Full wwPDB X-ray Structure Validation Report (i)

May 24, 2020 – 08:44 am BST

PDB ID	:	1GC0
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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

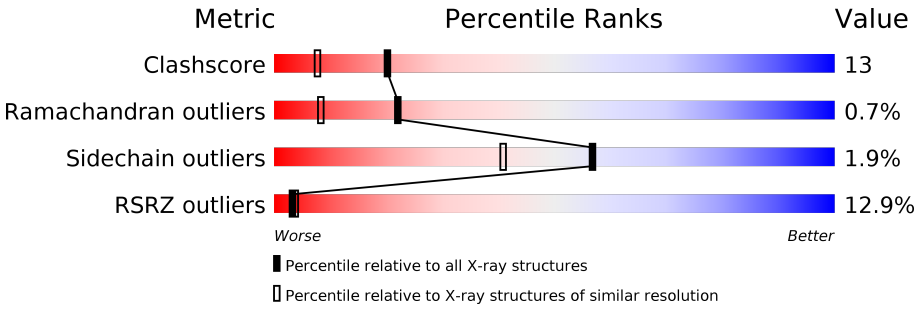
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (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 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 <=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	11% 71% 17% • 11%
1	B	398	11% 73% 15% • 10%
1	C	398	12% 70% 19% • 9%
1	D	398	12% 70% 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.

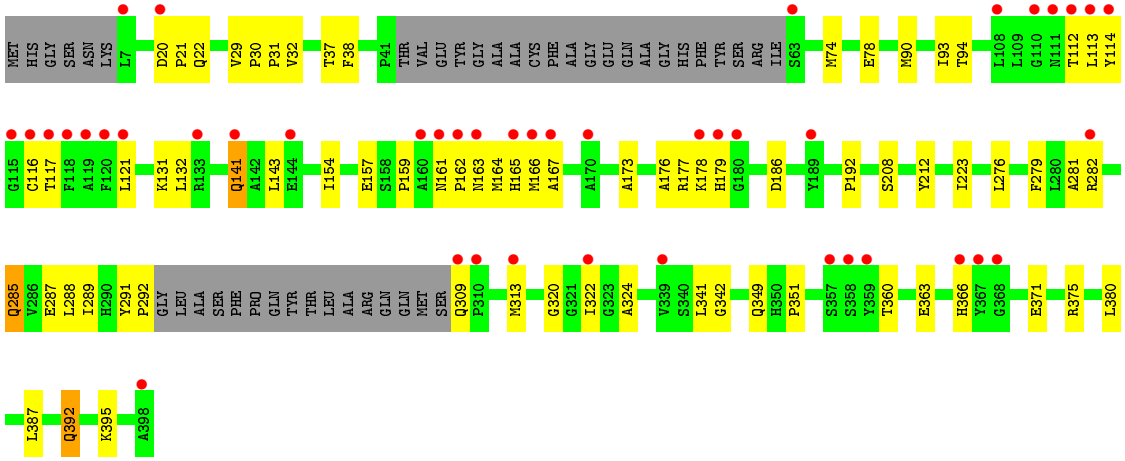
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	362	Total	O	0	0
			362	362		
2	B	310	Total	O	0	0
			310	310		
2	C	324	Total	O	0	0
			324	324		
2	D	262	Total	O	0	0
			262	262		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

