



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 04:49 PM GMT

PDB ID : 1GC0
Title : CRYSTAL STRUCTURE OF THE PYRIDOXAL-5'-PHOSPHATEDEPENDENT L-METHIONINE GAMMA-LYASE FROM PSEUDOMONAS PUTIDA
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Deposited on : 2000-07-06
Resolution : 1.70 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

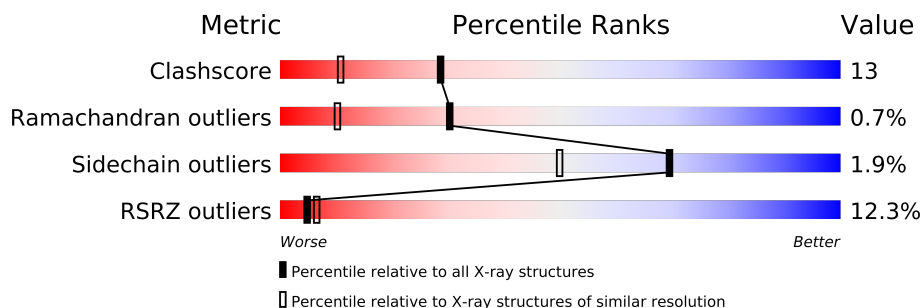
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.70 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))
Clashscore	79885	2929 (1.70-1.70)
Ramachandran outliers	78287	2878 (1.70-1.70)
Sidechain outliers	78261	2878 (1.70-1.70)
RSRZ outliers	66119	2456 (1.70-1.70)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	398	
1	B	398	
1	C	398	
1	D	398	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12053 atoms, of which 0 are hydrogen and 0 are deuterium.

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	355	Total	C	N	O	P	S	0	0	0
			2681	1690	474	501	1	15			
1	B	357	Total	C	N	O	P	S	0	0	0
			2695	1699	475	505	1	15			
1	C	363	Total	C	N	O	P	S	0	0	0
			2734	1721	483	513	1	16			
1	D	356	Total	C	N	O	P	S	0	0	0
			2685	1692	475	502	1	15			

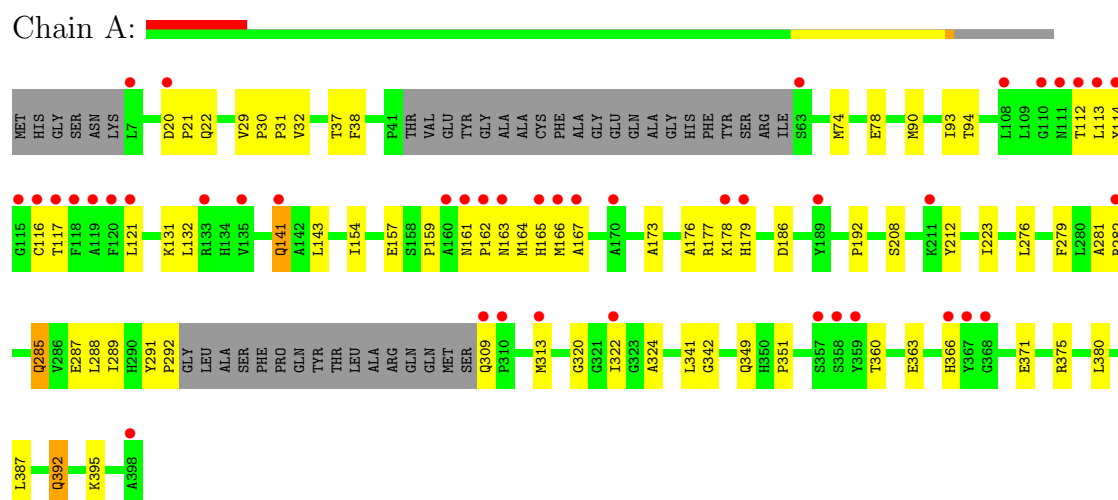
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	362	Total	O	0	0
			362	362		
2	B	310	Total	O	0	0
			310	310		
2	C	324	Total	O	0	0
			324	324		
2	D	262	Total	O	0	0
			262	262		

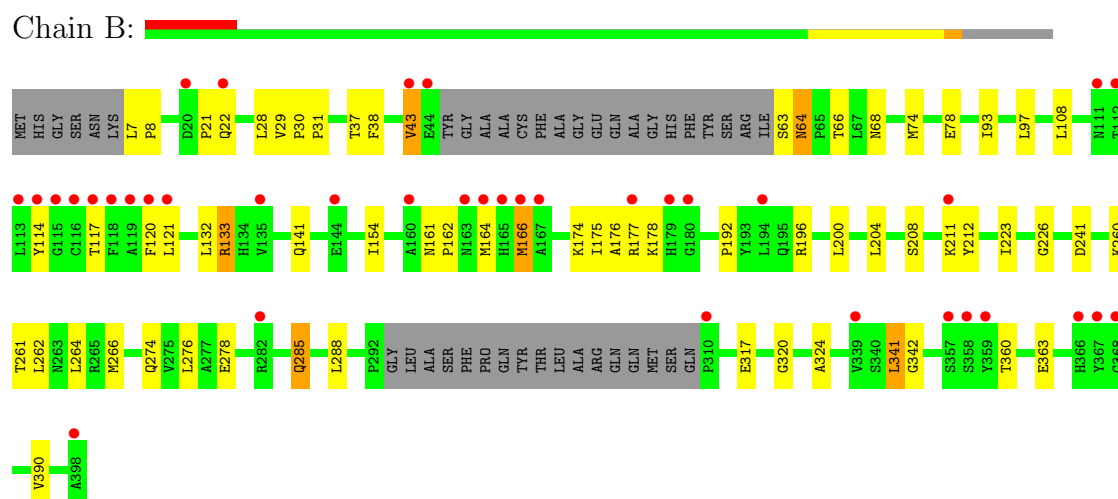
3 Residue-property plots

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.

