



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:44 AM UTC

PDB ID : 7CQL / pdb_00007cql
Title : Apo GmaS without ligand
Authors : Li, C.Y.; Zhang, Y.Z.
Deposited on : 2020-08-11
Resolution : 2.80 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
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

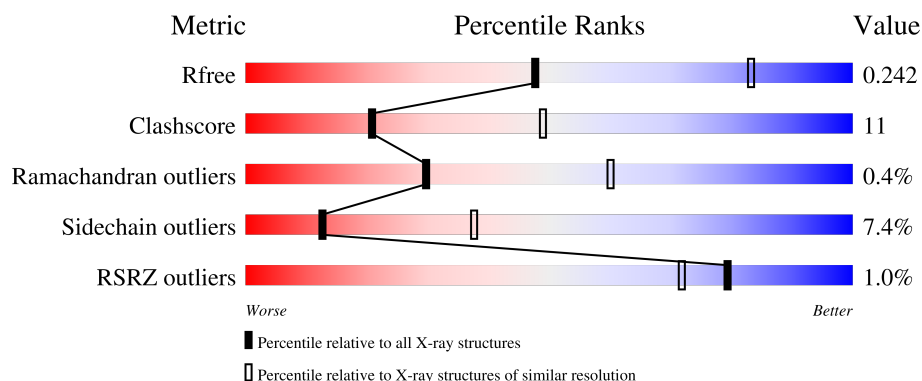
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	450	2% 69% 22% 6%
1	B	450	2% 71% 20% 6%
1	C	450	2% 69% 22% 6%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 9663 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 Type III glutamate–ammonia ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	421	Total	C	N	O	S	0	0	0
			3221	2046	557	600	18			
1	B	421	Total	C	N	O	S	0	0	0
			3221	2046	557	600	18			
1	C	421	Total	C	N	O	S	0	0	0
			3221	2046	557	600	18			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP A0A369R1N0
A	-18	GLY	-	expression tag	UNP A0A369R1N0
A	-17	SER	-	expression tag	UNP A0A369R1N0
A	-16	SER	-	expression tag	UNP A0A369R1N0
A	-15	HIS	-	expression tag	UNP A0A369R1N0
A	-14	HIS	-	expression tag	UNP A0A369R1N0
A	-13	HIS	-	expression tag	UNP A0A369R1N0
A	-12	HIS	-	expression tag	UNP A0A369R1N0
A	-11	HIS	-	expression tag	UNP A0A369R1N0
A	-10	HIS	-	expression tag	UNP A0A369R1N0
A	-9	SER	-	expression tag	UNP A0A369R1N0
A	-8	SER	-	expression tag	UNP A0A369R1N0
A	-7	GLY	-	expression tag	UNP A0A369R1N0
A	-6	LEU	-	expression tag	UNP A0A369R1N0
A	-5	VAL	-	expression tag	UNP A0A369R1N0
A	-4	PRO	-	expression tag	UNP A0A369R1N0
A	-3	ARG	-	expression tag	UNP A0A369R1N0
A	-2	GLY	-	expression tag	UNP A0A369R1N0
A	-1	SER	-	expression tag	UNP A0A369R1N0
A	0	HIS	-	expression tag	UNP A0A369R1N0
B	-19	MET	-	initiating methionine	UNP A0A369R1N0
B	-18	GLY	-	expression tag	UNP A0A369R1N0
B	-17	SER	-	expression tag	UNP A0A369R1N0

