Full wwPDB X-ray Structure Validation Report (i)

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PDB ID : 1GC2

Title : CRYSTAL STRUCTURE OF THE PYRIDOXAL-5'-PHOSPHATE DEPENDENT L-METHIONINE GAMMA-LYASE FROM PSEUDOMONAS PUTIDA

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Deposited on : 2000-07-06
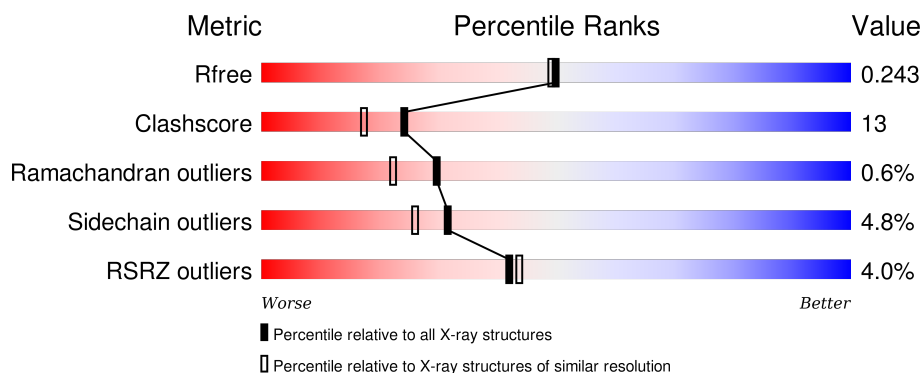
Resolution : 2.00 Å(reported)

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 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

Metric	Percentile Ranks	Value
Rfree		0.243
Clashscore		13
Ramachandran outliers		0.6%
Sidechain outliers		4.8%
RSRZ outliers		4.0%

Worse   *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	6% / 73% / 20% / • / 6%
1	B	398	% / 68% / 22% / • / 7%
1	C	398	3% / 71% / 20% / • / 6%
1	D	398	5% / 69% / 22% / • / 7%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 12444 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called METHIONINE GAMMA-LYASE.

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

- Molecule 2 is water.

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

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

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T148 P149 R152 V153 I154 E157 A160 N161 P162 N163 M164 D168 I169 L194 V172 A176 D186 L194 L198 V205 S208 K211 Y212 D218 L239 G244 H250 N263 R268 V275 L276 A277 E278 F279 L280 A281 R282 Q283 P284 L288

I289 H290 Y300 T301 L302 A303 R304 Q305 Q306 Q309 E317 G320 G321 A324 G325 R326 R327 F328 M329 N330 A331 V339 S340 L341 G342 Q349 A352 S353 M354 T355 H356 S357 S358 Y359 E363 R364 A365 H366 Y367 G368 I369 G372 R375 E381 D382 I383 L386

Q392 A393 L394 S397 A398

• Molecule 1: METHIONINE GAMMA-LYASE

Chain D:

5%

69% 22% 7%

MET HIS GLY SER ASN LYS L7 F10 Y19 Q22 L28 V29 P30 Q34 T37 F38 T39 F40 PRO THR VAL GLU TYR GLY ALA ALA CYS PHE ALA GLY GLU GLN ALA GLY HIS PHE TYR SER ARG ILE S63 N68 L69 L77 E78 L84 L100 E106

T112 L121 L132 R133 H134 V135 Q141 A142 L143 A146 M147 T148 P149 R152 E157 S158 P159 A160 N161 P162 N163 M164 H165 M166 I169 K178 H179 D186 M187 T188 Y189 P192 Y193 L194 L198 L204 V205 V206 H207 S208 K211 Y212 H216 G226

N263 L264 R265 R268 L276 L280 V286 E287 L288 I289 H290 Y291 P292 Y300 T301 L302 A303 R304 Q305 Q306 Q309 A315 F316 G320 G321 I322 G323 A324 G325 F328 M329 N330 A331 V339 S340 L341 G342 P351 A352 T355 H356 S357 S358 Y359 T360 P361 E362 E363

R364 A365 H366 Y367 G368 I369 S370 E371 G372 L373 L386 Q392 A393 L394 S397 A398

4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	133.58Å 133.58Å 213.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	83.43 – 2.00 94.45 – 2.00	Depositor EDS
% Data completeness (in resolution range)	94.9 (83.43-2.00) 95.0 (94.45-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.96 (at 2.00Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.211 , 0.243 0.211 , 0.243	Depositor DCC
R_{free} test set	12353 reflections (9.97%)	DCC
Wilson B-factor (Å^2)	29.9	Xtriage
Anisotropy	0.388	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 52.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.34$	Xtriage
Outliers	0 of 130029 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12444	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.
[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5   Model quality (i)