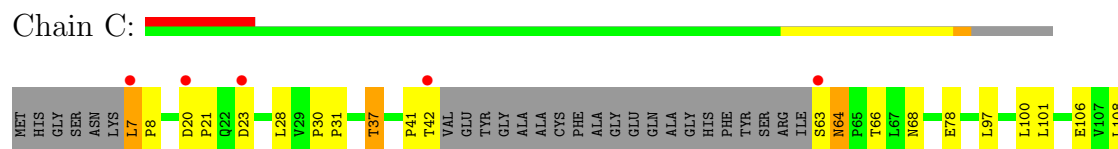
• Molecule 1: METHIONINE GAMMA-LYASE

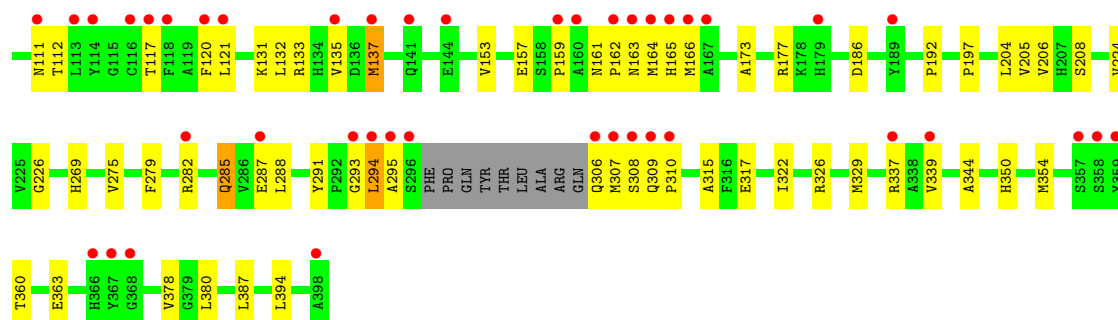


• Molecule 1: METHIONINE GAMMA-LYASE



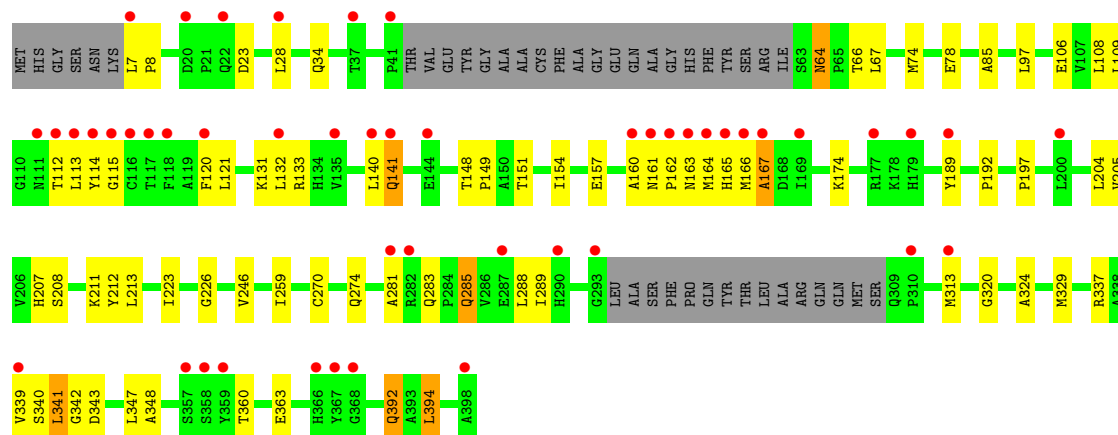
• Molecule 1: METHIONINE GAMMA-LYASE





• Molecule 1: METHIONINE GAMMA-LYASE

Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	72.86Å 81.03Å 81.28Å 70.56° 63.17° 63.38°	Depositor
Resolution (Å)	71.46 – 1.70 71.55 – 1.70	Depositor EDS
% Data completeness (in resolution range)	91.0 (71.46-1.70) 90.2 (71.55-1.70)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.54 (at 1.70Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.210 , 0.236 0.191 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	15.0	Xtriage
Anisotropy	0.364	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 35.8	EDS
Estimated twinning fraction	0.478 for h,h-k,h-l 0.478 for -h,-h+l,-h+k 0.477 for -h,-l,-k	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 149546 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12053	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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	0.28	0/2710	0.59	1/3677 (0.0%)
1	B	0.29	0/2724	0.58	1/3696 (0.0%)
1	C	0.28	0/2763	0.58	1/3748 (0.0%)
1	D	0.28	0/2714	0.59	1/3682 (0.0%)
All	All	0.29	0/10911	0.59	4/14803 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	208	SER	N-CA-C	-5.80	95.33	111.00
1	D	208	SER	N-CA-C	-5.65	95.74	111.00
1	C	208	SER	N-CA-C	-5.61	95.85	111.00
1	A	208	SER	N-CA-C	-5.51	96.12	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2681	0	2660	65	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2695	0	2674	61	0
1	C	2734	0	2712	73	0
1	D	2685	0	2662	73	0
2	A	362	0	0	14	0
2	B	310	0	0	15	0
2	C	324	0	0	9	0
2	D	262	0	0	15	0
All	All	12053	0	10708	269	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 13.