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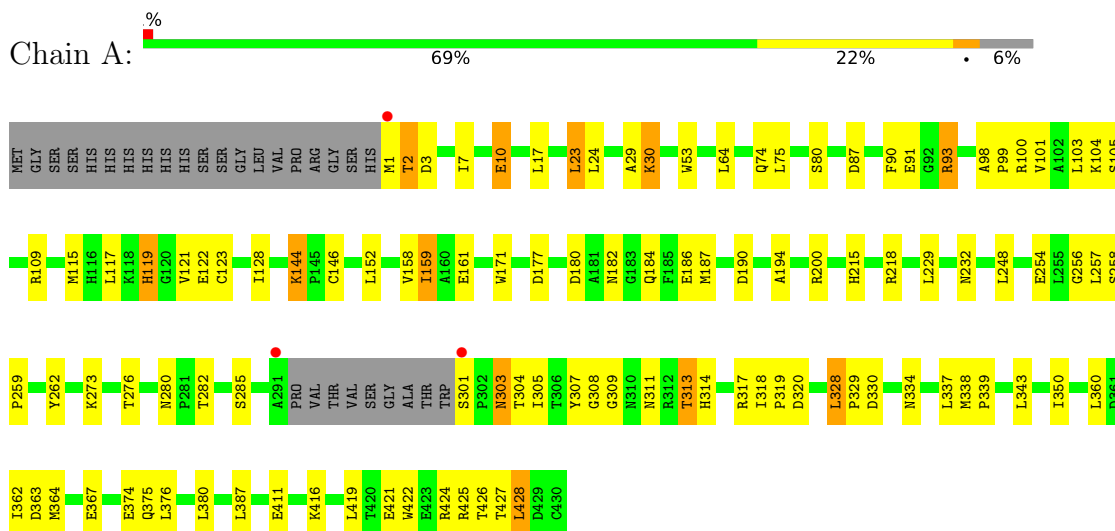
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	SER	-	expression tag	UNP A0A369R1N0
B	-15	HIS	-	expression tag	UNP A0A369R1N0
B	-14	HIS	-	expression tag	UNP A0A369R1N0
B	-13	HIS	-	expression tag	UNP A0A369R1N0
B	-12	HIS	-	expression tag	UNP A0A369R1N0
B	-11	HIS	-	expression tag	UNP A0A369R1N0
B	-10	HIS	-	expression tag	UNP A0A369R1N0
B	-9	SER	-	expression tag	UNP A0A369R1N0
B	-8	SER	-	expression tag	UNP A0A369R1N0
B	-7	GLY	-	expression tag	UNP A0A369R1N0
B	-6	LEU	-	expression tag	UNP A0A369R1N0
B	-5	VAL	-	expression tag	UNP A0A369R1N0
B	-4	PRO	-	expression tag	UNP A0A369R1N0
B	-3	ARG	-	expression tag	UNP A0A369R1N0
B	-2	GLY	-	expression tag	UNP A0A369R1N0
B	-1	SER	-	expression tag	UNP A0A369R1N0
B	0	HIS	-	expression tag	UNP A0A369R1N0
C	-19	MET	-	initiating methionine	UNP A0A369R1N0
C	-18	GLY	-	expression tag	UNP A0A369R1N0
C	-17	SER	-	expression tag	UNP A0A369R1N0
C	-16	SER	-	expression tag	UNP A0A369R1N0
C	-15	HIS	-	expression tag	UNP A0A369R1N0
C	-14	HIS	-	expression tag	UNP A0A369R1N0
C	-13	HIS	-	expression tag	UNP A0A369R1N0
C	-12	HIS	-	expression tag	UNP A0A369R1N0
C	-11	HIS	-	expression tag	UNP A0A369R1N0
C	-10	HIS	-	expression tag	UNP A0A369R1N0
C	-9	SER	-	expression tag	UNP A0A369R1N0
C	-8	SER	-	expression tag	UNP A0A369R1N0
C	-7	GLY	-	expression tag	UNP A0A369R1N0
C	-6	LEU	-	expression tag	UNP A0A369R1N0
C	-5	VAL	-	expression tag	UNP A0A369R1N0
C	-4	PRO	-	expression tag	UNP A0A369R1N0
C	-3	ARG	-	expression tag	UNP A0A369R1N0
C	-2	GLY	-	expression tag	UNP A0A369R1N0
C	-1	SER	-	expression tag	UNP A0A369R1N0
C	0	HIS	-	expression tag	UNP A0A369R1N0

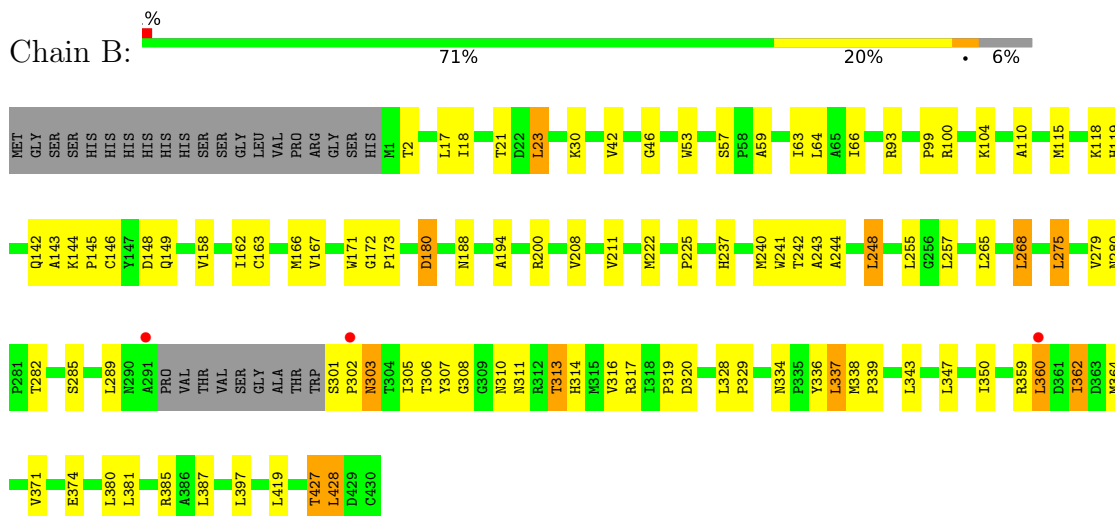
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Type III glutamate–ammonia ligase

