



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 02:02 PM UTC

PDB ID : 4TV7 / pdb_00004tv7
Title : Crystal structure of Bacillus subtilis GabR at 2.05 Angstroms resolution
Authors : Goto, M.; Okuda, K.; Yoshimura, T.
Deposited on : 2014-06-26
Resolution : 2.05 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

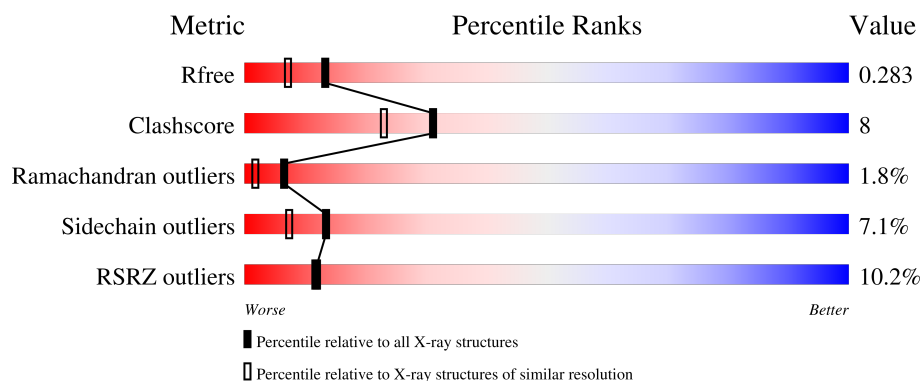
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	479	
1	B	479	
1	C	479	
1	D	479	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14499 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 HTH-type transcriptional regulatory protein GabR.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	432	Total	C	N	O	P	S	0	0	0
			3344	2135	570	621	1	17			
1	B	430	Total	C	N	O	P	S	0	0	0
			3373	2152	575	629	1	16			
1	C	452	Total	C	N	O	P	S	0	0	0
			3623	2303	623	679	1	17			
1	D	449	Total	C	N	O	P	S	0	0	0
			3596	2286	610	683	1	16			

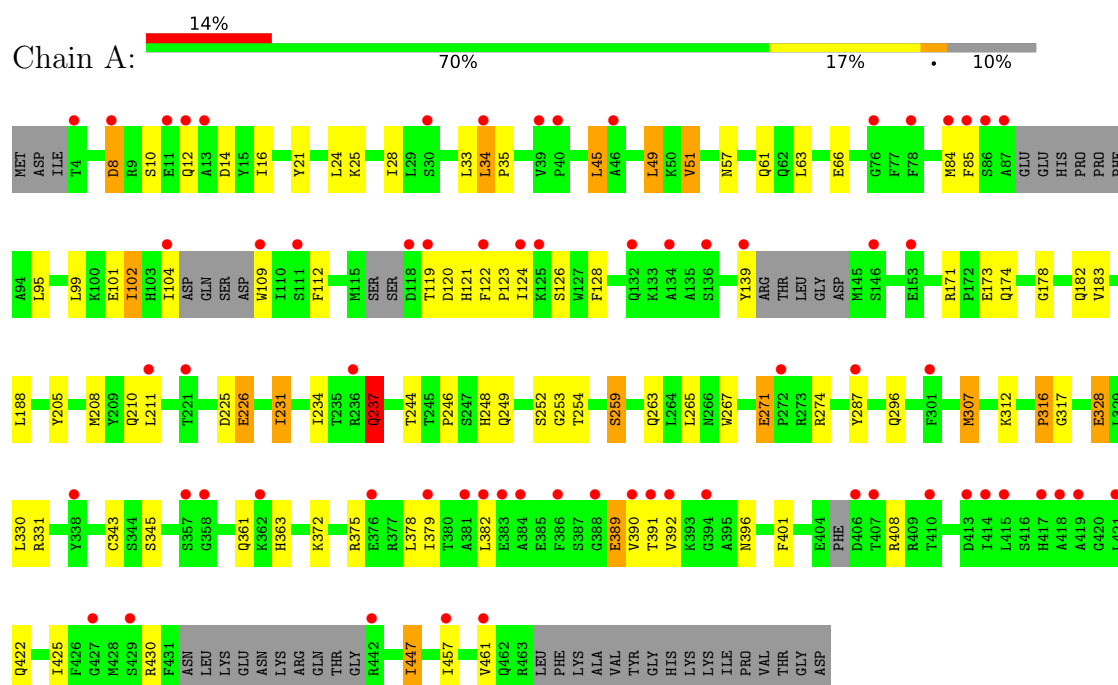
- Molecule 2 is water.

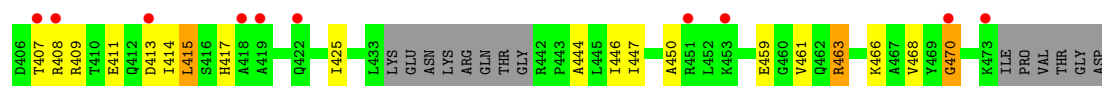
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	97	Total	O	0	0
			97	97		
2	B	120	Total	O	0	0
			120	120		
2	C	181	Total	O	0	0
			181	181		
2	D	165	Total	O	0	0
			165	165		