5.1   Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: LLP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	A	0.31	0/2853	0.60	1/3873 (0.0%)
1	B	0.32	0/2831	0.61	1/3841 (0.0%)
1	C	0.31	0/2870	0.61	1/3896 (0.0%)
1	D	0.31	0/2831	0.60	1/3841 (0.0%)
All	All	0.31	0/11385	0.60	4/15451 (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	D	208	SER	N-CA-C	-5.46	96.26	111.00
1	C	208	SER	N-CA-C	-5.43	96.33	111.00
1	B	208	SER	N-CA-C	-5.35	96.56	111.00
1	A	208	SER	N-CA-C	-5.14	97.12	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2   Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2820	0	2800	66	0
1	B	2799	0	2776	78	0
1	C	2837	0	2817	81	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2799	0	2777	90	0
2	A	274	0	0	1	0
2	B	346	0	0	5	0
2	C	307	0	0	7	0
2	D	262	0	0	10	0
All	All	12444	0	11170	291	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 (291) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:ASP:OD1	1:B:188:THR:HG23	1.74	0.88
1:C:169:ILE:H	1:C:306:GLN:HE22	1.19	0.86
1:A:7:LEU:HD12	1:A:8:PRO:HD2	1.56	0.85
1:C:161:ASN:H	1:C:161:ASN:HD22	1.22	0.84
1:D:286:VAL:HG11	1:D:289:ILE:HD11	1.60	0.83
1:A:361:PRO:HA	1:A:364:ARG:HH12	1.41	0.82
1:B:303:ALA:HB1	1:B:307:MET:HE2	1.60	0.82
1:B:169:ILE:H	1:B:306:GLN:HE22	1.26	0.82
1:D:186:ASP:OD1	1:D:188:THR:HG23	1.79	0.81
1:A:28:LEU:HD12	1:D:37:THR:OG1	1.81	0.80
1:B:198:LEU:HD13	1:B:205:VAL:HG23	1.64	0.80
1:C:161:ASN:N	1:C:161:ASN:HD22	1.78	0.77
1:A:286:VAL:HG11	1:A:289:ILE:HD11	1.65	0.77
1:C:161:ASN:H	1:C:161:ASN:ND2	1.80	0.77
1:A:300:TYR:O	1:A:304:ARG:HG3	1.86	0.76
1:B:303:ALA:HB1	1:B:307:MET:CE	2.14	0.76
1:D:198:LEU:HD13	1:D:205:VAL:HG23	1.67	0.76
1:B:327:ARG:HB3	1:B:397:SER:HA	1.69	0.74
1:C:162:PRO:HG2	2:C:580:HOH:O	1.88	0.74
1:A:354:MET:HG3	1:C:43:VAL:HG13	1.70	0.74
1:B:289:ILE:HD13	1:B:290:HIS:N	2.04	0.73
1:D:331:ALA:HB1	1:D:392:GLN:HE22	1.54	0.73
1:D:169:ILE:H	1:D:306:GLN:HE22	1.34	0.73
1:A:169:ILE:H	1:A:306:GLN:HE22	1.36	0.72
1:A:353:SER:OG	1:C:43:VAL:HG11	1.90	0.71
1:D:268:ARG:HH11	1:D:268:ARG:HA	1.55	0.71
1:D:265:ARG:CZ	2:D:630:HOH:O	2.39	0.71
1:D:276:LEU:O	1:D:280:LEU:HD23	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:265:ARG:NE	2:D:630:HOH:O	2.24	0.69
1:D:304:ARG:HB3	1:D:304:ARG:NH1	2.08	0.69
1:A:350:HIS:NE2	1:A:352:ALA:HB3	2.08	0.68
1:B:112:THR:HG21	1:B:162:PRO:HG2	1.76	0.68
1:D:304:ARG:HB3	1:D:304:ARG:HH11	1.59	0.67
1:B:338:ALA:HB2	1:D:39:THR:HG22	1.77	0.67
1:A:289:ILE:HD13	1:A:316:PHE:HB2	1.77	0.66
1:C:198:LEU:HD13	1:C:205:VAL:HG23	1.76	0.66
1:C:7:LEU:HD21	1:C:13:ARG:HD3	1.78	0.65
1:B:340:SER:HB2	1:D:37:THR:HG21	1.78	0.65
1:D:339:VAL:O	1:D:339:VAL:HG13	1.97	0.65
1:C:152:ARG:HA	1:C:152:ARG:NE	2.12	0.65
1:A:160:ALA:C	1:A:162:PRO:HD2	2.16	0.64
1:A:330:ASN:OD1	1:C:43:VAL:HG23	1.97	0.64
1:D:157:GLU:HG2	1:D:186:ASP:HB3	1.79	0.64
1:A:361:PRO:HA	1:A:364:ARG:NH1	2.14	0.62
1:C:327:ARG:HB3	1:C:397:SER:HA	1.82	0.62
1:D:331:ALA:HB1	1:D:392:GLN:NE2	2.13	0.61
1:A:290:HIS:HB2	1:A:315:ALA:HB3	1.81	0.61
1:A:37:THR:HB	1:D:28:LEU:HD12	1.81	0.61
1:A:321:GLY:HA2	1:A:371:GLU:HG2	1.82	0.61
1:C:349:GLN:NE2	1:C:375:ARG:NH2	2.47	0.61
1:C:40:PHE:HZ	1:C:62:ILE:HD11	1.66	0.61
1:D:364:ARG:HG3	1:D:371:GLU:OE2	2.00	0.61
1:C:331:ALA:HB1	1:C:392:GLN:HE22	1.66	0.61
1:D:398:ALA:HA	2:D:599:HOH:O	2.01	0.61
1:B:39:THR:HG23	1:C:28:LEU:HG	1.83	0.60
1:B:337:ARG:HD2	2:B:712:HOH:O	2.02	0.59
1:D:304:ARG:HH11	1:D:304:ARG:CB	2.15	0.59
1:C:7:LEU:HD23	1:C:8:PRO:HD2	1.85	0.59
