55	0.42
1:A:10:PRO:HA	1:A:11:PRO:HD3	1.95	0.41
1:A:36:ARG:HD3	1:A:278:LEU:HD13	2.02	0.41
1:A:312:LYS:O	1:A:314:PRO:HD3	2.21	0.41
1:A:145:GLN:HB3	1:A:146:HIS:CE1	2.56	0.41
1:A:183:ASP:OD1	1:A:183:ASP:C	2.64	0.41
1:A:297:TYR:CD2	1:A:370:ARG:HG2	2.55	0.41
1:A:53:MET:HE3	1:A:53:MET:O	2.22	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	384/392 (98%)	351 (91%)	28 (7%)	5 (1%)	9	21

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	99	SER
1	A	171	GLU
1	A	328	ALA
1	A	195	MET
1	A	28	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	317/326 (97%)	301 (95%)	16 (5%)	22	46

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LEU
1	A	136	LEU
1	A	164	GLN
1	A	208	GLN
1	A	211	LEU
1	A	247	LEU
1	A	273	ARG
1	A	274	GLU
1	A	278	LEU
1	A	284	LEU
1	A	292	ARG
1	A	323	THR
1	A	346	GLU
1	A	348	MET
1	A	351	LEU
1	A	381	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	HIS
1	A	32	ASN
1	A	72	ASN
1	A	110	GLN
1	A	155	HIS
1	A	208	GLN
1	A	290	GLN
1	A	299	HIS
1	A	308	GLN
1	A	367	ASN
1	A	386	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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$
1	LLP	A	209	1	23,24,25	3.24	8 (34%)	25,32,34	1.06	2 (8%)

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
1	LLP	A	209	1	-	7/16/17/19	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	209	LLP	C3-C2	9.08	1.50	1.41
1	A	209	LLP	C4-C5	8.03	1.53	1.42
1	A	209	LLP	P-OP1	5.02	1.66	1.50
1	A	209	LLP	C6-N1	4.63	1.43	1.34
1	A	209	LLP	P-OP3	3.59	1.68	1.54
1	A	209	LLP	P-OP4	2.46	1.68	1.60
1	A	209	LLP	CD-CE	2.16	1.58	1.51
1	A	209	LLP	C4-C3	-2.13	1.37	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	209	LLP	CE-NZ-C4'	2.49	126.68	118.72
1	A	209	LLP	OP3-P-OP4	2.29	112.65	106.67

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	209	LLP	C-CA-CB-CG
1	A	209	LLP	O-C-CA-CB
1	A	209	LLP	CA-CB-CG-CD
1	A	209	LLP	C3-C4-C4'-NZ
1	A	209	LLP	C5-C4-C4'-NZ
1	A	209	LLP	CD-CE-NZ-C4'
1	A	209	LLP	C4-C5-C5'-OP4

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	209	LLP	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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	$\# Z > 2$
3	GOL	A	1006	-	5,5,5	0.51	0	5,5,5	0.64	0
3	GOL	A	1003	-	5,5,5	0.47	0	5,5,5	0.64	0
3	GOL	A	1007	-	5,5,5	0.67	0	5,5,5	0.73	0
3	GOL	A	1009	-	5,5,5	0.68	0	5,5,5	0.78	0
2	AOA	A	1001	-	3,5,5	1.05	0	3,5,5	1.47	0
3	GOL	A	1002	-	5,5,5	0.66	0	5,5,5	0.68	0
3	GOL	A	1004	-	5,5,5	0.50	0	5,5,5	0.67	0
3	GOL	A	1008	-	5,5,5	0.64	0	5,5,5	0.76	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
3	GOL	A	1006	-	-	2/4/4/4	-
3	GOL	A	1003	-	-	0/4/4/4	-
3	GOL	A	1007	-	-	1/4/4/4	-
3	GOL	A	1009	-	-	3/4/4/4	-
2	AOA	A	1001	-	-	2/2/3/3	-
3	GOL	A	1002	-	-	2/4/4/4	-
3	GOL	A	1004	-	-	1/4/4/4	-
3	GOL	A	1008	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1008	GOL	O1-C1-C2-C3
3	A	1008	GOL	C1-C2-C3-O3
3	A	1008	GOL	O2-C2-C3-O3
3	A	1009	GOL	O1-C1-C2-C3
3	A	1008	GOL	O1-C1-C2-O2
3	A	1002	GOL	O1-C1-C2-C3
3	A	1006	GOL	C1-C2-C3-O3
3	A	1007	GOL	O1-C1-C2-C3
3	A	1002	GOL	O1-C1-C2-O2
3	A	1009	GOL	O1-C1-C2-O2
3	A	1006	GOL	O2-C2-C3-O3
2	A	1001	AOA	O1-C1-C2-O2
2	A	1001	AOA	O1-C1-C2-O3
3	A	1004	GOL	O1-C1-C2-O2
3	A	1009	GOL	O2-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1003	GOL	2	0
2	A	1001	AOA	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	386/392 (98%)	0.25	12 (3%)	51 45	23, 41, 57, 71	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	387	CYS	4.4
1	A	390	LYS	3.3
1	A	328	ALA	3.1
1	A	4	HIS	3.1
1	A	136	LEU	2.5
1	A	273	ARG	2.3
1	A	5	LYS	2.3
1	A	171	GLU	2.2
1	A	254	ASP	2.2
1	A	170	ARG	2.2
1	A	197	ARG	2.2
1	A	7	LEU	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q < 0.9
1	LLP	A	209	24/25	0.93	0.12	34,39,45,47	0

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
3	GOL	A	1009	6/6	0.53	0.26	67,70,70,70	0
3	GOL	A	1006	6/6	0.69	0.24	66,67,67,67	0
2	AOA	A	1001	6/6	0.70	0.20	66,67,67,68	0
3	GOL	A	1004	6/6	0.74	0.21	55,56,57,60	0
3	GOL	A	1008	6/6	0.77	0.19	61,62,62,63	0
3	GOL	A	1007	6/6	0.80	0.22	56,60,61,61	0
3	GOL	A	1003	6/6	0.84	0.20	63,63,64,65	0
3	GOL	A	1002	6/6	0.88	0.14	53,54,54,56	0

6.5 Other polymers [i](#)

There are no such residues in this entry.