



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:18 PM UTC

PDB ID : 1GC2 / pdb_00001gc2
Title : CRYSTAL STRUCTURE OF THE PYRIDOXAL-5'-PHOSPHATE
DEPENDENT L-METHIONINE GAMMA-LYASE FROM PSEUDOMONAS
PUTIDA
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T.; Esaki, N.; Soda, K.; Tanaka, N.; Yamamoto, M.; Tanaka, H.
Deposited on : 2000-07-06
Resolution : 2.00 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

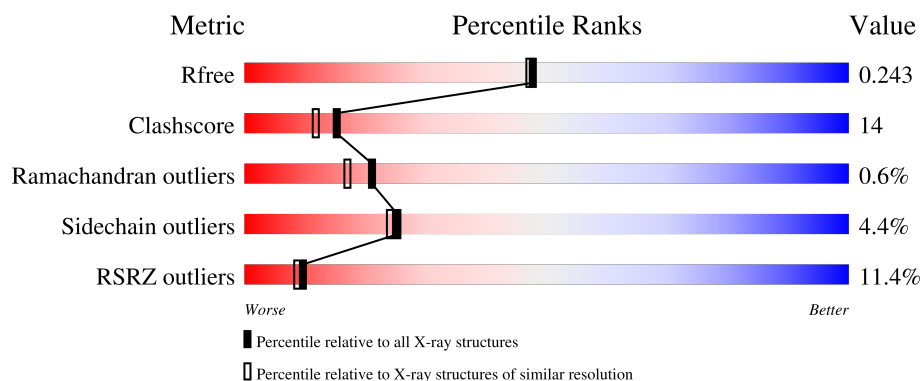
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	398	13% 69% 23% 6%
1	B	398	6% 67% 23% 7%
1	C	398	10% 69% 22% 6%
1	D	398	13% 67% 23% 7%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12444 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 METHIONINE GAMMA-LYASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	373	Total	C	N	O	P	S	0	0	0
			2820	1778	498	527	1	16			
1	B	370	Total	C	N	O	P	S	0	0	0
			2799	1764	495	523	1	16			
1	C	375	Total	C	N	O	P	S	0	0	0
			2837	1789	500	531	1	16			
1	D	370	Total	C	N	O	P	S	0	0	0
			2799	1764	495	523	1	16			

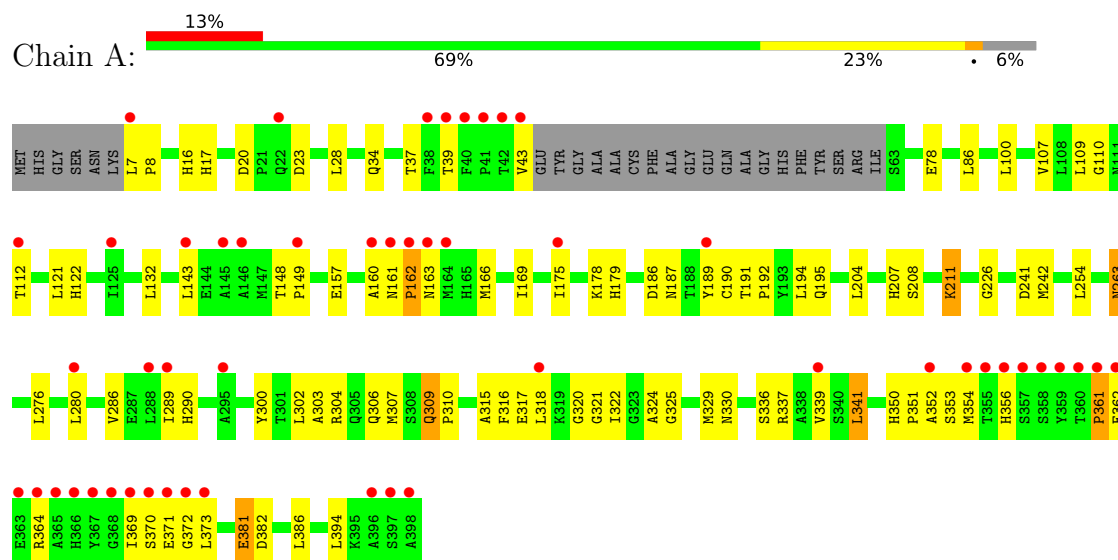
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	274	Total	O	0	0
			274	274		
2	B	346	Total	O	0	0
			346	346		
2	C	307	Total	O	0	0
			307	307		
2	D	262	Total	O	0	0
			262	262		