All (269) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:121:LEU:HB3	1:C:132:LEU:HD21	1.43	1.00
1:C:111:ASN:H	1:C:137:MET:HE2	1.33	0.93
1:A:313:MET:HG3	2:A:628:HOH:O	1.72	0.90
1:D:313:MET:HG3	2:D:581:HOH:O	1.75	0.86
1:C:380:LEU:HG	2:C:679:HOH:O	1.77	0.85
1:C:108:LEU:HD23	1:C:133:ARG:HG3	1.59	0.84
1:B:261:THR:HG22	2:B:678:HOH:O	1.81	0.80
1:D:270:CYS:O	1:D:274:GLN:HG3	1.84	0.76
1:D:112:THR:HG22	1:D:161:ASN:HD22	1.51	0.76
1:A:351:PRO:HD3	2:A:743:HOH:O	1.85	0.75
1:A:380:LEU:HD13	2:B:678:HOH:O	1.85	0.74
1:A:74:MET:HG2	1:A:223:ILE:HG21	1.70	0.73
1:A:287:GLU:HG3	1:A:288:LEU:HD22	1.72	0.71
1:C:137:MET:HE3	1:C:137:MET:H	1.53	0.71
1:A:349:GLN:HG3	2:A:743:HOH:O	1.90	0.71
1:D:7:LEU:HD13	1:D:8:PRO:O	1.90	0.71
1:D:74:MET:HG2	1:D:223:ILE:HG21	1.73	0.70
1:C:329:MET:HG3	1:C:354:MET:CE	2.21	0.70
1:D:112:THR:HG21	1:D:161:ASN:HB2	1.73	0.70
1:B:74:MET:HG2	1:B:223:ILE:HG21	1.73	0.70
1:C:117:THR:O	1:C:121:LEU:HD23	1.92	0.69
1:C:21:PRO:HG2	2:D:622:HOH:O	1.91	0.69
1:D:347:LEU:HB3	2:D:600:HOH:O	1.93	0.69
1:C:121:LEU:HB3	1:C:132:LEU:CD2	2.22	0.69
1:B:212:TYR:HB3	1:B:266:MET:HE3	1.74	0.69
1:C:173:ALA:HB1	1:C:177:ARG:HH22	1.58	0.68
1:B:175:ILE:O	1:B:178:LYS:HG2	1.95	0.67
1:B:174:LYS:HG2	1:B:177:ARG:NH2	2.10	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:117:THR:O	1:B:121:LEU:HD23	1.95	0.66
1:A:360:THR:OG1	1:A:363:GLU:HG3	1.95	0.65
1:C:137:MET:CE	1:C:137:MET:H	2.08	0.65
1:D:108:LEU:HD23	1:D:151:THR:HG23	1.78	0.65
1:B:29:VAL:HG13	2:B:701:HOH:O	1.96	0.65
1:C:350:HIS:HB3	1:C:354:MET:CE	2.27	0.64
1:C:63:SER:HB3	1:C:68:ASN:HD21	1.60	0.64
1:A:177:ARG:HH21	1:A:177:ARG:HG3	1.62	0.64
1:A:21:PRO:HG2	2:B:561:HOH:O	1.95	0.64
1:C:111:ASN:ND2	1:C:112:THR:HG23	2.13	0.64
1:C:205:VAL:HB	2:C:551:HOH:O	1.98	0.64
1:C:111:ASN:H	1:C:137:MET:CE	2.08	0.64
1:D:109:LEU:HD13	1:D:121:LEU:HD13	1.81	0.63
1:A:29:VAL:HG22	2:B:676:HOH:O	1.98	0.63
1:D:131:LYS:NZ	1:D:131:LYS:HB3	2.14	0.62
1:D:78:GLU:OE1	1:D:207:HIS:HE1	1.82	0.62
1:B:97:LEU:HD12	1:B:120:PHE:HE2	1.64	0.62
1:B:360:THR:OG1	1:B:363:GLU:HG3	1.99	0.61
1:D:7:LEU:HD22	1:D:8:PRO:HD2	1.81	0.61
1:B:28:LEU:HD12	1:C:37:THR:HB	1.83	0.61
1:B:37:THR:HB	1:C:28:LEU:HD22	1.83	0.60
1:D:360:THR:OG1	1:D:363:GLU:HG3	2.01	0.60
1:D:339:VAL:HB	2:D:601:HOH:O	2.02	0.60
1:C:387:LEU:HD21	2:C:721:HOH:O	2.01	0.59
1:B:211:LLP:HE3	1:B:341:LEU:CD1	2.33	0.59
1:C:101:LEU:HD21	1:C:153:VAL:HG21	1.85	0.59
1:C:360:THR:OG1	1:C:363:GLU:HG3	2.02	0.59
1:C:329:MET:HG3	1:C:354:MET:HE2	1.84	0.59
1:A:279:PHE:HA	1:A:282:ARG:NH2	2.17	0.59
1:B:174:LYS:HD3	1:B:174:LYS:C	2.23	0.59
1:D:78:GLU:OE1	1:D:207:HIS:CE1	2.56	0.58
2:A:698:HOH:O	1:B:21:PRO:HG2	2.03	0.58
1:C:111:ASN:N	1:C:137:MET:HE2	2.12	0.58
1:A:166:MET:O	1:A:167:ALA:HB3	2.04	0.57
1:A:292:PRO:HG3	2:A:726:HOH:O	2.03	0.57
1:A:121:LEU:HB3	1:A:132:LEU:HD21	1.85	0.57
1:D:392:GLN:NE2	2:D:659:HOH:O	2.38	0.57
1:A:309:GLN:HG3	2:A:704:HOH:O	2.03	0.57
1:D:160:ALA:O	1:D:164:MET:HA	2.05	0.57
1:D:339:VAL:O	1:D:339:VAL:HG13	2.05	0.57
1:D:74:MET:HE1	1:D:259:ILE:HD11	1.86	0.56
1:D:211:LLP:HE3	1:D:341:LEU:CD1	2.34	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:281:ALA:HB2	1:A:289:ILE:HD11	1.87	0.56
1:A:20:ASP:OD2	1:A:22:GLN:HB2	2.05	0.56
1:C:350:HIS:HB3	1:C:354:MET:HE3	1.88	0.56
1:B:121:LEU:HB3	1:B:132:LEU:HD13	1.88	0.56
1:A:117:THR:O	1:A:121:LEU:HD23	2.06	0.56
1:A:121:LEU:HB3	1:A:132:LEU:CD2	2.35	0.56
1:B:264:LEU:HD12	2:B:678:HOH:O	2.06	0.56
1:C:159:PRO:CG	1:C:164:MET:HG3	2.36	0.56
1:C:285:GLN:NE2	1:C:285:GLN:H	2.04	0.55
1:D:97:LEU:HD12	1:D:120:PHE:HE2	1.70	0.55
1:A:276:LEU:HD23	1:A:387:LEU:HD23	1.88	0.55
1:B:74:MET:HE2	1:B:192:PRO:HG3	1.89	0.55
1:A:178:LYS:HE3	1:A:179:HIS:HE1	1.70	0.55
2:A:520:HOH:O	1:D:34:GLN:HG2	2.06	0.55
1:B:22:GLN:HG3	2:B:507:HOH:O	2.06	0.55
1:B:74:MET:CE	1:B:192:PRO:HG3	2.37	0.55
1:B:320:GLY:HA3	1:B:324:ALA:HB2	1.89	0.55
1:C:106:GLU:OE1	1:C:133:ARG:HD3	2.07	0.55
1:B:285:GLN:H	1:B:285:GLN:NE2	2.05	0.55
1:C:339:VAL:HG13	1:C:339:VAL:O	2.08	0.54
1:D:112:THR:C	1:D:113:LEU:HD22	2.26	0.54