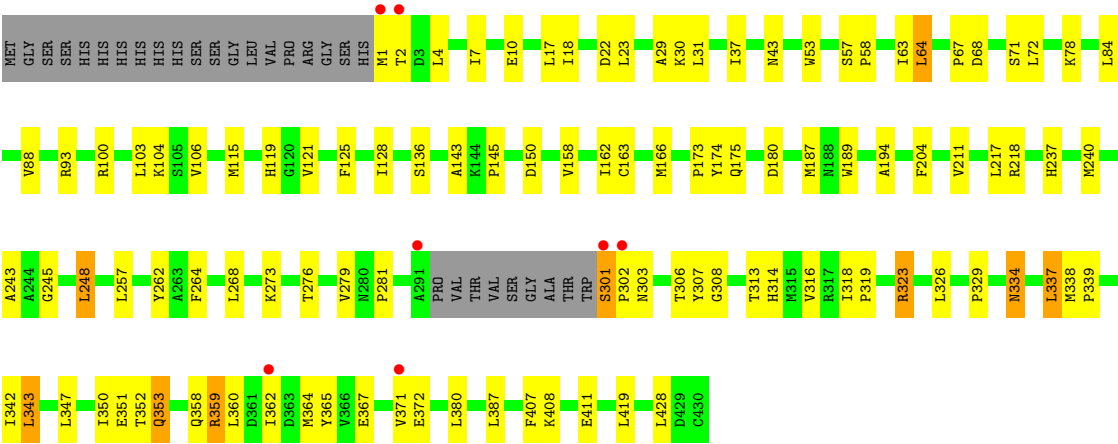


- Molecule 1: Type III glutamate–ammonia ligase



- Molecule 1: Type III glutamate–ammonia ligase





4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	115.91Å 179.02Å 192.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.57 – 2.80 40.57 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.6 (40.57-2.80) 97.7 (40.57-2.80)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	10.32 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.6.4_486	Depositor
R, R_{free}	0.200 , 0.251 0.195 , 0.242	Depositor DCC
R_{free} test set	2520 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	51.9	Xtriage
Anisotropy	0.897	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 24.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9663	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.57	0/3301	0.92	7/4486 (0.2%)
1	B	0.55	0/3301	0.89	4/4486 (0.1%)
1	C	0.54	0/3301	0.88	6/4486 (0.1%)
All	All	0.55	0/9903	0.90	17/13458 (0.1%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	144	LYS	CA-C-N	8.07	127.79	119.64
1	A	144	LYS	C-N-CA	8.07	127.79	119.64
1	C	334	ASN	CA-C-N	6.75	126.70	119.28
1	C	334	ASN	C-N-CA	6.75	126.70	119.28
1	C	307	TYR	N-CA-C	-6.39	100.74	110.14
1	C	78	LYS	CA-C-N	6.27	125.95	119.56
1	C	78	LYS	C-N-CA	6.27	125.95	119.56
1	A	109	ARG	N-CA-C	-5.71	104.96	111.07
1	A	119	HIS	N-CA-C	5.25	116.95	109.14
1	A	159	ILE	CB-CA-C	-5.23	105.27	111.97
1	B	66	ILE	CA-C-N	5.19	125.12	119.78
1	B	66	ILE	C-N-CA	5.19	125.12	119.78
1	B	172	GLY	CA-C-N	-5.19	114.61	119.85
1	B	172	GLY	C-N-CA	-5.19	114.61	119.85
1	C	359	ARG	N-CA-C	5.10	117.82	111.24
1	A	93	ARG	CA-C-N	5.08	125.08	119.90
1	A	93	ARG	C-N-CA	5.08	125.08	119.90

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	3221	0	3132	74	1
1	B	3221	0	3132	72	1
1	C	3221	0	3132	72	0
All	All	9663	0	9396	212	1

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 11.