3 Residue-property plots

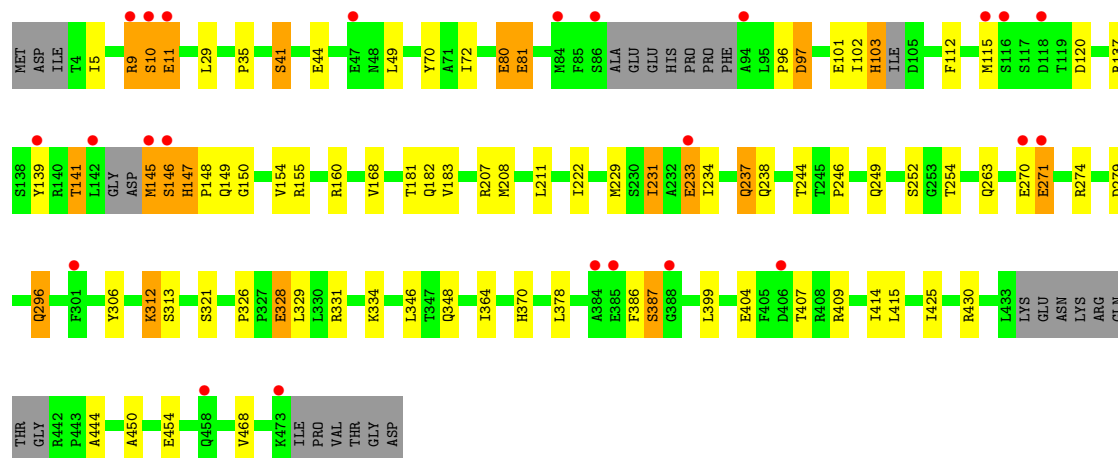
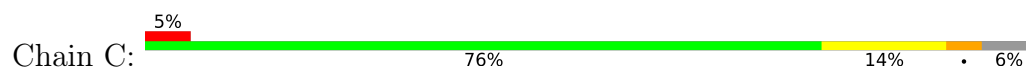
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: HTH-type transcriptional regulatory protein GabR

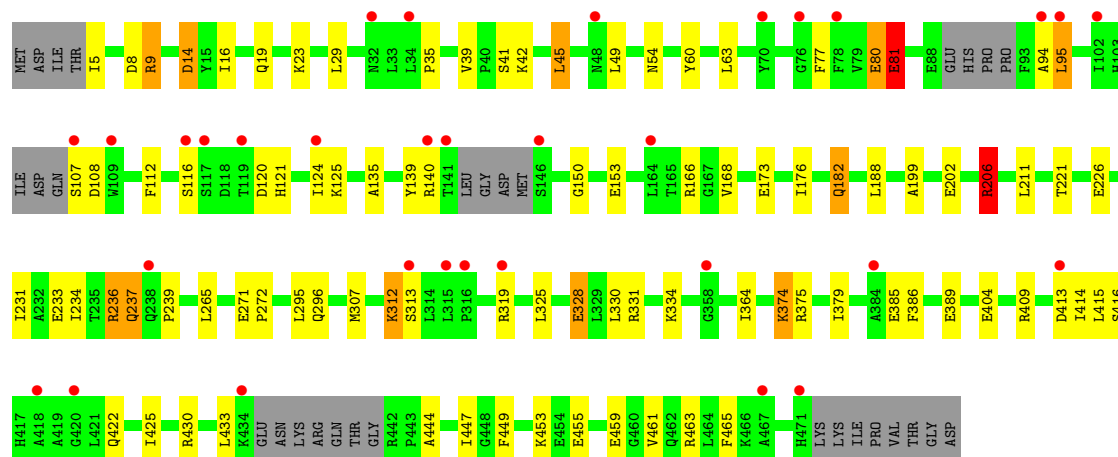
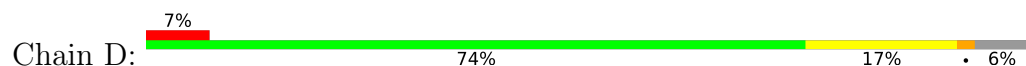




- Molecule 1: HTH-type transcriptional regulatory protein GabR



- Molecule 1: HTH-type transcriptional regulatory protein GabR



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	97.83Å 101.56Å 212.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.67 – 2.05 47.67 – 2.05	Depositor EDS
% Data completeness (in resolution range)	97.3 (47.67-2.05) 97.3 (47.67-2.05)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.53 (at 2.05Å)	Xtriage
Refinement program	REFMAC refmac_5.7.0032, REFMAC, REFMAC5	Depositor
R, R_{free}	0.231 , 0.284 0.230 , 0.283	Depositor DCC
R_{free} test set	6564 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	43.3	Xtriage
Anisotropy	0.473	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 45.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.013 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14499	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.81% 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	0.61	0/3380	0.91	4/4573 (0.1%)
1	B	0.62	0/3411	0.92	5/4606 (0.1%)
1	C	0.72	0/3666	0.96	7/4947 (0.1%)
1	D	0.72	0/3638	0.96	5/4910 (0.1%)
All	All	0.67	0/14095	0.94	21/19036 (0.1%)

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	80	GLU	N-CA-C	9.49	121.71	111.36
1	D	237	GLN	N-CA-C	-8.69	99.07	110.53
1	D	150	GLY	N-CA-C	-7.96	104.39	111.95
1	D	80	GLU	N-CA-C	7.79	120.86	111.82
1	A	237	GLN	N-CA-C	-6.86	100.83	110.50
1	B	80	GLU	N-CA-C	6.67	118.21	111.07
1	A	237	GLN	CA-C-N	-6.49	115.17	123.16
1	A	237	GLN	C-N-CA	-6.49	115.17	123.16
1	C	237	GLN	CA-C-N	-6.18	115.67	123.15
1	C	237	GLN	C-N-CA	-6.18	115.67	123.15
1	D	433	LEU	N-CA-C	-5.80	105.87	113.12
1	C	150	GLY	N-CA-C	-5.71	106.52	111.95
1	B	326	PRO	O-C-N	5.39	123.69	121.15
1	D	206	ARG	N-CA-C	5.27	116.71	111.07
1	C	181	THR	N-CA-C	5.25	117.00	111.28
1	C	155	ARG	NE-CZ-NH2	-5.24	114.48	119.20
1	C	9	ARG	N-CA-C	5.20	121.87	110.80
1	B	147	HIS	CA-C-N	5.17	124.96	119.28
1	B	147	HIS	C-N-CA	5.17	124.96	119.28
1	B	111	SER	N-CA-C	5.15	116.78	108.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	183	VAL	CB-CA-C	-5.03	105.35	112.14

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	3344	0	3212	68	0
1	B	3373	0	3265	63	0
1	C	3623	0	3576	59	0
1	D	3596	0	3537	46	0
2	A	97	0	0	2	0
2	B	120	0	0	6	0
2	C	181	0	0	14	0
2	D	165	0	0	6	0
All	All	14499	0	13590	225	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 8.