1:A:173:ALA:O	1:A:177:ARG:HG2	2.08	0.54
1:D:74:MET:HE3	1:D:223:ILE:HG13	1.90	0.54
1:A:285:GLN:H	1:A:285:GLN:NE2	2.06	0.53
1:C:135:VAL:O	1:C:137:MET:HE3	2.09	0.53
1:A:74:MET:CE	1:A:192:PRO:HG3	2.38	0.53
1:A:90:MET:HA	1:A:93:ILE:HG22	1.90	0.53
1:B:166:MET:CE	1:B:166:MET:H	2.23	0.52
1:A:281:ALA:HB2	1:A:289:ILE:CD1	2.39	0.52
1:D:281:ALA:HB2	1:D:289:ILE:HD12	1.92	0.52
1:C:329:MET:HG3	1:C:354:MET:HE1	1.92	0.52
1:A:166:MET:HA	2:A:510:HOH:O	2.10	0.52
1:C:131:LYS:NZ	1:C:133:ARG:HD2	2.24	0.51
1:B:114:TYR:HD1	1:B:117:THR:HG23	1.76	0.51
1:D:109:LEU:CD1	1:D:121:LEU:HD13	2.40	0.51
1:A:177:ARG:HG3	1:A:177:ARG:NH2	2.25	0.51
1:D:113:LEU:HD11	2:D:505:HOH:O	2.11	0.51
1:D:74:MET:CE	1:D:213:LEU:HD13	2.41	0.51
1:C:350:HIS:HB3	1:C:354:MET:HE1	1.92	0.51
1:B:154:ILE:HD12	1:B:176:ALA:HB2	1.91	0.51
1:C:161:ASN:HB3	1:C:162:PRO:HA	1.92	0.51
1:C:121:LEU:CB	1:C:132:LEU:HD21	2.29	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:43:VAL:HG12	1:B:43:VAL:O	2.11	0.51
1:B:196:ARG:O	1:B:200:LEU:HD23	2.10	0.51
1:B:121:LEU:HD12	1:B:132:LEU:HD22	1.93	0.51
1:B:174:LYS:HD2	2:B:575:HOH:O	2.11	0.51
1:B:22:GLN:NE2	2:B:641:HOH:O	2.44	0.50
1:A:161:ASN:HA	1:A:164:MET:CE	2.41	0.50
1:B:133:ARG:HG2	2:B:461:HOH:O	2.11	0.50
1:C:20:ASP:HB3	1:C:23:ASP:OD2	2.11	0.50
1:A:74:MET:HE2	1:A:192:PRO:HG3	1.94	0.50
1:C:63:SER:CB	1:C:68:ASN:HD21	2.23	0.50
1:B:212:TYR:HB3	1:B:266:MET:CE	2.40	0.50
1:A:322:ILE:HG13	1:A:371:GLU:HB3	1.94	0.50
1:D:132:LEU:N	1:D:132:LEU:HD12	2.27	0.50
1:C:106:GLU:CD	1:C:133:ARG:HD3	2.32	0.50
1:B:97:LEU:HD12	1:B:120:PHE:CE2	2.45	0.50
1:D:212:TYR:CE2	1:D:342:GLY:HA2	2.48	0.49
1:B:177:ARG:HG3	1:B:177:ARG:HH11	1.77	0.49
1:B:204:LEU:HD23	1:B:226:GLY:HA3	1.95	0.49
1:D:163:ASN:HB2	1:D:165:HIS:NE2	2.26	0.49
1:A:141:GLN:N	1:A:141:GLN:OE1	2.45	0.49
1:C:322:ILE:HG12	1:C:326:ARG:NH1	2.27	0.49
1:D:106:GLU:OE2	1:D:133:ARG:HD3	2.13	0.49
1:B:64:ASN:ND2	1:B:66:THR:H	2.11	0.49
1:D:343:ASP:HB3	2:D:654:HOH:O	2.12	0.49
1:A:163:ASN:HB2	1:A:165:HIS:NE2	2.28	0.49
1:D:166:MET:O	1:D:167:ALA:HB3	2.12	0.49
1:B:211:LLP:HE3	1:B:341:LEU:HD13	1.94	0.49
1:D:64:ASN:ND2	1:D:66:THR:H	2.11	0.49
1:D:281:ALA:HB2	1:D:289:ILE:CD1	2.42	0.48
1:C:204:LEU:HD23	1:C:226:GLY:HA3	1.96	0.48
1:C:293:GLY:HA3	1:C:306:GLN:HB2	1.95	0.48
1:C:7:LEU:HD23	1:C:8:PRO:HD2	1.95	0.48
1:B:166:MET:HB3	2:B:513:HOH:O	2.13	0.48
1:B:212:TYR:CE2	1:B:342:GLY:HA2	2.48	0.48
1:D:320:GLY:HA3	1:D:324:ALA:HB2	1.95	0.48
1:D:108:LEU:HD23	1:D:151:THR:CG2	2.43	0.48
1:D:74:MET:HE3	1:D:213:LEU:HD13	1.95	0.48
1:C:101:LEU:HD22	1:C:101:LEU:N	2.29	0.48
1:A:279:PHE:HA	1:A:282:ARG:HH22	1.79	0.47
1:C:287:GLU:HG3	1:C:288:LEU:HD22	1.95	0.47
1:A:117:THR:HG21	2:A:459:HOH:O	2.12	0.47
1:D:157:GLU:OE2	1:D:189:TYR:HE1	1.96	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:285:GLN:HE21	1:C:285:GLN:H	1.63	0.47
1:C:78:GLU:CD	1:C:192:PRO:HB3	2.34	0.47
1:C:97:LEU:HD12	1:C:120:PHE:HE2	1.81	0.46
1:C:269:HIS:HD2	1:C:378:VAL:O	1.99	0.46
1:A:395:LYS:HE2	2:A:501:HOH:O	2.16	0.46
1:B:63:SER:CB	1:B:68:ASN:HD21	2.29	0.46
1:B:108:LEU:HD23	1:B:133:ARG:HB3	1.98	0.46
1:A:157:GLU:HG2	1:A:186:ASP:HB3	1.97	0.46
1:A:37:THR:HG22	1:A:38:PHE:N	2.30	0.46
1:B:117:THR:HG21	2:B:466:HOH:O	2.16	0.46
1:D:108:LEU:HB2	1:D:154:ILE:CD1	2.45	0.46
1:A:285:GLN:H	1:A:285:GLN:HE21	1.64	0.46
1:C:64:ASN:ND2	1:C:66:THR:H	2.14	0.46
1:A:32:VAL:HB	2:C:423:HOH:O	2.15	0.46
1:D:74:MET:CE	1:D:259:ILE:HD11	2.46	0.46
1:B:141:GLN:OE1	1:B:141:GLN:N	2.49	0.46
1:D:246:VAL:HG23	2:D:437:HOH:O	2.15	0.45
1:C:269:HIS:HE1	2:C:399:HOH:O	1.98	0.45
1:D:108:LEU:HB2	1:D:154:ILE:HD12	1.99	0.45
1:A:159:PRO:HB2	1:A:164:MET:CA	2.46	0.45
1:D:285:GLN:NE2	1:D:285:GLN:H	2.15	0.45
1:A:143:LEU:C	1:A:143:LEU:HD13	2.37	0.45
1:A:113:LEU:N	1:A:113:LEU:HD22	2.32	0.45
1:D:288:LEU:HD12	1:D:288:LEU:C	2.38	0.45
1:C:206:VAL:HG12	1:C:224:VAL:HG22	1.99	0.45
1:C:344:ALA:HA	2:C:679:HOH:O	2.17	0.45
1:B:37:THR:HG22	1:B:38:PHE:N	2.31	0.45
1:C:288:LEU:HD23	1:C:317:GLU:HB3	1.99	0.45
1:A:161:ASN:HA	1:A:164:MET:HE2	1.98	0.44