All (212) 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:334:ASN:HB3	1:A:337:LEU:HB2	1.50	0.91
1:B:311:ASN:OD1	1:B:313:THR:HB	1.72	0.90
1:C:313:THR:HG22	1:C:364:MET:HB2	1.56	0.88
1:A:313:THR:HG21	1:A:364:MET:H	1.40	0.84
1:B:360:LEU:HD23	1:B:364:MET:HE1	1.60	0.83
1:A:313:THR:CG2	1:A:364:MET:H	1.93	0.81
1:C:334:ASN:HB3	1:C:337:LEU:HB2	1.61	0.81
1:A:338:MET:HB3	1:A:339:PRO:HD3	1.62	0.80
1:A:311:ASN:OD1	1:A:313:THR:HB	1.83	0.78
1:B:334:ASN:HB3	1:B:337:LEU:HB2	1.69	0.74
1:B:162:ILE:HG22	1:B:166:MET:HE2	1.69	0.73
1:C:17:LEU:HD22	1:C:29:ALA:HB1	1.71	0.72
1:C:279:VAL:HB	1:C:329:PRO:HB3	1.72	0.72
1:B:360:LEU:HD23	1:B:364:MET:CE	2.20	0.71
1:C:106:VAL:HG12	1:C:343:LEU:HG	1.73	0.71
1:B:110:ALA:HB2	1:B:347:LEU:HD11	1.73	0.71
1:C:313:THR:HG23	1:C:365:TYR:CD2	2.25	0.71
1:C:18:ILE:HD12	1:C:67:PRO:HG3	1.72	0.70
1:A:309:GLY:H	1:A:318:ILE:HD12	1.58	0.67
1:B:63:ILE:C	1:B:63:ILE:HD12	2.20	0.67
1:A:117:LEU:HD22	1:A:343:LEU:HD13	1.75	0.66
1:C:313:THR:HG21	1:C:364:MET:N	2.10	0.66
1:A:159:ILE:HG23	1:A:187:MET:HE2	1.76	0.66
1:A:115:MET:HE1	1:A:350:ILE:HG21	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:ALA:O	1:B:145:PRO:HD3	1.96	0.65
1:C:103:LEU:CD1	1:C:339:PRO:HB2	2.27	0.65
1:A:103:LEU:HD13	1:A:339:PRO:HB2	1.78	0.65
1:A:184:GLN:HE21	1:A:232:ASN:ND2	1.94	0.64
1:B:163:CYS:HA	1:B:166:MET:HE3	1.79	0.63
1:B:314:HIS:HE1	1:B:364:MET:HE2	1.64	0.62
1:C:359:ARG:O	1:C:360:LEU:HB2	1.98	0.62
1:B:115:MET:HE1	1:B:350:ILE:HD13	1.82	0.61
1:A:182:ASN:HD22	1:A:229:LEU:HD21	1.65	0.61
1:B:314:HIS:CE1	1:B:364:MET:CE	2.84	0.61
1:B:303:ASN:HD22	1:B:303:ASN:C	2.09	0.61
1:A:177:ASP:OD1	1:C:30:LYS:HE2	2.02	0.60
1:B:313:THR:HG22	1:B:314:HIS:CD2	2.35	0.60
1:C:103:LEU:HD13	1:C:339:PRO:HB2	1.83	0.60
1:A:184:GLN:HE21	1:A:232:ASN:HD22	1.49	0.60
1:B:307:TYR:CE2	1:B:359:ARG:HB2	2.35	0.60
1:C:119:HIS:HD2	1:C:194:ALA:HA	1.66	0.60
1:A:24:LEU:HD21	1:A:411:GLU:OE2	2.02	0.60
1:A:17:LEU:HD22	1:A:29:ALA:HB1	1.84	0.59
1:B:305:ILE:HD12	1:B:374:GLU:HB3	1.85	0.59
1:A:119:HIS:CD2	1:A:194:ALA:HA	2.36	0.59
1:B:242:THR:HG23	1:B:248:LEU:HD11	1.83	0.59
1:B:362:ILE:HD11	1:B:371:VAL:HG21	1.85	0.59
1:C:163:CYS:HA	1:C:166:MET:HE3	1.83	0.59
1:B:314:HIS:CE1	1:B:364:MET:HE2	2.39	0.58
1:C:100:ARG:O	1:C:104:LYS:HG3	2.02	0.58
1:A:119:HIS:CE1	1:A:339:PRO:HG3	2.38	0.58
1:A:334:ASN:CB	1:A:337:LEU:HB2	2.28	0.58
