Full wwPDB X-ray Structure Validation Report ⓘ

Oct 8, 2023 – 10:26 AM EDT

PDB ID	:	4R28
Title	:	MspJI Restriction Endonuclease in Complex with 27-mer Oligonucleotide
Authors	:	Horton, J.R.; Cheng, X.
Deposited on	:	2014-08-10
Resolution	:	3.06 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:

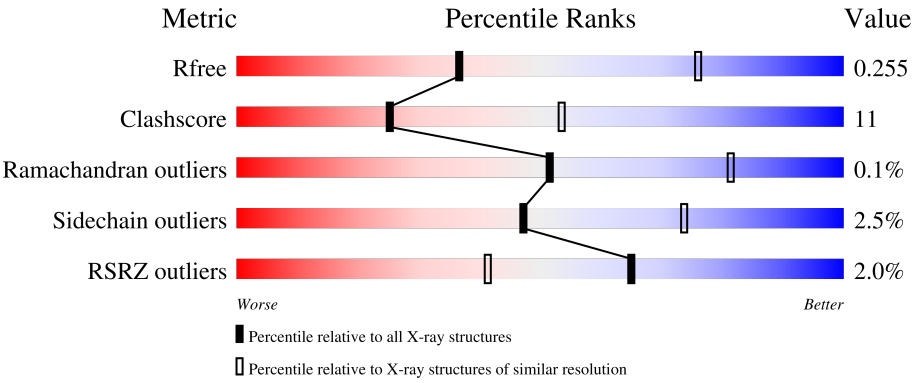
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.06 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}	130704	1754 (3.10-3.02)
Clashscore	141614	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)
RSRZ outliers	127900	1713 (3.10-3.02)

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 <=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	456	2% 75% 23%
1	B	456	2% 71% 27%
1	C	456	2% 74% 23%
1	D	456	% 71% 26%
2	X	27	41% 52% 7%

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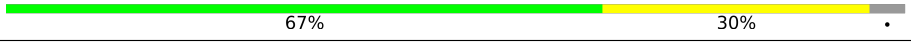
Mol	Chain	Length	Quality of chain
3	Y	27	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 14225 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 Restriction endonuclease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	449	Total	C	N	O	S	0	0	0
			3263	2048	607	604	4			
1	B	447	Total	C	N	O	S	0	0	0
			3274	2051	612	606	5			
1	C	449	Total	C	N	O	S	0	0	0
			3318	2082	619	612	5			
1	D	449	Total	C	N	O	S	0	0	0
			3328	2088	625	610	5			

- Molecule 2 is a DNA chain called DNA (25-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	X	25	Total	C	N	O	P	0	0	0
			512	244	99	145	24			

- Molecule 3 is a DNA chain called DNA (26-MER).

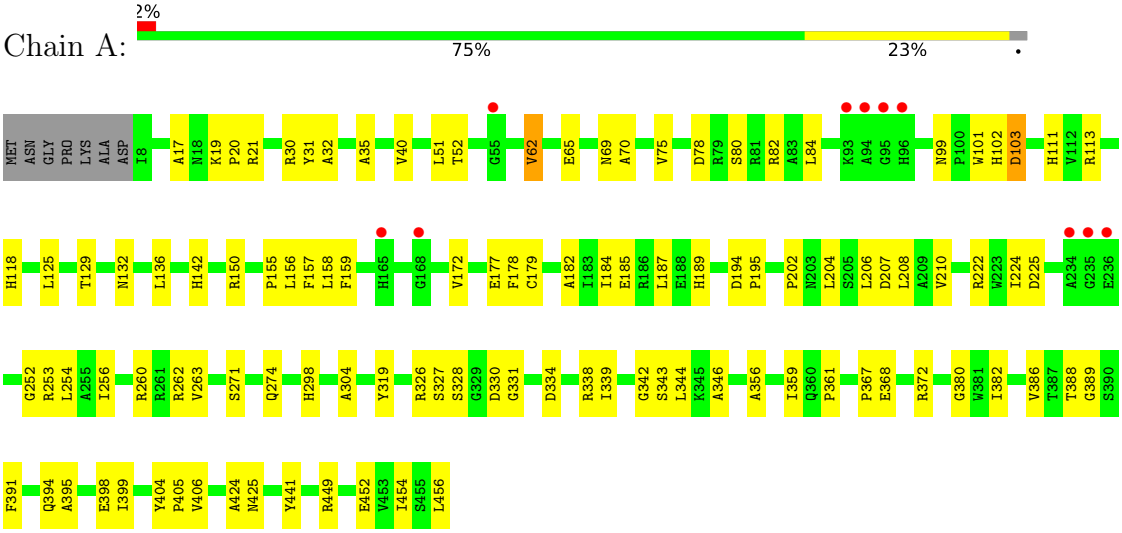
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	Y	26	Total	C	N	O	P	0	0	0
			530	252	93	159	26			

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.