1:C:163:ASN:HB2	1:C:165:HIS:CD2	2.52	0.44
1:A:212:TYR:CE2	1:A:342:GLY:HA2	2.52	0.44
1:A:366:HIS:HB2	2:A:530:HOH:O	2.15	0.44
1:D:141:GLN:OE1	1:D:141:GLN:N	2.49	0.44
1:B:285:GLN:H	1:B:285:GLN:HE21	1.65	0.44
1:C:279:PHE:HB2	2:C:721:HOH:O	2.18	0.44
1:D:140:LEU:HD12	1:D:140:LEU:N	2.32	0.44
1:C:350:HIS:N	1:C:354:MET:HE1	2.33	0.44
1:A:93:ILE:HG23	1:A:94:THR:N	2.33	0.44
1:D:329:MET:CE	1:D:337:ARG:HG2	2.48	0.44
1:D:161:ASN:HA	1:D:164:MET:CE	2.48	0.44
1:B:288:LEU:HD23	1:B:288:LEU:N	2.32	0.44
1:B:93:ILE:HD13	1:B:117:THR:HG22	1.99	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:78:GLU:CD	1:D:192:PRO:HB3	2.38	0.43
1:D:121:LEU:O	1:D:132:LEU:HD21	2.18	0.43
1:A:288:LEU:HD23	1:A:288:LEU:N	2.33	0.43
1:C:100:LEU:C	1:C:101:LEU:HD22	2.38	0.43
1:A:121:LEU:C	1:A:132:LEU:HD21	2.37	0.43
1:D:166:MET:HA	2:D:549:HOH:O	2.18	0.43
1:D:121:LEU:C	1:D:132:LEU:HD21	2.38	0.43
1:D:131:LYS:C	1:D:132:LEU:HD12	2.39	0.43
1:D:133:ARG:NE	2:D:642:HOH:O	2.52	0.43
1:B:161:ASN:HB3	1:B:162:PRO:HA	2.00	0.43
1:D:212:TYR:CD2	1:D:342:GLY:HA2	2.53	0.43
1:C:30:PRO:HA	1:C:31:PRO:HD3	1.88	0.43
1:C:157:GLU:HG2	1:C:186:ASP:HB3	2.00	0.43
1:A:313:MET:CE	1:A:341:LEU:HD22	2.49	0.43
1:B:212:TYR:CD2	1:B:342:GLY:HA2	2.54	0.43
1:B:174:LYS:HD3	1:B:175:ILE:N	2.34	0.43
1:A:178:LYS:HG2	1:A:179:HIS:ND1	2.34	0.42
1:D:7:LEU:HD22	1:D:8:PRO:CD	2.48	0.42
1:A:159:PRO:HB2	1:A:164:MET:HA	2.01	0.42
1:B:7:LEU:HD12	1:B:8:PRO:HD2	2.00	0.42
1:B:260:LYS:NZ	2:B:701:HOH:O	2.49	0.42
1:B:276:LEU:HD11	1:B:390:VAL:HG21	2.02	0.42
1:D:112:THR:CG2	1:D:161:ASN:HD22	2.27	0.42
1:D:348:ALA:N	2:D:600:HOH:O	2.53	0.42
1:A:178:LYS:HG2	1:A:179:HIS:CE1	2.55	0.42
1:A:116:CYS:HB3	2:C:674:HOH:O	2.19	0.42
1:A:154:ILE:HD12	1:A:176:ALA:HB2	2.01	0.42
1:C:329:MET:CE	1:C:337:ARG:HG2	2.49	0.42
1:B:30:PRO:HA	1:B:31:PRO:HD3	1.89	0.42
1:A:112:THR:C	1:A:113:LEU:HD22	2.40	0.42
1:A:78:GLU:CD	1:A:192:PRO:HB3	2.39	0.42
1:C:282:ARG:NH2	1:C:282:ARG:HB2	2.35	0.42
1:D:204:LEU:HD23	1:D:226:GLY:HA3	2.02	0.42
1:D:109:LEU:HB3	2:D:505:HOH:O	2.19	0.42
1:C:64:ASN:HD21	1:C:66:THR:HB	1.84	0.42
1:B:200:LEU:HD22	1:B:200:LEU:N	2.35	0.41
1:A:392:GLN:HE21	1:A:392:GLN:HB2	1.68	0.41
1:C:350:HIS:H	1:C:354:MET:CE	2.33	0.41
1:B:63:SER:HB2	1:B:68:ASN:HD21	1.86	0.41
1:D:28:LEU:HD12	2:D:489:HOH:O	2.21	0.41
1:C:41:PRO:O	1:C:42:THR:C	2.58	0.41
2:B:533:HOH:O	1:D:339:VAL:HG12	2.21	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:133:ARG:HG2	2:D:502:HOH:O	2.21	0.41
1:C:64:ASN:ND2	1:C:66:THR:HB	2.36	0.41
1:D:67:LEU:HD12	1:D:85:ALA:HB3	2.02	0.41
1:B:78:GLU:CD	1:B:192:PRO:HB3	2.40	0.41
1:C:197:PRO:HB2	1:C:205:VAL:CG1	2.51	0.41
1:A:282:ARG:NH2	2:A:655:HOH:O	2.54	0.41
1:D:174:LYS:C	1:D:174:LYS:HD3	2.41	0.41
1:C:291:TYR:CZ	1:C:315:ALA:HB2	2.55	0.41
1:A:320:GLY:HA3	1:A:324:ALA:HB2	2.02	0.41
1:A:30:PRO:HA	1:A:31:PRO:HD3	1.88	0.41
1:A:375:ARG:HB2	2:A:743:HOH:O	2.21	0.41
1:C:329:MET:HE3	1:C:337:ARG:HG2	2.02	0.41
1:C:275:VAL:HG12	2:C:721:HOH:O	2.20	0.41
1:C:159:PRO:HD3	1:C:166:MET:SD	2.60	0.41
1:B:274:GLN:O	1:B:278:GLU:HG3	2.21	0.41
1:D:148:THR:HB	1:D:149:PRO:HD2	2.02	0.41
1:D:131:LYS:HZ3	1:D:131:LYS:HB3	1.82	0.41
1:A:159:PRO:HG2	1:A:164:MET:SD	2.61	0.41
1:D:283:GLN:HG3	1:D:394:LEU:HD23	2.02	0.41
1:C:288:LEU:HD23	1:C:288:LEU:N	2.35	0.40
1:C:294:LEU:HD12	1:C:294:LEU:C	2.41	0.40
1:A:131:LYS:HD3	2:A:569:HOH:O	2.21	0.40
1:D:132:LEU:HD13	2:D:421:HOH:O	2.20	0.40
1:A:164:MET:HG2	1:A:291:TYR:CD2	2.56	0.40
1:B:288:LEU:HD23	1:B:317:GLU:HB3	2.04	0.40
1:B:262:LEU:HD12	1:B:266:MET:CE	2.51	0.40
1:B:241:ASP:O	1:D:120:PHE:CD1	2.74	0.40
1:D:197:PRO:HB2	1:D:205:VAL:HG12	2.03	0.40
1:C:309:GLN:HA	1:C:310:PRO:HD3	1.79	0.40
1:C:307:MET:O	1:C:308:SER:HB3	2.22	0.40
1:B:164:MET:HB3	2:B:648:HOH:O	2.22	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	348/398 (87%)	334 (96%)	12 (3%)	2 (1%)	33	13
1	B	350/398 (88%)	339 (97%)	10 (3%)	1 (0%)	50	27
1	C	356/398 (89%)	345 (97%)	9 (2%)	2 (1%)	33	13
1	D	349/398 (88%)	335 (96%)	9 (3%)	5 (1%)	16	2
All	All	1403/1592 (88%)	1353 (96%)	40 (3%)	10 (1%)	30	10