1:C:313:THR:CG2	1:C:364:MET:HB2	2.33	0.58
1:C:313:THR:HG21	1:C:364:MET:H	1.69	0.58
1:A:305:ILE:HD12	1:A:374:GLU:HB3	1.84	0.58
1:C:313:THR:HG23	1:C:365:TYR:CE2	2.39	0.58
1:B:313:THR:HG21	1:B:364:MET:H	1.68	0.57
1:A:338:MET:HB3	1:A:339:PRO:CD	2.34	0.57
1:C:119:HIS:CD2	1:C:194:ALA:HA	2.39	0.57
1:A:100:ARG:O	1:A:104:LYS:HG3	2.04	0.57
1:C:257:LEU:HB2	1:C:262:TYR:CE2	2.41	0.56
1:A:303:ASN:HD22	1:A:375:GLN:HG3	1.70	0.56
1:C:128:ILE:HG13	1:C:218:ARG:HB3	1.88	0.56
1:A:424:ARG:O	1:A:428:LEU:HB2	2.06	0.54
1:C:319:PRO:HB2	1:C:323:ARG:NH2	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:HIS:HD2	1:B:194:ALA:HA	1.73	0.54
1:A:119:HIS:HD2	1:A:194:ALA:HA	1.72	0.54
1:B:314:HIS:CE1	1:B:364:MET:HE3	2.44	0.53
1:B:30:LYS:NZ	1:B:46:GLY:O	2.39	0.53
1:B:305:ILE:O	1:B:306:THR:HG23	2.08	0.53
1:C:4:LEU:HD23	1:C:7:ILE:HD12	1.91	0.52
1:B:280:ASN:HD22	1:B:289:LEU:HD11	1.75	0.52
1:B:142:GLN:OE1	1:B:148:ASP:OD1	2.28	0.51
1:C:162:ILE:HG21	1:C:187:MET:HE1	1.92	0.51
1:C:257:LEU:CB	1:C:262:TYR:CE2	2.93	0.51
1:C:326:LEU:HD23	1:C:342:ILE:CD1	2.41	0.51
1:C:360:LEU:HD21	1:C:371:VAL:HG11	1.91	0.51
1:A:161:GLU:OE1	1:A:215:HIS:HE1	1.93	0.51
1:C:143:ALA:O	1:C:145:PRO:HD3	2.10	0.51
1:B:282:THR:O	1:B:285:SER:HB2	2.11	0.51
1:B:240:MET:HE1	1:B:343:LEU:CD1	2.40	0.50
1:C:115:MET:HE1	1:C:350:ILE:HG21	1.91	0.50
1:A:146:CYS:HB2	1:A:180:ASP:HB3	1.94	0.50
1:C:163:CYS:HA	1:C:166:MET:CE	2.41	0.50
1:A:276:THR:OG1	1:A:376:LEU:HD22	2.12	0.50
1:B:313:THR:CG2	1:B:364:MET:H	2.24	0.50
1:B:240:MET:HE1	1:B:343:LEU:HD13	1.94	0.50
1:B:158:VAL:HG23	1:B:211:VAL:HG12	1.93	0.49
1:A:1:MET:O	1:A:1:MET:HG3	2.12	0.49
1:C:240:MET:HE2	1:C:264:PHE:HE2	1.76	0.49
1:B:328:LEU:N	1:B:329:PRO:CD	2.75	0.49
1:C:119:HIS:HA	1:C:237:HIS:O	2.13	0.49
1:B:119:HIS:CD2	1:B:194:ALA:HA	2.48	0.49
1:A:182:ASN:HD22	1:A:229:LEU:CD2	2.25	0.49
1:C:136:SER:HB2	1:C:217:LEU:HD22	1.94	0.49
1:C:308:GLY:HA2	1:C:316:VAL:O	2.13	0.49
1:C:338:MET:HB3	1:C:339:PRO:HD3	1.94	0.49
1:B:23:LEU:HB2	1:B:53:TRP:O	2.13	0.48
1:B:242:THR:HG23	1:B:248:LEU:CD1	2.43	0.48
1:A:171:TRP:CZ2	1:A:200:ARG:HG2	2.48	0.48
1:A:313:THR:HG23	1:A:364:MET:HB2	1.93	0.48
1:A:317:ARG:O	1:A:319:PRO:HD3	2.13	0.48
1:B:314:HIS:HE1	1:B:364:MET:CE	2.25	0.48
1:A:314:HIS:CE1	1:A:364:MET:HG2	2.49	0.48
1:C:106:VAL:CG1	1:C:343:LEU:HG	2.42	0.48