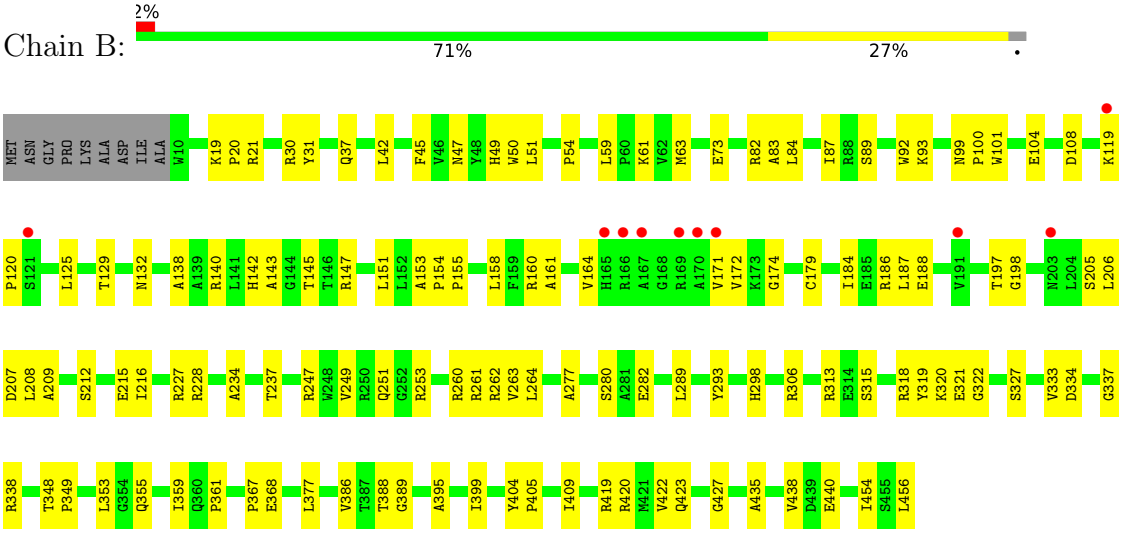
• Molecule 1: Restriction endonuclease

Chain A:



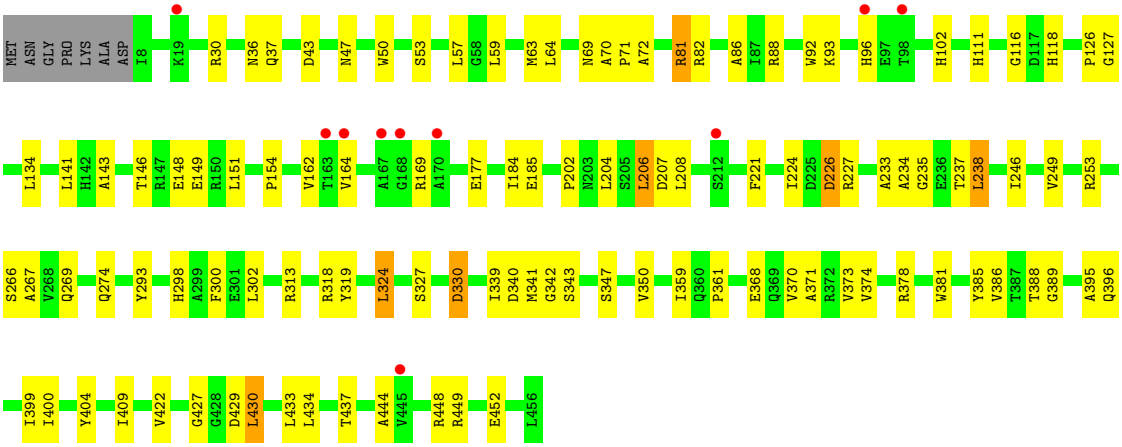
• Molecule 1: Restriction endonuclease

Chain B:



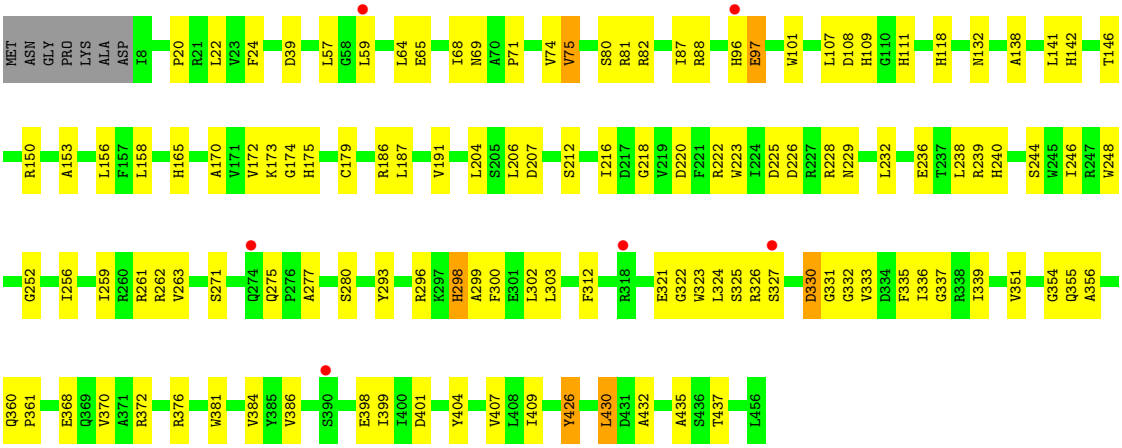
• Molecule 1: Restriction endonuclease

Chain C:



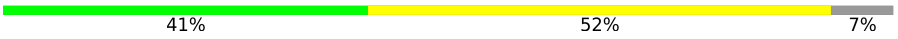
• Molecule 1: Restriction endonuclease

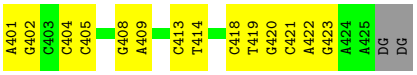
Chain D:



• Molecule 2: DNA (25-MER)

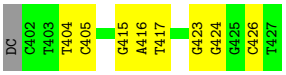
Chain X:





• Molecule 3: DNA (26-MER)

Chain Y:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	88.54Å 88.54Å 511.97Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	35.03 – 3.06 35.03 – 3.05	Depositor EDS
% Data completeness (in resolution range)	99.8 (35.03-3.06) 98.0 (35.03-3.05)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.20 (at 3.06Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.227 , 0.258 0.226 , 0.255	Depositor DCC
R_{free} test set	2128 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	80.1	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 33.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.407 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	14225	wwPDB-VP
Average B, all atoms (Å^2)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5CM

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	0.20	0/3332	0.37	0/4546
1	B	0.21	0/3342	0.38	0/4554
1	C	0.21	0/3386	0.38	0/4610
1	D	0.21	0/3398	0.39	0/4626
2	X	0.53	0/552	0.82	0/848
3	Y	0.51	0/592	0.88	0/911
All	All	0.25	0/14602	0.44	0/20095

There are no bond length outliers.

There are no bond angle outliers.

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	3263	0	3091	71	0
1	B	3274	0	3114	81	0
1	C	3318	0	3188	69	0
1	D	3328	0	3198	81	0
2	X	512	0	283	12	0
3	Y	530	0	294	10	0
All	All	14225	0	13168	294	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 11.