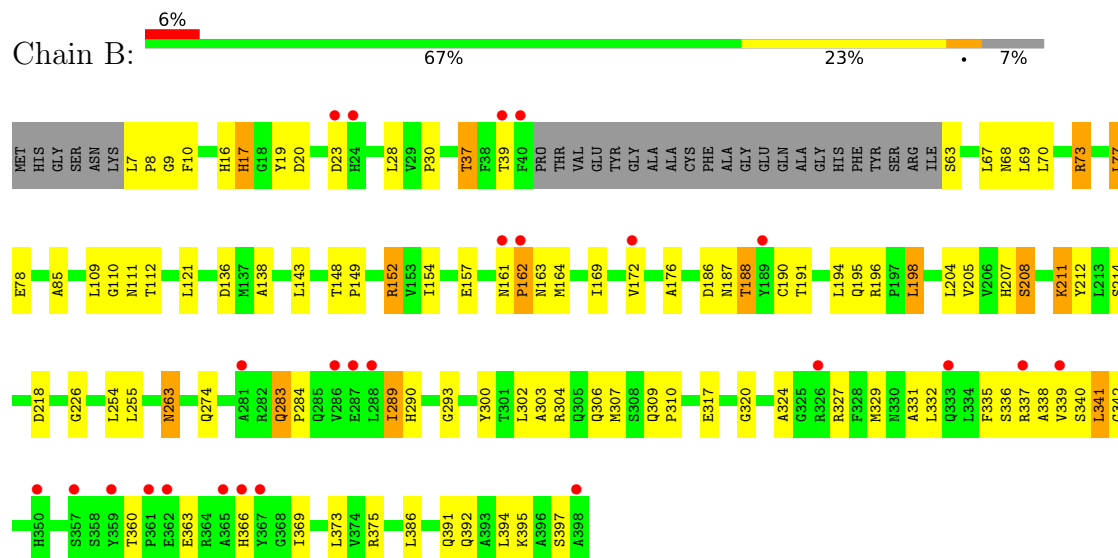
3 Residue-property plots

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: METHIONINE GAMMA-LYASE

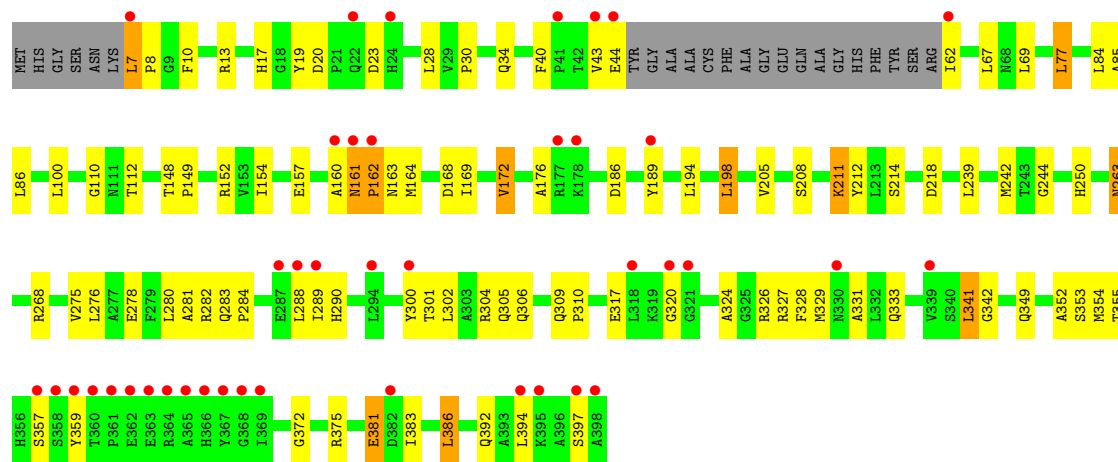


• Molecule 1: METHIONINE GAMMA-LYASE

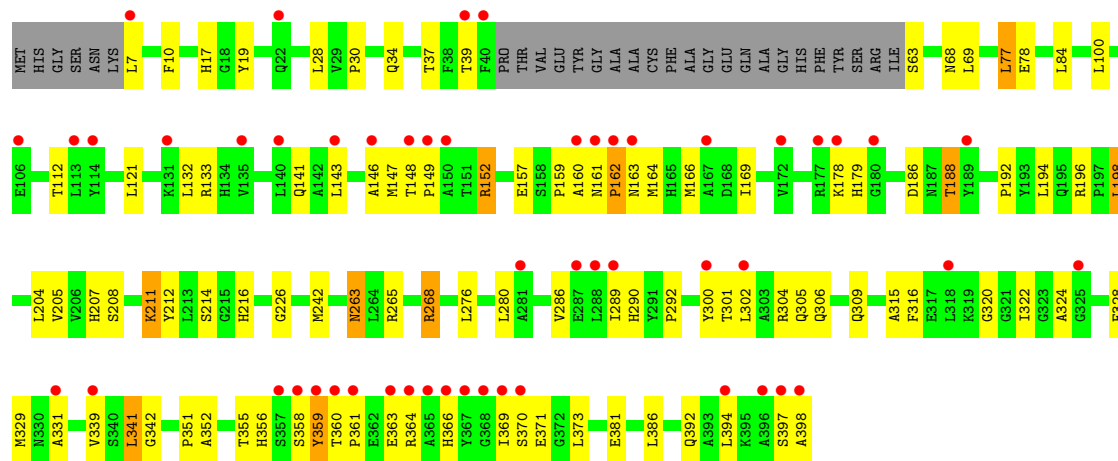


• Molecule 1: METHIONINE GAMMA-LYASE





• Molecule 1: METHIONINE GAMMA-LYASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	133.58Å 133.58Å 213.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	83.43 – 2.00 83.43 – 2.00	Depositor EDS
% Data completeness (in resolution range)	94.9 (83.43-2.00) 95.0 (83.43-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.96 (at 2.00Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.211 , 0.243 0.211 , 0.243	Depositor DCC
R_{free} test set	12954 reflections (9.96%)	wwPDB-VP
Wilson B-factor (Å ²)	29.9	Xtriage
Anisotropy	0.388	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 48.9	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	12444	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.37	0/2853	0.90	11/3873 (0.3%)
1	B	0.40	0/2831	0.91	9/3841 (0.2%)
1	C	0.39	0/2870	0.90	7/3896 (0.2%)
1	D	0.37	0/2831	0.87	6/3841 (0.2%)
All	All	0.38	0/11385	0.90	33/15451 (0.2%)

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	16	HIS	N-CA-C	6.73	122.16	113.88
1	A	110	GLY	N-CA-C	-6.65	104.28	111.93
1	B	283	GLN	CA-C-N	6.62	126.56	119.28
1	B	283	GLN	C-N-CA	6.62	126.56	119.28
1	A	242	MET	N-CA-C	6.51	121.39	113.38
1	B	110	GLY	N-CA-C	-6.42	105.26	112.33
1	C	110	GLY	N-CA-C	-6.32	104.66	111.93
1	D	214	SER	N-CA-C	-6.26	104.38	111.14
1	D	242	MET	N-CA-C	6.03	120.80	113.38
1	D	208	SER	N-CA-C	-5.83	96.26	107.57
1	C	208	SER	N-CA-C	-5.80	96.33	107.57
1	A	16	HIS	N-CA-C	5.79	121.00	113.88
1	A	208	SER	N-CA-C	-5.71	97.12	107.75
1	B	208	SER	N-CA-C	-5.67	96.56	107.57
1	B	17	HIS	N-CA-C	5.66	118.56	110.24
1	A	309	GLN	CA-C-N	5.63	125.34	119.82
1	A	309	GLN	C-N-CA	5.63	125.34	119.82
1	A	122	HIS	N-CA-C	5.61	117.48	111.36
1	C	310	PRO	N-CA-C	5.59	120.90	114.20
1	C	17	HIS	N-CA-C	5.38	118.27	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	214	SER	N-CA-C	-5.34	105.37	111.14
1	B	138	ALA	N-CA-C	-5.34	106.94	113.50
1	C	242	MET	N-CA-C	5.32	120.78	113.97
1	D	196	ARG	CA-C-N	5.30	125.36	119.32
1	D	196	ARG	C-N-CA	5.30	125.36	119.32
1	A	189	TYR	N-CA-C	5.20	116.95	111.28
1	C	189	TYR	N-CA-C	5.20	116.63	111.07
1	B	214	SER	N-CA-C	-5.18	105.54	111.14
1	A	17	HIS	N-CA-C	5.17	117.97	110.42
1	D	17	HIS	N-CA-C	5.16	117.96	110.42
1	A	241	ASP	N-CA-C	5.15	120.22	113.88
1	B	310	PRO	N-CA-C	5.15	120.38	114.20
1	A	310	PRO	N-CA-C	5.01	120.45	113.98

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	2820	0	2798	71	0
1	B	2799	0	2775	82	0
1	C	2837	0	2815	83	0
1	D	2799	0	2775	92	0
2	A	274	0	0	1	0
2	B	346	0	0	6	0
2	C	307	0	0	7	0
2	D	262	0	0	10	0
All	All	12444	0	11163	304	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 14.

