



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 10:54 PM UTC

PDB ID : 3VK3 / pdb_00003vk3
Title : Crystal Structure of L-Methionine gamma-Lyase from Pseudomonas putida C116H Mutant Complexed with L-methionine
Authors : Fukumoto, M.; Kudou, D.; Murano, S.; Shiba, T.; Sato, D.; Tamura, T.; Harada, S.; Inagaki, K.
Deposited on : 2011-11-07
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

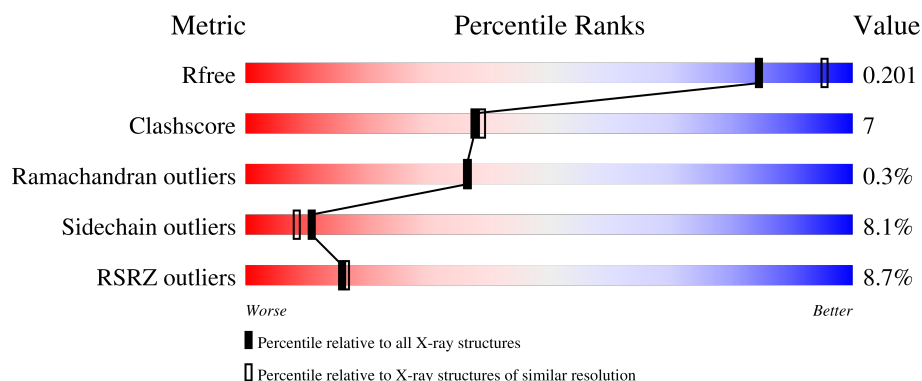
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	11% 85% 13% .
1	B	398	7% 83% 13% ..
1	C	398	10% 81% 13% ..
1	D	398	7% 80% 15% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12329 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.

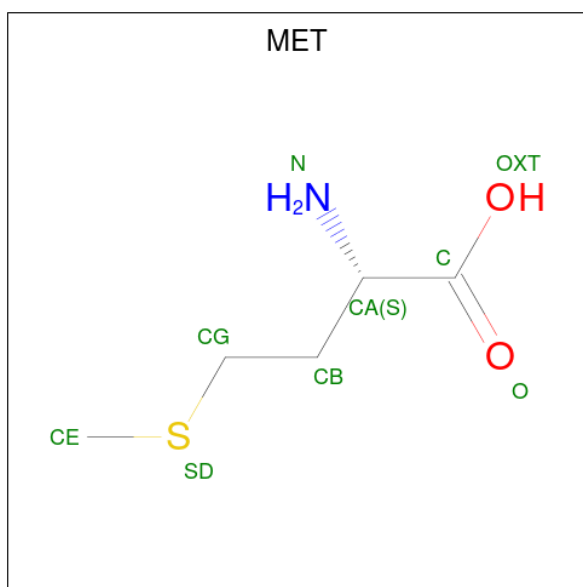
- Molecule 1 is a protein called Methionine gamma-lyase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	397	Total	C	N	O	P	S	0	0	0
			3007	1895	534	561	1	16			
1	B	392	Total	C	N	O	P	S	0	0	0
			2970	1874	525	554	1	16			
1	C	392	Total	C	N	O	P	S	0	0	0
			2970	1874	525	554	1	16			
1	D	392	Total	C	N	O	P	S	0	0	0
			2970	1874	525	554	1	16			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	116	HIS	CYS	engineered mutation	UNP P13254
B	116	HIS	CYS	engineered mutation	UNP P13254
C	116	HIS	CYS	engineered mutation	UNP P13254
D	116	HIS	CYS	engineered mutation	UNP P13254

- Molecule 2 is METHIONINE (CCD ID: MET) (formula: C₅H₁₁NO₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			9	5	1	2	1		
2	B	1	Total	C	N	O	S	0	0
			9	5	1	2	1		
2	C	1	Total	C	N	O	S	0	0
			9	5	1	2	1		
2	D	1	Total	C	N	O	S	0	0
			9	5	1	2	1		

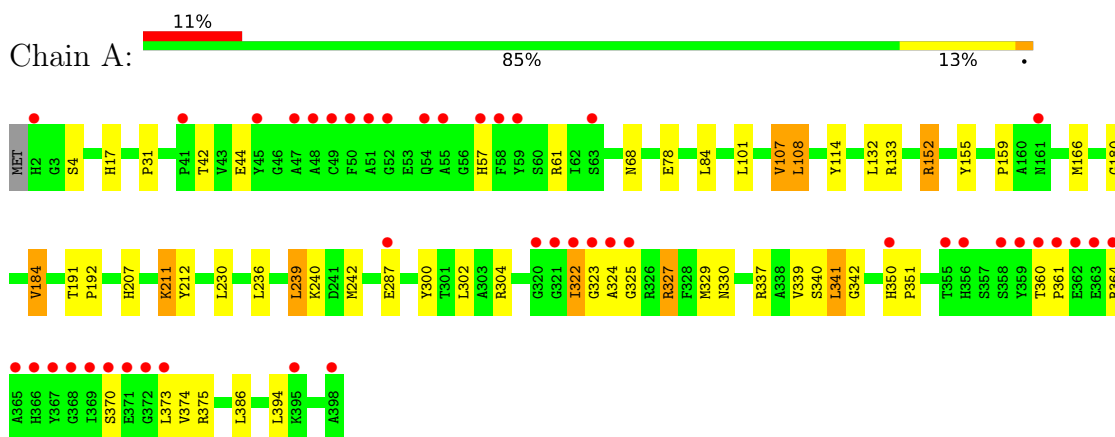
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	109	Total	O	0	0
			109	109		
3	B	103	Total	O	0	0
			103	103		
3	C	66	Total	O	0	0
			66	66		
3	D	98	Total	O	0	0
			98	98		