All (294) 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:433:LEU:O	1:C:437:THR:HG23	1.75	0.86
1:D:322:GLY:H	1:D:337:GLY:HA2	1.53	0.72
1:B:59:LEU:HD22	1:B:228:ARG:HD3	1.72	0.72
1:C:63:MET:O	1:C:69:ASN:ND2	2.23	0.72
1:B:186:ARG:HB3	1:B:207:ASP:HB2	1.73	0.71
1:C:269:GLN:H	1:C:396:GLN:HE22	1.39	0.70
1:C:81:ARG:NH2	1:C:227:ARG:O	2.26	0.69
1:D:332:GLY:O	1:D:355:GLN:NE2	2.26	0.68
1:A:187:LEU:HD11	1:A:204:LEU:HB2	1.76	0.68
1:D:236:GLU:O	1:D:239:ARG:NH1	2.27	0.68
1:A:368:GLU:HG3	1:D:372:ARG:HD2	1.76	0.67
1:D:186:ARG:HB2	1:D:207:ASP:HB2	1.77	0.67
1:D:64:LEU:O	1:D:88:ARG:NH1	2.25	0.66
1:D:81:ARG:NH1	1:D:232:LEU:O	2.28	0.66
1:B:21:ARG:NH2	1:B:51:LEU:O	2.28	0.66
1:D:81:ARG:NH2	1:D:226:ASP:O	2.29	0.66
1:A:65:GLU:O	1:A:69:ASN:ND2	2.26	0.65
1:D:81:ARG:NH2	1:D:229:ASN:O	2.30	0.64
1:C:399:ILE:HG23	1:C:404:TYR:HB2	1.80	0.64
1:B:143:ALA:HB1	1:B:253:ARG:HH21	1.63	0.64
1:C:116:GLY:N	1:C:204:LEU:O	2.29	0.64
1:B:188:GLU:HB3	1:B:205:SER:HB3	1.79	0.64
1:C:318:ARG:NH1	1:C:342:GLY:O	2.31	0.63
1:B:37:GLN:NE2	1:B:54:PRO:O	2.32	0.63
1:D:223:TRP:HB3	1:D:240:HIS:HB2	1.81	0.62
1:D:138:ALA:O	1:D:142:HIS:ND1	2.32	0.62
1:D:74:VAL:HG21	1:D:228:ARG:HA	1.82	0.62
1:D:150:ARG:HH22	1:D:252:GLY:HA2	1.65	0.62
1:B:129:THR:OG1	1:B:132:ASN:ND2	2.32	0.62
1:A:334:ASP:OD2	1:A:356:ALA:N	2.25	0.61
1:B:99:ASN:ND2	1:B:101:TRP:O	2.33	0.61
1:B:89:SER:OG	1:B:161:ALA:N	2.27	0.60
1:B:399:ILE:HG23	1:B:404:TYR:HB2	1.81	0.60
1:C:64:LEU:HG	1:C:88:ARG:HD2	1.83	0.60
1:D:75:VAL:HA	1:D:80:SER:HA	1.82	0.60
1:A:103:ASP:OD1	1:A:103:ASP:N	2.34	0.60
1:A:187:LEU:HD13	1:A:206:LEU:HG	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:226:ASP:OD1	1:C:226:ASP:N	2.34	0.59
1:A:330:ASP:OD1	1:A:331:GLY:N	2.35	0.59
1:C:224:ILE:HA	1:C:227:ARG:HB2	1.85	0.59
1:A:319:TYR:O	1:B:260:ARG:NH2	2.33	0.59
1:B:37:GLN:HB2	1:B:61:LYS:HE2	1.83	0.59
1:A:21:ARG:NH2	1:A:51:LEU:O	2.33	0.59
1:D:324:LEU:HA	1:D:335:PHE:HA	1.84	0.59
1:D:430:LEU:HD22	1:D:430:LEU:H	1.68	0.59
1:A:368:GLU:OE2	1:D:372:ARG:NH1	2.36	0.58
1:A:75:VAL:HA	1:A:80:SER:HA	1.84	0.58
1:D:20:PRO:HB3	1:D:222:ARG:HH21	1.68	0.58
1:D:212:SER:N	1:D:259:ILE:O	2.36	0.58
1:D:354:GLY:HA2	1:D:384:VAL:HG13	1.86	0.58
1:B:320:LYS:NZ	1:B:456:LEU:O	2.31	0.57
1:C:146:THR:HB	1:C:149:GLU:HG2	1.85	0.57