All (304) 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:B:186:ASP:OD1	1:B:188:THR:HG23	1.74	0.88
1:C:169:ILE:H	1:C:306:GLN:HE22	1.19	0.86
1:A:7:LEU:HD12	1:A:8:PRO:HD2	1.56	0.85
1:C:161:ASN:H	1:C:161:ASN:HD22	1.22	0.84
1:D:286:VAL:HG11	1:D:289:ILE:HD11	1.60	0.83
1:A:361:PRO:HA	1:A:364:ARG:HH12	1.41	0.82
1:B:169:ILE:H	1:B:306:GLN:HE22	1.26	0.82
1:D:186:ASP:OD1	1:D:188:THR:HG23	1.79	0.81
1:A:28:LEU:HD12	1:D:37:THR:OG1	1.81	0.80
1:B:198:LEU:HD13	1:B:205:VAL:HG23	1.64	0.80
1:C:161:ASN:HD22	1:C:161:ASN:N	1.78	0.77
1:A:286:VAL:HG11	1:A:289:ILE:HD11	1.65	0.77
1:C:161:ASN:H	1:C:161:ASN:ND2	1.80	0.77
1:A:300:TYR:O	1:A:304:ARG:HG3	1.86	0.76
1:B:303:ALA:HB1	1:B:307:MET:CE	2.14	0.76
1:D:198:LEU:HD13	1:D:205:VAL:HG23	1.67	0.76
1:B:327:ARG:HB3	1:B:397:SER:HA	1.69	0.74
1:C:162:PRO:HG2	2:C:580:HOH:O	1.88	0.74
1:A:354:MET:HG3	1:C:43:VAL:HG13	1.70	0.74
1:B:289:ILE:HD13	1:B:290:HIS:N	2.04	0.73
1:D:169:ILE:H	1:D:306:GLN:HE22	1.34	0.73
1:D:331:ALA:HB1	1:D:392:GLN:HE22	1.54	0.73
1:A:169:ILE:H	1:A:306:GLN:HE22	1.36	0.72
1:A:353:SER:OG	1:C:43:VAL:HG11	1.90	0.71
1:D:268:ARG:HA	1:D:268:ARG:HH11	1.55	0.71
1:D:265:ARG:CZ	2:D:630:HOH:O	2.39	0.71
1:B:307:MET:HE3	2:B:649:HOH:O	1.91	0.70
1:D:276:LEU:O	1:D:280:LEU:HD23	1.91	0.70
1:A:160:ALA:C	1:A:162:PRO:HD2	2.16	0.70
1:B:303:ALA:HB1	1:B:307:MET:HE2	1.73	0.69
1:D:265:ARG:NE	2:D:630:HOH:O	2.24	0.69
1:D:304:ARG:HB3	1:D:304:ARG:NH1	2.08	0.69
1:A:350:HIS:NE2	1:A:352:ALA:HB3	2.08	0.68
1:B:112:THR:HG21	1:B:162:PRO:HG2	1.76	0.68
1:D:304:ARG:HB3	1:D:304:ARG:HH11	1.59	0.67
1:B:338:ALA:HB2	1:D:39:THR:HG22	1.77	0.67
1:A:289:ILE:HD13	1:A:316:PHE:HB2	1.77	0.66
1:C:198:LEU:HD13	1:C:205:VAL:HG23	1.76	0.66
1:C:7:LEU:HD21	1:C:13:ARG:HD3	1.78	0.65
1:B:340:SER:HB2	1:D:37:THR:HG21	1.78	0.65
1:C:152:ARG:HA	1:C:152:ARG:NE	2.12	0.65
1:A:330:ASN:OD1	1:C:43:VAL:HG23	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:MET:HE3	1:B:337:ARG:HG2	1.80	0.64
1:D:157:GLU:HG2	1:D:186:ASP:HB3	1.79	0.64
1:D:339:VAL:HG13	1:D:339:VAL:O	1.97	0.64
1:A:361:PRO:HA	1:A:364:ARG:NH1	2.14	0.62
1:C:327:ARG:HB3	1:C:397:SER:HA	1.82	0.62
1:A:37:THR:HB	1:D:28:LEU:HD12	1.81	0.61
1:A:290:HIS:HB2	1:A:315:ALA:HB3	1.81	0.61
1:A:321:GLY:HA2	1:A:371:GLU:HG2	1.82	0.61
1:D:331:ALA:HB1	1:D:392:GLN:NE2	2.13	0.61
1:C:349:GLN:NE2	1:C:375:ARG:NH2	2.47	0.61
1:C:40:PHE:HZ	1:C:62:ILE:HD11	1.66	0.61
1:D:364:ARG:HG3	1:D:371:GLU:OE2	2.00	0.61
1:C:331:ALA:HB1	1:C:392:GLN:HE22	1.66	0.61
1:D:398:ALA:HA	2:D:599:HOH:O	2.01	0.61
1:B:39:THR:HG23	1:C:28:LEU:HG	1.83	0.60
1:B:337:ARG:HD2	2:B:712:HOH:O	2.02	0.59
1:D:304:ARG:HH11	1:D:304:ARG:CB	2.15	0.59
1:A:381:GLU:CG	1:A:386:LEU:HD21	2.33	0.59
1:C:7:LEU:HD23	1:C:8:PRO:HD2	1.85	0.59
1:D:160:ALA:C	1:D:162:PRO:HD2	2.28	0.58
1:A:351:PRO:HB3	1:A:356:HIS:HD2	1.68	0.58
1:D:286:VAL:HG11	1:D:289:ILE:CD1	2.32	0.58
1:D:351:PRO:HB3	1:D:356:HIS:HD2	1.68	0.58
1:C:263:ASN:HD22	1:C:263:ASN:H	1.52	0.58
1:D:359:TYR:HD2	1:D:363:GLU:HB3	1.69	0.58
1:B:157:GLU:HG2	1:B:186:ASP:HB3	1.85	0.58
1:D:204:LEU:HD23	1:D:226:GLY:HA3	1.86	0.58
1:B:19:TYR:CE1	1:B:30:PRO:HB3	2.38	0.58
1:D:198:LEU:HB2	2:D:407:HOH:O	2.03	0.58
1:D:300:TYR:CE2	1:D:304:ARG:HD2	2.39	0.57
1:C:276:LEU:O	1:C:280:LEU:HD23	2.04	0.57
1:B:339:VAL:O	1:B:339:VAL:HG13	2.03	0.57
1:D:320:GLY:HA3	1:D:324:ALA:HB2	1.86	0.57
1:C:211:LLP:HE3	1:C:341:LEU:CD1	2.35	0.57
1:D:10:PHE:CZ	1:D:77:LEU:HG	2.40	0.57
1:A:371:GLU:H	1:A:371:GLU:CD	2.13	0.57
1:D:289:ILE:HD13	1:D:316:PHE:HB2	1.86	0.57
1:D:328:PHE:HD2	1:D:329:MET:HE2	1.70	0.57
1:C:194:LEU:HD22	1:C:309:GLN:HB2	1.86	0.56
1:D:152:ARG:HB2	1:D:152:ARG:NH1	2.20	0.56
1:A:78:GLU:OE2	1:A:207:HIS:HE1	1.89	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:LEU:HD13	1:B:121:LEU:HD13	1.87	0.56
1:D:198:LEU:CD1	1:D:205:VAL:HG23	2.35	0.56
1:B:263:ASN:H	1:B:263:ASN:HD22	1.54	0.55
1:D:370:SER:HB3	1:D:373:LEU:HB2	1.89	0.55
1:A:300:TYR:CE2	1:A:304:ARG:HD2	2.42	0.55
1:C:157:GLU:HG2	1:C:186:ASP:HB3	1.88	0.55
1:B:198:LEU:HB2	2:B:399:HOH:O	2.07	0.55
1:A:289:ILE:HD13	1:A:316:PHE:CB	2.37	0.54
1:A:320:GLY:HA3	1:A:324:ALA:HB2	1.89	0.54
1:B:186:ASP:OD1	1:B:188:THR:CG2	2.53	0.54
1:C:67:LEU:HD12	1:C:85:ALA:HB3	1.89	0.54
1:D:78:GLU:OE2	1:D:192:PRO:HG3	2.08	0.54
1:D:186:ASP:OD1	1:D:188:THR:CG2	2.54	0.54
1:C:169:ILE:H	1:C:306:GLN:NE2	1.97	0.54
1:A:354:MET:HG3	1:C:43:VAL:CG1	2.36	0.54
1:B:7:LEU:HD12	1:B:8:PRO:HD2	1.90	0.54
1:C:7:LEU:HD23	1:C:8:PRO:CD	2.37	0.54
1:B:37:THR:HG23	1:C:28:LEU:HD12	1.90	0.54
1:B:204:LEU:HD23	1:B:226:GLY:HA3	1.90	0.54