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	162	PRO
1	D	114	TYR
1	D	162	PRO
1	A	114	TYR
1	C	294	LEU
1	C	295	ALA
1	D	115	GLY
1	D	167	ALA
1	D	340	SER
1	B	43	VAL

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	274/306 (90%)	271 (99%)	3 (1%)	84	72
1	B	276/306 (90%)	271 (98%)	5 (2%)	71	53
1	C	280/306 (92%)	274 (98%)	6 (2%)	66	45
1	D	274/306 (90%)	267 (97%)	7 (3%)	59	35
All	All	1104/1224 (90%)	1083 (98%)	21 (2%)	69	50

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	141	GLN
1	A	285	GLN

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Mol	Chain	Res	Type
1	A	392	GLN
1	B	64	ASN
1	B	133	ARG
1	B	166	MET
1	B	285	GLN
1	B	341	LEU
1	C	7	LEU
1	C	37	THR
1	C	64	ASN
1	C	137	MET
1	C	285	GLN
1	C	394	LEU
1	D	23	ASP
1	D	64	ASN
1	D	141	GLN
1	D	285	GLN
1	D	341	LEU
1	D	392	GLN
1	D	394	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	111	ASN
1	A	179	HIS
1	A	228	GLN
1	A	237	GLN
1	A	272	ASN
1	A	274	GLN
1	A	285	GLN
1	A	330	ASN
1	A	366	HIS
1	A	392	GLN
1	B	22	GLN
1	B	34	GLN
1	B	64	ASN
1	B	111	ASN
1	B	228	GLN
1	B	272	ASN
1	B	285	GLN
1	B	330	ASN

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Mol	Chain	Res	Type
1	C	64	ASN
1	C	68	ASN
1	C	228	GLN
1	C	269	HIS
1	C	272	ASN
1	C	274	GLN
1	C	285	GLN
1	C	290	HIS
1	C	306	GLN
1	C	330	ASN
1	C	391	GLN
1	D	22	GLN
1	D	64	ASN
1	D	111	ASN
1	D	161	ASN
1	D	207	HIS
1	D	228	GLN
1	D	250	HIS
1	D	272	ASN
1	D	274	GLN
1	D	285	GLN
1	D	290	HIS
1	D	309	GLN
1	D	330	ASN
1	D	392	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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	A	211	1	24,24,25	3.93	6 (25%)	30,32,34	2.40	11 (36%)
1	LLP	B	211	1	24,24,25	3.95	6 (25%)	30,32,34	2.37	10 (33%)
1	LLP	C	211	1	24,24,25	3.91	6 (25%)	30,32,34	2.39	10 (33%)
1	LLP	D	211	1	24,24,25	3.86	5 (20%)	30,32,34	2.38	11 (36%)

