Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:37 PM GMT

PDB ID	:	4TV7
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)

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

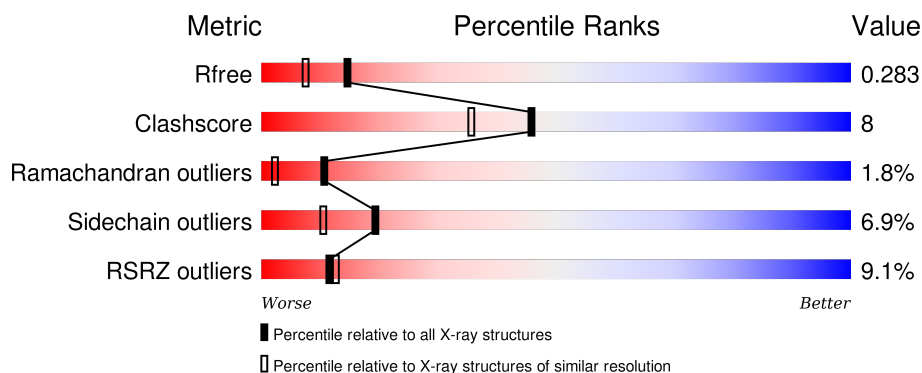|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.05 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	Percentile Ranks	Value
Rfree		0.283
Clashscore		8
Ramachandran outliers		1.8%
Sidechain outliers		6.9%
RSRZ outliers		9.1%

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	1192 (2.04-2.04)
Clashscore	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)
RSRZ outliers	91569	1194 (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 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	479	12% 71% 15% • 10%
1	B	479	11% 68% 19% • 10%
1	C	479	6% 77% 14% • 6%
1	D	479	5% 74% 17% • 6%

2 Entry composition (i)

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 3344	C 2135	N 570	O 621	P 1	S 17	0	0	0
1	B	430	Total 3373	C 2152	N 575	O 629	P 1	S 16	0	0	0
1	C	452	Total 3623	C 2303	N 623	O 679	P 1	S 17	0	0	0
1	D	449	Total 3596	C 2286	N 610	O 683	P 1	S 16	0	0	0

- Molecule 2 is water.

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

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: HTH-type transcriptional regulatory protein GabR
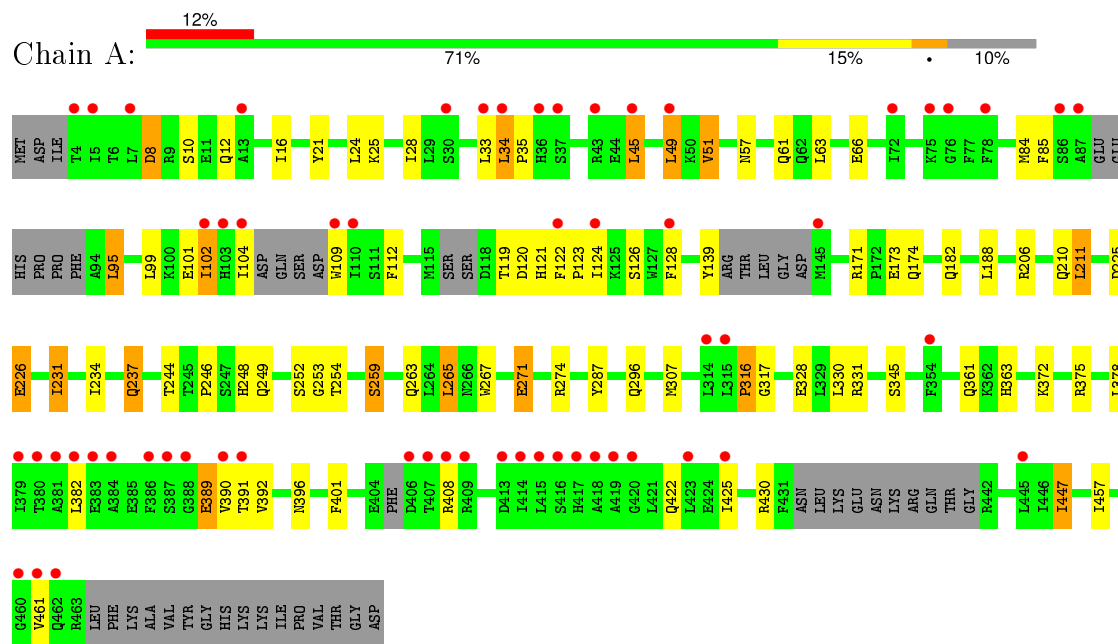
Chain A:

- Molecule 1: HTH-type transcriptional regulatory protein GabR

Chain B:

• Molecule 1: HTH-type transcriptional regulatory protein GabR

Chain C:

• Molecule 1: HTH-type transcriptional regulatory protein GabR

Chain D:
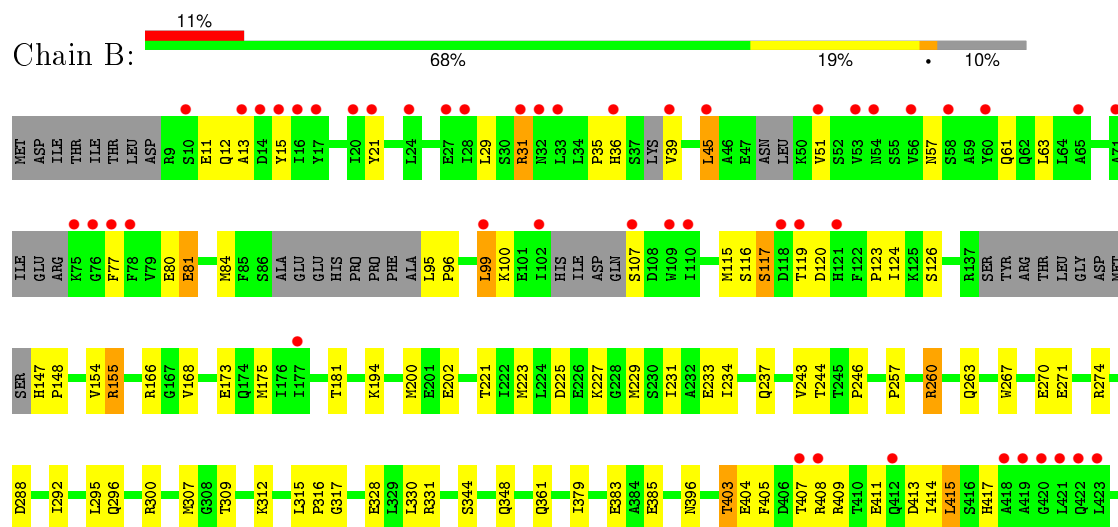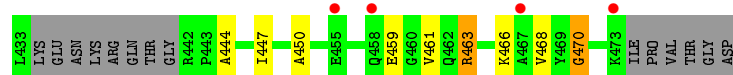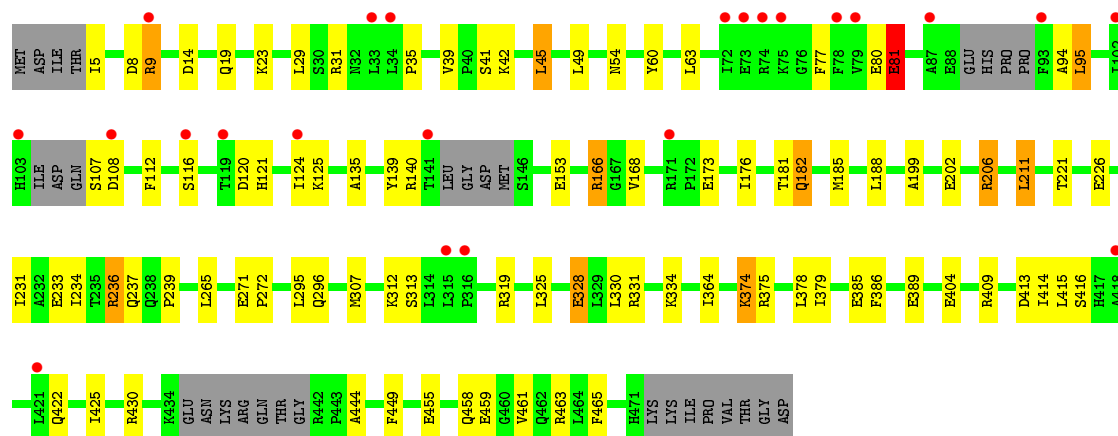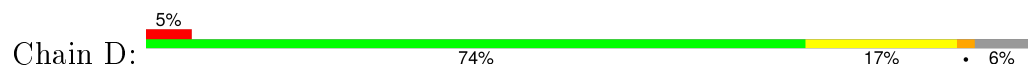
4   Data and refinement statistics (i)

