



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:36 AM UTC

PDB ID : 1GC0 / pdb_00001gc0
Title : CRYSTAL STRUCTURE OF THE PYRIDOXAL-5'-PHOSPHATE
DEPENDENT L-METHIONINE GAMMA-LYASE FROM PSEUDOMONAS
PUTIDA
Authors : Motoshima, H.; Inagaki, K.; Kumasaka, T.; Furuichi, M.; Inoue, H.; Tamura,
T.; Esaki, N.; Soda, K.; Tanaka, N.; Yamamoto, M.; Tanaka, H.
Deposited on : 2000-07-06
Resolution : 1.70 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

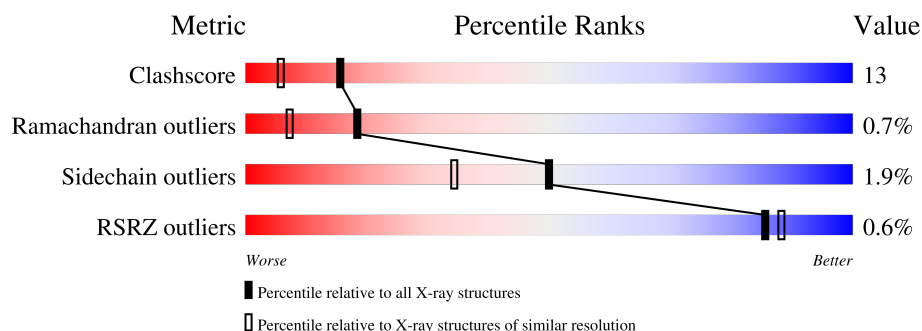
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (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 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	% 70% 18% • 11%
1	B	398	% 71% 17% • 10%
1	C	398	% 69% 20% • 9%
1	D	398	% 69% 18% • 11%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12053 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.

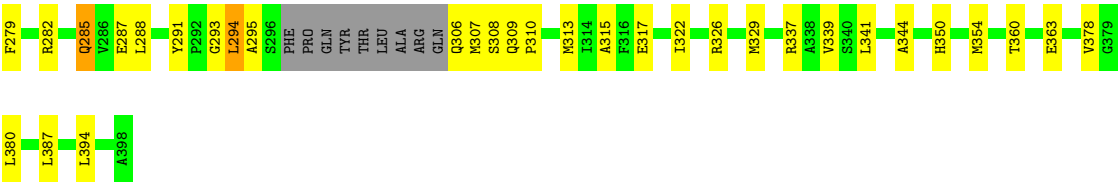
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	355	Total	C	N	O	P	S	0	0	0
			2681	1690	474	501	1	15			
1	B	357	Total	C	N	O	P	S	0	0	0
			2695	1699	475	505	1	15			
1	C	363	Total	C	N	O	P	S	0	0	0
			2734	1721	483	513	1	16			
1	D	356	Total	C	N	O	P	S	0	0	0
			2685	1692	475	502	1	15			

- Molecule 2 is water.