1:B:143:ALA:C	1:B:145:PRO:HD3	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:LEU:H	1:A:329:PRO:CD	2.27	0.47
1:C:63:ILE:HD12	1:C:63:ILE:C	2.39	0.47
1:A:128:ILE:HG13	1:A:218:ARG:HB3	1.96	0.47
1:A:362:ILE:HG23	1:A:367:GLU:HB2	1.96	0.47
1:B:308:GLY:HA2	1:B:316:VAL:O	2.14	0.47
1:B:171:TRP:CE2	1:B:200:ARG:HG2	2.50	0.47
1:C:326:LEU:HD23	1:C:342:ILE:HD11	1.97	0.47
1:A:276:THR:O	1:A:280:ASN:HB2	2.14	0.47
1:A:307:TYR:HB2	1:A:308:GLY:HA3	1.97	0.46
1:A:363:ASP:OD1	1:A:363:ASP:C	2.58	0.46
1:B:242:THR:CG2	1:B:248:LEU:HD11	2.44	0.46
1:B:317:ARG:O	1:B:319:PRO:HD3	2.14	0.46
1:C:187:MET:HE3	1:C:204:PHE:CZ	2.50	0.46
1:A:171:TRP:CE2	1:A:200:ARG:HG2	2.50	0.46
1:B:21:THR:O	1:B:99:PRO:HD2	2.15	0.46
1:C:281:PRO:O	1:C:408:LYS:HD2	2.15	0.46
1:A:362:ILE:HD12	1:A:362:ILE:H	1.81	0.46
1:B:100:ARG:O	1:B:104:LYS:HG3	2.15	0.46
1:B:173:PRO:HA	1:B:188:ASN:O	2.15	0.46
1:B:255:LEU:HG	1:B:359:ARG:NH1	2.30	0.46
1:B:162:ILE:HD13	1:B:208:VAL:HG22	1.98	0.46
1:C:173:PRO:HA	1:C:189:TRP:HA	1.98	0.46
1:A:30:LYS:HB2	1:A:30:LYS:HE2	1.64	0.45
1:A:23:LEU:HD13	1:A:99:PRO:HD3	1.98	0.45
1:B:146:CYS:HB2	1:B:180:ASP:HA	1.98	0.45
1:C:240:MET:HE2	1:C:264:PHE:CE2	2.50	0.45
1:C:352:THR:O	1:C:353:GLN:C	2.60	0.45
1:C:63:ILE:HD13	1:C:88:VAL:HG13	1.98	0.45
1:B:275:LEU:HD12	1:B:275:LEU:HA	1.72	0.45
1:C:57:SER:OG	1:C:58:PRO:HD2	2.17	0.45
1:A:362:ILE:HD12	1:A:362:ILE:N	2.32	0.45
1:B:381:LEU:HD21	1:B:385:ARG:NH2	2.30	0.45
1:B:338:MET:HB3	1:B:339:PRO:HD3	1.98	0.45
1:A:1:MET:O	1:A:2:THR:C	2.59	0.45
1:A:338:MET:HE2	1:A:339:PRO:HD3	1.99	0.45
1:A:152:LEU:HD21	1:C:31:LEU:HB2	1.99	0.45
1:A:362:ILE:HG22	1:A:363:ASP:N	2.31	0.45
1:C:43:ASN:O	1:C:64:LEU:HG	2.17	0.44
1:B:222:MET:O	1:B:225:PRO:HD3	2.18	0.44
1:C:22:ASP:OD1	1:C:22:ASP:C	2.60	0.44
1:C:273:LYS:O	1:C:276:THR:HB	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:ALA:O	1:A:99:PRO:C	2.60	0.44
1:C:372:GLU:OE2	1:C:372:GLU:HA	2.16	0.44
1:C:248:LEU:HD12	1:C:248:LEU:HA	1.85	0.43
1:B:23:LEU:HD12	1:B:23:LEU:HA	1.81	0.43
1:B:30:LYS:HE3	1:B:30:LYS:HB2	1.84	0.43
1:C:319:PRO:HB2	1:C:323:ARG:HH21	1.81	0.43
1:A:303:ASN:ND2	1:A:375:GLN:HG3	2.34	0.43
1:B:21:THR:OG1	1:B:336:TYR:HE2	2.01	0.43
1:C:306:THR:O	1:C:314:HIS:HB3	2.18	0.43
1:A:29:ALA:CB	1:B:149:GLN:HG3	2.49	0.43
1:A:87:ASP:OD1	1:A:100:ARG:NH1	2.48	0.43
1:A:338:MET:O	1:A:339:PRO:C	2.62	0.43