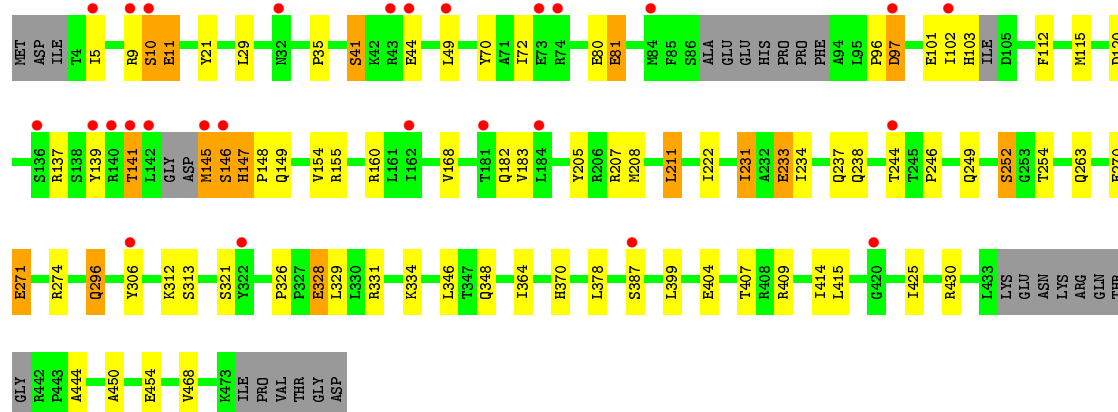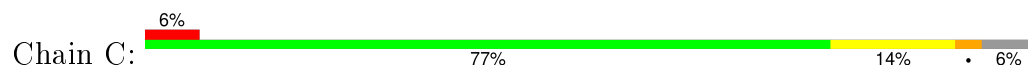| Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	97.83Å 101.56Å 212.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.67 – 2.05 47.67 – 2.05	Depositor EDS
% Data completeness (in resolution range)	97.3 (47.67-2.05) 97.3 (47.67-2.05)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.53 (at 2.05Å)	Xtriage
Refinement program	REFMAC5	Depositor
R, R_{free}	0.231 , 0.284 0.230 , 0.283	Depositor DCC
R_{free} test set	6558 reflections (5.32%)	DCC
Wilson B-factor (Å^2)	43.3	Xtriage
Anisotropy	0.473	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 54.9	EDS
Estimated twinning fraction	0.013 for k,h,-l	Xtriage
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Outliers	0 of 130063 reflections	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.*

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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 ⓘ

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	0.44	0/3380	0.66	3/4573 (0.1%)
1	B	0.46	0/3411	0.66	1/4606 (0.0%)
1	C	0.55	0/3666	0.75	3/4947 (0.1%)
1	D	0.54	0/3638	0.74	3/4910 (0.1%)
All	All	0.50	0/14095	0.71	10/19036 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	155	ARG	NE-CZ-NH2	-11.63	114.48	120.30
1	C	155	ARG	NE-CZ-NH1	10.31	125.46	120.30
1	D	211	LEU	CA-CB-CG	6.83	131.02	115.30
1	A	211	LEU	CA-CB-CG	6.45	130.12	115.30
1	C	211	LEU	CA-CB-CG	6.43	130.09	115.30
1	B	315	LEU	CA-CB-CG	6.22	129.61	115.30
1	D	185	MET	CG-SD-CE	-5.82	90.89	100.20
1	A	265	LEU	CA-CB-CG	5.53	128.01	115.30
1	A	95	LEU	CA-CB-CG	5.13	127.09	115.30
1	D	378	LEU	CA-CB-CG	5.01	126.83	115.30