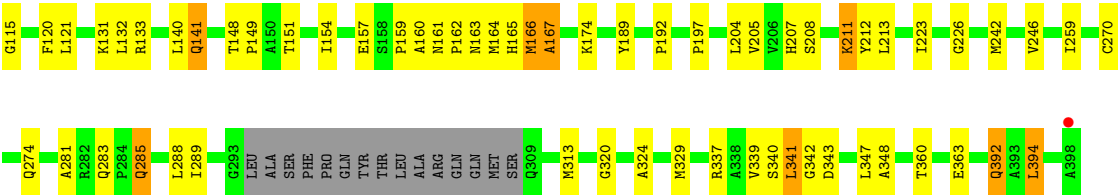
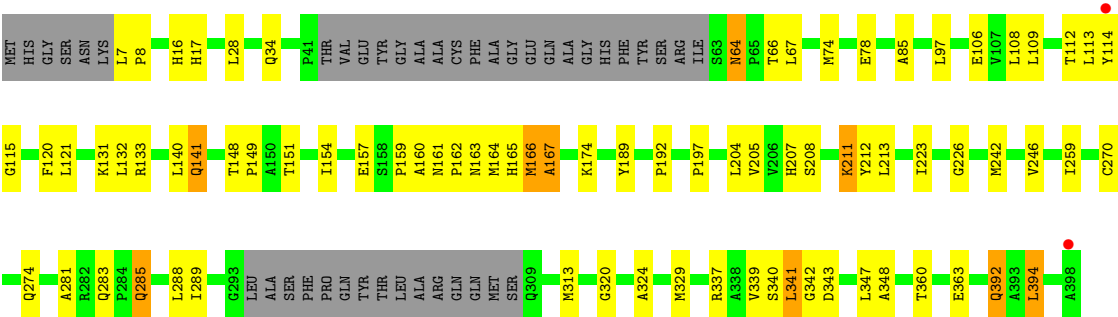
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	362	Total	O	0	0
			362	362		
2	B	310	Total	O	0	0
			310	310		
2	C	324	Total	O	0	0
			324	324		
2	D	262	Total	O	0	0
			262	262		

- Molecule 1: METHIONINE GAMMA-LYASE





• Molecule 1: METHIONINE GAMMA-LYASE



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 71.46 – 1.70	Depositor EDS
% Data completeness (in resolution range)	91.0 (71.46-1.70) 90.2 (71.46-1.70)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.18 (at 1.70Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.210 , 0.236 0.217 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	14.7	Xtriage
Anisotropy	0.359	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 33.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.479 for h,h-k,h-l 0.479 for -h,-h+l,-h+k 0.477 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.95	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.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.34	0/2710	0.86	6/3677 (0.2%)
1	B	0.36	0/2724	0.85	7/3696 (0.2%)
1	C	0.34	0/2763	0.85	5/3748 (0.1%)
1	D	0.34	0/2714	0.87	5/3682 (0.1%)
All	All	0.35	0/10911	0.86	23/14803 (0.2%)

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	208	SER	N-CA-C	-6.67	95.33	107.75
1	D	242	MET	N-CA-C	6.66	122.37	113.72
1	A	242	MET	N-CA-C	6.62	122.33	113.72
1	D	208	SER	N-CA-C	-6.46	95.74	107.75
1	C	208	SER	N-CA-C	-6.40	95.85	107.75
1	B	16	HIS	N-CA-C	6.34	121.90	114.04
1	A	208	SER	N-CA-C	-6.25	96.12	107.75
1	C	242	MET	N-CA-C	6.22	121.81	113.72
1	B	242	MET	N-CA-C	6.15	121.72	113.72
1	B	17	HIS	N-CA-C	6.04	119.11	110.24
1	C	16	HIS	N-CA-C	6.03	121.52	114.04
1	C	17	HIS	N-CA-C	6.02	119.08	110.24
1	D	166	MET	N-CA-C	5.97	117.79	111.28
1	D	16	HIS	N-CA-C	5.94	121.40	114.04
1	A	16	HIS	N-CA-C	5.90	121.36	114.04
1	A	309	GLN	CA-C-N	5.83	127.12	119.84
1	A	309	GLN	C-N-CA	5.83	127.12	119.84
1	A	17	HIS	N-CA-C	5.76	118.71	110.24
1	B	122	HIS	N-CA-C	5.63	117.42	111.28
1	D	17	HIS	N-CA-C	5.48	118.29	110.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	283	GLN	CA-C-N	5.45	125.27	119.28
1	B	283	GLN	C-N-CA	5.45	125.27	119.28
1	C	100	LEU	N-CA-C	5.21	119.36	112.89

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	2681	0	2658	70	0
1	B	2695	0	2673	69	0
1	C	2734	0	2711	77	0
1	D	2685	0	2661	75	0
2	A	362	0	0	14	0
2	B	310	0	0	15	0
2	C	324	0	0	10	0
2	D	262	0	0	15	0
All	All	12053	0	10703	288	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 13.