1:D:216:HIS:CE1	1:D:265:ARG:HH21	2.26	0.54
1:C:163:ASN:HB2	1:C:290:HIS:CD2	2.43	0.53
1:A:300:TYR:CZ	1:A:304:ARG:HD2	2.43	0.53
1:A:317:GLU:HA	1:A:372:GLY:O	2.07	0.53
1:A:353:SER:O	1:C:43:VAL:HG12	2.09	0.53
1:A:322:ILE:HA	1:A:371:GLU:O	2.07	0.53
1:D:356:HIS:CD2	1:D:369:ILE:HD13	2.43	0.53
1:C:84:LEU:HD11	1:C:239:LEU:HD22	1.90	0.53
1:D:328:PHE:CD2	1:D:329:MET:HE2	2.43	0.53
1:C:20:ASP:HB3	1:C:23:ASP:OD2	2.09	0.53
1:C:300:TYR:CZ	1:C:304:ARG:HD2	2.44	0.53
1:D:78:GLU:OE2	1:D:207:HIS:HE1	1.92	0.53
1:B:320:GLY:HA3	1:B:324:ALA:HB2	1.90	0.53
1:A:370:SER:HB3	1:A:373:LEU:HB2	1.90	0.53
1:D:148:THR:HB	1:D:149:PRO:HD2	1.90	0.53
1:B:67:LEU:HD12	1:B:85:ALA:HB3	1.91	0.53
1:D:161:ASN:N	1:D:162:PRO:HD2	2.24	0.52
1:B:196:ARG:NE	2:B:681:HOH:O	2.41	0.52
1:A:211:LLP:HE3	1:A:341:LEU:HD13	1.91	0.52
1:A:263:ASN:H	1:A:263:ASN:HD22	1.56	0.52
1:B:391:GLN:NE2	1:B:395:LYS:HE3	2.24	0.52
1:A:20:ASP:HB3	1:A:23:ASP:OD2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:GLU:OE2	1:B:207:HIS:HE1	1.92	0.52
1:C:112:THR:OG1	1:C:162:PRO:HG3	2.08	0.52
1:D:198:LEU:HD13	1:D:205:VAL:CG2	2.37	0.52
1:D:352:ALA:HA	1:D:364:ARG:HE	1.75	0.52
1:C:198:LEU:HB2	2:C:404:HOH:O	2.10	0.52
1:D:268:ARG:HH11	1:D:268:ARG:CA	2.21	0.52
1:D:211:LLP:HE3	1:D:341:LEU:HD13	1.90	0.51
1:C:300:TYR:O	1:C:304:ARG:HG3	2.10	0.51
1:B:112:THR:CB	1:B:162:PRO:HG2	2.41	0.51
1:B:17:HIS:O	1:B:73:ARG:HD3	2.10	0.51
1:B:161:ASN:HB3	1:B:162:PRO:HD3	1.93	0.51
1:A:329:MET:HE3	1:A:337:ARG:HG2	1.92	0.51
1:B:196:ARG:CZ	2:B:681:HOH:O	2.57	0.51
1:B:289:ILE:HD13	1:B:289:ILE:C	2.36	0.51
1:B:300:TYR:CZ	1:B:304:ARG:HD2	2.45	0.51
1:D:355:THR:HG23	2:D:603:HOH:O	2.11	0.51
1:A:276:LEU:O	1:A:280:LEU:HD13	2.10	0.51
1:C:211:LLP:HE3	1:C:341:LEU:HD13	1.92	0.51
1:C:278:GLU:O	1:C:282:ARG:HD3	2.11	0.51
1:C:34:GLN:HE22	1:C:250:HIS:H	1.59	0.50
1:D:143:LEU:O	1:D:147:MET:HG2	2.11	0.50
1:D:152:ARG:HD2	2:D:542:HOH:O	2.11	0.50
1:A:254:LEU:HD21	1:B:254:LEU:HD21	1.93	0.50
1:C:168:ASP:O	1:C:172:VAL:HG13	2.10	0.50
1:A:286:VAL:HG11	1:A:289:ILE:CD1	2.37	0.50
1:B:341:LEU:HD22	1:B:341:LEU:C	2.35	0.50
1:A:204:LEU:HD23	1:A:226:GLY:HA3	1.92	0.50
1:D:178:LYS:HE2	1:D:179:HIS:CE1	2.46	0.50
1:A:34:GLN:HG3	1:C:218:ASP:O	2.12	0.50
1:A:190:CYS:SG	1:A:307:MET:HE3	2.52	0.50
1:C:84:LEU:HD12	1:C:86:LEU:HD11	1.92	0.50
1:D:263:ASN:H	1:D:263:ASN:HD22	1.60	0.50
1:B:112:THR:CG2	1:B:162:PRO:HG2	2.41	0.49
1:B:360:THR:OG1	1:B:363:GLU:HG3	2.11	0.49
1:A:161:ASN:N	1:A:162:PRO:HD2	2.26	0.49
1:B:211:LLP:HE3	1:B:341:LEU:HD13	1.94	0.49
1:C:160:ALA:C	1:C:162:PRO:HD2	2.37	0.49
1:D:268:ARG:NE	2:D:611:HOH:O	2.17	0.49
1:B:211:LLP:HE3	1:B:341:LEU:CD1	2.42	0.49
1:C:288:LEU:HD12	1:C:289:ILE:H	1.78	0.49
1:B:39:THR:CG2	1:C:28:LEU:HG	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:LEU:HD22	1:B:309:GLN:HB2	1.94	0.49
1:B:303:ALA:CB	1:B:307:MET:HE2	2.43	0.49
1:D:164:MET:O	1:D:166:MET:HE2	2.13	0.49
1:B:111:ASN:HB2	2:B:479:HOH:O	2.13	0.48
1:A:157:GLU:HG2	1:A:186:ASP:HB3	1.95	0.48
1:B:188:THR:HG22	1:B:207:HIS:HA	1.94	0.48
1:C:7:LEU:CD2	1:C:13:ARG:HD3	2.42	0.48
1:C:154:ILE:HD12	1:C:176:ALA:HB2	1.96	0.48
1:D:363:GLU:O	1:D:366:HIS:HB3	2.14	0.48
1:A:39:THR:HG23	1:D:28:LEU:HG	1.95	0.48
1:C:244:GLY:HA2	2:C:510:HOH:O	2.13	0.48
1:C:328:PHE:CD2	1:C:329:MET:HE2	2.49	0.48
1:C:320:GLY:HA3	1:C:324:ALA:HB2	1.96	0.48
1:B:63:SER:HG	1:B:68:ASN:HD21	1.59	0.47
1:C:19:TYR:CE1	1:C:30:PRO:HB3	2.49	0.47
1:A:178:LYS:HE2	1:A:179:HIS:CE1	2.49	0.47
1:A:187:ASN:ND2	1:A:195:GLN:HE21	2.13	0.47
1:A:325:GLY:O	1:A:329:MET:HG2	2.14	0.47
1:B:20:ASP:HB3	1:B:23:ASP:OD2	2.15	0.47
1:B:109:LEU:CD1	1:B:121:LEU:HD13	2.44	0.47
1:B:263:ASN:HD22	1:B:263:ASN:N	2.13	0.47
1:B:154:ILE:HD12	1:B:176:ALA:HB2	1.96	0.47
1:B:187:ASN:ND2	1:B:195:GLN:HE21	2.12	0.47
1:C:288:LEU:HD12	2:C:446:HOH:O	2.14	0.47
1:D:7:LEU:C	1:D:7:LEU:HD13	2.39	0.47
1:A:148:THR:HB	1:A:149:PRO:HD2	1.95	0.47
1:A:369:ILE:N	1:A:369:ILE:HD12	2.30	0.47
1:A:382:ASP:OD2	1:B:9:GLY:HA3	2.13	0.47
1:B:152:ARG:NE	1:B:152:ARG:HA	2.29	0.47
1:B:161:ASN:O	1:B:162:PRO:C	2.58	0.47
1:B:164:MET:HA	1:B:164:MET:HE3	1.97	0.47
1:D:359:TYR:HD2	1:D:363:GLU:CB	2.27	0.47
1:D:7:LEU:HD13	1:D:7:LEU:O	2.15	0.47
1:A:163:ASN:HB2	1:A:290:HIS:CG	2.49	0.47
1:C:148:THR:HB	1:C:149:PRO:HD2	1.97	0.47
1:A:112:THR:OG1	1:A:162:PRO:HG3	2.15	0.47
1:C:328:PHE:HD2	1:C:329:MET:HE2	1.79	0.47
1:D:301:THR:HG22	1:D:305:GLN:HE21	1.80	0.46
1:B:10:PHE:CZ	1:B:77:LEU:HG	2.50	0.46
1:B:163:ASN:O	1:B:164:MET:HB2	2.15	0.46
1:B:212:TYR:CE2	1:B:342:GLY:HA2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:211:LLP:HE3	1:D:341:LEU:CD1	2.45	0.46