1:A:449:ARG:HH22	1:D:111:HIS:HB3	1.69	0.57
1:A:359:ILE:O	1:A:388:THR:OG1	2.23	0.57
1:D:232:LEU:HD21	1:D:239:ARG:HH22	1.70	0.57
1:B:262:ARG:NH1	1:B:263:VAL:O	2.38	0.56
1:B:84:LEU:H	1:B:227:ARG:HH22	1.53	0.56
1:C:302:LEU:HD23	1:C:437:THR:HB	1.86	0.56
1:C:361:PRO:HA	1:C:389:GLY:HA2	1.87	0.56
1:C:448:ARG:NH1	1:C:452:GLU:OE2	2.38	0.56
1:D:24:PHE:HD1	1:D:218:GLY:HA3	1.70	0.56
1:D:57:LEU:HD11	1:D:225:ASP:HB3	1.86	0.56
1:A:254:LEU:O	1:B:306:ARG:NH1	2.38	0.56
1:A:202:PRO:HB3	1:B:140:ARG:HD3	1.88	0.56
1:B:89:SER:HB3	1:B:160:ARG:HA	1.87	0.56
1:A:32:ALA:HB3	1:A:35:ALA:HB2	1.88	0.56
1:C:169:ARG:NH1	3:Y:416:DA:OP2	2.38	0.56
1:B:158:LEU:HB2	1:B:179:CYS:HB2	1.87	0.56
1:D:262:ARG:NH2	1:D:401:ASP:OD2	2.39	0.56
1:B:100:PRO:HG3	1:B:423:GLN:HG3	1.87	0.56
1:D:298:HIS:NE2	1:D:327:SER:O	2.39	0.56
1:A:262:ARG:NH1	1:A:263:VAL:O	2.39	0.55
1:B:30:ARG:NH1	1:B:31:TYR:O	2.39	0.55
1:A:343:SER:OG	1:A:344:LEU:N	2.40	0.55
1:C:313:ARG:NH1	1:C:319:TYR:O	2.40	0.55
1:C:81:ARG:HH22	1:C:227:ARG:HA	1.72	0.55
1:A:361:PRO:HA	1:A:389:GLY:HA2	1.89	0.54
1:C:57:LEU:HB3	1:C:59:LEU:HD23	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:416:DA:H2"	3:Y:417:DT:H5"	1.89	0.54
1:A:398:GLU:OE2	1:D:376:ARG:NH1	2.40	0.54
1:A:111:HIS:CE1	1:B:318:ARG:HH12	2.26	0.54
1:B:338:ARG:NH1	1:B:454:ILE:O	2.41	0.54
1:B:197:THR:N	1:B:198:GLY:HA2	2.24	0.53
1:C:118:HIS:ND1	1:C:202:PRO:O	2.41	0.53
1:B:367:PRO:HB3	1:B:395:ALA:HA	1.89	0.53
1:B:277:ALA:HB3	1:B:280:SER:HB3	1.90	0.53
1:A:125:LEU:H	1:A:125:LEU:HD23	1.74	0.53
1:A:449:ARG:NH2	1:D:109:HIS:HB2	2.24	0.53
1:C:359:ILE:O	1:C:388:THR:OG1	2.24	0.53
1:D:293:TYR:HB3	1:D:300:PHE:HB2	1.90	0.53
1:A:326:ARG:CZ	1:A:331:GLY:HA3	2.38	0.53
1:B:87:ILE:HD13	1:B:158:LEU:HD23	1.89	0.53
1:D:107:LEU:HB3	1:D:261:ARG:HH21	1.74	0.53
1:D:172:VAL:O	1:D:173:LYS:HB2	2.08	0.53
1:A:184:ILE:HA	1:A:208:LEU:HB3	1.92	0.52
1:B:361:PRO:HA	1:B:389:GLY:HA2	1.91	0.52
1:C:238:LEU:HD21	1:C:249:VAL:HG21	1.90	0.52
2:X:413:DC:H2"	2:X:414:DT:O5'	2.09	0.52
2:X:418:DC:H2"	2:X:419:DT:C5	2.44	0.52
1:A:189:HIS:HB3	1:B:187:LEU:HD22	1.91	0.52
1:D:330:ASP:N	1:D:330:ASP:OD1	2.43	0.52
1:A:372:ARG:HD2	1:D:368:GLU:HB3	1.91	0.52
1:B:30:ARG:NH1	1:B:174:GLY:O	2.41	0.52
1:C:237:THR:HG23	1:C:238:LEU:HD13	1.92	0.52