All (288) 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:C:121:LEU:HB3	1:C:132:LEU:HD21	1.43	1.00
1:A:313:MET:HG3	2:A:628:HOH:O	1.72	0.90
1:C:111:ASN:H	1:C:137:MET:HE2	1.38	0.88
1:D:313:MET:HG3	2:D:581:HOH:O	1.75	0.86
1:C:350:HIS:HB3	1:C:354:MET:HE3	1.56	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:C:137:MET:HE3	1:C:137:MET:H	1.45	0.82
1:B:261:THR:HG22	2:B:678:HOH:O	1.81	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:329:MET:HG3	1:C:354:MET:HE1	1.67	0.76
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:C:329:MET:HE3	1:C:337:ARG:HG2	1.68	0.75
1:A:380:LEU:HD13	2:B:678:HOH:O	1.85	0.74
1:C:136:ASP:HA	1:C:137:MET:HE3	1.70	0.73
1:D:329:MET:HE3	1:D:337:ARG:HG2	1.69	0.73
1:A:74:MET:HG2	1:A:223:ILE:HG21	1.70	0.73
1:B:262:LEU:HD12	1:B:266:MET:HE3	1.72	0.72
1:A:287:GLU:HG3	1:A:288:LEU:HD22	1.72	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:HE1	1:D:259:ILE:HD11	1.72	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:21:PRO:HG2	2:D:622:HOH:O	1.91	0.69
1:C:117:THR:O	1:C:121:LEU:HD23	1.92	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:C:173:ALA:HB1	1:C:177:ARG:HH22	1.58	0.68
1:B:166:MET:HE3	1:B:166:MET:H	1.57	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
1:C:111:ASN:H	1:C:137:MET:CE	2.08	0.66
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:H	1:C:137:MET:CE	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:B:262:LEU:CD1	1:B:266:MET:HE3	2.27	0.64
1:C:350:HIS:HB3	1:C:354:MET:CE	2.27	0.64
1:A:177:ARG:HH21	1:A:177:ARG:HG3	1.62	0.64
1:C:63:SER:HB3	1:C:68:ASN:HD21	1.60	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:B:174:LYS:HD3	1:B:174:LYS:C	2.23	0.63
1:D:74:MET:HE3	1:D:213:LEU:HD13	1.79	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HB3	1:D:131:LYS:NZ	2.14	0.62
1:D:78:GLU:OE1	1:D:207:HIS:HE1	1.82	0.62
1:B:166:MET:HE3	1:B:166:MET:N	2.15	0.62
1:A:161:ASN:HA	1:A:164:MET:HE2	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:D:161:ASN:HA	1:D:164:MET:HE2	1.82	0.60
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:D:112:THR:C	1:D:113:LEU:HD22	2.26	0.60
1:B:211:LLP:HE3	1:B:341:LEU:CD1	2.33	0.59
1:C:387:LEU:HD21	2:C:721:HOH:O	2.01	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:A:279:PHE:HA	1:A:282:ARG:NH2	2.17	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: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:A:309:GLN:HG3	2:A:704:HOH:O	2.03	0.57
1:D:392:GLN:NE2	2:D:659:HOH:O	2.38	0.57