1:D:121:LEU:O	1:D:132:LEU:HD11	2.14	0.46
1:D:169:ILE:H	1:D:306:GLN:NE2	2.09	0.46
1:D:363:GLU:CD	1:D:363:GLU:H	2.23	0.46
1:A:28:LEU:HG	1:D:39:THR:HG23	1.98	0.46
1:A:78:GLU:OE2	1:A:192:PRO:HG3	2.15	0.46
1:B:28:LEU:HD13	1:B:28:LEU:C	2.41	0.46
1:B:212:TYR:CD2	1:B:342:GLY:HA2	2.51	0.46
1:B:198:LEU:HD13	1:B:205:VAL:CG2	2.41	0.46
1:B:332:LEU:HD22	1:B:335:PHE:HB2	1.97	0.46
1:D:360:THR:O	1:D:364:ARG:HG2	2.17	0.45
1:A:39:THR:CG2	1:D:28:LEU:HG	2.47	0.45
1:C:301:THR:HG22	1:C:305:GLN:HE21	1.82	0.45
1:C:381:GLU:HG2	1:C:386:LEU:CD1	2.47	0.45
1:B:111:ASN:ND2	1:B:136:ASP:HA	2.32	0.45
1:C:112:THR:CB	1:C:162:PRO:HG3	2.46	0.45
1:D:300:TYR:CZ	1:D:304:ARG:HD2	2.52	0.45
1:B:70:LEU:HD21	1:B:255:LEU:HD23	1.99	0.45
1:D:159:PRO:HB2	1:D:164:MET:HA	1.98	0.44
1:D:290:HIS:HB2	1:D:315:ALA:HB3	1.99	0.44
1:A:43:VAL:HG23	1:C:354:MET:HG3	1.99	0.44
1:C:44:GLU:OE1	1:C:44:GLU:HA	2.18	0.44
1:C:157:GLU:OE1	1:C:161:ASN:ND2	2.50	0.44
1:D:363:GLU:HA	1:D:366:HIS:CB	2.47	0.44
1:A:318:LEU:N	1:A:318:LEU:HD22	2.32	0.44
1:C:352:ALA:O	1:C:357:SER:HA	2.17	0.44
1:A:339:VAL:O	1:A:339:VAL:HG22	2.16	0.44
1:A:143:LEU:HD12	1:A:175:ILE:HD12	2.00	0.43
1:B:303:ALA:HB1	1:B:307:MET:HE1	1.99	0.43
1:C:349:GLN:NE2	1:C:375:ARG:HH21	2.14	0.43
1:B:148:THR:HB	1:B:149:PRO:HD2	1.99	0.43
1:D:19:TYR:CE1	1:D:30:PRO:HB3	2.53	0.43
1:C:161:ASN:N	1:C:162:PRO:HD2	2.32	0.43
1:C:381:GLU:H	1:C:381:GLU:CD	2.26	0.43
1:B:169:ILE:H	1:B:306:GLN:NE2	2.05	0.43
1:A:190:CYS:C	1:A:191:THR:HG23	2.44	0.43
1:B:188:THR:CG2	1:B:208:SER:H	2.31	0.43
1:C:317:GLU:HA	1:C:372:GLY:O	2.18	0.43
1:B:369:ILE:HG23	1:B:373:LEU:HD23	2.00	0.43
1:C:10:PHE:CZ	1:C:77:LEU:HG	2.53	0.43
1:C:300:TYR:CE2	1:C:304:ARG:HD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:289:ILE:HD13	1:D:316:PHE:CB	2.47	0.43
1:D:164:MET:HG2	1:D:292:PRO:HD3	2.00	0.43
1:D:322:ILE:HG22	2:D:600:HOH:O	2.19	0.43
1:B:290:HIS:HE1	1:B:317:GLU:OE2	2.02	0.42
1:C:276:LEU:O	1:C:280:LEU:CD2	2.66	0.42
1:A:166:MET:HE3	1:A:303:ALA:HB2	2.00	0.42
1:A:109:LEU:HD13	1:A:121:LEU:HD13	2.00	0.42
1:C:268:ARG:NH2	2:C:481:HOH:O	2.51	0.42
1:D:188:THR:HG22	1:D:207:HIS:HA	2.00	0.42
1:A:194:LEU:HD22	1:A:309:GLN:HB2	2.02	0.42
1:C:40:PHE:CZ	1:C:62:ILE:HD11	2.51	0.42
1:C:112:THR:HG21	1:C:162:PRO:HG3	2.01	0.42
1:C:212:TYR:CE2	1:C:342:GLY:HA2	2.54	0.42
1:D:360:THR:HB	1:D:361:PRO:HD2	2.00	0.42
1:A:107:VAL:CG1	1:A:132:LEU:HD23	2.49	0.42
1:A:339:VAL:HG12	2:C:437:HOH:O	2.20	0.42
1:B:336:SER:HB3	1:D:39:THR:HG21	2.01	0.42
1:D:211:LLP:HB2	1:D:341:LEU:HD22	2.01	0.42
1:D:143:LEU:HD13	1:D:143:LEU:C	2.44	0.42
1:C:275:VAL:HG11	1:C:383:ILE:HG12	2.00	0.42
1:C:283:GLN:HA	1:C:284:PRO:HD3	1.86	0.42
1:D:78:GLU:HG3	2:D:407:HOH:O	2.19	0.42
1:C:349:GLN:HE21	1:C:375:ARG:HH21	1.67	0.42
1:D:359:TYR:HB3	1:D:363:GLU:HB2	2.01	0.42
1:C:281:ALA:HA	1:C:289:ILE:CD1	2.50	0.42
1:B:363:GLU:O	1:B:366:HIS:HB3	2.20	0.41
1:D:63:SER:CB	1:D:68:ASN:HD21	2.33	0.41
1:A:43:VAL:HG11	1:C:326:ARG:HA	2.01	0.41
1:D:341:LEU:HD22	1:D:341:LEU:C	2.45	0.41
1:D:141:GLN:OE1	1:D:141:GLN:N	2.51	0.41
1:D:194:LEU:HD22	1:D:309:GLN:HB2	2.01	0.41
1:B:190:CYS:C	1:B:191:THR:HG23	2.45	0.41
1:A:321:GLY:CA	1:A:371:GLU:HG2	2.48	0.41
1:B:331:ALA:HB1	1:B:392:GLN:HE22	1.85	0.41
1:C:355:THR:HG23	2:C:485:HOH:O	2.20	0.41
1:D:133:ARG:NH1	1:D:146:ALA:HA	2.35	0.41
1:A:341:LEU:C	1:A:341:LEU:HD22	2.46	0.41
1:A:364:ARG:NH1	2:A:663:HOH:O	2.54	0.41
1:D:207:HIS:HD2	2:D:406:HOH:O	2.03	0.41
1:A:86:LEU:N	1:A:86:LEU:HD12	2.36	0.41
1:B:78:GLU:OE2	1:B:207:HIS:CE1	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:328:PHE:HD2	1:C:329:MET:CE	2.34	0.41
1:B:169:ILE:O	1:B:172:VAL:HG22	2.21	0.41
1:B:218:ASP:O	1:D:34:GLN:HG3	2.21	0.41
1:D:178:LYS:HD2	1:D:178:LYS:O	2.21	0.41
1:A:354:MET:CG	1:C:43:VAL:HG13	2.47	0.40
1:B:329:MET:CE	1:B:337:ARG:HG2	2.49	0.40
1:A:381:GLU:HG2	1:A:386:LEU:HD21	2.03	0.40
1:B:274:GLN:HE22	1:B:293:GLY:HA3	1.86	0.40
1:B:283:GLN:HA	1:B:284:PRO:HD3	1.78	0.40
1:A:43:VAL:HG21	1:C:353:SER:OG	2.20	0.40
1:B:161:ASN:HD21	1:B:375:ARG:HD3	1.85	0.40
1:C:381:GLU:HG2	1:C:386:LEU:HD13	2.03	0.40
1:C:7:LEU:HD22	1:C:8:PRO:O	2.22	0.40
1:D:112:THR:OG1	1:D:162:PRO:HG3	2.20	0.40
1:D:212:TYR:CE2	1:D:342:GLY:HA2	2.56	0.40
1:C:163:ASN:O	1:C:164:MET:HB2	2.21	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	368/398 (92%)	353 (96%)	13 (4%)	2 (0%)	24	21
1	B	365/398 (92%)	351 (96%)	13 (4%)	1 (0%)	36	35
1	C	370/398 (93%)	357 (96%)	11 (3%)	2 (0%)	24	21
1	D	365/398 (92%)	347 (95%)	14 (4%)	4 (1%)	11	7
All	All	1468/1592 (92%)	1408 (96%)	51 (4%)	9 (1%)	21	17