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	211	1	-	0/15/17/19	0/1/1/1
1	LLP	B	211	1	-	0/15/17/19	0/1/1/1
1	LLP	C	211	1	-	0/15/17/19	0/1/1/1
1	LLP	D	211	1	-	0/15/17/19	0/1/1/1

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	211	LLP	O-C	17.84	1.23	1.11
1	A	211	LLP	O-C	17.77	1.23	1.11
1	C	211	LLP	O-C	17.61	1.23	1.11
1	D	211	LLP	O-C	17.35	1.23	1.11
1	A	211	LLP	C3-C2	4.25	1.43	1.40
1	D	211	LLP	C3-C2	4.22	1.43	1.40
1	B	211	LLP	C3-C2	4.17	1.43	1.40
1	C	211	LLP	C3-C2	3.95	1.43	1.40
1	C	211	LLP	C4'-NZ	-3.02	1.30	1.45
1	C	211	LLP	CA-C	2.99	1.53	1.48
1	B	211	LLP	C4'-NZ	-2.99	1.30	1.45
1	D	211	LLP	C4'-NZ	-2.96	1.30	1.45
1	A	211	LLP	C4'-NZ	-2.96	1.30	1.45
1	D	211	LLP	CA-C	2.89	1.53	1.48
1	B	211	LLP	CA-C	2.89	1.53	1.48
1	A	211	LLP	CA-C	2.84	1.53	1.48
1	C	211	LLP	C3-C4	2.67	1.44	1.40
1	D	211	LLP	C3-C4	2.63	1.44	1.40
1	A	211	LLP	C3-C4	2.53	1.44	1.40
1	B	211	LLP	C3-C4	2.46	1.44	1.40
1	B	211	LLP	O3-C3	-2.12	1.31	1.37
1	C	211	LLP	O3-C3	-2.09	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	211	LLP	O3-C3	-2.06	1.32	1.37

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	211	LLP	C4-C4'-NZ	5.34	121.47	111.52
1	C	211	LLP	C4-C4'-NZ	5.34	121.46	111.52
1	D	211	LLP	C4-C4'-NZ	5.33	121.45	111.52
1	B	211	LLP	C4-C4'-NZ	5.09	121.00	111.52
1	A	211	LLP	C4'-C4-C5	4.82	124.12	119.70
1	C	211	LLP	C4'-C4-C5	4.76	124.07	119.70
1	D	211	LLP	C4'-C4-C5	4.74	124.05	119.70
1	B	211	LLP	C4'-C4-C5	4.69	124.00	119.70
1	B	211	LLP	C4'-NZ-CE	4.45	129.85	113.47
1	C	211	LLP	C4'-NZ-CE	4.38	129.59	113.47
1	A	211	LLP	C4'-NZ-CE	4.34	129.45	113.47
1	D	211	LLP	C4'-NZ-CE	4.34	129.43	113.47
1	B	211	LLP	C6-N1-C2	3.92	127.67	119.28
1	C	211	LLP	C6-N1-C2	3.91	127.66	119.28
1	A	211	LLP	C6-N1-C2	3.89	127.61	119.28
1	D	211	LLP	C6-N1-C2	3.87	127.57	119.28
1	B	211	LLP	C4'-C4-C3	-3.83	115.44	120.31
1	C	211	LLP	C4'-C4-C3	-3.82	115.45	120.31
1	D	211	LLP	C4'-C4-C3	-3.78	115.50	120.31
1	A	211	LLP	C4'-C4-C3	-3.70	115.60	120.31
1	C	211	LLP	C5-C6-N1	-3.69	117.20	123.86
1	B	211	LLP	C5-C6-N1	-3.67	117.24	123.86
1	D	211	LLP	C5-C6-N1	-3.65	117.28	123.86
1	A	211	LLP	C5-C6-N1	-3.62	117.34	123.86
1	A	211	LLP	OP4-C5'-C5	3.56	116.51	109.26
1	C	211	LLP	OP4-C5'-C5	3.38	116.14	109.26
1	D	211	LLP	OP4-C5'-C5	3.38	116.13	109.26
1	B	211	LLP	OP4-C5'-C5	3.24	115.84	109.26
1	A	211	LLP	C5'-C5-C6	-3.23	113.17	119.28
1	A	211	LLP	C2'-C2-C3	3.15	124.85	121.02
1	B	211	LLP	C2'-C2-C3	3.09	124.77	121.02
1	D	211	LLP	C5'-C5-C6	-3.06	113.48	119.28
1	C	211	LLP	C5'-C5-C6	-3.02	113.57	119.28
1	D	211	LLP	C2'-C2-C3	3.01	124.67	121.02
1	C	211	LLP	C2'-C2-C3	2.94	124.59	121.02
1	B	211	LLP	C5'-C5-C6	-2.94	113.72	119.28
1	B	211	LLP	C3-C2-N1	-2.60	117.09	120.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	211	LLP	C3-C2-N1	-2.54	117.17	120.66
1	C	211	LLP	C3-C2-N1	-2.52	117.21	120.66
1	D	211	LLP	C3-C2-N1	-2.49	117.25	120.66
1	D	211	LLP	P-OP4-C5'	2.07	128.70	121.22
1	A	211	LLP	C5'-C5-C4	2.03	127.25	123.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

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 ⓘ

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	355/398 (89%)	0.94	43 (12%) 5 7	8, 16, 35, 42	0
1	B	357/398 (89%)	0.91	38 (10%) 7 9	8, 16, 35, 42	0
1	C	363/398 (91%)	1.04	47 (12%) 4 6	8, 17, 37, 47	0
1	D	356/398 (89%)	0.98	48 (13%) 4 5	8, 16, 35, 42	0
All	All	1431/1592 (89%)	0.97	176 (12%) 5 6	8, 16, 36, 47	0