1:D:160:ALA:O	1:D:164:MET:HA	2.05	0.57
1:D:339:VAL:HG13	1:D:339:VAL:O	2.05	0.57
1:C:111:ASN:N	1:C:137:MET:HE2	2.15	0.56
1:A:281:ALA:HB2	1:A:289:ILE:HD11	1.87	0.56
1:D:211:LLP:HE3	1:D:341:LEU:CD1	2.34	0.56
1:A:20:ASP:OD2	1:A:22:GLN:HB2	2.05	0.56
1:B:121:LEU:HB3	1:B:132:LEU:HD13	1.88	0.56
1:C:137:MET:HE3	1:C:137:MET:N	2.17	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:A:276:LEU:HD23	1:A:387:LEU:HD23	1.88	0.55
1:C:285:GLN:NE2	1:C:285:GLN:H	2.04	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:97:LEU:HD12	1:D:120:PHE:HE2	1.70	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:C:354:MET:HE2	2:C:589:HOH:O	2.07	0.55
1:B:74:MET:CE	1:B:192:PRO:HG3	2.37	0.55
1:B:74:MET:HE2	1:B:192:PRO:HG3	1.89	0.55
1:B:320:GLY:HA3	1:B:324:ALA:HB2	1.89	0.55
1:B:285:GLN:H	1:B:285:GLN:NE2	2.05	0.55
1:C:106:GLU:OE1	1:C:133:ARG:HD3	2.07	0.55
1:C:106:GLU:CD	1:C:133:ARG:HD3	2.32	0.54
1:C:339:VAL:O	1:C:339:VAL:HG13	2.08	0.54
1:C:329:MET:HE2	1:C:354:MET:HE1	1.87	0.54
1:A:173:ALA:O	1:A:177:ARG:HG2	2.08	0.54
1:A:285:GLN:H	1:A:285:GLN:NE2	2.06	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:H	1:B:166:MET:CE	2.23	0.52
1:C:111:ASN:OD1	1:C:137:MET:HE1	2.09	0.52
1:A:281:ALA:HB2	1:A:289:ILE:CD1	2.39	0.52
1:A:313:MET:HE2	1:A:341:LEU:HD22	1.92	0.52
1:D:281:ALA:HB2	1:D:289:ILE:HD12	1.92	0.52
1:A:166:MET:HA	2:A:510:HOH:O	2.10	0.52
1:B:212:TYR:HB3	1:B:266:MET:CE	2.40	0.52
1:C:78:GLU:CD	1:C:192:PRO:HB3	2.34	0.52
1:B:114:TYR:HD1	1:B:117:THR:HG23	1.76	0.51
1:C:131:LYS:NZ	1:C:133:ARG:HD2	2.24	0.51
1:A:177:ARG:HG3	1:A:177:ARG:NH2	2.25	0.51
1:C:164:MET:HE2	1:C:291:TYR:CZ	2.45	0.51
1:D:109:LEU:CD1	1:D:121:LEU:HD13	2.40	0.51
1:D:74:MET:CE	1:D:213:LEU:HD13	2.41	0.51
1:D:113:LEU:HD11	2:D:505:HOH:O	2.11	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:B:43:VAL:HG12	1:B:43:VAL:O	2.11	0.51
1:C:121:LEU:CB	1:C:132:LEU:HD21	2.29	0.51
1:B:196:ARG:O	1:B:200:LEU:HD23	2.10	0.51
1:C:329:MET:CG	1:C:354:MET:HE1	2.40	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:97:LEU:HD12	1:B:120:PHE:CE2	2.45	0.50
1:A:143:LEU:HD13	1:A:143:LEU:C	2.37	0.49
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:288:LEU:HD12	1:D:288:LEU:C	2.38	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:B:64:ASN:ND2	1:B:66:THR:H	2.11	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:A:163:ASN:HB2	1:A:165:HIS:NE2	2.28	0.49