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	162	PRO
1	A	361	PRO
1	B	162	PRO
1	C	359	TYR
1	D	162	PRO
1	D	358	SER
1	D	359	TYR
1	C	162	PRO
1	D	397	SER

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	289/306 (94%)	281 (97%)	8 (3%)	38	41
1	B	286/306 (94%)	272 (95%)	14 (5%)	22	20
1	C	291/306 (95%)	277 (95%)	14 (5%)	23	21
1	D	286/306 (94%)	271 (95%)	15 (5%)	21	18
All	All	1152/1224 (94%)	1101 (96%)	51 (4%)	25	24

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	LEU
1	A	263	ASN
1	A	302	LEU
1	A	336	SER
1	A	341	LEU
1	A	362	GLU
1	A	381	GLU
1	A	394	LEU
1	B	37	THR
1	B	69	LEU
1	B	73	ARG
1	B	77	LEU
1	B	143	LEU

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Mol	Chain	Res	Type
1	B	152	ARG
1	B	188	THR
1	B	198	LEU
1	B	263	ASN
1	B	289	ILE
1	B	302	LEU
1	B	341	LEU
1	B	386	LEU
1	B	394	LEU
1	C	7	LEU
1	C	69	LEU
1	C	77	LEU
1	C	100	LEU
1	C	161	ASN
1	C	172	VAL
1	C	198	LEU
1	C	263	ASN
1	C	302	LEU
1	C	333	GLN
1	C	341	LEU
1	C	381	GLU
1	C	386	LEU
1	C	394	LEU
1	D	69	LEU
1	D	77	LEU
1	D	84	LEU
1	D	100	LEU
1	D	152	ARG
1	D	163	ASN
1	D	188	THR
1	D	198	LEU
1	D	263	ASN
1	D	268	ARG
1	D	302	LEU
1	D	341	LEU
1	D	381	GLU
1	D	386	LEU
1	D	394	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	34	GLN
1	A	187	ASN
1	A	195	GLN
1	A	207	HIS
1	A	228	GLN
1	A	263	ASN
1	A	272	ASN
1	A	274	GLN
1	A	305	GLN
1	A	306	GLN
1	A	356	HIS
1	B	34	GLN
1	B	111	ASN
1	B	141	GLN
1	B	161	ASN
1	B	187	ASN
1	B	195	GLN
1	B	207	HIS
1	B	237	GLN
1	B	263	ASN
1	B	272	ASN
1	B	274	GLN
1	B	290	HIS
1	B	306	GLN
1	B	349	GLN
1	B	392	GLN
1	C	34	GLN
1	C	161	ASN
1	C	187	ASN
1	C	207	HIS
1	C	228	GLN
1	C	237	GLN
1	C	263	ASN
1	C	272	ASN
1	C	274	GLN
1	C	290	HIS
1	C	305	GLN
1	C	306	GLN
1	C	349	GLN
1	C	392	GLN
1	D	34	GLN
1	D	68	ASN