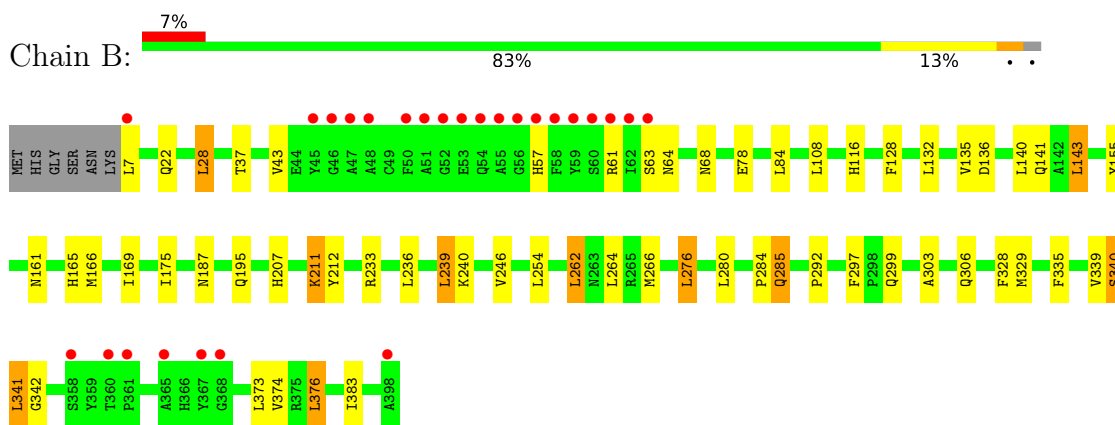
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

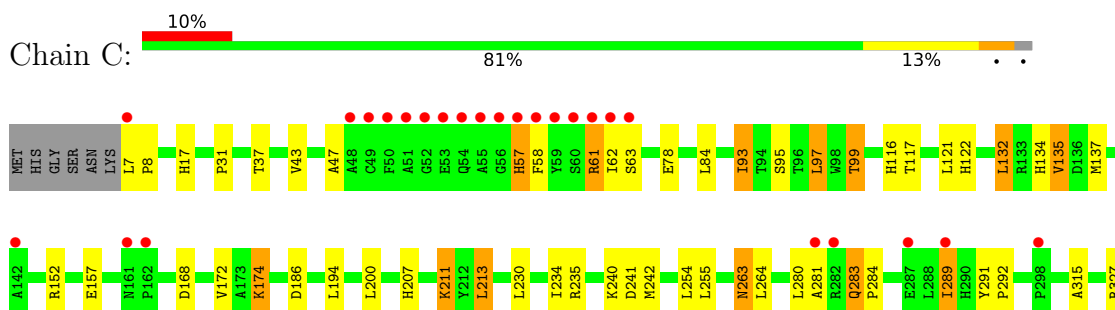
- Molecule 1: Methionine gamma-lyase

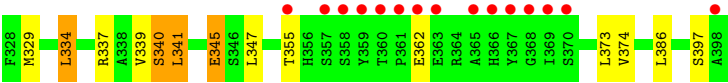


- Molecule 1: Methionine gamma-lyase

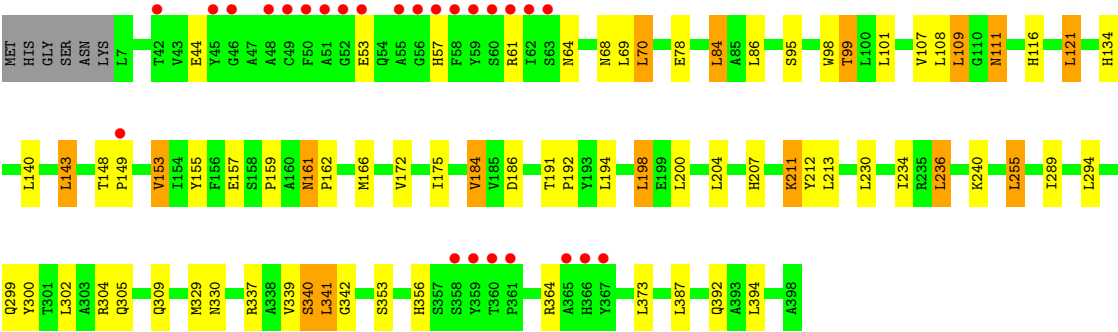
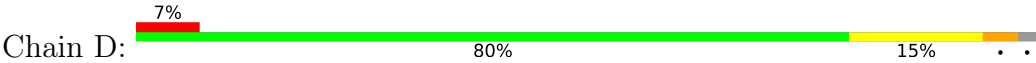