1:A:425:ASN:OD1	1:B:253:ARG:N	2.43	0.52
1:C:71:PRO:O	1:C:82:ARG:NH1	2.38	0.52
1:D:68:ILE:HG22	1:D:87:ILE:HG23	1.92	0.52
1:C:430:LEU:O	1:C:434:LEU:HG	2.09	0.51
2:X:423:DG:H1	3:Y:405:DC:H42	1.57	0.51
1:D:244:SER:HB3	1:D:259:ILE:HB	1.92	0.51
1:D:426:TYR:HE1	1:D:430:LEU:HD13	1.76	0.51
1:B:104:GLU:OE2	1:B:420:ARG:NH2	2.42	0.51
1:C:340:ASP:HB3	1:C:347:SER:HB2	1.92	0.50
1:B:386:VAL:HG22	1:B:409:ILE:HD12	1.93	0.50
1:C:69:ASN:O	1:C:86:ALA:N	2.44	0.50
1:B:30:ARG:HG2	1:B:42:LEU:HB3	1.92	0.50
1:C:298:HIS:NE2	1:C:327:SER:O	2.44	0.50
1:C:206:LEU:HD13	1:C:208:LEU:HD21	1.94	0.50
1:C:422:VAL:O	1:C:427:GLY:N	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:233:ALA:O	1:C:235:GLY:N	2.45	0.50
1:C:396:GLN:O	1:C:400:ILE:HG12	2.12	0.50
2:X:404:DC:N4	3:Y:423:DG:O6	2.45	0.50
1:B:108:ASP:HA	1:B:263:VAL:HB	1.94	0.49
1:B:184:ILE:HG23	1:B:206:LEU:HD11	1.93	0.49
1:D:141:LEU:HD23	1:D:153:ALA:HA	1.93	0.49
1:D:22:LEU:HG	1:D:220:ASP:HB3	1.95	0.49
1:D:296:ARG:HG3	1:D:299:ALA:H	1.77	0.49
1:A:298:HIS:CD2	1:A:327:SER:HA	2.47	0.49
1:A:182:ALA:HB2	1:A:210:VAL:HG22	1.95	0.49
1:A:158:LEU:HB2	1:A:179:CYS:HB2	1.94	0.49
1:A:406:VAL:O	1:B:348:THR:OG1	2.24	0.48
1:C:185:GLU:N	1:C:207:ASP:O	2.42	0.48
1:A:21:ARG:NH1	1:A:225:ASP:OD2	2.46	0.48
1:A:338:ARG:HH11	1:A:454:ILE:HA	1.79	0.48
1:A:449:ARG:HB2	1:A:452:GLU:HG3	1.93	0.48
1:B:186:ARG:NH1	1:B:207:ASP:OD2	2.46	0.48
1:C:92:TRP:N	1:C:93:LYS:HA	2.28	0.48
1:A:150:ARG:HD3	1:A:252:GLY:HA2	1.94	0.48
1:C:30:ARG:NH2	1:C:43:ASP:OD2	2.46	0.48
1:B:83:ALA:HA	1:B:227:ARG:HH12	1.79	0.48
1:B:298:HIS:NE2	1:B:327:SER:O	2.46	0.48
1:D:325:SER:OG	1:D:333:VAL:O	2.31	0.48
1:A:380:GLY:HA3	1:B:405:PRO:HG3	1.95	0.48
1:D:398:GLU:HG2	1:D:404:TYR:HE2	1.78	0.48
1:D:238:LEU:HD23	1:D:246:ILE:HG22	1.95	0.48
1:A:84:LEU:HD11	1:A:224:ILE:HG23	1.96	0.48
1:A:382:ILE:HG22	1:A:405:PRO:HB2	1.96	0.48
1:A:319:TYR:HD1	1:A:339:ILE:HG12	1.77	0.48
1:B:92:TRP:N	1:B:93:LYS:HA	2.29	0.47
1:C:339:ILE:HB	1:C:350:VAL:HB	1.95	0.47
1:D:277:ALA:O	1:D:280:SER:OG	2.22	0.47
1:A:84:LEU:HD11	1:A:224:ILE:HD12	1.96	0.47
1:A:99:ASN:O	1:A:102:HIS:ND1	2.34	0.47
1:B:322:GLY:H	1:B:337:GLY:HA2	1.79	0.47
1:D:71:PRO:O	1:D:82:ARG:NH1	2.46	0.47
1:D:158:LEU:HB2	1:D:179:CYS:HB2	1.96	0.47