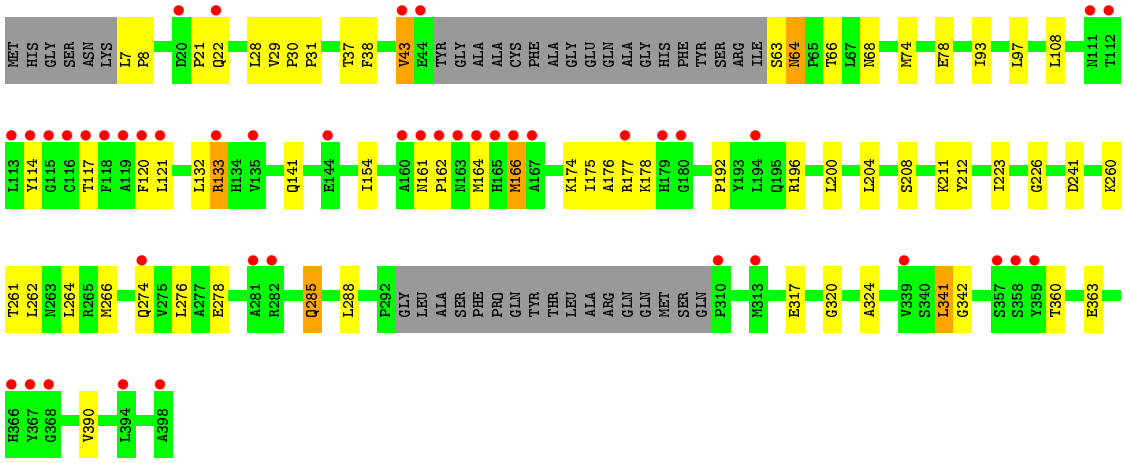
- Molecule 1: METHIONINE GAMMA-LYASE

Chain A:



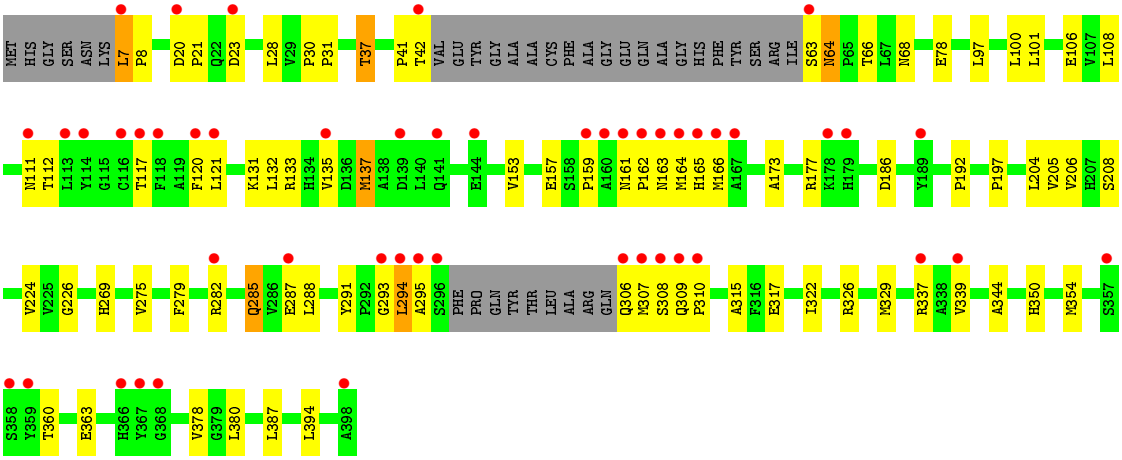
- Molecule 1: METHIONINE GAMMA-LYASE

Chain B:



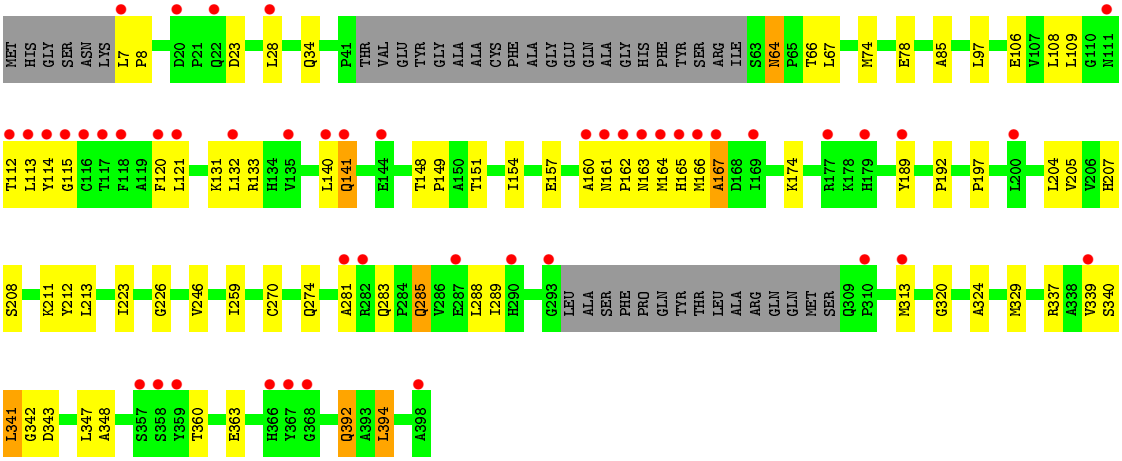
- Molecule 1: METHIONINE GAMMA-LYASE

Chain C:



- Molecule 1: METHIONINE GAMMA-LYASE

Chain D:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	4.18 (at 1.70Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.210 , 0.236 0.211 , (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 , 39.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	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	0.94	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.28	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(^{o})	Ideal(^{o})
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 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	65	0
1	B	2695	0	2672	61	0
1	C	2734	0	2710	73	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2685	0	2660	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	10700	269	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 (269) 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: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:A:349:GLN:HG3	2:A:743:HOH:O	1.90	0.71
1:C:137:MET:HE3	1:C:137:MET:H	1.53	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:B:212:TYR:HB3	1:B:266:MET:HE3	1.74	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: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	Interatomic distance (Å)	Clash overlap (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: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: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: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:C:329:MET:HG3	1:C:354:MET:HE2	1.84	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: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:O	1:D:339:VAL:HG13	2.05	0.57
1:D:74:MET:HE1	1:D:259:ILE:HD11	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
1:D:97:LEU:HD12	1:D:120:PHE:HE2	1.70	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: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: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: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:D:109:LEU:CD1	1:D:121:LEU:HD13	2.40	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:350:HIS:HB3	1:C:354:MET:HE1	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: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:A:161:ASN:HA	1:A:164:MET:CE	2.41	0.50
1:B:22:GLN:NE2	2:B:641:HOH:O	2.44	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:A:322:ILE:HG13	1:A:371:GLU:HB3	1.94	0.50
1:B:212:TYR:HB3	1:B:266:MET:CE	2.40	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:C:269:HIS:HD2	1:C:378:VAL:O	1.99	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: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: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:B:141:GLN:OE1	1:B:141:GLN:N	2.49	0.46
1:D:74:MET:CE	1:D:259:ILE:HD11	2.46	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:C:206:VAL:HG12	1:C:224:VAL:HG22	1.99	0.45
1:D:288:LEU:HD12	1:D:288:LEU:C	2.38	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: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:A:93:ILE:HG23	1:A:94:THR:N	2.33	0.44
1:C:350:HIS:N	1:C:354:MET:HE1	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:329:MET:CE	1:D:337:ARG:HG2	2.48	0.44
1:B:288:LEU:HD23	1:B:288:LEU:N	2.32	0.44
1:D:161:ASN:HA	1:D:164:MET:CE	2.48	0.44
1:B:93:ILE:HD13	1:B:117:THR:HG22	1.99	0.43
1:D:78:GLU:CD	1:D:192:PRO:HB3	2.38	0.43
1:A:121:LEU:C	1:A:132:LEU:HD21	2.37	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: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:D:121:LEU:C	1:D:132:LEU:HD21	2.38	0.43
1:B:161:ASN:HB3	1:B:162:PRO:HA	2.00	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: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: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: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:A:178:LYS:HG2	1:A:179:HIS:ND1	2.34	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: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:B:30:PRO:HA	1:B:31:PRO:HD3	1.89	0.42
1:C:329:MET:CE	1:C:337:ARG:HG2	2.49	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: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:HD22	1:B:200:LEU:N	2.35	0.41