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Mol	Chain	Res	Type
1	D	111	ASN
1	D	161	ASN
1	D	179	HIS
1	D	187	ASN
1	D	207	HIS
1	D	237	GLN
1	D	263	ASN
1	D	272	ASN
1	D	274	GLN
1	D	305	GLN
1	D	306	GLN
1	D	356	HIS
1	D	392	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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$
1	LLP	C	211	1	23,24,25	1.25	3 (13%)	25,32,34	2.27	9 (36%)
1	LLP	B	211	1	23,24,25	1.30	3 (13%)	25,32,34	2.22	10 (40%)
1	LLP	A	211	1	23,24,25	1.23	4 (17%)	25,32,34	2.27	10 (40%)
1	LLP	D	211	1	23,24,25	1.25	4 (17%)	25,32,34	2.27	10 (40%)

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	C	211	1	-	10/16/17/19	0/1/1/1
1	LLP	B	211	1	-	9/16/17/19	0/1/1/1
1	LLP	A	211	1	-	10/16/17/19	0/1/1/1
1	LLP	D	211	1	-	9/16/17/19	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	211	LLP	C3-C2	2.62	1.43	1.41
1	B	211	LLP	C3-C2	2.58	1.43	1.41
1	C	211	LLP	C3-C2	2.52	1.43	1.41
1	D	211	LLP	C4-C4'	2.51	1.52	1.46
1	B	211	LLP	C4-C4'	2.48	1.51	1.46
1	C	211	LLP	O3-C3	-2.45	1.31	1.36
1	A	211	LLP	O3-C3	-2.28	1.31	1.36
1	B	211	LLP	O3-C3	-2.28	1.31	1.36
1	A	211	LLP	C3-C2	2.20	1.43	1.41
1	A	211	LLP	OP4-C5'	-2.11	1.37	1.44
1	D	211	LLP	OP4-C5'	-2.08	1.37	1.44
1	D	211	LLP	O3-C3	-2.08	1.32	1.36
1	C	211	LLP	C4-C4'	2.06	1.51	1.46
1	A	211	LLP	C4-C4'	2.06	1.51	1.46

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	211	LLP	C6-N1-C2	4.76	127.82	119.20
1	A	211	LLP	C6-N1-C2	4.75	127.81	119.20
1	D	211	LLP	C6-N1-C2	4.72	127.75	119.20
1	B	211	LLP	C6-N1-C2	4.69	127.69	119.20
1	B	211	LLP	C5-C6-N1	-4.28	116.87	123.83
1	C	211	LLP	C5-C6-N1	-4.27	116.88	123.83
1	D	211	LLP	C5-C6-N1	-4.24	116.93	123.83
1	A	211	LLP	C5-C6-N1	-4.23	116.94	123.83
1	D	211	LLP	C4-C3-C2	-3.99	117.90	120.14
1	C	211	LLP	C4-C3-C2	-3.95	117.92	120.14
1	A	211	LLP	C4-C3-C2	-3.94	117.93	120.14
1	B	211	LLP	C4-C3-C2	-3.67	118.08	120.14
1	A	211	LLP	CE-NZ-C4'	3.47	129.84	118.72
1	D	211	LLP	CE-NZ-C4'	3.44	129.75	118.72
1	C	211	LLP	CE-NZ-C4'	3.44	129.73	118.72
1	D	211	LLP	C2'-C2-C3	3.33	124.69	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	211	LLP	CE-NZ-C4'	3.31	129.33	118.72
1	C	211	LLP	C2'-C2-C3	3.31	124.67	120.80
1	C	211	LLP	C3-C4-C5	3.28	120.91	118.28
1	B	211	LLP	C2'-C2-C3	3.24	124.59	120.80
1	C	211	LLP	C3-C2-N1	-3.17	116.97	120.96
1	B	211	LLP	C3-C2-N1	-3.15	116.99	120.96
1	D	211	LLP	C5'-C5-C6	-3.15	114.23	119.36
1	A	211	LLP	C2'-C2-C3	3.12	124.45	120.80
1	A	211	LLP	C3-C2-N1	-3.04	117.13	120.96
1	A	211	LLP	C3-C4-C5	3.02	120.70	118.28
1	B	211	LLP	C3-C4-C5	3.01	120.69	118.28
1	D	211	LLP	C3-C2-N1	-3.00	117.17	120.96
1	C	211	LLP	C3-C4-C4'	-2.91	115.15	120.40
1	D	211	LLP	C3-C4-C5	2.86	120.57	118.28
1	A	211	LLP	C5'-C5-C6	-2.85	114.72	119.36
1	A	211	LLP	C3-C4-C4'	-2.82	115.31	120.40
1	D	211	LLP	C3-C4-C4'	-2.76	115.42	120.40
1	B	211	LLP	C3-C4-C4'	-2.69	115.54	120.40
1	B	211	LLP	C5'-C5-C6	-2.63	115.08	119.36
1	C	211	LLP	C5'-C5-C6	-2.61	115.10	119.36
1	A	211	LLP	OP4-C5'-C5	2.57	114.17	109.36
1	D	211	LLP	OP4-C5'-C5	2.27	113.60	109.36
1	B	211	LLP	OP4-C5'-C5	2.18	113.44	109.36

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	211	LLP	O-C-CA-CB
1	B	211	LLP	C4-C4'-NZ-CE
1	B	211	LLP	O-C-CA-CB
1	C	211	LLP	C4-C4'-NZ-CE
1	C	211	LLP	C5'-OP4-P-OP2
1	C	211	LLP	C5'-OP4-P-OP3
1	C	211	LLP	O-C-CA-CB
1	D	211	LLP	C5'-OP4-P-OP2
1	D	211	LLP	C5'-OP4-P-OP3
1	D	211	LLP	O-C-CA-CB
1	D	211	LLP	C4-C4'-NZ-CE
1	A	211	LLP	C4-C4'-NZ-CE
1	A	211	LLP	C3-C4-C4'-NZ
1	B	211	LLP	C3-C4-C4'-NZ

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Mol	Chain	Res	Type	Atoms
1	C	211	LLP	C3-C4-C4'-NZ
1	D	211	LLP	C3-C4-C4'-NZ
1	C	211	LLP	C5'-OP4-P-OP1
1	A	211	LLP	CA-CB-CG-CD
1	D	211	LLP	C5-C4-C4'-NZ
1	A	211	LLP	C5'-OP4-P-OP2
1	A	211	LLP	C5'-OP4-P-OP3
1	B	211	LLP	C5'-OP4-P-OP2
1	B	211	LLP	C5'-OP4-P-OP3
1	B	211	LLP	CA-CB-CG-CD
1	C	211	LLP	C5-C4-C4'-NZ
1	C	211	LLP	C4-C5-C5'-OP4
1	D	211	LLP	CD-CE-NZ-C4'
1	B	211	LLP	CD-CE-NZ-C4'
1	A	211	LLP	C5'-OP4-P-OP1
1	B	211	LLP	C5'-OP4-P-OP1
1	D	211	LLP	C5'-OP4-P-OP1
1	A	211	LLP	CD-CE-NZ-C4'
1	C	211	LLP	CD-CE-NZ-C4'
1	D	211	LLP	CA-CB-CG-CD
1	A	211	LLP	CG-CD-CE-NZ
1	B	211	LLP	C5-C4-C4'-NZ
1	C	211	LLP	CA-CB-CG-CD
1	A	211	LLP	C5-C4-C4'-NZ