All (225) 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:312:LLP:H6	2:C:666:HOH:O	1.48	1.11
1:A:16:ILE:HG21	1:A:51:VAL:HG11	1.42	0.99
1:D:328:GLU:HG3	2:D:646:HOH:O	1.62	0.97
1:A:51:VAL:HG12	2:A:576:HOH:O	1.70	0.90
1:D:80:GLU:O	1:D:81:GLU:HB3	1.73	0.89
1:C:208:MET:CE	2:C:636:HOH:O	2.22	0.88
1:B:379:ILE:O	1:B:383:GLU:HG2	1.78	0.84
1:D:331:ARG:NH1	2:D:658:HOH:O	2.01	0.81
1:A:267:TRP:NE1	1:A:274:ARG:NH1	2.29	0.81
1:A:267:TRP:CE2	1:A:274:ARG:NH1	2.49	0.80
1:C:370:HIS:HE1	2:C:676:HOH:O	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:103:HIS:HB2	2:C:672:HOH:O	1.82	0.78
1:A:271:GLU:HG3	1:A:274:ARG:HH21	1.48	0.78
1:C:407:THR:HG22	1:C:409:ARG:H	1.50	0.77
1:C:147:HIS:HD2	1:C:149:GLN:H	1.30	0.77
1:A:57:ASN:O	1:A:61:GLN:HG2	1.83	0.77
1:C:312:LLP:C6	2:C:666:HOH:O	2.16	0.75
1:C:80:GLU:O	1:C:81:GLU:HB3	1.87	0.73
1:B:417:HIS:CE1	1:B:470:GLY:HA2	2.24	0.73
1:A:328:GLU:HA	1:A:331:ARG:HG3	1.69	0.73
1:B:185:MET:HE1	1:B:277:ILE:HD13	1.72	0.71
1:C:244:THR:HG23	1:C:246:PRO:HD3	1.72	0.70
1:B:80:GLU:O	1:B:81:GLU:HB3	1.92	0.70
1:D:233:GLU:CG	1:D:237:GLN:HE21	2.05	0.70
1:C:208:MET:HE1	2:C:636:HOH:O	1.88	0.69
1:D:5:ILE:N	2:D:640:HOH:O	2.25	0.69
1:C:249:GLN:HB3	1:C:252:SER:O	1.94	0.67
1:A:378:LEU:HD12	1:A:401:PHE:HZ	1.60	0.67
1:D:42:LYS:HD3	2:D:649:HOH:O	1.94	0.66
1:D:234:ILE:O	1:D:237:GLN:O	2.12	0.66
1:B:411:GLU:O	1:B:415:LEU:HD22	1.96	0.66
1:C:234:ILE:O	1:C:237:GLN:O	2.13	0.66
1:B:403:THR:HG23	1:B:405:PHE:CE2	2.31	0.66
1:C:182:GLN:HG3	1:C:183:VAL:H	1.62	0.65
1:D:236:ARG:NE	1:D:236:ARG:HA	2.12	0.64
1:A:271:GLU:HB2	1:A:274:ARG:HE	1.63	0.64
1:C:182:GLN:HG3	1:C:183:VAL:N	2.12	0.64
1:A:120:ASP:O	1:A:122:PHE:N	2.28	0.64
1:B:57:ASN:O	1:B:61:GLN:HG2	1.98	0.63
1:B:459:GLU:OE1	1:B:463:ARG:NH1	2.32	0.63
1:A:99:LEU:HD21	1:B:331:ARG:HG2	1.82	0.60
1:C:222:ILE:HG23	1:C:233:GLU:HG2	1.84	0.60
1:A:378:LEU:HD12	1:A:401:PHE:CZ	2.37	0.58
1:B:403:THR:HG23	1:B:405:PHE:CZ	2.38	0.58
1:A:84:MET:HE3	1:B:266:ASN:HD21	1.67	0.58
1:D:271:GLU:HG3	1:D:272:PRO:HD2	1.86	0.57
1:A:109:TRP:CD1	1:A:422:GLN:HG3	2.39	0.57
1:D:409:ARG:HD3	1:D:413:ASP:HB3	1.87	0.57
1:D:45:LEU:HD23	1:D:49:LEU:HG	1.86	0.57
1:D:135:ALA:O	1:D:139:TYR:HB2	2.05	0.57
1:C:80:GLU:O	1:C:80:GLU:OE2	2.22	0.56
1:D:233:GLU:HG3	1:D:237:GLN:HE21	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:8:ASP:O	1:D:9:ARG:HB2	2.06	0.56
1:A:112:PHE:HB2	1:A:425:ILE:HD13	1.87	0.56
1:A:234:ILE:O	1:A:237:GLN:O	2.23	0.56
1:A:267:TRP:CZ2	1:A:274:ARG:NH1	2.70	0.56
1:C:145:MET:O	1:C:146:SER:C	2.48	0.56
1:A:101:GLU:HB2	1:B:173:GLU:HG3	1.86	0.55
1:A:123:PRO:HB2	1:A:126:SER:OG	2.06	0.55
1:B:166:ARG:HB2	1:B:168:VAL:HG23	1.89	0.55
1:D:374:LYS:HE3	1:D:449:PHE:O	2.07	0.55
1:D:5:ILE:HG12	1:D:23:LYS:HG2	1.89	0.55
1:B:233:GLU:HG2	1:B:237:GLN:HE21	1.72	0.55
1:C:10:SER:O	1:C:11:GLU:O	2.25	0.55
1:A:244:THR:HG23	1:A:246:PRO:HD3	1.89	0.55
1:C:145:MET:SD	1:D:319:ARG:HD3	2.46	0.55
1:C:312:LLP:OP1	1:C:321:SER:OG	2.24	0.55
1:D:112:PHE:HD2	1:D:425:ILE:HD12	1.72	0.54
1:C:29:LEU:HD11	2:C:645:HOH:O	2.07	0.54
1:C:252:SER:O	1:C:252:SER:OG	2.26	0.54
1:A:45:LEU:HD22	1:A:49:LEU:HD22	1.89	0.54
1:B:154:VAL:HG21	1:B:348:GLN:HB3	1.89	0.54
1:C:399:LEU:HD13	1:C:450:ALA:HB2	1.90	0.54
1:A:389:GLU:O	1:A:391:THR:N	2.38	0.54
1:B:119:THR:CG2	1:B:316:PRO:HG2	2.38	0.54
1:A:10:SER:O	1:A:12:GLN:OE1	2.26	0.53
1:D:404:GLU:HG2	1:D:444:ALA:HB2	1.90	0.53