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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:C:41:PRO:O	1:C:42:THR:C	2.58	0.41
1:D:28:LEU:HD12	2:D:489:HOH:O	2.21	0.41
1:C:64:ASN:ND2	1:C:66:THR:HB	2.36	0.41
1:D:133:ARG:HG2	2:D:502:HOH:O	2.21	0.41
2:B:533:HOH:O	1:D:339:VAL:HG12	2.21	0.41
1:D:67:LEU:HD12	1:D:85:ALA:HB3	2.02	0.41
1:A:282:ARG:NH2	2:A:655:HOH:O	2.54	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:D:174:LYS:C	1:D:174:LYS:HD3	2.41	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:C:329:MET:HE3	1:C:337:ARG:HG2	2.02	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:131:LYS:HZ3	1:D:131:LYS:HB3	1.82	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:C:294:LEU:HD12	1:C:294:LEU:C	2.41	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:B:262:LEU:HD12	1:B:266:MET:CE	2.51	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: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%)	25 11
1	B	350/398 (88%)	339 (97%)	10 (3%)	1 (0%)	41 24
1	C	356/398 (89%)	345 (97%)	9 (2%)	2 (1%)	25 11
1	D	349/398 (88%)	335 (96%)	9 (3%)	5 (1%)	11 2
All	All	1403/1592 (88%)	1353 (96%)	40 (3%)	10 (1%)	22 8

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%)	73 63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	276/306 (90%)	271 (98%)	5 (2%)	59 43
1	C	280/306 (92%)	274 (98%)	6 (2%)	53 36
1	D	274/306 (90%)	267 (97%)	7 (3%)	46 28
All	All	1104/1224 (90%)	1083 (98%)	21 (2%)	57 41

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	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

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Mol	Chain	Res	Type
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
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 molecules in this entry.

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

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	B	211	1	23,24,25	1.29	4 (17%)	25,32,34	2.26	10 (40%)
1	LLP	D	211	1	23,24,25	1.31	4 (17%)	25,32,34	2.25	10 (40%)
1	LLP	A	211	1	23,24,25	1.31	4 (17%)	25,32,34	2.27	10 (40%)
1	LLP	C	211	1	23,24,25	1.30	4 (17%)	25,32,34	2.26	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	B	211	1	-	10/16/17/19	0/1/1/1
1	LLP	D	211	1	-	10/16/17/19	0/1/1/1
1	LLP	A	211	1	-	8/16/17/19	0/1/1/1
1	LLP	C	211	1	-	8/16/17/19	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	211	LLP	C3-C2	2.91	1.43	1.40
1	D	211	LLP	C3-C2	2.89	1.43	1.40
1	B	211	LLP	C3-C2	2.85	1.43	1.40
1	C	211	LLP	C3-C2	2.69	1.43	1.40
1	A	211	LLP	C4-C4'	2.65	1.51	1.46
1	C	211	LLP	C4-C3	2.61	1.44	1.40
1	D	211	LLP	C4-C3	2.55	1.44	1.40
1	C	211	LLP	C4-C4'	2.51	1.51	1.46
1	D	211	LLP	C4-C4'	2.49	1.51	1.46
1	B	211	LLP	C4-C4'	2.45	1.51	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	211	LLP	C4-C3	2.44	1.44	1.40
1	B	211	LLP	C4-C3	2.36	1.44	1.40
1	B	211	LLP	O3-C3	-2.16	1.31	1.37
1	C	211	LLP	O3-C3	-2.14	1.32	1.37
1	A	211	LLP	O3-C3	-2.10	1.32	1.37
1	D	211	LLP	O3-C3	-2.00	1.32	1.37