1:D:187:LEU:HD12	1:D:206:LEU:HD11	1.95	0.47
1:B:154:PRO:HA	1:B:155:PRO:HD3	1.82	0.47
1:C:141:LEU:HD12	1:C:154:PRO:HD3	1.95	0.47
1:D:312:PHE:HB3	1:D:339:ILE:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:419:DT:H2'	2:X:420:DG:C8	2.48	0.47
1:A:342:GLY:O	1:B:315:SER:OG	2.26	0.47
1:D:432:ALA:HA	1:D:435:ALA:HB3	1.96	0.47
1:B:99:ASN:HD21	1:B:101:TRP:HB2	1.80	0.47
1:C:371:ALA:HA	1:C:374:VAL:HG22	1.97	0.47
1:D:335:PHE:CE2	1:D:354:GLY:HA3	2.50	0.47
1:A:424:ALA:HA	1:B:145:THR:HG22	1.96	0.47
1:B:138:ALA:O	1:B:142:HIS:ND1	2.29	0.46
1:D:312:PHE:HE1	1:D:407:VAL:HG21	1.80	0.46
1:C:37:GLN:NE2	1:C:53:SER:O	2.45	0.46
1:A:30:ARG:NH1	1:A:31:TYR:O	2.47	0.46
1:B:349:PRO:HG3	1:B:454:ILE:HG23	1.96	0.46
2:X:421:DC:H2'	2:X:422:DA:C8	2.51	0.46
1:C:72:ALA:HB2	3:Y:426:DC:H5'	1.96	0.46
2:X:414:DT:O2	3:Y:415:DG:N2	2.48	0.46
1:C:274:GLN:NE2	1:C:396:GLN:OE1	2.48	0.46
1:D:271:SER:O	1:D:275:GLN:NE2	2.48	0.46
1:C:293:TYR:HB3	1:C:300:PHE:HD2	1.81	0.46
1:B:359:ILE:O	1:B:388:THR:OG1	2.21	0.46
1:A:17:ALA:O	1:A:222:ARG:NH1	2.49	0.46
1:B:264:LEU:N	1:D:191:VAL:O	2.48	0.46
1:C:70:ALA:HB3	1:C:134:LEU:HD13	1.98	0.46
1:D:323:TRP:O	1:D:335:PHE:HB2	2.16	0.46
1:B:184:ILE:HA	1:B:208:LEU:HD23	1.98	0.45
1:C:324:LEU:HB3	1:C:444:ALA:HB2	1.98	0.45
1:B:247:ARG:HE	1:B:251:GLN:NE2	2.14	0.45
1:B:353:LEU:HD13	1:B:377:LEU:HD23	1.99	0.45
1:C:64:LEU:HD11	1:C:88:ARG:HB2	1.98	0.45
1:C:126:PRO:HA	1:C:127:GLY:HA2	1.69	0.45
1:D:108:ASP:HA	1:D:263:VAL:HB	1.99	0.45
1:D:336:ILE:HD11	1:D:351:VAL:HG13	1.99	0.45
2:X:423:DG:H1	3:Y:405:DC:N4	2.13	0.45
2:X:413:DC:H4'	2:X:414:DT:OP1	2.16	0.45
1:D:370:VAL:HG11	1:D:399:ILE:HD11	1.97	0.45
1:C:378:ARG:H	1:C:381:TRP:HB2	1.81	0.45
1:A:136:LEU:HD12	1:B:125:LEU:HD13	1.99	0.45
1:B:368:GLU:HB3	1:C:368:GLU:HB3	1.99	0.45
1:C:47:ASN:OD1	1:C:50:TRP:N	2.45	0.45
1:A:274:GLN:HE22	1:A:391:PHE:HD2	1.65	0.44
1:D:24:PHE:CD1	1:D:218:GLY:HA3	2.52	0.44
1:D:256:ILE:HA	1:D:259:ILE:HG12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:SER:HB2	1:B:261:ARG:HA	2.00	0.44
1:C:422:VAL:HG22	1:C:433:LEU:HD13	2.00	0.44
1:D:303:LEU:HB2	1:D:437:THR:HG21	2.00	0.44
1:D:87:ILE:HD11	1:D:156:LEU:HD23	1.98	0.44
1:B:333:VAL:HG21	1:B:353:LEU:HD23	1.99	0.44
1:C:330:ASP:OD1	1:C:330:ASP:N	2.51	0.44