1:D:343:ASP:HB3	2:D:654:HOH:O	2.12	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:A:161:ASN:HA	1:A:164:MET:CE	2.41	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:B:212:TYR:CD2	1:B:266:MET:HE1	2.48	0.48
1:A:121:LEU:C	1:A:132:LEU:HD21	2.37	0.48
1:C:204:LEU:HD23	1:C:226:GLY:HA3	1.96	0.48
1:D:78:GLU:CD	1:D:192:PRO:HB3	2.38	0.48
1:C:7:LEU:HD23	1:C:8:PRO:HD2	1.95	0.48
1:C:100:LEU:C	1:C:101:LEU:HD22	2.38	0.48
1:C:293:GLY:HA3	1:C:306:GLN:HB2	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:121:LEU:C	1:D:132:LEU:HD21	2.38	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: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:131:LYS:C	1:D:132:LEU:HD12	2.39	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:157:GLU:OE2	1:D:189:TYR:HE1	1.96	0.47
1:C:285:GLN:H	1:C:285:GLN:HE21	1.63	0.47
1:A:78:GLU:CD	1:A:192:PRO:HB3	2.39	0.47
1:A:112:THR:C	1:A:113:LEU:HD22	2.40	0.47
1:C:97:LEU:HD12	1:C:120:PHE:HE2	1.81	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:78:GLU:CD	1:B:192:PRO:HB3	2.40	0.46
1:C:269:HIS:HD2	1:C:378:VAL:O	1.99	0.46
1:A:37:THR:HG22	1:A:38:PHE:N	2.30	0.46
1:A:157:GLU:HG2	1:A:186:ASP:HB3	1.97	0.46
1:B:108:LEU:HD23	1:B:133:ARG:HB3	1.98	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:C:41:PRO:O	1:C:42:THR:C	2.58	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:C:294:LEU:C	1:C:294:LEU:HD12	2.41	0.46
1:A:32:VAL:HB	2:C:423:HOH:O	2.15	0.46
1:B:141:GLN:OE1	1:B:141:GLN:N	2.49	0.46
1:D:174:LYS:C	1:D:174:LYS:HD3	2.41	0.45
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:H	1:D:285:GLN:NE2	2.15	0.45
1:A:113:LEU:HD22	1:A:113:LEU:N	2.32	0.45
1:C:206:VAL:HG12	1:C:224:VAL:HG22	1.99	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:C:344:ALA:HA	2:C:679:HOH:O	2.17	0.45
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:N	1:D:140:LEU:HD12	2.32	0.44
1:A:93:ILE:HG23	1:A:94:THR:N	2.33	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:PRO:HB2	1:A:164:MET:C	2.42	0.43
1:A:288:LEU:N	1:A:288:LEU:HD23	2.33	0.43
1:D:121:LEU:O	1:D:132:LEU:HD21	2.18	0.43
1:D:166:MET:HA	2:D:549:HOH:O	2.18	0.43
1:B:161:ASN:HB3	1:B:162:PRO:HA	2.00	0.43
1:D:133:ARG:NE	2:D:642:HOH:O	2.52	0.43
1:C:30:PRO:HA	1:C:31:PRO:HD3	1.88	0.43
1:D:212:TYR:CD2	1:D:342:GLY:HA2	2.53	0.43
1:B:341:LEU:HD22	1:B:341:LEU:C	2.44	0.43
1:C:157:GLU:HG2	1:C:186:ASP:HB3	2.00	0.43
1:A:161:ASN:O	1:A:162:PRO:C	2.62	0.43
1:B:174:LYS:HD3	1:B:175:ILE:N	2.34	0.43
1:B:212:TYR:CD2	1:B:342:GLY:HA2	2.54	0.43
1:C:136:ASP:CA	1:C:137:MET:HE3	2.44	0.43
1:A:178:LYS:HG2	1:A:179:HIS:ND1	2.34	0.42