1:C:71:SER:O	1:C:72:LEU:C	2.61	0.43
1:C:243:ALA:C	1:C:245:GLY:H	2.27	0.43
1:A:144:LYS:HG3	1:C:53:TRP:CZ2	2.53	0.43
1:A:258:SER:HB2	1:A:259:PRO:HD2	2.01	0.43
1:C:358:GLN:HG2	1:C:359:ARG:H	1.83	0.43
1:C:103:LEU:HD11	1:C:339:PRO:HB2	2.00	0.42
1:A:309:GLY:H	1:A:318:ILE:CD1	2.28	0.42
1:C:162:ILE:HD11	1:C:211:VAL:HB	2.01	0.42
1:A:285:SER:OG	1:A:330:ASP:OD2	2.33	0.42
1:B:301:SER:HB3	1:B:302:PRO:HD3	2.01	0.42
1:C:301:SER:HB3	1:C:302:PRO:HD3	2.01	0.42
1:A:422:TRP:O	1:A:426:THR:HG23	2.20	0.42
1:A:421:GLU:O	1:A:425:ARG:HG3	2.19	0.42
1:B:57:SER:C	1:B:59:ALA:H	2.27	0.42
1:A:7:ILE:HA	1:A:10:GLU:HG3	2.02	0.42
1:A:74:GLN:O	1:A:75:LEU:C	2.62	0.42
1:A:103:LEU:CD1	1:A:339:PRO:HB2	2.46	0.42
1:A:144:LYS:HE2	1:C:53:TRP:CZ3	2.54	0.42
1:B:347:LEU:HD23	1:B:347:LEU:HA	1.86	0.42
1:C:318:ILE:HA	1:C:319:PRO:HD3	1.84	0.42
1:B:119:HIS:HA	1:B:237:HIS:O	2.19	0.42
1:A:159:ILE:HD13	1:A:187:MET:CE	2.50	0.41
1:C:68:ASP:OD1	1:C:68:ASP:C	2.63	0.41
1:C:407:PHE:O	1:C:411:GLU:HG3	2.20	0.41
1:A:273:LYS:HE3	1:A:374:GLU:HG3	2.01	0.41
1:B:328:LEU:H	1:B:329:PRO:CD	2.33	0.41
1:B:397:LEU:HD23	1:B:397:LEU:HA	1.80	0.41
1:B:427:THR:O	1:B:428:LEU:C	2.62	0.41
1:C:358:GLN:HG2	1:C:359:ARG:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:PRO:O	1:B:148:ASP:HB2	2.20	0.41
1:C:174:TYR:CE2	1:C:175:GLN:HG2	2.55	0.41
1:A:53:TRP:CZ2	1:B:144:LYS:HG3	2.56	0.41
1:A:282:THR:O	1:A:285:SER:HB2	2.20	0.41
1:B:313:THR:HG23	1:B:364:MET:HB2	2.02	0.41
1:C:347:LEU:O	1:C:351:GLU:HG3	2.21	0.41
1:B:243:ALA:O	1:B:244:ALA:C	2.62	0.41
1:B:268:LEU:HA	1:B:268:LEU:HD12	1.86	0.41
1:C:67:PRO:HB3	1:C:84:LEU:HD13	2.02	0.41
1:B:63:ILE:C	1:B:63:ILE:CD1	2.91	0.41
1:C:257:LEU:HB3	1:C:262:TYR:CE2	2.56	0.41
1:A:90:PHE:O	1:A:91:GLU:HB2	2.21	0.41
1:A:146:CYS:HB2	1:A:180:ASP:HA	2.03	0.41
1:A:257:LEU:HB2	1:A:262:TYR:CE2	2.56	0.41
1:B:280:ASN:ND2	1:B:289:LEU:HD11	2.35	0.41
1:B:118:LYS:HD2	1:B:241:TRP:NE1	2.36	0.40
1:A:146:CYS:HB2	1:A:180:ASP:CB	2.51	0.40
1:A:254:GLU:C	1:A:256:GLY:H	2.30	0.40
1:B:265:LEU:HD11	1:B:316:VAL:HG11	2.03	0.40
1:C:187:MET:HE3	1:C:204:PHE:HZ	1.86	0.40
1:C:362:ILE:HG23	1:C:367:GLU:HB2	2.04	0.40
1:A:122:GLU:HB3	1:A:186:GLU:OE2	2.22	0.40
1:B:328:LEU:H	1:B:329:PRO:HD3	1.85	0.40
1:C:125:PHE:CZ	1:C:187:MET:HE2	2.57	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:ARG:NH1	1:B:225:PRO:O[3_455]	2.19	0.01