- Molecule 1: Methionine gamma-lyase





● Molecule 1: Methionine gamma-lyase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	153.17Å 152.95Å 80.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.23 – 2.10 29.23 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.6 (29.23-2.10) 99.5 (29.23-2.10)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.88 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.172 , 0.201 0.174 , 0.201	Depositor DCC
R_{free} test set	5545 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	22.1	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 36.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.013 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12329	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% 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	0.70	0/3048	0.86	1/4136 (0.0%)
1	B	0.68	0/3010	0.85	0/4086
1	C	0.65	0/3010	0.87	3/4086 (0.1%)
1	D	0.70	0/3010	0.91	0/4086
All	All	0.68	0/12078	0.87	4/16394 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	57	HIS	N-CA-C	8.20	119.06	108.24
1	A	107	VAL	CB-CA-C	-6.48	101.17	110.83
1	C	283	GLN	CA-C-N	5.17	126.30	119.84
1	C	283	GLN	C-N-CA	5.17	126.30	119.84

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	3007	0	2961	44	0
1	B	2970	0	2927	42	0
1	C	2970	0	2927	50	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2970	0	2928	48	0
2	A	9	0	8	5	0
2	B	9	0	8	0	0
2	C	9	0	8	0	0
2	D	9	0	8	1	0
3	A	109	0	0	1	0
3	B	103	0	0	4	0
3	C	66	0	0	1	0
3	D	98	0	0	1	0
All	All	12329	0	11775	167	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 7.