1:C:97:ASP:OD1	1:C:97:ASP:N	2.42	0.53
1:B:312:LLP:H4'1	2:B:601:HOH:O	2.09	0.52
1:B:403:THR:HB	1:B:447:ILE:HD13	1.92	0.52
1:A:119:THR:HA	1:A:316:PRO:HG3	1.91	0.52
1:C:137:ARG:NH2	2:C:530:HOH:O	2.43	0.52
1:A:226:GLU:CD	1:A:226:GLU:H	2.17	0.51
1:B:119:THR:HG22	1:B:316:PRO:HG2	1.92	0.51
1:B:267:TRP:CZ2	1:B:274:ARG:HD2	2.45	0.51
1:A:287:TYR:HB3	1:A:372:LYS:HG3	1.93	0.51
1:C:35:PRO:HB3	1:C:81:GLU:HB2	1.92	0.51
1:C:296:GLN:HG2	1:C:306:TYR:HB2	1.91	0.51
1:A:21:TYR:CD1	1:A:25:LYS:HE3	2.46	0.51
1:B:270:GLU:HG3	1:B:274:ARG:HH21	1.75	0.51
1:B:361:GLN:HG2	2:B:578:HOH:O	2.10	0.51
1:A:84:MET:HE3	1:A:85:PHE:H	1.75	0.50
1:A:112:PHE:CB	1:A:425:ILE:HD13	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:ILE:HG13	1:A:263:GLN:HB3	1.92	0.50
1:A:378:LEU:CD1	1:A:401:PHE:HZ	2.22	0.50
1:C:414:ILE:HG12	1:C:468:VAL:HA	1.92	0.50
1:D:45:LEU:HD12	1:D:60:TYR:OH	2.10	0.50
1:A:252:SER:O	1:A:252:SER:OG	2.29	0.50
1:A:259:SER:HB3	2:B:549:HOH:O	2.11	0.50
1:B:95:LEU:HB3	1:B:100:LYS:HE3	1.93	0.50
1:B:288:ASP:CG	1:B:396:ASN:HD22	2.19	0.50
1:C:404:GLU:HG2	1:C:444:ALA:HB2	1.94	0.50
1:C:154:VAL:HG21	1:C:348:GLN:HB3	1.94	0.50
1:A:84:MET:HG3	1:A:85:PHE:N	2.27	0.50
1:B:260:ARG:NH1	2:B:602:HOH:O	2.45	0.49
1:A:252:SER:O	1:A:254:THR:N	2.33	0.49
1:A:361:GLN:HG3	2:A:551:HOH:O	2.12	0.49
1:C:101:GLU:HB2	1:D:173:GLU:HG3	1.93	0.49
1:A:317:GLY:O	1:B:344:SER:HA	2.13	0.49
1:B:35:PRO:HB3	1:B:81:GLU:HB2	1.95	0.49
1:D:385:GLU:HG3	1:D:461:VAL:HG12	1.95	0.49
1:D:422:GLN:NE2	2:D:501:HOH:O	2.27	0.49
1:A:123:PRO:HD3	1:A:363:HIS:ND1	2.28	0.49
1:B:225:ASP:OD2	1:B:260:ARG:NH2	2.46	0.49
1:D:459:GLU:O	1:D:463:ARG:HG3	2.13	0.48
1:A:8:ASP:C	1:A:10:SER:H	2.21	0.48
1:A:389:GLU:O	1:A:389:GLU:HG3	2.11	0.48
1:A:447:ILE:O	1:A:447:ILE:HG13	2.13	0.48
1:C:146:SER:HB2	2:C:664:HOH:O	2.12	0.48
1:B:331:ARG:HD2	2:B:588:HOH:O	2.13	0.48
1:D:35:PRO:HB3	1:D:81:GLU:HB2	1.95	0.48
1:C:182:GLN:NE2	2:C:641:HOH:O	2.46	0.48
1:B:31:ARG:HE	1:B:84:MET:HG2	1.78	0.48
1:A:66:GLU:HG2	1:B:292:ILE:HG12	1.95	0.47
1:D:312:LLP:P	1:D:319:ARG:HE	2.37	0.47
1:D:120:ASP:O	1:D:121:HIS:HB2	2.13	0.47
1:D:39:VAL:CG2	1:D:77:PHE:HB2	2.44	0.47
1:A:375:ARG:NH1	1:A:396:ASN:OD1	2.48	0.47
1:A:248:HIS:O	1:A:249:GLN:C	2.57	0.47
1:C:346:LEU:HB3	2:C:623:HOH:O	2.14	0.47
1:C:168:VAL:HG22	1:C:296:GLN:HG3	1.96	0.47
1:C:182:GLN:HG2	2:C:659:HOH:O	2.13	0.47
1:D:202:GLU:HB2	1:D:221:THR:HB	1.97	0.47
1:C:270:GLU:O	1:C:271:GLU:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:VAL:N	1:B:77:PHE:O	2.48	0.47
1:A:225:ASP:HB2	1:A:226:GLU:OE2	2.15	0.46
1:C:145:MET:HE3	1:C:145:MET:N	2.30	0.46
1:C:274:ARG:HG2	1:C:274:ARG:HH11	1.80	0.46
1:A:331:ARG:HG2	1:B:99:LEU:HD21	1.96	0.46
1:B:260:ARG:NH1	1:B:263:GLN:OE1	2.46	0.46
1:A:120:ASP:C	1:A:122:PHE:H	2.19	0.46
1:B:181:THR:HG23	1:B:307:MET:HE2	1.98	0.46
1:A:21:TYR:HD1	1:A:25:LYS:HE3	1.79	0.46
1:B:123:PRO:HB2	1:B:126:SER:OG	2.15	0.46
1:B:403:THR:O	1:B:403:THR:CG2	2.63	0.46
1:C:231:ILE:HG13	1:C:263:GLN:HB3	1.98	0.46
1:A:101:GLU:HB2	1:B:173:GLU:CG	2.45	0.46
1:B:155:ARG:CG	1:B:175:MET:HB3	2.46	0.46
1:B:244:THR:HG23	1:B:246:PRO:HD3	1.98	0.46
1:C:96:PRO:HD3	2:C:648:HOH:O	2.16	0.46
1:C:115:MET:SD	1:C:207:ARG:NH2	2.89	0.45
1:A:249:GLN:HB3	1:A:252:SER:O	2.16	0.45
1:C:279:ASP:OD2	1:C:312:LLP:H2'3	2.17	0.45
1:B:404:GLU:HG2	1:B:444:ALA:HB2	1.99	0.45
1:B:200:MET:HG2	1:B:243:VAL:HB	1.99	0.45