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	3213	63	0
1	B	3373	0	3267	57	0
1	C	3623	0	3578	55	0
1	D	3596	0	3538	46	0
2	A	97	0	0	2	0
2	B	120	0	0	5	0
2	C	181	0	0	14	0
2	D	165	0	0	6	0
All	All	14499	0	13596	211	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 (211) 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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:5:ILE:N	2:D:640:HOH:O	2.25	0.69
1:C:208:MET:HE1	2:C:636:HOH:O	1.89	0.67
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:234:ILE:O	1:D:237:GLN:O	2.12	0.66
1:D:42:LYS:HD3	2:D:649:HOH:O	1.94	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:A:84:MET:HE2	1:A:85:PHE:H	1.60	0.65
1:D:236:ARG:HA	1:D:236:ARG:NE	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: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:OE2	1:C:80:GLU:O	2.22	0.56
1:D:233:GLU:HG3	1:D:237:GLN:HE21	1.69	0.56
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:267:TRP:CZ2	1:A:274:ARG:NH1	2.70	0.56
1:A:234:ILE:O	1:A:237:GLN:O	2.23	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:D:374:LYS:HE3	1:D:449:PHE:O	2.07	0.55
1:B:166:ARG:HB2	1:B:168:VAL:HG23	1.89	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:252:SER:OG	1:C:252:SER:O	2.26	0.54
1:C:29:LEU:HD11	2:C:645:HOH:O	2.07	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:N	1:C:97:ASP:OD1	2.42	0.53
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: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:C:35:PRO:HB3	1:C:81:GLU:HB2	1.92	0.51
1:C:145:MET:O	1:C:146:SER:C	2.48	0.51
1:A:287:TYR:HB3	1:A:372:LYS:HG3	1.93	0.51
1:C:296:GLN:HG2	1:C:306:TYR:HB2	1.91	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:21:TYR:CD1	1:A:25:LYS:HE3	2.46	0.51
1:A:378:LEU:CD1	1:A:401:PHE:HZ	2.22	0.50
1:A:112:PHE:CB	1:A:425:ILE:HD13	2.41	0.50
1:A:231:ILE:HG13	1:A:263:GLN:HB3	1.92	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:B:95:LEU:HB3	1:B:100:LYS:HE3	1.93	0.50
1:A:252:SER:OG	1:A:252:SER:O	2.29	0.50
1:A:259:SER:HB3	2:B:549:HOH:O	2.11	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:C:205:TYR:CD2	1:C:312:LLP:H2'3	2.47	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:C:101:GLU:HB2	1:D:173:GLU:HG3	1.93	0.49
1:A:361:GLN:HG3	2:A:551:HOH:O	2.12	0.49
1:B:35:PRO:HB3	1:B:81:GLU:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:422:GLN:NE2	2:D:501:HOH:O	2.27	0.49
1:D:385:GLU:HG3	1:D:461:VAL:HG12	1.95	0.49
1:A:317:GLY:O	1:B:344:SER:HA	2.13	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:447:ILE:O	1:A:447:ILE:HG13	2.13	0.48
1:A:389:GLU:O	1:A:389:GLU:HG3	2.11	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:D:312:LLP:P	1:D:319:ARG:HE	2.37	0.47
1:A:66:GLU:HG2	1:B:292:ILE:HG12	1.95	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:C:346:LEU:HB3	2:C:623:HOH:O	2.14	0.47
1:C:182:GLN:HG2	2:C:659:HOH:O	2.13	0.47
1:C:168:VAL:HG22	1:C:296:GLN:HG3	1.96	0.47
1:A:226:GLU:H	1:A:226:GLU:CD	2.17	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
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:274:ARG:HH11	1:C:274:ARG:HG2	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: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:244:THR:HG23	1:B:246:PRO:HD3	1.98	0.46