All (167) 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:A:327:ARG:HG2	1:A:327:ARG:HH11	1.22	1.04
1:B:166:MET:HE2	1:B:303:ALA:HA	1.49	0.94
1:D:166:MET:H	1:D:299:GLN:HE22	1.14	0.94
1:C:240:LYS:HD3	1:D:116:HIS:ND1	1.84	0.92
1:C:43:VAL:H	1:D:330:ASN:HD21	1.18	0.91
1:D:57:HIS:HE1	1:D:68:ASN:ND2	1.68	0.91
1:D:148:THR:HB	1:D:149:PRO:HD2	1.55	0.88
1:D:57:HIS:HE1	1:D:68:ASN:HD21	1.19	0.84
1:A:42:THR:HG22	1:A:44:GLU:H	1.42	0.84
1:D:339:VAL:HB	2:D:501:MET:HA	1.59	0.84
1:C:281:ALA:HA	1:C:289:ILE:HD11	1.59	0.83
1:C:99:THR:HG21	1:C:234:ILE:HA	1.62	0.82
1:D:70:LEU:HD21	1:D:255:LEU:HD13	1.64	0.80
1:B:169:ILE:H	1:B:306:GLN:HE22	1.28	0.79
1:D:57:HIS:CE1	1:D:68:ASN:ND2	2.50	0.79
1:D:57:HIS:CE1	1:D:68:ASN:HD21	2.00	0.79
1:D:339:VAL:O	1:D:340:SER:CB	2.29	0.76
1:D:99:THR:HG21	1:D:234:ILE:HA	1.68	0.76
1:D:339:VAL:O	1:D:340:SER:HB3	1.86	0.76
1:D:78:GLU:OE2	1:D:207:HIS:HE1	1.70	0.74
1:A:340:SER:HA	2:A:501:MET:HB3	1.69	0.74
1:B:166:MET:H	1:B:299:GLN:HE22	1.34	0.73
1:B:236:LEU:O	1:B:240:LYS:HE3	1.88	0.73
1:B:61:ARG:HG2	1:B:246:VAL:HG21	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:ARG:HH11	1:A:327:ARG:CG	2.01	0.72
1:B:63:SER:HA	3:B:479:HOH:O	1.90	0.72
1:B:166:MET:CE	1:B:303:ALA:HA	2.21	0.69
1:C:7:LEU:HB3	1:C:8:PRO:HD3	1.75	0.69
1:C:281:ALA:HA	1:C:289:ILE:CD1	2.24	0.68
1:D:78:GLU:OE2	1:D:207:HIS:CE1	2.47	0.68
1:C:57:HIS:CG	1:C:58:PHE:H	2.13	0.67
1:C:240:LYS:HD3	1:D:116:HIS:CE1	2.29	0.67
1:A:339:VAL:HG23	1:A:339:VAL:O	1.95	0.67
1:D:95:SER:O	1:D:99:THR:CG2	2.43	0.67
1:C:122:HIS:NE2	1:C:134:HIS:HE1	1.93	0.67
1:D:101:LEU:HD21	1:D:153:VAL:HG13	1.77	0.65
1:A:325:GLY:HA3	1:A:350:HIS:CE1	2.31	0.65
1:C:95:SER:O	1:C:99:THR:CG2	2.45	0.65
1:C:211:LLP:HD3	1:C:341:LEU:HG	1.79	0.64
1:A:17:HIS:HD2	3:A:449:HOH:O	1.82	0.63
1:D:166:MET:H	1:D:299:GLN:NE2	1.93	0.63
1:A:330:ASN:HD21	1:B:43:VAL:H	1.47	0.63
1:B:166:MET:HE2	1:B:303:ALA:CA	2.27	0.62
1:C:240:LYS:HD2	1:C:241:ASP:OD1	1.99	0.62
1:B:285:GLN:H	1:B:285:GLN:HE21	1.48	0.62
1:D:159:PRO:HG3	1:D:166:MET:HE2	1.83	0.60
1:A:155:TYR:CD1	1:A:184:VAL:HG22	2.37	0.60
1:C:61:ARG:HD3	1:D:211:LLP:OP3	2.02	0.60
1:A:78:GLU:OE1	1:A:207:HIS:HE1	1.86	0.59
1:A:42:THR:HG22	1:A:44:GLU:N	2.15	0.58
1:A:300:TYR:CZ	1:A:304:ARG:HD2	2.38	0.58
1:A:211:LLP:HD3	1:A:341:LEU:HG	1.86	0.58
1:B:166:MET:H	1:B:299:GLN:NE2	2.01	0.58
1:B:276:LEU:HD13	1:B:383:ILE:HD11	1.86	0.58
1:C:339:VAL:O	1:C:340:SER:CB	2.52	0.58
1:A:114:TYR:HE1	2:A:501:MET:HG3	1.69	0.57
1:A:327:ARG:HG2	1:A:327:ARG:NH1	2.03	0.57
1:A:159:PRO:HG3	1:A:166:MET:HE2	1.86	0.56
1:A:61:ARG:HH22	1:B:116:HIS:HD2	1.53	0.56
1:C:78:GLU:OE2	1:C:207:HIS:CE1	2.58	0.56
1:C:17:HIS:HD2	3:C:453:HOH:O	1.89	0.56
1:D:95:SER:O	1:D:99:THR:HG22	2.06	0.56
1:A:114:TYR:CE1	2:A:501:MET:HG3	2.41	0.56
1:C:174:LYS:NZ	1:C:174:LYS:HB3	2.20	0.56
1:A:61:ARG:HH12	1:B:116:HIS:CD2	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:HIS:HE1	1:B:68:ASN:ND2	2.05	0.55
1:B:328:PHE:HD2	1:B:329:MET:HE2	1.71	0.55
1:A:236:LEU:O	1:A:240:LYS:HE3	2.08	0.54
1:C:174:LYS:HB3	1:C:174:LYS:HZ3	1.71	0.54
1:A:324:ALA:HA	1:A:327:ARG:HD3	1.89	0.53
1:C:95:SER:O	1:C:99:THR:HG22	2.07	0.53
1:A:322:ILE:HD12	1:A:364:ARG:HH21	1.72	0.53
1:C:93:ILE:HD12	1:C:97:LEU:HD22	1.91	0.53
1:A:329:MET:HE3	1:A:337:ARG:HG2	1.91	0.53
1:C:213:LEU:HB3	1:C:255:LEU:HD11	1.89	0.53
1:B:262:LEU:HD22	1:B:266:MET:HG2	1.90	0.53
1:D:155:TYR:CD1	1:D:184:VAL:HG22	2.44	0.53
1:A:78:GLU:OE1	1:A:207:HIS:CE1	2.62	0.52
1:D:95:SER:O	1:D:99:THR:HG23	2.08	0.52
1:B:28:LEU:CD2	1:C:345:GLU:HG3	2.41	0.51
1:B:328:PHE:CD2	1:B:329:MET:HE2	2.45	0.51
1:C:116:HIS:HD2	1:D:61:ARG:HH22	1.59	0.51
1:D:111:ASN:HD22	1:D:134:HIS:HB3	1.76	0.51
1:B:292:PRO:HA	1:B:297:PHE:CD2	2.47	0.50
1:A:370:SER:HB3	1:A:373:LEU:HB2	1.94	0.50
1:C:7:LEU:HB3	1:C:8:PRO:CD	2.40	0.50
1:B:22:GLN:HA	1:B:22:GLN:OE1	2.12	0.49