1:D:206:ARG:HG3	1:D:430:ARG:O	2.17	0.45
1:A:124:ILE:HG12	1:A:128:PHE:CE2	2.52	0.45
1:A:307:MET:HE2	1:A:307:MET:HB3	1.81	0.45
1:B:446:ILE:C	1:B:447:ILE:HD12	2.42	0.45
1:D:409:ARG:HD3	1:D:413:ASP:CB	2.46	0.45
1:D:80:GLU:O	1:D:80:GLU:OE2	2.35	0.44
1:A:205:TYR:HD2	1:A:208:MET:HE2	1.82	0.44
1:A:267:TRP:CZ2	1:A:274:ARG:HD3	2.53	0.44
1:B:227:LYS:HG2	1:B:257:PRO:HG3	2.00	0.44
1:C:5:ILE:HB	1:C:49:LEU:HD11	2.00	0.44
1:C:112:PHE:HB2	1:C:425:ILE:HG22	2.00	0.44
1:D:166:ARG:HB2	1:D:168:VAL:HG23	1.99	0.44
1:D:313:SER:HB2	1:D:364:ILE:HD11	1.99	0.44
1:A:174:GLN:HA	1:A:330:LEU:HD22	2.00	0.44
1:A:378:LEU:HD11	1:A:447:ILE:HD11	1.99	0.44
1:B:80:GLU:O	1:B:81:GLU:CB	2.65	0.44
1:C:41:SER:HB2	1:C:44:GLU:CD	2.42	0.44
1:A:12:GLN:C	1:A:14:ASP:H	2.26	0.43
1:C:160:ARG:NH1	2:C:502:HOH:O	2.48	0.43
1:D:233:GLU:CD	1:D:237:GLN:HE21	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:375:ARG:O	1:D:379:ILE:HG12	2.18	0.43
1:C:270:GLU:O	1:C:271:GLU:CB	2.66	0.43
1:B:414:ILE:HG12	1:B:468:VAL:HA	2.00	0.43
1:C:147:HIS:HA	1:C:148:PRO:HD3	1.96	0.43
1:D:135:ALA:O	1:D:139:TYR:CB	2.66	0.43
1:C:80:GLU:O	1:C:81:GLU:CB	2.55	0.43
1:C:328:GLU:O	1:C:331:ARG:HB2	2.17	0.43
1:B:45:LEU:HD22	2:B:589:HOH:O	2.18	0.43
1:B:147:HIS:HA	1:B:148:PRO:HD3	1.85	0.43
1:C:326:PRO:HD2	1:C:329:LEU:HD12	2.01	0.43
1:D:386:PHE:CZ	1:D:465:PHE:HA	2.53	0.43
1:B:158:ILE:HG22	1:B:175:MET:HE1	2.00	0.43
1:A:375:ARG:NH1	1:A:396:ASN:HA	2.34	0.42
1:D:182:GLN:HG3	1:D:319:ARG:HH22	1.84	0.42
1:B:117:SER:HB3	1:B:450:ALA:HB1	2.01	0.42
1:A:34:LEU:HA	1:A:35:PRO:HD3	1.94	0.42
1:A:171:ARG:HB3	1:A:173:GLU:OE1	2.19	0.42
1:B:168:VAL:HG13	1:B:296:GLN:CD	2.44	0.42
1:B:202:GLU:HB2	1:B:221:THR:HB	2.02	0.42
1:C:252:SER:O	1:C:254:THR:N	2.50	0.42
1:A:457:ILE:O	1:A:461:VAL:HG23	2.20	0.42
1:B:12:GLN:O	1:B:13:ALA:HB3	2.20	0.42
1:A:178:GLY:C	1:A:343:CYS:SG	3.03	0.42
1:A:345:SER:OG	1:B:317:GLY:HA3	2.20	0.42
1:D:14:ASP:HB2	1:D:19:GLN:HG3	2.02	0.42
1:A:24:LEU:O	1:A:28:ILE:HG13	2.20	0.41
1:A:267:TRP:HE1	1:A:274:ARG:HH12	1.68	0.41
1:B:11:GLU:HG2	1:B:15:TYR:HA	2.01	0.41
1:B:96:PRO:HG2	1:B:99:LEU:HD22	2.01	0.41
1:B:385:GLU:HG3	1:B:461:VAL:HG12	2.02	0.41
1:B:466:LYS:O	1:B:470:GLY:N	2.54	0.41
1:C:41:SER:HB3	1:C:44:GLU:H	1.85	0.41
1:C:313:SER:HB3	1:C:364:ILE:HD11	2.03	0.41
1:A:389:GLU:C	1:A:391:THR:H	2.26	0.41
1:B:229:MET:HG2	1:B:234:ILE:HD11	2.03	0.41
1:B:307:MET:HE2	1:B:307:MET:HB3	1.96	0.41
1:D:176:ILE:HD11	1:D:325:LEU:HD11	2.02	0.41
1:D:307:MET:HE2	1:D:307:MET:HB3	1.68	0.41
1:C:70:TYR:HE1	1:C:72:ILE:HD11	1.86	0.41
1:D:233:GLU:OE1	1:D:237:GLN:NE2	2.51	0.41
1:D:409:ARG:HD2	1:D:414:ILE:HG13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:TYR:CE1	1:B:124:ILE:HD12	2.56	0.40
1:A:102:ILE:H	1:A:102:ILE:HG13	1.60	0.40
1:D:199:ALA:HB2	1:D:239:PRO:HB3	2.03	0.40
1:B:309:THR:HG21	1:B:312:LLP:H5'2	2.03	0.40
1:C:222:ILE:HG13	1:C:229:MET:HE2	2.02	0.40
1:C:386:PHE:O	1:C:387:SER:C	2.64	0.40
1:B:409:ARG:CZ	1:B:413:ASP:HB3	2.52	0.40
1:C:328:GLU:H	1:C:328:GLU:HG3	1.37	0.40
1:D:182:GLN:HG3	2:D:642:HOH:O	2.20	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	417/479 (87%)	377 (90%)	33 (8%)	7 (2%)	7	2
1	B	413/479 (86%)	384 (93%)	21 (5%)	8 (2%)	6	2
1	C	441/479 (92%)	418 (95%)	14 (3%)	9 (2%)	6	1
1	D	438/479 (91%)	411 (94%)	20 (5%)	7 (2%)	7	2
All	All	1709/1916 (89%)	1590 (93%)	88 (5%)	31 (2%)	6	2