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	211	LLP	C6-N1-C2	4.59	127.67	119.17
1	C	211	LLP	C6-N1-C2	4.58	127.66	119.17
1	A	211	LLP	C6-N1-C2	4.56	127.61	119.17
1	D	211	LLP	C6-N1-C2	4.53	127.57	119.17
1	C	211	LLP	C5-C6-N1	-3.97	117.20	123.82
1	B	211	LLP	C5-C6-N1	-3.95	117.24	123.82
1	D	211	LLP	C5-C6-N1	-3.92	117.28	123.82
1	A	211	LLP	C5-C6-N1	-3.89	117.34	123.82
1	A	211	LLP	C5'-C5-C6	-3.77	113.17	119.37
1	A	211	LLP	OP4-C5'-C5	3.76	116.51	109.35
1	D	211	LLP	C5'-C5-C6	-3.58	113.48	119.37
1	D	211	LLP	C4-C3-C2	-3.57	117.98	120.19
1	B	211	LLP	CE-NZ-C4'	3.57	129.85	118.90
1	C	211	LLP	OP4-C5'-C5	3.56	116.14	109.35
1	D	211	LLP	OP4-C5'-C5	3.56	116.13	109.35
1	C	211	LLP	C5'-C5-C6	-3.53	113.57	119.37
1	C	211	LLP	C4-C3-C2	-3.52	118.01	120.19
1	A	211	LLP	C4-C3-C2	-3.48	118.03	120.19
1	C	211	LLP	CE-NZ-C4'	3.48	129.59	118.90
1	B	211	LLP	C4-C3-C2	-3.48	118.03	120.19
1	A	211	LLP	CE-NZ-C4'	3.44	129.45	118.90
1	B	211	LLP	C5'-C5-C6	-3.44	113.72	119.37
1	D	211	LLP	CE-NZ-C4'	3.43	129.43	118.90
1	B	211	LLP	OP4-C5'-C5	3.41	115.84	109.35
1	A	211	LLP	C2'-C2-C3	3.20	124.85	120.89
1	B	211	LLP	C2'-C2-C3	3.14	124.77	120.89
1	D	211	LLP	C2'-C2-C3	3.07	124.67	120.89
1	B	211	LLP	C3-C4-C5	3.00	120.56	118.26
1	C	211	LLP	C2'-C2-C3	3.00	124.59	120.89
1	C	211	LLP	C3-C4-C5	2.89	120.48	118.26
1	D	211	LLP	C3-C4-C5	2.86	120.45	118.26
1	B	211	LLP	C3-C2-N1	-2.84	117.09	120.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	211	LLP	C3-C2-N1	-2.78	117.17	120.77
1	C	211	LLP	C3-C2-N1	-2.76	117.21	120.77
1	D	211	LLP	C3-C2-N1	-2.72	117.25	120.77
1	B	211	LLP	C3-C4-C4'	-2.67	115.44	120.41
1	C	211	LLP	C3-C4-C4'	-2.66	115.45	120.41
1	D	211	LLP	C3-C4-C4'	-2.64	115.50	120.41
1	A	211	LLP	C3-C4-C5	2.62	120.27	118.26
1	A	211	LLP	C3-C4-C4'	-2.58	115.60	120.41

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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	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	A	211	LLP	C5'-OP4-P-OP2
1	A	211	LLP	C5'-OP4-P-OP3
1	A	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-C4'-NZ-CE
1	C	211	LLP	C4-C4'-NZ-CE
1	B	211	LLP	C4-C4'-NZ-CE
1	B	211	LLP	C3-C4-C4'-NZ
1	D	211	LLP	C3-C4-C4'-NZ
1	A	211	LLP	C3-C4-C4'-NZ
1	C	211	LLP	C3-C4-C4'-NZ
1	D	211	LLP	CA-CB-CG-CD
1	B	211	LLP	C5'-OP4-P-OP1
1	D	211	LLP	C5'-OP4-P-OP1
1	A	211	LLP	C5'-OP4-P-OP1
1	C	211	LLP	C5'-OP4-P-OP1
1	B	211	LLP	CA-CB-CG-CD
1	D	211	LLP	C6-C5-C5'-OP4
1	C	211	LLP	CA-CB-CG-CD