1:B:155:ARG:CG	1:B:175:MET:HB3	2.46	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:B:288:ASP:CG	1:B:396:ASN:HD22	2.19	0.45
1:A:249:GLN:HB3	1:A:252:SER:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:404:GLU:HG2	1:B:444:ALA:HB2	1.99	0.45
1:D:181:THR:HG23	1:D:307:MET:HE2	1.98	0.45
1:D:206:ARG:HG3	1:D:430:ARG:O	2.17	0.45
1:B:200:MET:HG2	1:B:243:VAL:HB	1.99	0.45
1:D:409:ARG:HD3	1:D:413:ASP:CB	2.46	0.45
1:A:124:ILE:HG12	1:A:128:PHE:CE2	2.52	0.45
1:D:80:GLU:O	1:D:80:GLU:OE2	2.35	0.44
1:A:267:TRP:CZ2	1:A:274:ARG:HD3	2.53	0.44
1:C:5:ILE:HB	1:C:49:LEU:HD11	2.00	0.44
1:B:227:LYS:HG2	1:B:257:PRO:HG3	2.00	0.44
1:C:112:PHE:HB2	1:C:425:ILE:HG22	2.00	0.44
1:D:313:SER:HB2	1:D:364:ILE:HD11	1.99	0.44
1:D:166:ARG:HB2	1:D:168:VAL:HG23	1.99	0.44
1:B:80:GLU:O	1:B:81:GLU:CB	2.65	0.44
1:A:378:LEU:HD11	1:A:447:ILE:HD11	1.99	0.44
1:A:8:ASP:C	1:A:10:SER:H	2.21	0.44
1:A:174:GLN:HA	1:A:330:LEU:HD22	2.00	0.44
1:C:160:ARG:NH1	2:C:502:HOH:O	2.48	0.43
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: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:B:414:ILE:HG12	1:B:468:VAL:HA	2.00	0.43
1:A:307:MET:HE2	1:A:307:MET:HB3	1.97	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:D:386:PHE:CZ	1:D:465:PHE:HA	2.53	0.43
1:C:326:PRO:HD2	1:C:329:LEU:HD12	2.01	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:D:307:MET:HB3	1:D:307:MET:HE2	1.89	0.42
1:A:248:HIS:O	1:A:249:GLN:C	2.57	0.42
1:B:117:SER:HB3	1:B:450:ALA:HB1	2.01	0.42
1:C:252:SER:O	1:C:254:THR:N	2.50	0.42
1:B:202:GLU:HB2	1:B:221:THR:HB	2.02	0.42
1:A:171:ARG:HB3	1:A:173:GLU:OE1	2.19	0.42
1:A:34:LEU:HA	1:A:35:PRO:HD3	1.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:267:TRP:HE1	1:A:274:ARG:HH12	1.68	0.41
1:A:24:LEU:O	1:A:28:ILE:HG13	2.20	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:466:LYS:O	1:B:470:GLY:N	2.54	0.41
1:A:120:ASP:C	1:A:122:PHE:H	2.19	0.41
1:B:385:GLU:HG3	1:B:461:VAL:HG12	2.02	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: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:B:229:MET:HG2	1:B:234:ILE:HD11	2.03	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
1:C:70:TYR:HE1	1:C:72:ILE:HD11	1.86	0.41
1:A:139:TYR:CE1	1:B:124:ILE:HD12	2.56	0.40
1:D:199:ALA:HB2	1:D:239:PRO:HB3	2.03	0.40
1:A:102:ILE:HG13	1:A:102:ILE:H	1.60	0.40
1:B:309:THR:HG21	1:B:312:LLP:H5'2	2.03	0.40
1:D:182:GLN:HG3	2:D:642:HOH:O	2.20	0.40
1:C:328:GLU:H	1:C:328:GLU:HG3	1.37	0.40
1:B:409:ARG:CZ	1:B:413:ASP:HB3	2.52	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%)	11	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	413/479 (86%)	384 (93%)	21 (5%)	8 (2%)	10	2
1	C	441/479 (92%)	418 (95%)	14 (3%)	9 (2%)	9	2
1	D	438/479 (91%)	411 (94%)	20 (5%)	7 (2%)	12	3
All	All	1709/1916 (89%)	1590 (93%)	88 (5%)	31 (2%)	11	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
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 (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	335/424 (79%)	310 (92%)	25 (8%)	17	7
1	B	347/424 (82%)	324 (93%)	23 (7%)	21	11
1	C	386/424 (91%)	366 (95%)	20 (5%)	29	18
1	D	383/424 (90%)	351 (92%)	32 (8%)	14	6
All	All	1451/1696 (86%)	1351 (93%)	100 (7%)	19	10