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	HIS
1	A	390	VAL
1	B	407	THR
1	C	11	GLU
1	C	139	TYR
1	C	387	SER

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Mol	Chain	Res	Type
1	D	94	ALA
1	D	140	ARG
1	A	253	GLY
1	B	36	HIS
1	B	120	ASP
1	B	271	GLU
1	C	81	GLU
1	C	146	SER
1	D	108	ASP
1	B	81	GLU
1	C	271	GLU
1	D	9	ARG
1	D	116	SER
1	A	316	PRO
1	C	141	THR
1	C	147	HIS
1	D	81	GLU
1	D	95	LEU
1	A	34	LEU
1	A	408	ARG
1	B	116	SER
1	B	408	ARG
1	C	9	ARG
1	B	470	GLY
1	A	271	GLU

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	335/424 (79%)	308 (92%)	27 (8%)	11	5
1	B	347/424 (82%)	323 (93%)	24 (7%)	14	8
1	C	386/424 (91%)	367 (95%)	19 (5%)	22	15
1	D	383/424 (90%)	350 (91%)	33 (9%)	10	4
All	All	1451/1696 (86%)	1348 (93%)	103 (7%)	13	7

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ASP
1	A	33	LEU
1	A	45	LEU
1	A	49	LEU
1	A	51	VAL
1	A	63	LEU
1	A	95	LEU
1	A	102	ILE
1	A	104	ILE
1	A	182	GLN
1	A	188	LEU
1	A	210	GLN
1	A	211	LEU
1	A	226	GLU
1	A	231	ILE
1	A	237	GLN
1	A	259	SER
1	A	265	LEU
1	A	296	GLN
1	A	307	MET
1	A	328	GLU
1	A	379	ILE
1	A	382	LEU
1	A	389	GLU
1	A	392	VAL
1	A	430	ARG
1	A	447	ILE
1	B	21	TYR
1	B	29	LEU
1	B	33	LEU
1	B	45	LEU
1	B	51	VAL
1	B	63	LEU
1	B	99	LEU
1	B	107	SER
1	B	115	MET
1	B	117	SER
1	B	155	ARG
1	B	207	ARG
1	B	223	MET
1	B	231	ILE
1	B	295	LEU

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Mol	Chain	Res	Type
1	B	296	GLN
1	B	300	ARG
1	B	327	PRO
1	B	328	GLU
1	B	330	LEU
1	B	403	THR
1	B	415	LEU
1	B	425	ILE
1	B	463	ARG
1	C	10	SER
1	C	41	SER
1	C	97	ASP
1	C	102	ILE
1	C	103	HIS
1	C	120	ASP
1	C	141	THR
1	C	145	MET
1	C	211	LEU
1	C	231	ILE
1	C	233	GLU
1	C	238	GLN
1	C	296	GLN
1	C	328	GLU
1	C	334	LYS
1	C	378	LEU
1	C	415	LEU
1	C	430	ARG
1	C	454	GLU
1	D	14	ASP
1	D	16	ILE
1	D	29	LEU
1	D	41	SER
1	D	45	LEU
1	D	54	ASN
1	D	63	LEU
1	D	81	GLU
1	D	95	LEU
1	D	107	SER
1	D	124	ILE
1	D	125	LYS
1	D	153	GLU
1	D	182	GLN

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Mol	Chain	Res	Type
1	D	188	LEU
1	D	206	ARG
1	D	211	LEU
1	D	226	GLU
1	D	231	ILE
1	D	236	ARG
1	D	265	LEU
1	D	295	LEU
1	D	296	GLN
1	D	328	GLU
1	D	330	LEU
1	D	334	LYS
1	D	374	LYS
1	D	389	GLU
1	D	415	LEU
1	D	416	SER
1	D	447	ILE
1	D	453	LYS
1	D	455	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	61	GLN
1	A	121	HIS
1	A	182	GLN
1	A	210	GLN
1	A	248	HIS
1	A	369	GLN
1	B	32	ASN
1	B	149	GLN
1	B	214	ASN
1	B	237	GLN
1	B	266	ASN
1	B	396	ASN
1	B	417	HIS
1	C	57	ASN
1	C	121	HIS
1	C	147	HIS
1	C	149	GLN
1	C	214	ASN

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Mol	Chain	Res	Type
1	C	218	GLN
1	C	370	HIS
1	C	462	GLN
1	D	22	GLN
1	D	32	ASN
1	D	57	ASN
1	D	61	GLN
1	D	214	ASN
1	D	218	GLN
1	D	335	GLN
1	D	422	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	312	1	23,24,25	2.76	5 (21%)	25,32,34	1.49	5 (20%)
1	LLP	B	312	1	23,24,25	2.71	5 (21%)	25,32,34	1.70	6 (24%)
1	LLP	D	312	1	23,24,25	2.93	6 (26%)	25,32,34	1.72	7 (28%)
1	LLP	A	312	1	23,24,25	2.72	5 (21%)	25,32,34	1.46	4 (16%)