1:A:381:GLU:CG	1:A:386:LEU:HD21	2.33	0.59
1:A:351:PRO:HB3	1:A:356:HIS:HD2	1.68	0.58
1:D:286:VAL:HG11	1:D:289:ILE:CD1	2.32	0.58
1:B:339:VAL:HG13	1:B:339:VAL:O	2.03	0.58
1:D:351:PRO:HB3	1:D:356:HIS:HD2	1.68	0.58
1:C:161:ASN:ND2	1:C:161:ASN:N	2.46	0.58
1:C:263:ASN:H	1:C:263:ASN:HD22	1.52	0.58
1:D:359:TYR:HD2	1:D:363:GLU:HB3	1.69	0.58
1:B:157:GLU:HG2	1:B:186:ASP:HB3	1.85	0.58
1:D:204:LEU:HD23	1:D:226:GLY:HA3	1.86	0.58
1:D:198:LEU:HB2	2:D:407:HOH:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:TYR:CE1	1:B:30:PRO:HB3	2.38	0.58
1:D:300:TYR:CE2	1:D:304:ARG:HD2	2.39	0.57
1:C:276:LEU:O	1:C:280:LEU:HD23	2.04	0.57
1:D:320:GLY:HA3	1:D:324:ALA:HB2	1.86	0.57
1:C:211:LLP:HE3	1:C:341:LEU:CD1	2.35	0.57
1:D:10:PHE:CZ	1:D:77:LEU:HG	2.40	0.57
1:D:289:ILE:HD13	1:D:316:PHE:HB2	1.86	0.57
1:C:194:LEU:HD22	1:C:309:GLN:HB2	1.86	0.56
1:D:152:ARG:HB2	1:D:152:ARG:NH1	2.20	0.56
1:A:78:GLU:OE2	1:A:207:HIS:HE1	1.89	0.56
1:B:109:LEU:HD13	1:B:121:LEU:HD13	1.87	0.56
1:D:198:LEU:CD1	1:D:205:VAL:HG23	2.35	0.56
1:B:263:ASN:H	1:B:263:ASN:HD22	1.54	0.55
1:D:370:SER:HB3	1:D:373:LEU:HB2	1.89	0.55
1:A:300:TYR:CE2	1:A:304:ARG:HD2	2.42	0.55
1:C:157:GLU:HG2	1:C:186:ASP:HB3	1.88	0.55
1:B:198:LEU:HB2	2:B:399:HOH:O	2.07	0.55
1:B:186:ASP:OD1	1:B:188:THR:CG2	2.53	0.54
1:D:78:GLU:OE2	1:D:192:PRO:HG3	2.08	0.54
1:A:289:ILE:HD13	1:A:316:PHE:CB	2.37	0.54
1:A:320:GLY:HA3	1:A:324:ALA:HB2	1.89	0.54
1:C:67:LEU:HD12	1:C:85:ALA:HB3	1.89	0.54
1:D:186:ASP:OD1	1:D:188:THR:CG2	2.54	0.54
1:C:169:ILE:H	1:C:306:GLN:NE2	1.97	0.54
1:A:354:MET:HG3	1:C:43:VAL:CG1	2.36	0.54
1:B:7:LEU:HD12	1:B:8:PRO:HD2	1.90	0.54
1:C:7:LEU:HD23	1:C:8:PRO:CD	2.37	0.54
1:D:160:ALA:C	1:D:162:PRO:HD2	2.28	0.54
1:B:37:THR:HG23	1:C:28:LEU:HD12	1.90	0.54
1:B:204:LEU:HD23	1:B:226:GLY:HA3	1.90	0.54
1:D:216:HIS:CE1	1:D:265:ARG:HH21	2.26	0.54
1:C:163:ASN:HB2	1:C:290:HIS:CD2	2.43	0.53
1:A:300:TYR:CZ	1:A:304:ARG:HD2	2.43	0.53
1:A:353:SER:O	1:C:43:VAL:HG12	2.09	0.53
1:A:317:GLU:HA	1:A:372:GLY:O	2.07	0.53
1:A:322:ILE:HA	1:A:371:GLU:O	2.07	0.53
1:D:356:HIS:CD2	1:D:369:ILE:HD13	2.43	0.53
1:C:84:LEU:HD11	1:C:239:LEU:HD22	1.90	0.53
1:D:78:GLU:OE2	1:D:207:HIS:HE1	1.92	0.53
1:C:20:ASP:HB3	1:C:23:ASP:OD2	2.09	0.53
1:C:300:TYR:CZ	1:C:304:ARG:HD2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:GLY:HA3	1:B:324:ALA:HB2	1.90	0.53
1:A:370:SER:HB3	1:A:373:LEU:HB2	1.90	0.53
1:D:148:THR:HB	1:D:149:PRO:HD2	1.90	0.53
1:B:67:LEU:HD12	1:B:85:ALA:HB3	1.91	0.53
1:D:161:ASN:N	1:D:162:PRO:HD2	2.24	0.52
1:B:196:ARG:NE	2:B:681:HOH:O	2.41	0.52
1:A:211:LLP:HE3	1:A:341:LEU:HD13	1.91	0.52
1:A:263:ASN:H	1:A:263:ASN:HD22	1.56	0.52
1:B:391:GLN:NE2	1:B:395:LYS:HE3	2.24	0.52
1:B:78:GLU:OE2	1:B:207:HIS:HE1	1.92	0.52
1:C:112:THR:OG1	1:C:162:PRO:HG3	2.08	0.52
1:D:198:LEU:HD13	1:D:205:VAL:CG2	2.37	0.52
1:A:371:GLU:H	1:A:371:GLU:CD	2.13	0.52
1:A:20:ASP:HB3	1:A:23:ASP:OD2	2.09	0.52
1:D:352:ALA:HA	1:D:364:ARG:HE	1.75	0.52
1:D:268:ARG:HH11	1:D:268:ARG:CA	2.21	0.52
1:C:198:LEU:HB2	2:C:404:HOH:O	2.10	0.52
1:D:211:LLP:HE3	1:D:341:LEU:HD13	1.90	0.51
1:C:300:TYR:O	1:C:304:ARG:HG3	2.10	0.51
1:B:112:THR:CB	1:B:162:PRO:HG2	2.41	0.51
1:B:161:ASN:HB3	1:B:162:PRO:HD3	1.93	0.51
1:B:17:HIS:O	1:B:73:ARG:HD3	2.10	0.51
1:B:196:ARG:CZ	2:B:681:HOH:O	2.57	0.51
1:B:300:TYR:CZ	1:B:304:ARG:HD2	2.45	0.51
1:D:355:THR:HG23	2:D:603:HOH:O	2.11	0.51
1:C:211:LLP:HE3	1:C:341:LEU:HD13	1.92	0.51
1:C:278:GLU:O	1:C:282:ARG:HD3	2.11	0.51
1:A:276:LEU:O	1:A:280:LEU:HD13	2.10	0.51