1:D:84:LEU:HD13	1:D:86:LEU:HD11	1.95	0.49
1:D:109:LEU:HD21	1:D:121:LEU:HG	1.95	0.49
1:B:63:SER:HB3	3:B:480:HOH:O	2.13	0.49
1:D:107:VAL:HG22	1:D:109:LEU:HD13	1.95	0.49
1:B:28:LEU:HD21	1:C:345:GLU:HG3	1.94	0.48
1:A:360:THR:HB	1:A:361:PRO:HD2	1.96	0.48
1:C:57:HIS:CG	1:C:58:PHE:N	2.80	0.48
1:C:57:HIS:HE1	1:C:62:ILE:HB	1.77	0.48
1:C:116:HIS:CD2	1:D:61:ARG:HH12	2.31	0.48
1:D:300:TYR:CZ	1:D:304:ARG:HD2	2.50	0.47
1:C:132:LEU:N	1:C:132:LEU:HD12	2.30	0.47
1:B:57:HIS:CE1	1:B:68:ASN:ND2	2.81	0.47
1:B:339:VAL:O	1:B:340:SER:CB	2.61	0.47
1:C:95:SER:O	1:C:99:THR:HG23	2.12	0.47
1:D:157:GLU:HG2	1:D:186:ASP:HB3	1.97	0.47
1:A:57:HIS:NE2	1:A:68:ASN:ND2	2.62	0.47
1:C:157:GLU:HG2	1:C:186:ASP:HB3	1.97	0.47
1:B:233:ARG:HD2	3:B:475:HOH:O	2.14	0.47
1:C:211:LLP:O3	1:C:211:LLP:NZ	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:VAL:HG21	1:B:143:LEU:HD23	1.97	0.47
1:C:78:GLU:OE2	1:C:207:HIS:HE1	1.98	0.47
1:A:84:LEU:HD11	1:A:239:LEU:HD12	1.98	0.46
1:C:242:MET:HE2	1:D:98:TRP:HZ2	1.80	0.46
1:C:315:ALA:HB1	1:C:373:LEU:HD11	1.98	0.46
1:A:108:LEU:HD12	1:A:133:ARG:HB3	1.97	0.46
1:A:152:ARG:NH2	1:A:180:GLY:O	2.49	0.46
1:A:327:ARG:CG	1:A:327:ARG:NH1	2.69	0.45
1:A:322:ILE:HD12	1:A:364:ARG:NH2	2.31	0.45
1:A:339:VAL:O	1:A:339:VAL:CG2	2.64	0.45
1:D:161:ASN:HD22	1:D:161:ASN:HA	1.55	0.45
1:D:143:LEU:HD13	1:D:175:ILE:HG21	1.98	0.45
1:D:162:PRO:HB2	1:D:373:LEU:HD21	1.97	0.45
1:A:323:GLY:O	1:A:327:ARG:HD3	2.17	0.45
1:A:330:ASN:HD21	1:B:43:VAL:HG22	1.82	0.45
1:B:335:PHE:CE2	1:B:376:LEU:HG	2.52	0.45
1:B:136:ASP:OD1	1:B:165:HIS:HE1	2.00	0.45
1:C:329:MET:HE3	1:C:337:ARG:HG2	1.97	0.44
1:D:356:HIS:O	1:D:364:ARG:NH1	2.46	0.44
1:C:263:ASN:H	1:C:263:ASN:HD22	1.64	0.44
1:C:93:ILE:HD13	1:C:117:THR:HG23	1.99	0.43
1:D:329:MET:HE3	1:D:337:ARG:HG2	2.00	0.43
1:B:84:LEU:HD11	1:B:239:LEU:HD12	2.00	0.43
1:D:198:LEU:HB2	3:D:407:HOH:O	2.17	0.43
1:B:285:GLN:H	1:B:285:GLN:NE2	2.14	0.43
1:C:47:ALA:HB2	1:D:353:SER:O	2.18	0.43
1:D:107:VAL:HG23	1:D:153:VAL:HG22	1.99	0.43
1:B:143:LEU:HD13	1:B:175:ILE:HG21	2.01	0.43
1:A:31:PRO:HB2	1:C:31:PRO:HB2	2.01	0.43
1:A:375:ARG:HH22	2:A:501:MET:HA	1.83	0.43
1:D:211:LLP:HD3	1:D:341:LEU:HG	2.01	0.43
1:B:211:LLP:O3	1:B:211:LLP:NZ	2.52	0.43
1:C:334:LEU:HD13	1:C:386:LEU:HD23	2.00	0.43
1:B:284:PRO:HD2	1:B:285:GLN:NE2	2.34	0.42
1:A:211:LLP:O3	1:A:211:LLP:NZ	2.52	0.42
1:D:191:THR:HB	1:D:192:PRO:HD2	2.01	0.42
1:C:339:VAL:O	1:C:340:SER:HB3	2.19	0.42
1:D:212:TYR:CE1	1:D:342:GLY:HA2	2.54	0.42
1:C:62:ILE:O	1:C:235:ARG:NH1	2.52	0.42
1:C:135:VAL:HG22	1:C:137:MET:HE2	2.02	0.42
1:A:340:SER:HA	2:A:501:MET:CB	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:327:ARG:NH2	1:C:397:SER:O	2.53	0.42
1:C:362:GLU:H	1:C:362:GLU:CD	2.28	0.42
1:B:78:GLU:OE2	1:B:207:HIS:NE2	2.49	0.42
1:B:63:SER:CA	3:B:479:HOH:O	2.58	0.41
1:C:291:TYR:HA	1:C:292:PRO:HD3	1.94	0.41
1:B:212:TYR:CE1	1:B:342:GLY:HA2	2.56	0.41
1:D:211:LLP:NZ	1:D:211:LLP:O3	2.45	0.41
1:A:351:PRO:HD2	1:A:373:LEU:O	2.20	0.41
1:A:242:MET:HE1	1:B:128:PHE:HE2	1.84	0.41
1:D:194:LEU:HD22	1:D:309:GLN:HB2	2.02	0.41
1:A:212:TYR:CE1	1:A:342:GLY:HA2	2.55	0.41
1:B:187:ASN:ND2	1:B:195:GLN:HE21	2.19	0.41
1:C:61:ARG:HD3	1:D:211:LLP:P	2.61	0.41
1:A:42:THR:CG2	1:A:44:GLU:OE1	2.69	0.40
1:B:211:LLP:HD3	1:B:341:LEU:HG	2.02	0.40
1:C:168:ASP:O	1:C:172:VAL:HG23	2.22	0.40
1:D:236:LEU:O	1:D:240:LYS:HE3	2.22	0.40
1:A:191:THR:HB	1:A:192:PRO:HD2	2.02	0.40
1:B:155:TYR:CD2	1:B:155:TYR:C	2.99	0.40
1:C:283:GLN:HA	1:C:284:PRO:HD2	1.73	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	394/398 (99%)	385 (98%)	8 (2%)	1 (0%)	36	36
1	B	389/398 (98%)	377 (97%)	11 (3%)	1 (0%)	36	36
1	C	389/398 (98%)	373 (96%)	15 (4%)	1 (0%)	36	36
1	D	389/398 (98%)	381 (98%)	7 (2%)	1 (0%)	36	36
All	All	1561/1592 (98%)	1516 (97%)	41 (3%)	4 (0%)	36	36