All (100) 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	206	ARG
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	382	LEU
1	A	389	GLU
1	A	392	VAL
1	A	430	ARG

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Mol	Chain	Res	Type
1	A	447	ILE
1	B	21	TYR
1	B	29	LEU
1	B	31	ARG
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	194	LYS
1	B	223	MET
1	B	231	ILE
1	B	260	ARG
1	B	295	LEU
1	B	296	GLN
1	B	300	ARG
1	B	328	GLU
1	B	330	LEU
1	B	403	THR
1	B	415	LEU
1	B	463	ARG
1	C	10	SER
1	C	21	TYR
1	C	41	SER
1	C	97	ASP
1	C	102	ILE
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	252	SER
1	C	296	GLN
1	C	328	GLU
1	C	334	LYS
1	C	378	LEU
1	C	415	LEU

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Mol	Chain	Res	Type
1	C	430	ARG
1	C	454	GLU
1	D	29	LEU
1	D	31	ARG
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	166	ARG
1	D	182	GLN
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	455	GLU
1	D	458	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	54	ASN
1	A	61	GLN
1	A	182	GLN

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Mol	Chain	Res	Type
1	A	210	GLN
1	A	248	HIS
1	A	369	GLN
1	B	32	ASN
1	B	214	ASN
1	B	237	GLN
1	B	266	ASN
1	B	370	HIS
1	B	417	HIS
1	C	121	HIS
1	C	147	HIS
1	C	214	ASN
1	C	218	GLN
1	C	370	HIS
1	C	462	GLN
1	D	32	ASN
1	D	214	ASN
1	D	218	GLN
1	D	237	GLN
1	D	335	GLN
1	D	422	GLN
1	D	432	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
1	LLP	A	312	1	23,24,25	3.42	5 (21%)	28,32,34	1.28	3 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
1	LLP	B	312	1	23,24,25	3.51	5 (21%)	28,32,34	1.63	7 (25%)
1	LLP	C	312	1	23,24,25	3.40	5 (21%)	28,32,34	1.51	5 (17%)
1	LLP	D	312	1	23,24,25	3.70	6 (26%)	28,32,34	1.67	5 (17%)

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	312	1	-	0/15/17/19	0/1/1/1
1	LLP	B	312	1	-	0/15/17/19	0/1/1/1
1	LLP	C	312	1	-	0/15/17/19	0/1/1/1
1	LLP	D	312	1	-	0/15/17/19	0/1/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	312	LLP	C6-C5	2.13	1.42	1.37
1	B	312	LLP	C4-C4'	2.71	1.51	1.46
1	C	312	LLP	C4-C4'	3.53	1.52	1.46
1	D	312	LLP	C4-C4'	3.56	1.52	1.46
1	A	312	LLP	C4-C4'	3.81	1.53	1.46
1	B	312	LLP	C4-C5	5.82	1.49	1.42
1	A	312	LLP	C4'-NZ	6.12	1.45	1.27
1	D	312	LLP	C4'-NZ	6.33	1.46	1.27
1	B	312	LLP	C4'-NZ	6.36	1.46	1.27
1	C	312	LLP	C4'-NZ	6.58	1.47	1.27
1	A	312	LLP	C4-C5	6.86	1.51	1.42
1	B	312	LLP	C4-C3	6.90	1.49	1.40
1	C	312	LLP	C4-C5	7.13	1.51	1.42
1	D	312	LLP	C4-C5	7.19	1.51	1.42
1	C	312	LLP	C4-C3	7.63	1.50	1.40
1	D	312	LLP	C4-C3	7.65	1.50	1.40
1	A	312	LLP	C4-C3	7.97	1.50	1.40
1	C	312	LLP	C3-C2	9.30	1.47	1.40
1	A	312	LLP	C3-C2	9.97	1.47	1.40
1	D	312	LLP	C3-C2	11.67	1.48	1.40
1	B	312	LLP	C3-C2	11.99	1.49	1.40