All (176) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	114	TYR	11.0
1	D	114	TYR	10.0
1	C	114	TYR	9.6
1	B	114	TYR	8.0
1	C	310	PRO	7.8
1	A	116	CYS	7.7
1	B	43	VAL	7.5
1	D	166	MET	7.2
1	B	165	HIS	7.1
1	C	306	GLN	7.1
1	C	307	MET	7.0
1	C	308	SER	6.8
1	C	116	CYS	6.7
1	C	163	ASN	6.6
1	B	359	TYR	6.4
1	D	165	HIS	6.3
1	B	358	SER	6.2
1	B	116	CYS	5.9
1	C	359	TYR	5.8
1	C	111	ASN	5.7
1	A	398	ALA	5.7

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Mol	Chain	Res	Type	RSRZ
1	C	166	MET	5.7
1	A	359	TYR	5.6
1	C	160	ALA	5.5
1	C	358	SER	5.4
1	C	296	SER	5.2
1	D	160	ALA	5.2
1	C	367	TYR	5.0
1	C	165	HIS	4.9
1	A	358	SER	4.9
1	D	358	SER	4.9
1	A	160	ALA	4.8
1	B	398	ALA	4.7
1	C	164	MET	4.7
1	B	120	PHE	4.7
1	A	165	HIS	4.7
1	C	294	LEU	4.7
1	B	368	GLY	4.6
1	D	310	PRO	4.6
1	A	166	MET	4.6
1	B	367	TYR	4.5
1	D	359	TYR	4.5
1	C	366	HIS	4.5
1	A	167	ALA	4.4
1	A	367	TYR	4.4
1	D	398	ALA	4.4
1	C	141	GLN	4.4
1	D	111	ASN	4.4
1	A	161	ASN	4.4
1	A	366	HIS	4.4
1	A	120	PHE	4.4
1	C	120	PHE	4.3
1	B	366	HIS	4.3
1	B	121	LEU	4.3
1	A	357	SER	4.2
1	C	42	THR	4.2
1	D	164	MET	4.2
1	D	117	THR	4.2
1	A	111	ASN	4.1
1	D	357	SER	4.1
1	A	113	LEU	4.0
1	B	177	ARG	4.0
1	B	164	MET	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	398	ALA	3.9
1	D	113	LEU	3.9
1	B	166	MET	3.9
1	D	163	ASN	3.9
1	B	160	ALA	3.9
1	D	367	TYR	3.8
1	B	111	ASN	3.8
1	B	357	SER	3.8
1	A	322	ILE	3.8
1	B	117	THR	3.8
1	B	20	ASP	3.8
1	A	121	LEU	3.7
1	D	116	CYS	3.7
1	D	366	HIS	3.6
1	B	163	ASN	3.5
1	C	113	LEU	3.5
1	D	20	ASP	3.5
1	D	179	HIS	3.5
1	C	295	ALA	3.4
1	D	339	VAL	3.4
1	A	310	PRO	3.4
1	B	310	PRO	3.4
1	B	113	LEU	3.3
1	C	293	GLY	3.3
1	A	163	ASN	3.3
1	D	120	PHE	3.3
1	C	159	PRO	3.3
1	C	179	HIS	3.3
1	D	177	ARG	3.2
1	D	115	GLY	3.2
1	A	141	GLN	3.2
1	B	167	ALA	3.2
1	C	368	GLY	3.2
1	D	161	ASN	3.2
1	C	121	LEU	3.1
1	A	117	THR	3.1
1	A	20	ASP	3.0
1	B	282	ARG	3.0
1	C	20	ASP	3.0
1	C	135	VAL	3.0
1	A	118	PHE	3.0
1	B	118	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	309	GLN	2.9
1	D	135	VAL	2.9
1	A	119	ALA	2.9
1	B	339	VAL	2.8
1	C	282	ARG	2.8
1	D	144	GLU	2.8
1	C	357	SER	2.8
1	C	167	ALA	2.8
1	C	162	PRO	2.8
1	C	117	THR	2.7
1	A	133	ARG	2.7
1	C	189	TYR	2.7
1	B	144	GLU	2.6
1	D	132	LEU	2.6
1	B	119	ALA	2.6
1	D	22	GLN	2.6
1	D	118	PHE	2.6
1	A	189	TYR	2.6
1	A	112	THR	2.6
1	C	339	VAL	2.5
1	A	7	LEU	2.5
1	A	162	PRO	2.5
1	B	44	GLU	2.5
1	D	167	ALA	2.5
1	A	368	GLY	2.5
1	B	135	VAL	2.4
1	D	281	ALA	2.4
1	B	22	GLN	2.4
1	C	7	LEU	2.4
1	D	293	GLY	2.4
1	A	110	GLY	2.4
1	B	180	GLY	2.4
1	D	282	ARG	2.4
1	D	189	TYR	2.4
1	D	141	GLN	2.3
1	B	112	THR	2.3
1	A	178	LYS	2.3
1	A	309	GLN	2.3
1	A	282	ARG	2.3
1	D	162	PRO	2.3
1	C	144	GLU	2.3
1	D	41	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	179	HIS	2.3
1	A	115	GLY	2.3
1	B	194	LEU	2.2
1	C	63	SER	2.2
1	C	287	GLU	2.2
1	D	112	THR	2.2
1	B	115	GLY	2.2
1	B	211	LLP	2.2
1	D	140	LEU	2.2
1	D	200	LEU	2.2
1	D	287	GLU	2.2
1	A	63	SER	2.2
1	A	211	LLP	2.2
1	A	135	VAL	2.2
1	D	28	LEU	2.1
1	D	169	ILE	2.1
1	D	37	THR	2.1
1	D	7	LEU	2.1
1	C	337	ARG	2.1
1	D	313	MET	2.1
1	D	290	HIS	2.1
1	C	23	ASP	2.1
1	C	118	PHE	2.0
1	D	368	GLY	2.0
1	C	137	MET	2.0
1	A	108	LEU	2.0
1	A	313	MET	2.0
1	A	170	ALA	2.0
1	A	179	HIS	2.0

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

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	LLP	B	211	24/25	0.19	0.71	9,19,22,23	0
1	LLP	A	211	24/25	0.19	0.41	10,20,23,24	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
1	LLP	D	211	24/25	0.16	0.20	10,19,22,23	0
1	LLP	C	211	24/25	0.14	0.02	9,20,22,23	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.