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	312	1	-	7/16/17/19	0/1/1/1
1	LLP	B	312	1	-	8/16/17/19	0/1/1/1
1	LLP	D	312	1	-	7/16/17/19	0/1/1/1
1	LLP	A	312	1	-	11/16/17/19	0/1/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	312	LLP	C3-C2	7.80	1.49	1.41
1	D	312	LLP	C3-C2	7.59	1.48	1.41
1	D	312	LLP	C4-C5	6.99	1.51	1.42
1	C	312	LLP	C4-C5	6.93	1.51	1.42
1	A	312	LLP	C4-C5	6.66	1.51	1.42
1	A	312	LLP	C3-C2	6.45	1.47	1.41
1	C	312	LLP	C3-C2	6.01	1.47	1.41
1	C	312	LLP	C4'-NZ	5.96	1.47	1.27
1	A	312	LLP	C4-C3	5.88	1.50	1.41
1	B	312	LLP	C4'-NZ	5.78	1.46	1.27
1	D	312	LLP	C4'-NZ	5.75	1.46	1.27
1	B	312	LLP	C4-C5	5.66	1.49	1.42
1	D	312	LLP	C4-C3	5.64	1.50	1.41
1	C	312	LLP	C4-C3	5.62	1.50	1.41
1	A	312	LLP	C4'-NZ	5.56	1.45	1.27
1	B	312	LLP	C4-C3	5.06	1.49	1.41
1	A	312	LLP	C4-C4'	3.14	1.53	1.46
1	D	312	LLP	C4-C4'	2.93	1.52	1.46
1	C	312	LLP	C4-C4'	2.91	1.52	1.46
1	D	312	LLP	C6-C5	2.34	1.42	1.37
1	B	312	LLP	C4-C4'	2.24	1.51	1.46

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	312	LLP	OP4-C5'-C5	4.72	118.20	109.36
1	D	312	LLP	OP4-C5'-C5	4.27	117.36	109.36
1	B	312	LLP	C4-C4'-NZ	-3.45	108.13	124.04
1	D	312	LLP	C4-C4'-NZ	-3.43	108.21	124.04
1	A	312	LLP	C4-C3-C2	-3.36	118.25	120.14
1	C	312	LLP	C4-C4'-NZ	-3.13	109.58	124.04
1	B	312	LLP	C4-C3-C2	-3.00	118.46	120.14
1	A	312	LLP	C6-N1-C2	2.71	124.11	119.20
1	C	312	LLP	OP4-C5'-C5	2.66	114.34	109.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	312	LLP	OP3-P-OP4	-2.65	99.77	106.67
1	A	312	LLP	C4-C4'-NZ	-2.57	112.20	124.04
1	C	312	LLP	C2'-C2-C3	-2.55	117.81	120.80
1	D	312	LLP	C4-C3-C2	-2.46	118.76	120.14
1	C	312	LLP	C2'-C2-N1	2.40	122.17	117.64
1	B	312	LLP	C6-N1-C2	2.38	123.51	119.20
1	D	312	LLP	C6-N1-C2	2.27	123.31	119.20
1	B	312	LLP	OP3-P-OP4	-2.25	100.80	106.67
1	D	312	LLP	OP3-P-OP2	2.25	116.24	107.80
1	D	312	LLP	C2'-C2-N1	2.13	121.65	117.64
1	B	312	LLP	OP3-P-OP2	2.10	115.66	107.80
1	A	312	LLP	C2'-C2-N1	2.08	121.56	117.64
1	C	312	LLP	C3-C4-C5	-2.01	116.66	118.28

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	312	LLP	C4-C4'-NZ-CE
1	A	312	LLP	O-C-CA-CB
1	A	312	LLP	CG-CD-CE-NZ
1	B	312	LLP	C4-C4'-NZ-CE
1	B	312	LLP	C4-C5-C5'-OP4
1	B	312	LLP	C6-C5-C5'-OP4
1	B	312	LLP	O-C-CA-CB
1	C	312	LLP	C5'-OP4-P-OP2
1	C	312	LLP	C5'-OP4-P-OP3
1	D	312	LLP	C5'-OP4-P-OP2
1	D	312	LLP	C5'-OP4-P-OP3
1	C	312	LLP	C4-C4'-NZ-CE
1	A	312	LLP	C3-C4-C4'-NZ
1	B	312	LLP	C3-C4-C4'-NZ
1	A	312	LLP	CA-CB-CG-CD
1	C	312	LLP	C3-C4-C4'-NZ
1	D	312	LLP	CA-CB-CG-CD
1	C	312	LLP	C5'-OP4-P-OP1
1	D	312	LLP	C5'-OP4-P-OP1
1	C	312	LLP	C5-C4-C4'-NZ
1	A	312	LLP	CE-CD-CG-CB
1	D	312	LLP	C3-C4-C4'-NZ
1	A	312	LLP	C5'-OP4-P-OP3
1	B	312	LLP	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
1	B	312	LLP	CD-CE-NZ-C4'
1	A	312	LLP	N-CA-CB-CG
1	C	312	LLP	CD-CE-NZ-C4'
1	A	312	LLP	CD-CE-NZ-C4'
1	B	312	LLP	CE-CD-CG-CB
1	D	312	LLP	C5-C4-C4'-NZ
1	A	312	LLP	C6-C5-C5'-OP4
1	D	312	LLP	CE-CD-CG-CB
1	A	312	LLP	C-CA-CB-CG

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	312	LLP	4	0
1	B	312	LLP	2	0
1	D	312	LLP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	431/479 (89%)	1.04	67 (15%) 5 4	32, 58, 98, 114	0
1	B	429/479 (89%)	0.93	57 (13%) 7 6	35, 56, 84, 115	1 (0%)
1	C	451/479 (94%)	0.51	24 (5%) 32 32	30, 45, 73, 99	1 (0%)
1	D	448/479 (93%)	0.61	32 (7%) 22 22	29, 46, 76, 105	1 (0%)
All	All	1759/1916 (91%)	0.77	180 (10%) 12 12	29, 50, 86, 115	3 (0%)