1:D:74:MET:HE3	1:D:223:ILE:HG13	2.01	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:D:7:LEU:HD22	1:D:8:PRO:CD	2.48	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:A:178:LYS:HG2	1:A:179:HIS:CE1	2.55	0.42
1:D:112:THR:CG2	1:D:161:ASN:HD22	2.27	0.42
1:D:161:ASN:HA	1:D:164:MET:CE	2.48	0.42
1:D:348:ALA:N	2:D:600:HOH:O	2.53	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:A:313:MET:CE	1:A:341:LEU:HD22	2.49	0.42
1:B:212:TYR:HB3	1:B:266:MET:HE1	2.00	0.42
1:B:30:PRO:HA	1:B:31:PRO:HD3	1.89	0.42
1:B:291:TYR:HA	1:B:292:PRO:C	2.45	0.42
1:C:313:MET:HE3	1:C:341:LEU:HD22	2.02	0.42
1:D:131:LYS:HB3	1:D:131:LYS:HZ3	1.81	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:A:177:ARG:O	1:A:178:LYS:C	2.63	0.42
1:C:64:ASN:HD21	1:C:66:THR:HB	1.84	0.42
1:D:109:LEU:HB3	2:D:505:HOH:O	2.19	0.42
1:A:392:GLN:HE21	1:A:392:GLN:HB2	1.68	0.41
1:B:200:LEU:N	1:B:200:LEU:HD22	2.35	0.41
1:B:212:TYR:HD2	1:B:266:MET:HE1	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:SER:HB2	1:B:68:ASN:HD21	1.86	0.41
1:C:350:HIS:H	1:C:354:MET:CE	2.33	0.41
1:D:28:LEU:HD12	2:D:489:HOH:O	2.21	0.41
2:B:533:HOH:O	1:D:339:VAL:HG12	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:D:74:MET:CE	1:D:259:ILE:HD11	2.46	0.41
1:D:133:ARG:HG2	2:D:502:HOH:O	2.21	0.41
1:D:159:PRO:HB2	1:D:164:MET:C	2.46	0.41
1:A:282:ARG:NH2	2:A:655:HOH:O	2.54	0.41
1:A:291:TYR:HA	1:A:292:PRO:C	2.46	0.41
1:C:197:PRO:HB2	1:C:205:VAL:CG1	2.51	0.41
1:A:320:GLY:HA3	1:A:324:ALA:HB2	2.02	0.41
1:C:291:TYR:CZ	1:C:315:ALA:HB2	2.55	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:B:274:GLN:O	1:B:278:GLU:HG3	2.21	0.41
1:C:159:PRO:HD3	1:C:166:MET:SD	2.60	0.41
1:C:275:VAL:HG12	2:C:721:HOH:O	2.20	0.41
1:D:148:THR:HB	1:D:149:PRO:HD2	2.02	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:A:131:LYS:HD3	2:A:569:HOH:O	2.21	0.40
1:C:288:LEU:HD23	1:C:288:LEU:N	2.35	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:D:132:LEU:HD13	2:D:421:HOH:O	2.20	0.40
1:B:241:ASP:O	1:D:120:PHE:CD1	2.74	0.40
1:C:309:GLN:HA	1:C:310:PRO:HD3	1.79	0.40
1:D:197:PRO:HB2	1:D:205:VAL:HG12	2.03	0.40
1:B:74:MET:HE3	1:B:77:LEU:HB2	2.03	0.40
1:B:164:MET:HB3	2:B:648:HOH:O	2.22	0.40
1:C:307:MET:O	1:C:308:SER:HB3	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%)	21	9
1	B	350/398 (88%)	339 (97%)	10 (3%)	1 (0%)	36	22
1	C	356/398 (89%)	345 (97%)	9 (2%)	2 (1%)	21	9
1	D	349/398 (88%)	335 (96%)	9 (3%)	5 (1%)	9	2
All	All	1403/1592 (88%)	1353 (96%)	40 (3%)	10 (1%)	18	7