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	340	SER
1	C	340	SER
1	D	340	SER
1	A	322	ILE

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	305/306 (100%)	289 (95%)	16 (5%)	21	20
1	B	301/306 (98%)	280 (93%)	21 (7%)	14	11
1	C	301/306 (98%)	274 (91%)	27 (9%)	9	6
1	D	301/306 (98%)	269 (89%)	32 (11%)	6	4
All	All	1208/1224 (99%)	1112 (92%)	96 (8%)	11	9

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	SER
1	A	101	LEU
1	A	107	VAL
1	A	108	LEU
1	A	132	LEU
1	A	152	ARG
1	A	184	VAL
1	A	230	LEU
1	A	239	LEU
1	A	287	GLU
1	A	302	LEU
1	A	327	ARG
1	A	341	LEU
1	A	374	VAL
1	A	386	LEU
1	A	394	LEU

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Mol	Chain	Res	Type
1	B	7	LEU
1	B	28	LEU
1	B	37	THR
1	B	64	ASN
1	B	108	LEU
1	B	132	LEU
1	B	140	LEU
1	B	141	GLN
1	B	143	LEU
1	B	161	ASN
1	B	239	LEU
1	B	254	LEU
1	B	262	LEU
1	B	264	LEU
1	B	276	LEU
1	B	280	LEU
1	B	285	GLN
1	B	341	LEU
1	B	373	LEU
1	B	374	VAL
1	B	376	LEU
1	C	37	THR
1	C	61	ARG
1	C	63	SER
1	C	84	LEU
1	C	93	ILE
1	C	97	LEU
1	C	99	THR
1	C	121	LEU
1	C	132	LEU
1	C	135	VAL
1	C	152	ARG
1	C	174	LYS
1	C	194	LEU
1	C	200	LEU
1	C	213	LEU
1	C	230	LEU
1	C	254	LEU
1	C	263	ASN
1	C	264	LEU
1	C	280	LEU
1	C	289	ILE

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Mol	Chain	Res	Type
1	C	334	LEU
1	C	341	LEU
1	C	345	GLU
1	C	347	LEU
1	C	355	THR
1	C	374	VAL
1	D	44	GLU
1	D	53	GLU
1	D	64	ASN
1	D	69	LEU
1	D	70	LEU
1	D	84	LEU
1	D	99	THR
1	D	108	LEU
1	D	109	LEU
1	D	111	ASN
1	D	121	LEU
1	D	140	LEU
1	D	143	LEU
1	D	153	VAL
1	D	161	ASN
1	D	172	VAL
1	D	184	VAL
1	D	198	LEU
1	D	200	LEU
1	D	204	LEU
1	D	213	LEU
1	D	230	LEU
1	D	236	LEU
1	D	255	LEU
1	D	289	ILE
1	D	294	LEU
1	D	302	LEU
1	D	305	GLN
1	D	341	LEU
1	D	387	LEU
1	D	392	GLN
1	D	394	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	HIS
1	A	22	GLN
1	A	34	GLN
1	A	54	GLN
1	A	68	ASN
1	A	116	HIS
1	A	141	GLN
1	A	161	ASN
1	A	187	ASN
1	A	207	HIS
1	A	274	GLN
1	A	330	ASN
1	A	392	GLN
1	B	34	GLN
1	B	54	GLN
1	B	57	HIS
1	B	64	ASN
1	B	68	ASN
1	B	116	HIS
1	B	165	HIS
1	B	187	ASN
1	B	195	GLN
1	B	237	GLN
1	B	263	ASN
1	B	285	GLN
1	B	290	HIS
1	B	299	GLN
1	B	305	GLN
1	B	306	GLN
1	B	366	HIS
1	C	17	HIS
1	C	22	GLN
1	C	111	ASN
1	C	116	HIS
1	C	134	HIS
1	C	207	HIS
1	C	250	HIS
1	C	305	GLN
1	D	22	GLN
1	D	57	HIS
1	D	64	ASN
1	D	68	ASN
1	D	111	ASN

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Mol	Chain	Res	Type
1	D	161	ASN
1	D	207	HIS
1	D	290	HIS
1	D	299	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	C	211	1	23,24,25	2.41	6 (26%)	25,32,34	1.81	4 (16%)
1	LLP	B	211	1	23,24,25	2.25	5 (21%)	25,32,34	2.10	5 (20%)
1	LLP	A	211	1	23,24,25	2.30	6 (26%)	25,32,34	1.67	3 (12%)
1	LLP	D	211	1	23,24,25	2.36	5 (21%)	25,32,34	1.61	3 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LLP	C	211	1	-	3/16/17/19	0/1/1/1
1	LLP	B	211	1	-	3/16/17/19	0/1/1/1
1	LLP	A	211	1	-	4/16/17/19	0/1/1/1
1	LLP	D	211	1	-	3/16/17/19	0/1/1/1

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	211	LLP	C4'-NZ	7.07	1.50	1.27
1	C	211	LLP	C4'-NZ	6.60	1.49	1.27
1	D	211	LLP	C4'-NZ	6.40	1.48	1.27
1	A	211	LLP	C4'-NZ	6.33	1.48	1.27
1	D	211	LLP	C2'-C2	-6.31	1.40	1.50
1	A	211	LLP	C2'-C2	-5.85	1.41	1.50
1	C	211	LLP	C2'-C2	-5.75	1.41	1.50
1	B	211	LLP	C2'-C2	-5.45	1.41	1.50
1	C	211	LLP	C6-N1	4.35	1.43	1.34
1	D	211	LLP	C6-N1	4.13	1.42	1.34
1	B	211	LLP	C6-N1	3.83	1.42	1.34
1	A	211	LLP	C5'-C5	-3.39	1.42	1.50
1	C	211	LLP	C5'-C5	-3.28	1.42	1.50
1	A	211	LLP	C6-N1	3.11	1.40	1.34
1	D	211	LLP	C5'-C5	-2.93	1.43	1.50
1	A	211	LLP	P-OP3	-2.57	1.45	1.54
1	A	211	LLP	C4-C4'	-2.47	1.41	1.46
1	B	211	LLP	P-OP2	-2.40	1.45	1.54
1	C	211	LLP	CB-CA	2.40	1.57	1.53
1	C	211	LLP	P-OP3	-2.21	1.46	1.54
1	D	211	LLP	P-OP3	-2.06	1.47	1.54
1	B	211	LLP	C5'-C5	-2.06	1.45	1.50