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	312	LLP	C4-C4'-NZ	-3.04	108.13	125.06
1	D	312	LLP	C4-C4'-NZ	-3.03	108.21	125.06
1	C	312	LLP	C4-C4'-NZ	-2.78	109.58	125.06
1	C	312	LLP	C2'-C2-C3	-2.68	117.81	121.04
1	D	312	LLP	OP3-P-OP4	-2.36	99.77	106.56
1	A	312	LLP	C4-C4'-NZ	-2.31	112.20	125.06
1	C	312	LLP	O-C-CA	-2.28	119.55	125.49
1	B	312	LLP	O-C-CA	-2.11	119.99	125.49
1	D	312	LLP	O-C-CA	-2.09	120.06	125.49
1	B	312	LLP	OP3-P-OP4	-2.00	100.80	106.56
1	C	312	LLP	CD-CE-NZ	2.06	114.36	110.98
1	B	312	LLP	O3-C3-C2	2.07	121.25	117.66
1	B	312	LLP	C6-N1-C2	2.07	123.51	119.28
1	B	312	LLP	OP3-P-OP2	2.18	115.66	107.38
1	D	312	LLP	OP3-P-OP2	2.33	116.24	107.38
1	A	312	LLP	C6-N1-C2	2.37	124.11	119.28
1	A	312	LLP	OP4-C5'-C5	2.45	113.04	108.99
1	C	312	LLP	OP4-C5'-C5	3.24	114.34	108.99
1	D	312	LLP	OP4-C5'-C5	5.06	117.36	108.99
1	B	312	LLP	OP4-C5'-C5	5.57	118.20	108.99

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (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	431/479 (89%)	0.86	59 (13%)	4	4	32, 58, 98, 114	0
1	B	429/479 (89%)	0.81	51 (11%)	6	6	35, 56, 84, 115	1 (0%)
1	C	451/479 (94%)	0.54	27 (5%)	25	28	30, 45, 73, 99	1 (0%)
1	D	448/479 (93%)	0.47	23 (5%)	32	36	29, 46, 76, 105	1 (0%)
All	All	1759/1916 (91%)	0.66	160 (9%)	11	12	29, 50, 86, 115	3 (0%)