All (180) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	34	LEU	5.4
1	D	315	LEU	5.4
1	D	316	PRO	5.2
1	A	413	ASP	4.7
1	D	94	ALA	4.5
1	C	270	GLU	4.2
1	A	390	VAL	4.2
1	B	21	TYR	4.1
1	D	124	ILE	4.0
1	A	104	ILE	4.0
1	B	39	VAL	3.9
1	A	85	PHE	3.9
1	B	118	ASP	3.8
1	D	434	LYS	3.6
1	C	139	TYR	3.6
1	A	388	GLY	3.6
1	A	386	PHE	3.6
1	A	376	GLU	3.5
1	C	142	LEU	3.5
1	C	388	GLY	3.5
1	D	418	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	406	ASP	3.4
1	A	381	ALA	3.4
1	A	442	ARG	3.3
1	B	27	GLU	3.3
1	B	50	LYS	3.3
1	A	358	GLY	3.3
1	B	37	SER	3.2
1	A	379	ILE	3.2
1	A	461	VAL	3.2
1	C	384	ALA	3.2
1	B	98	ASP	3.2
1	A	118	ASP	3.1
1	A	407	THR	3.1
1	A	109	TRP	3.1
1	A	383	GLU	3.1
1	A	429	SER	3.1
1	B	40	PRO	3.1
1	B	64	LEU	3.1
1	B	41	SER	3.1
1	D	141	THR	3.0
1	A	13	ALA	3.0
1	B	135	ALA	3.0
1	A	8	ASP	3.0
1	B	109	TRP	3.0
1	C	271	GLU	2.9
1	A	78	PHE	2.9
1	D	146	SER	2.9
1	A	87	ALA	2.9
1	B	407	THR	2.9
1	B	12	GLN	2.9
1	C	145	MET	2.9
1	D	238	GLN	2.9
1	B	473	LYS	2.8
1	D	117	SER	2.8
1	A	457	ILE	2.8
1	B	271	GLU	2.8
1	D	34	LEU	2.8
1	A	84	MET	2.7
1	A	419	ALA	2.7
1	D	471	HIS	2.7
1	B	451	ARG	2.7
1	D	140	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	134	ALA	2.7
1	B	134	ALA	2.7
1	A	4	THR	2.7
1	C	86	SER	2.7
1	C	146	SER	2.7
1	A	357	SER	2.6
1	B	70	TYR	2.6
1	C	473	LYS	2.6
1	B	137	ARG	2.6
1	A	427	GLY	2.6
1	B	19	GLN	2.6
1	A	384	ALA	2.6
1	B	119	THR	2.6
1	B	58	SER	2.6
1	A	139	TYR	2.6
1	B	355	ILE	2.6
1	C	118	ASP	2.6
1	D	116	SER	2.6
1	B	79	VAL	2.6
1	A	410	THR	2.6
1	D	413	ASP	2.6
1	B	54	ASN	2.5
1	A	272	PRO	2.5
1	B	422	GLN	2.5
1	D	164	LEU	2.5
1	B	51	VAL	2.5
1	A	136	SER	2.5
1	A	146	SER	2.5
1	B	59	ALA	2.5
1	B	327	PRO	2.5
1	D	102	ILE	2.5
1	A	12	GLN	2.5
1	C	116	SER	2.5
1	A	418	ALA	2.5
1	A	382	LEU	2.5
1	A	415	LEU	2.5
1	B	418	ALA	2.4
1	B	408	ARG	2.4
1	D	319	ARG	2.4
1	B	102	ILE	2.4
1	C	458	GLN	2.4
1	A	86	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	111	SER	2.4
1	A	119	THR	2.4
1	A	391	THR	2.4
1	D	119	THR	2.4
1	D	467	ALA	2.4
1	D	95	LEU	2.4
1	B	238	GLN	2.4
1	C	406	ASP	2.4
1	C	84	MET	2.4
1	C	47	GLU	2.3
1	A	76	GLY	2.3
1	B	76	GLY	2.3
1	B	78	PHE	2.3
1	A	221	THR	2.3
1	C	385	GLU	2.3
1	C	94	ALA	2.3
1	D	48	ASN	2.3
1	B	387	SER	2.3
1	D	107	SER	2.3
1	A	39	VAL	2.3
1	C	233	GLU	2.3
1	B	65	ALA	2.3
1	B	315	LEU	2.3
1	D	109	TRP	2.3
1	B	453	LYS	2.3
1	A	34	LEU	2.3
1	B	99	LEU	2.3
1	B	17	TYR	2.3
1	A	122	PHE	2.2
1	C	301	PHE	2.2
1	D	32	ASN	2.2
1	A	11	GLU	2.2
1	C	9	ARG	2.2
1	A	362	LYS	2.2
1	A	392	VAL	2.2
1	B	413	ASP	2.2
1	D	358	GLY	2.2
1	B	47	GLU	2.2
1	B	384	ALA	2.2
1	B	419	ALA	2.2
1	A	211	LEU	2.2
1	B	164	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	132	GLN	2.2
1	A	30	SER	2.2
1	C	115	MET	2.2
1	D	384	ALA	2.2
1	B	126	SER	2.2
1	C	10	SER	2.2
1	A	414	ILE	2.1
1	B	13	ALA	2.1
1	A	287	TYR	2.1
1	D	70	TYR	2.1
1	A	40	PRO	2.1
1	B	165	THR	2.1
1	B	301	PHE	2.1
1	D	76	GLY	2.1
1	A	46	ALA	2.1
1	A	153	GLU	2.1
1	A	417	HIS	2.1
1	D	78	PHE	2.1
1	A	421	LEU	2.1
1	C	11	GLU	2.1
1	A	236	ARG	2.1
1	A	301	PHE	2.1
1	B	71	ALA	2.1
1	B	136	SER	2.1
1	A	338	TYR	2.0
1	A	394	GLY	2.0
1	D	420	GLY	2.0
1	A	124	ILE	2.0
1	D	313	SER	2.0
1	A	125	LYS	2.0
1	B	316	PRO	2.0
1	B	470	GLY	2.0
1	B	15	TYR	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	LLP	D	312	24/25	0.76	0.24	51,75,83,85	0
1	LLP	C	312	24/25	0.78	0.21	44,72,82,87	0
1	LLP	A	312	24/25	0.78	0.19	64,85,95,103	0
1	LLP	B	312	24/25	0.80	0.17	50,73,83,87	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.