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%)	65	54

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	276/306 (90%)	271 (98%)	5 (2%)	51	36
1	C	280/306 (92%)	273 (98%)	7 (2%)	42	24
1	D	274/306 (90%)	268 (98%)	6 (2%)	45	29
All	All	1104/1224 (90%)	1083 (98%)	21 (2%)	50	34

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

Mol	Chain	Res	Type
1	A	141	GLN
1	A	285	GLN
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	28	LEU
1	C	37	THR
1	C	64	ASN
1	C	137	MET
1	C	285	GLN
1	C	394	LEU
1	D	64	ASN
1	D	141	GLN
1	D	285	GLN
1	D	341	LEU
1	D	392	GLN
1	D	394	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	34	GLN
1	A	111	ASN
1	A	179	HIS
1	A	228	GLN
1	A	237	GLN
1	A	272	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	274	GLN
1	A	283	GLN
1	A	285	GLN
1	A	290	HIS
1	A	330	ASN
1	A	391	GLN
1	A	392	GLN
1	B	22	GLN
1	B	34	GLN
1	B	64	ASN
1	B	111	ASN
1	B	123	HIS
1	B	161	ASN
1	B	272	ASN
1	B	285	GLN
1	B	290	HIS
1	B	330	ASN
1	B	349	GLN
1	B	391	GLN
1	C	64	ASN
1	C	68	ASN
1	C	123	HIS
1	C	228	GLN
1	C	237	GLN
1	C	269	HIS
1	C	272	ASN
1	C	274	GLN
1	C	283	GLN
1	C	285	GLN
1	C	290	HIS
1	C	306	GLN
1	C	330	ASN
1	C	391	GLN
1	D	64	ASN
1	D	111	ASN
1	D	161	ASN
1	D	207	HIS
1	D	228	GLN
1	D	272	ASN
1	D	274	GLN
1	D	283	GLN
1	D	285	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	290	HIS
1	D	309	GLN
1	D	330	ASN
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	A	211	1	23,24,25	1.25	4 (17%)	25,32,34	2.33	10 (40%)
1	LLP	D	211	1	23,24,25	1.25	3 (13%)	25,32,34	2.31	10 (40%)
1	LLP	B	211	1	23,24,25	1.23	3 (13%)	25,32,34	2.31	10 (40%)
1	LLP	C	211	1	23,24,25	1.24	4 (17%)	25,32,34	2.31	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	A	211	1	-	8/16/17/19	0/1/1/1
1	LLP	D	211	1	-	10/16/17/19	0/1/1/1
1	LLP	B	211	1	-	10/16/17/19	0/1/1/1
1	LLP	C	211	1	-	8/16/17/19	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	211	LLP	C3-C2	2.74	1.43	1.41
1	D	211	LLP	C3-C2	2.72	1.43	1.41
1	B	211	LLP	C3-C2	2.68	1.43	1.41
1	C	211	LLP	C3-C2	2.53	1.43	1.41
1	A	211	LLP	C4-C4'	2.37	1.51	1.46
1	C	211	LLP	C4-C4'	2.24	1.51	1.46
1	D	211	LLP	C4-C4'	2.22	1.51	1.46
1	C	211	LLP	C4-C3	2.20	1.44	1.41
1	B	211	LLP	C4-C4'	2.19	1.51	1.46
1	B	211	LLP	O3-C3	-2.16	1.31	1.36
1	D	211	LLP	C4-C3	2.16	1.44	1.41
1	C	211	LLP	O3-C3	-2.14	1.32	1.36
1	A	211	LLP	O3-C3	-2.10	1.32	1.36
1	A	211	LLP	C4-C3	2.05	1.44	1.41