1:A:161:ASN:N	1:A:162:PRO:HD2	2.26	0.50
1:D:152:ARG:HD2	2:D:542:HOH:O	2.11	0.50
1:D:143:LEU:O	1:D:147:MET:HG2	2.11	0.50
1:C:34:GLN:HE22	1:C:250:HIS:H	1.59	0.50
1:C:168:ASP:O	1:C:172:VAL:HG13	2.10	0.50
1:A:254:LEU:HD21	1:B:254:LEU:HD21	1.93	0.50
1:A:286:VAL:HG11	1:A:289:ILE:CD1	2.37	0.50
1:A:204:LEU:HD23	1:A:226:GLY:HA3	1.92	0.50
1:D:178:LYS:HE2	1:D:179:HIS:CE1	2.46	0.50
1:C:84:LEU:HD12	1:C:86:LEU:HD11	1.92	0.50
1:D:263:ASN:H	1:D:263:ASN:HD22	1.60	0.50
1:A:34:GLN:HG3	1:C:218:ASP:O	2.12	0.50
1:B:112:THR:CG2	1:B:162:PRO:HG2	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:360:THR:OG1	1:B:363:GLU:HG3	2.11	0.49
1:D:268:ARG:NE	2:D:611:HOH:O	2.17	0.49
1:B:211:LLP:HE3	1:B:341:LEU:HD13	1.94	0.49
1:B:303:ALA:CB	1:B:307:MET:HE2	2.35	0.49
1:B:211:LLP:HE3	1:B:341:LEU:CD1	2.42	0.49
1:C:288:LEU:HD12	1:C:289:ILE:H	1.78	0.49
1:B:39:THR:CG2	1:C:28:LEU:HG	2.42	0.49
1:B:329:MET:HE3	1:B:337:ARG:HG2	1.94	0.49
1:B:194:LEU:HD22	1:B:309:GLN:HB2	1.94	0.49
1:B:111:ASN:HB2	2:B:479:HOH:O	2.13	0.48
1:B:188:THR:HG22	1:B:207:HIS:HA	1.94	0.48
1:D:164:MET:O	1:D:166:MET:HE2	2.13	0.48
1:A:157:GLU:HG2	1:A:186:ASP:HB3	1.95	0.48
1:C:7:LEU:CD2	1:C:13:ARG:HD3	2.42	0.48
1:C:154:ILE:HD12	1:C:176:ALA:HB2	1.96	0.48
1:D:363:GLU:O	1:D:366:HIS:HB3	2.14	0.48
1:A:39:THR:HG23	1:D:28:LEU:HG	1.95	0.48
1:C:244:GLY:HA2	2:C:510:HOH:O	2.13	0.48
1:C:320:GLY:HA3	1:C:324:ALA:HB2	1.96	0.48
1:C:19:TYR:CE1	1:C:30:PRO:HB3	2.49	0.47
1:B:63:SER:HG	1:B:68:ASN:HD21	1.59	0.47
1:B:109:LEU:CD1	1:B:121:LEU:HD13	2.44	0.47
1:B:263:ASN:HD22	1:B:263:ASN:N	2.13	0.47
1:A:325:GLY:O	1:A:329:MET:HG2	2.14	0.47
1:A:178:LYS:HE2	1:A:179:HIS:CE1	2.49	0.47
1:A:187:ASN:ND2	1:A:195:GLN:HE21	2.13	0.47
1:B:20:ASP:HB3	1:B:23:ASP:OD2	2.15	0.47
1:C:288:LEU:HD12	2:C:446:HOH:O	2.14	0.47
1:B:187:ASN:ND2	1:B:195:GLN:HE21	2.12	0.47
1:B:154:ILE:HD12	1:B:176:ALA:HB2	1.96	0.47
1:A:369:ILE:HD12	1:A:369:ILE:N	2.30	0.47
1:A:148:THR:HB	1:A:149:PRO:HD2	1.95	0.47
1:D:359:TYR:HD2	1:D:363:GLU:CB	2.27	0.47
1:A:382:ASP:OD2	1:B:9:GLY:HA3	2.13	0.47
1:B:152:ARG:HA	1:B:152:ARG:NE	2.29	0.47
1:D:7:LEU:O	1:D:7:LEU:HD13	2.15	0.47
1:A:163:ASN:HB2	1:A:290:HIS:CG	2.49	0.47
1:C:148:THR:HB	1:C:149:PRO:HD2	1.97	0.47
1:A:112:THR:OG1	1:A:162:PRO:HG3	2.15	0.47
1:D:301:THR:HG22	1:D:305:GLN:HE21	1.80	0.46
1:B:10:PHE:CZ	1:B:77:LEU:HG	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:TYR:CE2	1:B:342:GLY:HA2	2.50	0.46
1:B:163:ASN:O	1:B:164:MET:HB2	2.15	0.46
1:D:211:LLP:HE3	1:D:341:LEU:CD1	2.45	0.46
1:B:289:ILE:HD13	1:B:289:ILE:C	2.36	0.46
1:D:169:ILE:H	1:D:306:GLN:NE2	2.09	0.46
1:D:121:LEU:O	1:D:132:LEU:HD11	2.14	0.46
1:A:28:LEU:HG	1:D:39:THR:HG23	1.98	0.46
1:A:78:GLU:OE2	1:A:192:PRO:HG3	2.15	0.46
1:B:212:TYR:CD2	1:B:342:GLY:HA2	2.51	0.46
1:B:198:LEU:HD13	1:B:205:VAL:CG2	2.41	0.46
1:B:341:LEU:HD22	1:B:341:LEU:C	2.35	0.46
1:B:332:LEU:HD22	1:B:335:PHE:HB2	1.97	0.46
1:D:360:THR:O	1:D:364:ARG:HG2	2.17	0.45
1:C:160:ALA:C	1:C:162:PRO:HD2	2.37	0.45
1:A:39:THR:CG2	1:D:28:LEU:HG	2.47	0.45
1:C:301:THR:HG22	1:C:305:GLN:HE21	1.82	0.45
1:C:381:GLU:HG2	1:C:386:LEU:CD1	2.47	0.45
1:C:112:THR:CB	1:C:162:PRO:HG3	2.46	0.45
1:D:300:TYR:CZ	1:D:304:ARG:HD2	2.52	0.45
1:B:111:ASN:ND2	1:B:136:ASP:HA	2.32	0.45
1:B:70:LEU:HD21	1:B:255:LEU:HD23	1.99	0.45
1:D:159:PRO:HB2	1:D:164:MET:HA	1.98	0.44
1:D:290:HIS:HB2	1:D:315:ALA:HB3	1.99	0.44
1:A:43:VAL:HG23	1:C:354:MET:HG3	1.99	0.44
1:C:44:GLU:HA	1:C:44:GLU:OE1	2.18	0.44
1:C:157:GLU:OE1	1:C:161:ASN:ND2	2.50	0.44