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	417/450 (93%)	395 (95%)	20 (5%)	2 (0%)	24	55
1	B	417/450 (93%)	396 (95%)	19 (5%)	2 (0%)	24	55
1	C	417/450 (93%)	388 (93%)	28 (7%)	1 (0%)	43	72
All	All	1251/1350 (93%)	1179 (94%)	67 (5%)	5 (0%)	30	60

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	310	ASN
1	A	190	ASP
1	C	150	ASP
1	A	328	LEU
1	B	362	ILE

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	324/348 (93%)	298 (92%)	26 (8%)	11	34
1	B	324/348 (93%)	300 (93%)	24 (7%)	13	37
1	C	324/348 (93%)	302 (93%)	22 (7%)	14	42
All	All	972/1044 (93%)	900 (93%)	72 (7%)	13	37

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	3	ASP
1	A	10	GLU
1	A	23	LEU
1	A	30	LYS
1	A	64	LEU

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Mol	Chain	Res	Type
1	A	80	SER
1	A	93	ARG
1	A	101	VAL
1	A	105	SER
1	A	121	VAL
1	A	123	CYS
1	A	158	VAL
1	A	248	LEU
1	A	301	SER
1	A	303	ASN
1	A	304	THR
1	A	313	THR
1	A	320	ASP
1	A	360	LEU
1	A	380	LEU
1	A	387	LEU
1	A	416	LYS
1	A	419	LEU
1	A	427	THR
1	A	428	LEU
1	B	2	THR
1	B	17	LEU
1	B	18	ILE
1	B	23	LEU
1	B	42	VAL
1	B	64	LEU
1	B	93	ARG
1	B	167	VAL
1	B	180	ASP
1	B	248	LEU
1	B	257	LEU
1	B	268	LEU
1	B	275	LEU
1	B	279	VAL
1	B	303	ASN
1	B	313	THR
1	B	320	ASP
1	B	337	LEU
1	B	360	LEU
1	B	380	LEU
1	B	387	LEU
1	B	419	LEU

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Mol	Chain	Res	Type
1	B	427	THR
1	B	428	LEU
1	C	1	MET
1	C	2	THR
1	C	10	GLU
1	C	23	LEU
1	C	37	ILE
1	C	64	LEU
1	C	93	ARG
1	C	121	VAL
1	C	158	VAL
1	C	180	ASP
1	C	248	LEU
1	C	268	LEU
1	C	301	SER
1	C	303	ASN
1	C	323	ARG
1	C	337	LEU
1	C	343	LEU
1	C	353	GLN
1	C	380	LEU
1	C	387	LEU
1	C	419	LEU
1	C	428	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	GLN
1	A	142	GLN
1	A	149	GLN
1	A	176	ASN
1	A	182	ASN
1	A	184	GLN
1	A	201	HIS
1	A	215	HIS
1	A	290	ASN
1	A	303	ASN
1	A	375	GLN
1	B	119	HIS
1	B	142	GLN
1	B	182	ASN

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Mol	Chain	Res	Type
1	B	215	HIS
1	B	232	ASN
1	B	237	HIS
1	B	280	ASN
1	B	290	ASN
1	B	303	ASN
1	B	314	HIS
1	C	89	HIS
1	C	119	HIS
1	C	142	GLN
1	C	175	GLN
1	C	176	ASN
1	C	188	ASN
1	C	215	HIS
1	C	232	ASN
1	C	237	HIS
1	C	290	ASN
1	C	353	GLN
1	C	375	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

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 [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	421/450 (93%)	-0.28	3 (0%) 84 77	42, 51, 74, 115	0
1	B	421/450 (93%)	-0.14	3 (0%) 84 77	40, 53, 87, 119	0
1	C	421/450 (93%)	-0.13	7 (1%) 69 60	45, 55, 87, 120	0
All	All	1263/1350 (93%)	-0.19	13 (1%) 79 72	40, 53, 84, 120	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	291	ALA	4.4
1	B	291	ALA	3.0
1	C	301	SER	2.7
1	C	362	ILE	2.7
1	A	291	ALA	2.7
1	C	1	MET	2.4
1	A	1	MET	2.3
1	C	302	PRO	2.3
1	B	360	LEU	2.3
1	A	301	SER	2.2
1	B	302	PRO	2.1
1	C	2	THR	2.1
1	C	371	VAL	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.