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Mol	Chain	Res	Type	Atoms
1	D	211	LLP	CD-CE-NZ-C4'
1	A	211	LLP	CD-CE-NZ-C4'
1	C	211	LLP	CD-CE-NZ-C4'
1	B	211	LLP	CG-CD-CE-NZ
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	B	211	LLP	2	0
1	D	211	LLP	1	0

5.5 Carbohydrates (i)

There are no carbohydrates 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, 95^{th} 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%)	0.92	44 (12%)	4 4	8, 16, 35, 42	0
1	B	356/398 (89%)	0.89	44 (12%)	4 4	8, 16, 35, 42	0
1	C	362/398 (90%)	1.03	49 (13%)	3 3	8, 17, 37, 47	0
1	D	355/398 (89%)	0.96	47 (13%)	3 3	8, 16, 35, 42	0
All	All	1427/1592 (89%)	0.95	184 (12%)	3 4	8, 16, 36, 47	0

All (184) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	114	TYR	10.8
1	D	114	TYR	9.9
1	C	114	TYR	9.2
1	A	116	CYS	8.5
1	C	310	PRO	8.0
1	D	166	MET	8.0
1	B	43	VAL	7.7
1	C	308	SER	7.5
1	B	114	TYR	7.4
1	C	306	GLN	7.4
1	C	307	MET	7.4
1	C	116	CYS	7.3
1	B	116	CYS	7.0
1	C	163	ASN	6.6
1	B	359	TYR	6.6
1	B	165	HIS	6.5
1	C	160	ALA	6.4
1	C	166	MET	5.8
1	D	165	HIS	5.8
1	A	359	TYR	5.8
1	C	359	TYR	5.8