1:D:363:GLU:HA	1:D:366:HIS:CB	2.47	0.44
1:C:352:ALA:O	1:C:357:SER:HA	2.17	0.44
1:A:318:LEU:HD22	1:A:318:LEU:N	2.32	0.44
1:A:339:VAL:O	1:A:339:VAL:HG22	2.16	0.44
1:C:349:GLN:NE2	1:C:375:ARG:HH21	2.14	0.43
1:A:143:LEU:HD12	1:A:175:ILE:HD12	2.00	0.43
1:D:19:TYR:CE1	1:D:30:PRO:HB3	2.53	0.43
1:B:148:THR:HB	1:B:149:PRO:HD2	1.99	0.43
1:C:161:ASN:N	1:C:162:PRO:HD2	2.32	0.43
1:B:169:ILE:H	1:B:306:GLN:NE2	2.05	0.43
1:B:188:THR:CG2	1:B:208:SER:H	2.31	0.43
1:C:317:GLU:HA	1:C:372:GLY:O	2.18	0.43
1:B:369:ILE:HG23	1:B:373:LEU:HD23	2.00	0.43
1:C:10:PHE:CZ	1:C:77:LEU:HG	2.53	0.43
1:D:289:ILE:HD13	1:D:316:PHE:CB	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:300:TYR:CE2	1:C:304:ARG:HD2	2.53	0.43
1:D:328:PHE:CD2	1:D:329:MET:HE2	2.54	0.43
1:D:164:MET:HG2	1:D:292:PRO:HD3	2.00	0.43
1:D:322:ILE:HG22	2:D:600:HOH:O	2.19	0.43
1:B:290:HIS:HE1	1:B:317:GLU:OE2	2.02	0.42
1:C:276:LEU:O	1:C:280:LEU:CD2	2.66	0.42
1:D:7:LEU:C	1:D:7:LEU:HD13	2.39	0.42
1:D:188:THR:HG22	1:D:207:HIS:HA	2.00	0.42
1:B:161:ASN:O	1:B:162:PRO:C	2.58	0.42
1:C:268:ARG:NH2	2:C:481:HOH:O	2.51	0.42
1:A:109:LEU:HD13	1:A:121:LEU:HD13	2.00	0.42
1:C:112:THR:HG21	1:C:162:PRO:HG3	2.01	0.42
1:C:40:PHE:CZ	1:C:62:ILE:HD11	2.51	0.42
1:D:360:THR:HB	1:D:361:PRO:HD2	2.00	0.42
1:A:194:LEU:HD22	1:A:309:GLN:HB2	2.02	0.42
1:C:212:TYR:CE2	1:C:342:GLY:HA2	2.54	0.42
1:B:336:SER:HB3	1:D:39:THR:HG21	2.01	0.42
1:D:211:LLP:HB2	1:D:341:LEU:HD22	2.01	0.42
1:A:339:VAL:HG12	2:C:437:HOH:O	2.20	0.42
1:A:107:VAL:CG1	1:A:132:LEU:HD23	2.49	0.42
1:D:78:GLU:HG3	2:D:407:HOH:O	2.19	0.42
1:C:283:GLN:HA	1:C:284:PRO:HD3	1.86	0.42
1:C:275:VAL:HG11	1:C:383:ILE:HG12	2.00	0.42
1:C:349:GLN:HE21	1:C:375:ARG:HH21	1.67	0.42
1:D:359:TYR:HB3	1:D:363:GLU:HB2	2.01	0.42
1:C:281:ALA:HA	1:C:289:ILE:CD1	2.50	0.42
1:B:363:GLU:O	1:B:366:HIS:HB3	2.20	0.41
1:D:63:SER:CB	1:D:68:ASN:HD21	2.33	0.41
1:D:363:GLU:H	1:D:363:GLU:CD	2.23	0.41
1:A:43:VAL:HG11	1:C:326:ARG:HA	2.01	0.41
1:D:328:PHE:HD2	1:D:329:MET:CE	2.33	0.41
1:B:28:LEU:HD13	1:B:28:LEU:C	2.41	0.41
1:D:141:GLN:N	1:D:141:GLN:OE1	2.51	0.41
1:D:194:LEU:HD22	1:D:309:GLN:HB2	2.01	0.41
1:A:321:GLY:CA	1:A:371:GLU:HG2	2.48	0.41
1:C:355:THR:HG23	2:C:485:HOH:O	2.20	0.41
1:B:331:ALA:HB1	1:B:392:GLN:HE22	1.85	0.41
1:D:133:ARG:NH1	1:D:146:ALA:HA	2.35	0.41
1:A:364:ARG:NH1	2:A:663:HOH:O	2.54	0.41
1:D:207:HIS:HD2	2:D:406:HOH:O	2.03	0.41
1:B:78:GLU:OE2	1:B:207:HIS:CE1	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:328:PHE:HD2	1:C:329:MET:CE	2.34	0.41
1:A:86:LEU:HD12	1:A:86:LEU:N	2.36	0.41
1:B:169:ILE:O	1:B:172:VAL:HG22	2.21	0.41
1:D:178:LYS:O	1:D:178:LYS:HD2	2.21	0.41
1:B:218:ASP:O	1:D:34:GLN:HG3	2.21	0.41
1:A:354:MET:CG	1:C:43:VAL:HG13	2.47	0.40
1:B:329:MET:CE	1:B:337:ARG:HG2	2.49	0.40
1:A:381:GLU:HG2	1:A:386:LEU:HD21	2.03	0.40
1:B:274:GLN:HE22	1:B:293:GLY:HA3	1.86	0.40
1:B:283:GLN:HA	1:B:284:PRO:HD3	1.78	0.40
1:B:161:ASN:HD21	1:B:375:ARG:HD3	1.85	0.40
1:C:381:GLU:HG2	1:C:386:LEU:HD13	2.03	0.40
1:A:43:VAL:HG21	1:C:353:SER:OG	2.20	0.40
1:C:7:LEU:HD22	1:C:8:PRO:O	2.22	0.40
1:D:112:THR:OG1	1:D:162:PRO:HG3	2.20	0.40
1:D:212:TYR:CE2	1:D:342:GLY:HA2	2.56	0.40
1:C:163:ASN:O	1:C:164:MET:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	368/398 (92%)	353 (96%)	13 (4%)	2 (0%)	34	26
1	B	365/398 (92%)	351 (96%)	13 (4%)	1 (0%)	46	41
1	C	370/398 (93%)	357 (96%)	11 (3%)	2 (0%)	34	26
1	D	365/398 (92%)	347 (95%)	14 (4%)	4 (1%)	17	9
All	All	1468/1592 (92%)	1408 (96%)	51 (4%)	9 (1%)	30	22