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	211	LLP	C4-C3-C2	7.24	124.22	120.14
1	C	211	LLP	C4-C3-C2	6.97	124.07	120.14
1	D	211	LLP	C4-C3-C2	5.35	123.15	120.14
1	A	211	LLP	C4-C3-C2	5.06	122.99	120.14
1	B	211	LLP	OP4-P-OP1	-3.28	97.59	106.44
1	B	211	LLP	CE-NZ-C4'	-3.26	108.28	118.72
1	D	211	LLP	OP4-P-OP1	-2.56	99.52	106.44
1	A	211	LLP	C4-C4'-NZ	-2.26	113.59	124.04
1	A	211	LLP	C3-C2-N1	-2.26	118.11	120.96
1	B	211	LLP	C3-C2-N1	-2.21	118.17	120.96
1	C	211	LLP	C4-C4'-NZ	-2.16	114.07	124.04
1	C	211	LLP	OP2-P-OP4	-2.13	101.12	106.67
1	B	211	LLP	OP4-C5'-C5	2.06	113.21	109.36
1	C	211	LLP	C3-C2-N1	-2.05	118.38	120.96
1	D	211	LLP	OP4-C5'-C5	2.02	113.14	109.36

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	211	LLP	O-C-CA-CB
1	B	211	LLP	O-C-CA-CB
1	C	211	LLP	O-C-CA-CB
1	D	211	LLP	O-C-CA-CB
1	A	211	LLP	C4-C4'-NZ-CE
1	B	211	LLP	C4-C4'-NZ-CE
1	D	211	LLP	C4-C4'-NZ-CE
1	C	211	LLP	C4-C4'-NZ-CE
1	A	211	LLP	CD-CE-NZ-C4'
1	C	211	LLP	CD-CE-NZ-C4'
1	A	211	LLP	N-CA-CB-CG
1	B	211	LLP	N-CA-CB-CG
1	D	211	LLP	N-CA-CB-CG

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	211	LLP	2	0
1	B	211	LLP	2	0
1	A	211	LLP	2	0
1	D	211	LLP	4	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands 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
2	MET	D	501	-	7,8,8	0.93	1 (14%)	5,9,9	1.36	1 (20%)
2	MET	A	501	-	7,8,8	0.94	1 (14%)	5,9,9	1.36	1 (20%)
2	MET	C	501	-	7,8,8	0.95	1 (14%)	5,9,9	1.59	1 (20%)
2	MET	B	501	-	7,8,8	0.99	1 (14%)	5,9,9	1.44	1 (20%)

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
2	MET	D	501	-	-	4/8/8/8	-
2	MET	A	501	-	-	6/8/8/8	-
2	MET	C	501	-	-	3/8/8/8	-
2	MET	B	501	-	-	3/8/8/8	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	MET	OXT-C	-2.43	1.22	1.30
2	B	501	MET	OXT-C	-2.41	1.23	1.30
2	C	501	MET	OXT-C	-2.35	1.23	1.30
2	D	501	MET	OXT-C	-2.20	1.23	1.30

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	MET	OXT-C-O	-3.44	116.27	124.08
2	B	501	MET	OXT-C-O	-3.15	116.93	124.08
2	A	501	MET	OXT-C-O	-2.99	117.30	124.08
2	D	501	MET	OXT-C-O	-2.93	117.43	124.08

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	MET	CA-CB-CG-SD
2	C	501	MET	CA-CB-CG-SD
2	A	501	MET	CA-CB-CG-SD

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Mol	Chain	Res	Type	Atoms
2	A	501	MET	O-C-CA-N
2	D	501	MET	CB-CG-SD-CE
2	B	501	MET	OXT-C-CA-CB
2	C	501	MET	C-CA-CB-CG
2	C	501	MET	N-CA-CB-CG
2	D	501	MET	N-CA-CB-CG
2	B	501	MET	O-C-CA-CB
2	D	501	MET	O-C-CA-CB
2	D	501	MET	OXT-C-CA-CB
2	A	501	MET	C-CA-CB-CG
2	A	501	MET	OXT-C-CA-N
2	A	501	MET	O-C-CA-CB
2	A	501	MET	OXT-C-CA-CB

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	501	MET	1	0
2	A	501	MET	5	0

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	396/398 (99%)	0.08	44 (11%)	10 10	8, 18, 63, 76	0
1	B	391/398 (98%)	0.02	26 (6%)	24 26	9, 20, 56, 75	0
1	C	391/398 (98%)	0.43	40 (10%)	12 12	11, 27, 64, 79	0
1	D	391/398 (98%)	-0.05	26 (6%)	24 26	8, 19, 52, 74	0
All	All	1569/1592 (98%)	0.12	136 (8%)	16 16	8, 21, 59, 79	0