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Mol	Chain	Res	Type	RSRZ
1	A	398	ALA	5.7
1	C	111	ASN	5.7
1	B	358	SER	5.7
1	D	160	ALA	5.6
1	A	160	ALA	5.4
1	C	294	LEU	5.3
1	C	296	SER	5.2
1	C	367	TYR	5.2
1	C	358	SER	5.1
1	B	368	GLY	5.0
1	A	161	ASN	4.9
1	C	141	GLN	4.8
1	A	166	MET	4.8
1	C	366	HIS	4.8
1	A	358	SER	4.7
1	B	398	ALA	4.7
1	D	359	TYR	4.6
1	A	165	HIS	4.6
1	C	165	HIS	4.6
1	B	367	TYR	4.6
1	B	160	ALA	4.5
1	A	366	HIS	4.4
1	D	117	THR	4.4
1	B	177	ARG	4.4
1	D	111	ASN	4.4
1	A	367	TYR	4.4
1	D	398	ALA	4.3
1	C	42	THR	4.3
1	B	366	HIS	4.3
1	B	121	LEU	4.3
1	D	358	SER	4.3
1	D	310	PRO	4.3
1	B	120	PHE	4.2
1	D	116	CYS	4.2
1	C	164	MET	4.2
1	A	121	LEU	4.2
1	A	120	PHE	4.2
1	B	20	ASP	4.1
1	B	166	MET	4.1
1	C	120	PHE	4.1
1	D	367	TYR	4.0
1	A	167	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	398	ALA	4.0
1	D	366	HIS	4.0
1	D	164	MET	4.0
1	A	111	ASN	3.9
1	B	117	THR	3.9
1	A	357	SER	3.9
1	D	357	SER	3.9
1	B	164	MET	3.9
1	D	339	VAL	3.9
1	D	161	ASN	3.8
1	D	20	ASP	3.8
1	D	163	ASN	3.7
1	B	111	ASN	3.7
1	C	293	GLY	3.7
1	D	179	HIS	3.7
1	B	163	ASN	3.6
1	C	368	GLY	3.6
1	D	177	ARG	3.6
1	B	118	PHE	3.5
1	C	179	HIS	3.5
1	A	118	PHE	3.5
1	A	310	PRO	3.5
1	A	322	ILE	3.5
1	A	117	THR	3.5
1	A	141	GLN	3.5
1	A	113	LEU	3.4
1	D	144	GLU	3.4
1	C	113	LEU	3.4
1	D	113	LEU	3.4
1	B	167	ALA	3.4
1	B	357	SER	3.4
1	C	162	PRO	3.3
1	A	20	ASP	3.3
1	C	309	GLN	3.3
1	D	115	GLY	3.3
1	C	121	LEU	3.2
1	B	310	PRO	3.2
1	C	159	PRO	3.2
1	C	20	ASP	3.2
1	A	163	ASN	3.1
1	C	295	ALA	3.1
1	B	339	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	189	TYR	3.1
1	C	117	THR	3.1
1	A	189	TYR	3.1
1	D	118	PHE	3.0
1	D	162	PRO	3.0
1	C	339	VAL	3.0
1	C	282	ARG	3.0
1	B	144	GLU	3.0
1	B	113	LEU	2.9
1	D	120	PHE	2.9
1	D	22	GLN	2.9
1	A	133	ARG	2.9
1	B	282	ARG	2.8
1	A	119	ALA	2.8
1	B	119	ALA	2.8
1	B	44	GLU	2.8
1	D	135	VAL	2.7
1	C	144	GLU	2.7
1	C	135	VAL	2.7
1	D	189	TYR	2.6
1	A	162	PRO	2.6
1	B	22	GLN	2.6
1	A	110	GLY	2.5
1	A	178	LYS	2.5
1	D	281	ALA	2.5
1	D	141	GLN	2.5
1	D	293	GLY	2.5
1	C	118	PHE	2.5
1	C	167	ALA	2.5
1	A	368	GLY	2.5
1	A	112	THR	2.5
1	A	309	GLN	2.4
1	C	357	SER	2.4
1	C	7	LEU	2.4
1	D	132	LEU	2.4
1	B	180	GLY	2.4
1	C	63	SER	2.4
1	D	282	ARG	2.4
1	C	287	GLU	2.4
1	B	179	HIS	2.4
1	D	28	LEU	2.3
1	A	115	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	337	ARG	2.3
1	B	162	PRO	2.3
1	B	115	GLY	2.3
1	D	140	LEU	2.3
1	D	313	MET	2.3
1	B	194	LEU	2.3
1	D	167	ALA	2.2
1	D	287	GLU	2.2
1	A	170	ALA	2.2
1	A	7	LEU	2.2
1	D	200	LEU	2.2
1	D	112	THR	2.2
1	A	313	MET	2.2
1	B	274	GLN	2.2
1	A	179	HIS	2.2
1	B	112	THR	2.2
1	A	63	SER	2.1
1	A	339	VAL	2.1
1	D	290	HIS	2.1
1	C	23	ASP	2.1
1	A	282	ARG	2.1
1	C	161	ASN	2.1
1	C	139	ASP	2.1
1	A	144	GLU	2.1
1	B	161	ASN	2.1
1	A	108	LEU	2.1
1	D	121	LEU	2.1
1	B	133	ARG	2.1
1	A	180	GLY	2.1
1	D	368	GLY	2.1
1	B	313	MET	2.1
1	D	169	ILE	2.1
1	C	178	LYS	2.0
1	B	281	ALA	2.0
1	B	394	LEU	2.0
1	B	135	VAL	2.0
1	D	7	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, 95^{th} 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	B	211	24/25	0.88	0.18	9,19,22,23	0
1	LLP	D	211	24/25	0.90	0.16	10,19,22,23	0
1	LLP	A	211	24/25	0.90	0.18	10,20,23,24	0
1	LLP	C	211	24/25	0.91	0.13	9,20,22,23	0

6.3 Carbohydrates (i)

There are no carbohydrates 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.