All (9) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	289/306 (94%)	280 (97%)	9 (3%)	47	46
1	B	286/306 (94%)	268 (94%)	18 (6%)	22	16
1	C	291/306 (95%)	277 (95%)	14 (5%)	31	26
1	D	286/306 (94%)	272 (95%)	14 (5%)	31	25
All	All	1152/1224 (94%)	1097 (95%)	55 (5%)	31	26

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	LEU
1	A	164	MET
1	A	263	ASN
1	A	302	LEU
1	A	336	SER
1	A	341	LEU
1	A	362	GLU
1	A	371	GLU
1	A	394	LEU
1	B	37	THR
1	B	69	LEU
1	B	73	ARG
1	B	77	LEU

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Mol	Chain	Res	Type
1	B	143	LEU
1	B	152	ARG
1	B	161	ASN
1	B	164	MET
1	B	178	LYS
1	B	188	THR
1	B	198	LEU
1	B	263	ASN
1	B	289	ILE
1	B	302	LEU
1	B	341	LEU
1	B	345	GLU
1	B	386	LEU
1	B	394	LEU
1	C	7	LEU
1	C	69	LEU
1	C	77	LEU
1	C	100	LEU
1	C	152	ARG
1	C	161	ASN
1	C	164	MET
1	C	172	VAL
1	C	198	LEU
1	C	263	ASN
1	C	302	LEU
1	C	341	LEU
1	C	386	LEU
1	C	394	LEU
1	D	69	LEU
1	D	77	LEU
1	D	84	LEU
1	D	100	LEU
1	D	152	ARG
1	D	163	ASN
1	D	164	MET
1	D	188	THR
1	D	263	ASN
1	D	268	ARG
1	D	302	LEU
1	D	341	LEU
1	D	386	LEU
1	D	394	LEU