All (160) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	390	VAL	7.9
1	A	419	ALA	7.4
1	C	142	LEU	7.1
1	A	386	PHE	6.9
1	D	316	PRO	6.8
1	B	33	LEU	6.1
1	A	104	ILE	6.0
1	B	78	PHE	5.9
1	A	4	THR	5.9
1	A	381	ALA	5.8
1	A	379	ILE	5.6
1	A	382	LEU	5.4
1	A	388	GLY	5.3
1	B	13	ALA	5.0
1	A	5	ILE	4.8
1	A	413	ASP	4.8
1	A	383	GLU	4.7
1	A	315	LEU	4.7
1	A	461	VAL	4.7
1	B	77	PHE	4.6
1	D	87	ALA	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	380	THR	4.5
1	B	21	TYR	4.5
1	B	24	LEU	4.5
1	A	420	GLY	4.5
1	A	109	TRP	4.4
1	B	15	TYR	4.4
1	B	75	LYS	4.3
1	B	56	VAL	4.3
1	B	54	ASN	4.2
1	A	33	LEU	4.1
1	A	407	THR	4.1
1	C	102	ILE	4.0
1	A	384	ALA	4.0
1	C	43	ARG	4.0
1	B	418	ALA	4.0
1	A	423	LEU	3.9
1	A	416	SER	3.9
1	B	109	TRP	3.9
1	B	408	ARG	3.9
1	A	408	ARG	3.8
1	D	315	LEU	3.7
1	A	72	ILE	3.7
1	B	53	VAL	3.7
1	A	13	ALA	3.7
1	B	39	VAL	3.6
1	A	43	ARG	3.5
1	D	93	PHE	3.4
1	B	421	LEU	3.4
1	C	139	TYR	3.4
1	A	415	LEU	3.3
1	A	110	ILE	3.3
1	A	76	GLY	3.3
1	B	423	LEU	3.3
1	A	49	LEU	3.3
1	D	34	LEU	3.2
1	C	74	ARG	3.2
1	D	124	ILE	3.2
1	D	73	GLU	3.1
1	B	20	ILE	3.1
1	D	74	ARG	3.1
1	B	17	TYR	3.1
1	A	124	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	418	ALA	3.0
1	A	417	HIS	3.0
1	B	31	ARG	3.0
1	C	97	ASP	3.0
1	B	407	THR	3.0
1	A	409	ARG	3.0
1	A	102	ILE	3.0
1	A	78	PHE	3.0
1	B	10	SER	2.9
1	B	455	GLU	2.9
1	B	119	THR	2.9
1	D	102	ILE	2.9
1	A	391	THR	2.9
1	A	145	MET	2.8
1	A	445	LEU	2.8
1	C	322	TYR	2.8
1	C	140	ARG	2.8
1	C	145	MET	2.7
1	A	462	GLN	2.7
1	A	86	SER	2.7
1	B	76	GLY	2.7
1	C	84	MET	2.7
1	A	34	LEU	2.7
1	A	314	LEU	2.7
1	C	49	LEU	2.7
1	C	5	ILE	2.6
1	B	473	LYS	2.6
1	D	78	PHE	2.6
1	A	460	GLY	2.6
1	D	116	SER	2.6
1	D	79	VAL	2.6
1	B	60	TYR	2.5
1	C	306	TYR	2.5
1	C	10	SER	2.5
1	B	99	LEU	2.5
1	B	16	ILE	2.5
1	B	58	SER	2.5
1	D	119	THR	2.5
1	A	387	SER	2.5
1	B	177	ILE	2.5
1	A	103	HIS	2.5
1	B	71	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	406	ASP	2.4
1	A	414	ILE	2.4
1	B	51	VAL	2.4
1	D	72	ILE	2.4
1	B	65	ALA	2.4
1	A	36	HIS	2.4
1	B	467	ALA	2.4
1	C	162	ILE	2.4
1	D	75	LYS	2.4
1	D	421	LEU	2.4
1	D	108	ASP	2.4
1	C	387	SER	2.4
1	B	27	GLU	2.4
1	D	171	ARG	2.3
1	B	121	HIS	2.3
1	A	122	PHE	2.3
1	B	102	ILE	2.3
1	B	118	ASP	2.3
1	B	14	ASP	2.3
1	B	422	GLN	2.3
1	B	107	SER	2.3
1	A	425	ILE	2.3
1	B	36	HIS	2.3
1	A	37	SER	2.2
1	C	136	SER	2.2
1	A	45	LEU	2.2
1	C	9	ARG	2.2
1	A	87	ALA	2.2
1	C	32	ASN	2.2
1	C	44	GLU	2.2
1	B	412	GLN	2.2
1	B	45	LEU	2.2
1	D	141	THR	2.2
1	D	9	ARG	2.2
1	C	141	THR	2.2
1	A	128	PHE	2.2
1	B	32	ASN	2.2
1	B	419	ALA	2.1
1	B	28	ILE	2.1
1	C	184	LEU	2.1
1	A	30	SER	2.1
1	B	458	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	73	GLU	2.1
1	D	33	LEU	2.1
1	D	418	ALA	2.1
1	C	420	GLY	2.1
1	A	7	LEU	2.1
1	A	354	PHE	2.1
1	C	146	SER	2.0
1	C	244	THR	2.0
1	A	75	LYS	2.0
1	C	181	THR	2.0
1	D	103	HIS	2.0
1	B	420	GLY	2.0
1	B	110	ILE	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. 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	312	24/25	0.78	0.29	-	51,75,83,85	0
1	LLP	C	312	24/25	0.80	0.25	-	44,72,82,87	0
1	LLP	B	312	24/25	0.79	0.22	-	50,73,83,87	0
1	LLP	A	312	24/25	0.78	0.26	-	64,85,95,103	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.