All (136) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	58	PHE	9.0
1	D	51	ALA	8.8
1	A	51	ALA	7.2
1	B	55	ALA	7.2
1	C	62	ILE	7.1
1	C	59	TYR	7.0
1	D	55	ALA	6.8
1	C	63	SER	6.6
1	B	58	PHE	6.5
1	B	62	ILE	6.1
1	A	367	TYR	5.7
1	C	55	ALA	5.6
1	C	60	SER	5.6
1	C	52	GLY	5.5
1	B	63	SER	5.5
1	C	61	ARG	5.4
1	A	366	HIS	5.3
1	B	51	ALA	5.3
1	A	55	ALA	5.3
1	D	367	TYR	5.2
1	D	58	PHE	5.2

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Mol	Chain	Res	Type	RSRZ
1	C	365	ALA	5.0
1	B	59	TYR	4.9
1	B	52	GLY	4.8
1	C	360	THR	4.8
1	A	365	ALA	4.8
1	B	57	HIS	4.7
1	C	54	GLN	4.5
1	A	369	ILE	4.4
1	D	60	SER	4.4
1	A	360	THR	4.3
1	A	361	PRO	4.2
1	B	50	PHE	4.2
1	A	58	PHE	4.2
1	C	57	HIS	4.2
1	A	398	ALA	3.9
1	A	52	GLY	3.9
1	A	368	GLY	3.9
1	A	321	GLY	3.9
1	B	398	ALA	3.9
1	C	361	PRO	3.8
1	B	60	SER	3.8
1	A	364	ARG	3.7
1	C	56	GLY	3.7
1	A	49	CYS	3.6
1	C	362	GLU	3.6
1	D	61	ARG	3.6
1	A	59	TYR	3.6
1	D	63	SER	3.6
1	D	48	ALA	3.5
1	A	359	TYR	3.5
1	C	359	TYR	3.5
1	C	367	TYR	3.5
1	A	322	ILE	3.5
1	C	53	GLU	3.5
1	D	57	HIS	3.4
1	D	59	TYR	3.4
1	A	54	GLN	3.3
1	A	47	ALA	3.2
1	D	365	ALA	3.2
1	A	45	TYR	3.2
1	B	61	ARG	3.1
1	D	358	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	357	SER	3.0
1	B	56	GLY	3.0
1	A	363	GLU	3.0
1	A	48	ALA	3.0
1	A	63	SER	3.0
1	D	52	GLY	3.0
1	A	362	GLU	3.0
1	C	142	ALA	2.9
1	C	366	HIS	2.9
1	A	324	ALA	2.9
1	B	361	PRO	2.9
1	D	53	GLU	2.9
1	B	45	TYR	2.9
1	D	45	TYR	2.9
1	C	51	ALA	2.9
1	D	49	CYS	2.8
1	C	369	ILE	2.8
1	B	367	TYR	2.8
1	C	363	GLU	2.8
1	A	371	GLU	2.8
1	C	398	ALA	2.8
1	A	323	GLY	2.8
1	C	48	ALA	2.8
1	B	7	LEU	2.8
1	A	57	HIS	2.7
1	B	47	ALA	2.7
1	D	50	PHE	2.6
1	C	358	SER	2.6
1	B	54	GLN	2.6
1	B	358	SER	2.6
1	D	62	ILE	2.5
1	D	359	TYR	2.5
1	A	370	SER	2.5
1	D	366	HIS	2.5
1	B	360	THR	2.4
1	D	149	PRO	2.4
1	A	2	HIS	2.4
1	A	325	GLY	2.4
1	C	368	GLY	2.4
1	A	287	GLU	2.4
1	A	161	ASN	2.4
1	C	161	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	289	ILE	2.4
1	C	370	SER	2.4
1	B	365	ALA	2.3
1	C	281	ALA	2.3
1	A	350	HIS	2.3
1	B	368	GLY	2.3
1	C	287	GLU	2.2
1	A	41	PRO	2.2
1	A	395	LYS	2.2
1	A	320	GLY	2.2
1	A	50	PHE	2.2
1	A	356	HIS	2.2
1	D	361	PRO	2.2
1	A	373	LEU	2.2
1	D	42	THR	2.2
1	C	7	LEU	2.1
1	C	282	ARG	2.1
1	C	49	CYS	2.1
1	A	355	THR	2.1
1	C	162	PRO	2.1
1	C	50	PHE	2.1
1	B	48	ALA	2.1
1	D	360	THR	2.1
1	A	372	GLY	2.1
1	B	46	GLY	2.1
1	A	358	SER	2.1
1	B	53	GLU	2.0
1	C	298	PRO	2.0
1	D	46	GLY	2.0
1	C	355	THR	2.0
1	D	56	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	LLP	C	211	24/25	0.97	0.07	14,18,21,22	0
1	LLP	D	211	24/25	0.97	0.06	10,16,17,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	LLP	A	211	24/25	0.98	0.05	9,13,15,15	0
1	LLP	B	211	24/25	0.98	0.04	11,14,16,19	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MET	D	501	9/9	0.52	0.38	94,94,95,95	0
2	MET	B	501	9/9	0.61	0.39	73,73,76,76	0
2	MET	A	501	9/9	0.68	0.30	82,82,83,83	0
2	MET	C	501	9/9	0.73	0.30	68,69,71,71	0

6.5 Other polymers [i](#)

There are no such residues in this entry.