Some 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	161	ASN
1	A	187	ASN
1	A	207	HIS
1	A	228	GLN
1	A	263	ASN
1	A	272	ASN
1	A	274	GLN
1	A	305	GLN
1	A	306	GLN
1	A	356	HIS
1	B	34	GLN
1	B	111	ASN
1	B	141	GLN
1	B	161	ASN
1	B	187	ASN
1	B	207	HIS
1	B	228	GLN
1	B	263	ASN
1	B	272	ASN
1	B	274	GLN
1	B	290	HIS
1	B	306	GLN
1	B	349	GLN
1	B	356	HIS
1	B	391	GLN
1	B	392	GLN
1	C	34	GLN
1	C	161	ASN
1	C	187	ASN
1	C	207	HIS
1	C	228	GLN
1	C	263	ASN
1	C	272	ASN
1	C	274	GLN
1	C	290	HIS
1	C	305	GLN
1	C	306	GLN
1	C	349	GLN
1	C	392	GLN

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Mol	Chain	Res	Type
1	D	34	GLN
1	D	111	ASN
1	D	161	ASN
1	D	187	ASN
1	D	207	HIS
1	D	263	ASN
1	D	272	ASN
1	D	274	GLN
1	D	305	GLN
1	D	306	GLN
1	D	356	HIS
1	D	392	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
1	LLP	A	211	1	23,24,25	1.43	4 (17%)	28,32,34	2.14	12 (42%)
1	LLP	B	211	1	23,24,25	1.53	4 (17%)	28,32,34	2.09	11 (39%)
1	LLP	C	211	1	23,24,25	1.47	4 (17%)	28,32,34	2.11	11 (39%)
1	LLP	D	211	1	23,24,25	1.50	4 (17%)	28,32,34	2.13	12 (42%)

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 (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	211	LLP	O3-C3	-2.46	1.31	1.37
1	A	211	LLP	O3-C3	-2.29	1.31	1.37
1	B	211	LLP	O3-C3	-2.29	1.31	1.37
1	D	211	LLP	O3-C3	-2.09	1.32	1.37
1	A	211	LLP	C4-C4'	2.49	1.51	1.46
1	C	211	LLP	C4-C4'	2.49	1.51	1.46
1	B	211	LLP	C4-C3	2.72	1.44	1.40
1	D	211	LLP	C4-C3	2.74	1.44	1.40
1	A	211	LLP	C4-C3	2.83	1.44	1.40
1	C	211	LLP	C4-C3	2.87	1.44	1.40
1	B	211	LLP	C4-C4'	3.00	1.51	1.46
1	D	211	LLP	C4-C4'	3.05	1.52	1.46
1	A	211	LLP	C3-C2	3.59	1.43	1.40
1	C	211	LLP	C3-C2	4.07	1.43	1.40
1	B	211	LLP	C3-C2	4.16	1.43	1.40
1	D	211	LLP	C3-C2	4.22	1.43	1.40