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	211	LLP	C6-N1-C2	4.67	127.67	119.20
1	C	211	LLP	C6-N1-C2	4.67	127.66	119.20
1	A	211	LLP	C6-N1-C2	4.64	127.61	119.20
1	D	211	LLP	C6-N1-C2	4.62	127.57	119.20
1	C	211	LLP	C5-C6-N1	-4.08	117.20	123.83
1	B	211	LLP	C5-C6-N1	-4.05	117.24	123.83
1	D	211	LLP	C5-C6-N1	-4.02	117.28	123.83
1	A	211	LLP	C5-C6-N1	-3.99	117.34	123.83
1	D	211	LLP	C4-C3-C2	-3.85	117.98	120.14
1	A	211	LLP	OP4-C5'-C5	3.82	116.51	109.36
1	A	211	LLP	C5'-C5-C6	-3.80	113.17	119.36
1	C	211	LLP	C4-C3-C2	-3.79	118.01	120.14
1	A	211	LLP	C4-C3-C2	-3.75	118.03	120.14
1	B	211	LLP	C4-C3-C2	-3.75	118.03	120.14
1	C	211	LLP	OP4-C5'-C5	3.62	116.14	109.36
1	D	211	LLP	OP4-C5'-C5	3.61	116.13	109.36
1	D	211	LLP	C5'-C5-C6	-3.61	113.48	119.36
1	C	211	LLP	C5'-C5-C6	-3.55	113.57	119.36
1	B	211	LLP	CE-NZ-C4'	3.48	129.85	118.72
1	B	211	LLP	OP4-C5'-C5	3.46	115.84	109.36
1	B	211	LLP	C5'-C5-C6	-3.46	113.72	119.36
1	A	211	LLP	C2'-C2-C3	3.46	124.85	120.80
1	B	211	LLP	C2'-C2-C3	3.40	124.77	120.80
1	C	211	LLP	CE-NZ-C4'	3.40	129.59	118.72
1	A	211	LLP	CE-NZ-C4'	3.35	129.45	118.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	211	LLP	CE-NZ-C4'	3.35	129.43	118.72
1	D	211	LLP	C2'-C2-C3	3.31	124.67	120.80
1	C	211	LLP	C2'-C2-C3	3.24	124.59	120.80
1	B	211	LLP	C3-C2-N1	-3.06	117.09	120.96
1	A	211	LLP	C3-C2-N1	-3.00	117.17	120.96
1	C	211	LLP	C3-C2-N1	-2.98	117.21	120.96
1	D	211	LLP	C3-C2-N1	-2.94	117.25	120.96
1	B	211	LLP	C3-C4-C5	2.85	120.56	118.28
1	B	211	LLP	C3-C4-C4'	-2.75	115.44	120.40
1	C	211	LLP	C3-C4-C5	2.74	120.48	118.28
1	C	211	LLP	C3-C4-C4'	-2.74	115.45	120.40
1	D	211	LLP	C3-C4-C4'	-2.72	115.50	120.40
1	D	211	LLP	C3-C4-C5	2.71	120.45	118.28
1	A	211	LLP	C3-C4-C4'	-2.66	115.60	120.40
1	A	211	LLP	C3-C4-C5	2.49	120.27	118.28

There are no chirality outliers.

All (36) torsion outliers are listed below:

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	A	211	LLP	C5'-OP4-P-OP1
1	B	211	LLP	C5'-OP4-P-OP1
1	C	211	LLP	C5'-OP4-P-OP1
1	D	211	LLP	C5'-OP4-P-OP1
1	D	211	LLP	C6-C5-C5'-OP4
1	B	211	LLP	CA-CB-CG-CD
1	C	211	LLP	CA-CB-CG-CD
1	D	211	LLP	CD-CE-NZ-C4'
1	B	211	LLP	CG-CD-CE-NZ
1	C	211	LLP	CD-CE-NZ-C4'
1	A	211	LLP	CD-CE-NZ-C4'
1	A	211	LLP	CA-CB-CG-CD
1	B	211	LLP	CD-CE-NZ-C4'
1	B	211	LLP	C5-C4-C4'-NZ

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	211	LLP	1	0
1	B	211	LLP	2	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	354/398 (88%)	-0.68	3 (0%) 82 85	8, 16, 35, 42	0
1	B	356/398 (89%)	-0.71	2 (0%) 85 88	8, 16, 35, 42	0
1	C	362/398 (90%)	-0.64	2 (0%) 85 88	8, 17, 37, 47	0
1	D	355/398 (89%)	-0.67	2 (0%) 85 88	8, 16, 35, 42	0
All	All	1427/1592 (89%)	-0.67	9 (0%) 85 88	8, 16, 36, 47	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	398	ALA	3.3
1	A	114	TYR	2.9
1	B	114	TYR	2.8
1	A	116	CYS	2.6
1	B	368	GLY	2.2
1	D	114	TYR	2.1
1	C	160	ALA	2.1
1	D	398	ALA	2.1
1	C	163	ASN	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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	LLP	A	211	24/25	0.98	0.06	10,20,23,24	0
1	LLP	B	211	24/25	0.99	0.05	9,19,22,23	0
1	LLP	C	211	24/25	0.99	0.05	9,20,22,23	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	LLP	D	211	24/25	0.99	0.05	10,19,22,23	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.