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	211	LLP	2	0
1	B	211	LLP	2	0
1	A	211	LLP	1	0
1	D	211	LLP	3	0

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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	372/398 (93%)	0.80	51 (13%) 6 6	21, 33, 59, 88	0
1	B	369/398 (92%)	0.62	25 (6%) 23 22	20, 32, 46, 58	0
1	C	374/398 (93%)	0.66	41 (10%) 10 9	21, 33, 51, 79	0
1	D	369/398 (92%)	0.94	52 (14%) 6 5	23, 37, 56, 89	0
All	All	1484/1592 (93%)	0.76	169 (11%) 10 9	20, 33, 53, 89	0

All (169) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	161	ASN	9.0
1	B	161	ASN	7.6
1	A	367	TYR	7.0
1	A	43	VAL	6.4
1	C	43	VAL	6.1
1	D	367	TYR	5.8
1	A	161	ASN	5.8
1	B	40	PHE	5.6
1	A	359	TYR	5.6
1	C	161	ASN	5.2
1	A	360	THR	5.1
1	D	40	PHE	4.9
1	C	367	TYR	4.8
1	C	361	PRO	4.7
1	D	365	ALA	4.6
1	A	41	PRO	4.6
1	A	364	ARG	4.5
1	A	42	THR	4.5
1	A	366	HIS	4.4
1	A	40	PHE	4.2
1	D	39	THR	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	354	MET	4.2
1	A	355	THR	4.1
1	A	372	GLY	4.1
1	D	398	ALA	4.1
1	A	371	GLU	4.0
1	C	359	TYR	4.0
1	D	288	LEU	4.0
1	D	358	SER	4.0
1	D	361	PRO	3.9
1	A	163	ASN	3.9
1	B	39	THR	3.9
1	D	359	TYR	3.8
1	C	41	PRO	3.8
1	D	189	TYR	3.8
1	A	145	ALA	3.7
1	C	398	ALA	3.7
1	A	22	GLN	3.7
1	A	357	SER	3.6
1	B	367	TYR	3.5
1	B	162	PRO	3.5
1	C	189	TYR	3.5
1	D	363	GLU	3.5
1	B	333	GLN	3.5
1	A	370	SER	3.5
1	B	189	TYR	3.3
1	D	162	PRO	3.3
1	D	289	ILE	3.3
1	D	300	TYR	3.3
1	D	364	ARG	3.3
1	C	364	ARG	3.3
1	B	398	ALA	3.2
1	D	178	LYS	3.2
1	D	366	HIS	3.2
1	C	339	VAL	3.2
1	A	365	ALA	3.2
1	D	368	GLY	3.2
1	C	369	ILE	3.1
1	C	44	GLU	3.1
1	A	368	GLY	3.1
1	D	360	THR	3.1
1	A	369	ILE	3.1
1	C	360	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	365	ALA	3.1
1	A	7	LEU	3.1
1	D	287	GLU	3.0
1	A	160	ALA	3.0
1	A	396	ALA	3.0
1	C	394	LEU	3.0
1	D	140	LEU	3.0
1	D	22	GLN	3.0
1	C	289	ILE	3.0
1	C	363	GLU	3.0
1	A	398	ALA	3.0
1	A	143	LEU	3.0
1	C	395	LYS	3.0
1	A	356	HIS	3.0
1	D	143	LEU	2.9
1	B	287	GLU	2.9
1	B	357	SER	2.9
1	D	325	GLY	2.9
1	D	394	LEU	2.9
1	B	23	ASP	2.9
1	B	286	VAL	2.8
1	C	330	ASN	2.8
1	A	339	VAL	2.8
1	C	366	HIS	2.8
1	B	359	TYR	2.8
1	B	339	VAL	2.8
1	D	163	ASN	2.8
1	A	318	LEU	2.8
1	C	288	LEU	2.8
1	C	318	LEU	2.8
1	D	7	LEU	2.8
1	A	189	TYR	2.7
1	B	288	LEU	2.7
1	A	361	PRO	2.7
1	D	369	ILE	2.7
1	C	320	GLY	2.7
1	B	365	ALA	2.7
1	A	358	SER	2.7
1	C	62	ILE	2.7
1	D	135	VAL	2.7
1	A	289	ILE	2.6
1	C	368	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	149	PRO	2.6
1	A	288	LEU	2.6
1	B	361	PRO	2.6
1	D	113	LEU	2.6
1	D	177	ARG	2.6
1	A	112	THR	2.6
1	C	22	GLN	2.5
1	C	287	GLU	2.5
1	C	178	LYS	2.5
1	C	382	ASP	2.5
1	C	358	SER	2.5
1	C	362	GLU	2.5
1	C	24	HIS	2.5
1	C	321	GLY	2.5
1	D	396	ALA	2.5
1	A	162	PRO	2.4
1	A	362	GLU	2.4
1	D	370	SER	2.4
1	D	146	ALA	2.4
1	D	160	ALA	2.4
1	D	180	GLY	2.4
1	D	339	VAL	2.4
1	B	337	ARG	2.4
1	D	331	ALA	2.4
1	A	280	LEU	2.4
1	C	300	TYR	2.3
1	A	295	ALA	2.3
1	B	281	ALA	2.3
1	B	366	HIS	2.3
1	D	106	GLU	2.3
1	D	318	LEU	2.3
1	A	175	ILE	2.3
1	A	146	ALA	2.3
1	C	160	ALA	2.3
1	D	281	ALA	2.3
1	C	177	ARG	2.3
1	D	131	LYS	2.3
1	D	149	PRO	2.3
1	C	7	LEU	2.3
1	A	39	THR	2.2
1	D	148	THR	2.2
1	D	172	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	172	VAL	2.2
1	A	373	LEU	2.2
1	A	363	GLU	2.2
1	A	352	ALA	2.2
1	D	167	ALA	2.2
1	C	397	SER	2.1
1	D	397	SER	2.1
1	B	24	HIS	2.1
1	C	294	LEU	2.1
1	A	164	MET	2.1
1	B	362	GLU	2.1
1	A	125	ILE	2.1
1	D	150	ALA	2.1
1	D	357	SER	2.1
1	A	38	PHE	2.1
1	A	397	SER	2.1
1	B	326	ARG	2.0
1	B	350	HIS	2.0
1	C	162	PRO	2.0
1	D	114	TYR	2.0
1	C	357	SER	2.0
1	D	302	LEU	2.0

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($\text{\AA}^2$)	Q<0.9
1	LLP	A	211	24/25	0.95	0.09	24,31,33,34	0
1	LLP	B	211	24/25	0.95	0.09	24,30,30,32	0
1	LLP	C	211	24/25	0.95	0.09	23,29,29,30	0
1	LLP	D	211	24/25	0.95	0.08	26,33,34,35	0

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.