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	211	LLP	C5-C6-N1	-4.03	116.87	123.86
1	C	211	LLP	C5-C6-N1	-4.02	116.88	123.86
1	D	211	LLP	C5-C6-N1	-3.99	116.93	123.86
1	A	211	LLP	C5-C6-N1	-3.98	116.94	123.86
1	C	211	LLP	C3-C4-C4'	-3.87	115.15	120.16
1	A	211	LLP	C3-C4-C4'	-3.75	115.31	120.16
1	D	211	LLP	C3-C4-C4'	-3.66	115.42	120.16
1	B	211	LLP	C3-C4-C4'	-3.57	115.54	120.16
1	D	211	LLP	C5'-C5-C6	-2.67	114.23	119.28
1	C	211	LLP	C3-C2-N1	-2.64	116.97	120.61
1	B	211	LLP	C3-C2-N1	-2.62	116.99	120.61
1	A	211	LLP	C3-C2-N1	-2.52	117.13	120.61
1	D	211	LLP	C3-C2-N1	-2.49	117.17	120.61
1	A	211	LLP	C5'-C5-C6	-2.41	114.72	119.28
1	B	211	LLP	C5'-C5-C6	-2.22	115.08	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	211	LLP	C5'-C5-C6	-2.21	115.10	119.28
1	A	211	LLP	O-C-CA	-2.09	120.06	125.49
1	D	211	LLP	O-C-CA	-2.03	120.19	125.49
1	C	211	LLP	CD-CE-NZ	2.00	114.25	110.98
1	D	211	LLP	CD-CE-NZ	2.11	114.43	110.98
1	A	211	LLP	CD-CE-NZ	2.14	114.49	110.98
1	C	211	LLP	OP4-C5'-C5	2.23	112.68	108.99
1	B	211	LLP	C5'-C5-C4	2.24	125.23	121.47
1	C	211	LLP	C5'-C5-C4	2.34	125.40	121.47
1	B	211	LLP	CD-CE-NZ	2.45	114.98	110.98
1	A	211	LLP	C5'-C5-C4	2.58	125.80	121.47
1	B	211	LLP	OP4-C5'-C5	2.69	113.44	108.99
1	D	211	LLP	C5'-C5-C4	2.75	126.09	121.47
1	D	211	LLP	OP4-C5'-C5	2.79	113.60	108.99
1	A	211	LLP	C2'-C2-C3	2.83	124.45	121.04
1	B	211	LLP	C2'-C2-C3	2.94	124.59	121.04
1	C	211	LLP	C2'-C2-C3	3.01	124.67	121.04
1	D	211	LLP	C2'-C2-C3	3.03	124.69	121.04
1	A	211	LLP	OP4-C5'-C5	3.13	114.17	108.99
1	D	211	LLP	C3-C4-C5	3.29	120.57	118.11
1	B	211	LLP	C3-C4-C5	3.45	120.69	118.11
1	A	211	LLP	C3-C4-C5	3.47	120.70	118.11
1	B	211	LLP	CE-NZ-C4'	3.59	129.33	118.97
1	C	211	LLP	CE-NZ-C4'	3.73	129.73	118.97
1	D	211	LLP	CE-NZ-C4'	3.73	129.75	118.97
1	C	211	LLP	C3-C4-C5	3.75	120.91	118.11
1	A	211	LLP	CE-NZ-C4'	3.77	129.84	118.97
1	B	211	LLP	C6-N1-C2	4.12	127.69	119.28
1	D	211	LLP	C6-N1-C2	4.15	127.75	119.28
1	A	211	LLP	C6-N1-C2	4.18	127.81	119.28
1	C	211	LLP	C6-N1-C2	4.19	127.82	119.28

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	211	LLP	3	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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB($Å^2$)	Q<0.9
1	A	372/398 (93%)	0.35	25 (6%)	21	22	21, 33, 59, 88	0
1	B	369/398 (92%)	0.18	5 (1%)	78	78	20, 32, 46, 58	0
1	C	374/398 (93%)	0.21	11 (2%)	55	56	21, 33, 51, 79	0
1	D	369/398 (92%)	0.36	19 (5%)	32	33	23, 37, 56, 89	0
All	All	1484/1592 (93%)	0.27	60 (4%)	42	44	20, 33, 53, 89	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	161	ASN	8.3
1	A	367	TYR	8.2
1	A	161	ASN	7.4
1	D	367	TYR	6.4
1	A	43	VAL	6.4
1	B	161	ASN	6.2
1	A	360	THR	5.7
1	C	43	VAL	5.3
1	A	366	HIS	4.6
1	C	367	TYR	4.5
1	A	368	GLY	4.5
1	A	359	TYR	4.4
1	D	40	PHE	4.2
1	A	362	GLU	4.0
1	A	41	PRO	3.8
1	D	366	HIS	3.8
1	A	365	ALA	3.7
1	C	366	HIS	3.7
1	A	398	ALA	3.5
1	C	359	TYR	3.5
1	A	372	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	358	SER	3.4
1	D	359	TYR	3.4
1	D	189	TYR	3.4
1	C	369	ILE	3.2
1	D	364	ARG	3.2
1	A	22	GLN	3.2
1	D	178	LYS	3.1
1	A	364	ARG	3.1
1	C	365	ALA	3.1
1	A	357	SER	3.0
1	A	42	THR	3.0
1	A	363	GLU	2.9
1	C	161	ASN	2.9
1	A	339	VAL	2.8
1	D	22	GLN	2.8
1	C	363	GLU	2.7
1	D	288	LEU	2.7
1	D	39	THR	2.6
1	D	369	ILE	2.6
1	A	149	PRO	2.6
1	A	354	MET	2.6
1	B	367	TYR	2.6
1	B	398	ALA	2.6
1	D	398	ALA	2.6
1	A	356	HIS	2.5
1	A	40	PHE	2.5
1	A	7	LEU	2.4
1	B	189	TYR	2.3
1	D	365	ALA	2.3
1	B	40	PHE	2.3
1	A	371	GLU	2.3
1	D	106	GLU	2.3
1	D	325	GLY	2.2
1	C	339	VAL	2.2
1	A	143	LEU	2.2
1	D	28	LEU	2.1
1	C	321	GLY	2.1
1	C	7	LEU	2.1
1	D	135	VAL	2.1

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. 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	RSCC	RSR	LLDF	B-factors($Å^2$)	Q<0.9
1	LLP	D	211	24/25	0.97	0.12	-	26,33,34,35	0
1	LLP	C	211	24/25	0.96	0.14	-	23,29,29,30	0
1	LLP	B	211	24/25	0.97	0.13	-	24,30,30,32	0
1	LLP	A	211	24/25	0.96	0.14	-	24,31,33,34	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.