1:A:298:HIS:CG	1:A:327:SER:HA	2.53	0.44
1:A:118:HIS:HB2	1:A:132:ASN:HD21	1.81	0.44
1:D:226:ASP:OD2	1:D:239:ARG:NH2	2.51	0.44
1:D:300:PHE:CE2	1:D:356:ALA:HB1	2.53	0.44
1:A:142:HIS:CE1	1:A:156:LEU:HD13	2.53	0.43
1:C:370:VAL:HG11	1:C:399:ILE:HD11	2.00	0.43
1:C:395:ALA:O	1:C:399:ILE:HG13	2.17	0.43
1:B:313:ARG:NH2	1:B:319:TYR:O	2.51	0.43
1:C:96:HIS:HA	1:C:102:HIS:CB	2.48	0.43
1:C:449:ARG:H	1:C:449:ARG:HG2	1.59	0.43
1:B:422:VAL:O	1:B:427:GLY:N	2.52	0.43
1:B:30:ARG:HB2	1:B:45:PHE:HB2	2.00	0.43
1:C:234:ALA:O	1:C:237:THR:HG22	2.18	0.43
1:D:165:HIS:HA	1:D:170:ALA:HA	2.01	0.43
1:C:429:ASP:OD1	1:C:429:ASP:N	2.52	0.43
1:D:65:GLU:H	1:D:69:ASN:ND2	2.16	0.43
1:A:70:ALA:HB1	1:A:82:ARG:HH21	1.83	0.43
1:B:147:ARG:HG3	1:B:249:VAL:HG12	2.00	0.43
1:C:318:ARG:NH1	1:C:347:SER:HB3	2.33	0.43
1:C:386:VAL:HA	1:C:409:ILE:HB	2.01	0.43
1:A:253:ARG:HA	1:A:256:ILE:HG13	2.00	0.43
1:B:49:HIS:NE2	1:B:63:MET:SD	2.87	0.43
1:B:334:ASP:HB2	1:B:355:GLN:HA	2.01	0.43
1:A:113:ARG:HH21	1:B:318:ARG:HH21	1.67	0.42
3:Y:404:DT:H4'	3:Y:405:DC:OP1	2.19	0.42
1:B:47:ASN:HB3	1:B:50:TRP:HB3	2.00	0.42
1:C:36:ASN:OD1	1:C:37:GLN:N	2.52	0.42
1:C:143:ALA:HA	1:C:253:ARG:HD2	2.00	0.42
1:C:266:SER:OG	1:C:267:ALA:N	2.53	0.42
1:D:59:LEU:HB3	1:D:228:ARG:HH21	1.84	0.42
1:D:248:TRP:HB2	1:D:259:ILE:HD13	2.00	0.42
1:D:187:LEU:HD11	1:D:204:LEU:HD23	2.02	0.42
1:A:367:PRO:HB3	1:A:395:ALA:HA	2.01	0.42
1:B:215:GLU:HG2	1:B:216:ILE:HG23	2.01	0.42
1:B:19:LYS:HA	1:B:20:PRO:HD3	1.79	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:THR:HG21	1:A:62:VAL:HG11	2.02	0.42
1:A:159:PHE:HA	1:A:177:GLU:O	2.20	0.42
1:B:234:ALA:O	1:B:237:THR:HG22	2.19	0.42
1:D:174:GLY:C	1:D:175:HIS:ND1	2.73	0.42
2:X:404:DC:H42	3:Y:424:DG:H1	1.68	0.42
1:B:151:LEU:HB3	1:B:249:VAL:HG11	2.02	0.42
1:C:341:MET:O	1:C:347:SER:HA	2.20	0.42
1:B:73:GLU:HG3	1:B:82:ARG:CZ	2.50	0.42
1:B:84:LEU:HB3	1:B:227:ARG:NH2	2.35	0.42
1:D:326:ARG:NH1	1:D:331:GLY:HA3	2.35	0.42
1:A:343:SER:N	1:A:346:ALA:O	2.53	0.41
1:A:404:TYR:OH	1:D:376:ARG:HD3	2.19	0.41
1:B:171:VAL:HA	1:B:172:VAL:HA	1.64	0.41
1:C:238:LEU:HG	1:C:246:ILE:HG22	2.02	0.41
1:A:101:TRP:HZ2	1:A:424:ALA:HB2	1.86	0.41
1:A:101:TRP:CZ2	1:A:424:ALA:HB2	2.55	0.41
1:B:142:HIS:CE1	1:B:153:ALA:HB1	2.55	0.41
1:D:107:LEU:HD21	1:D:179:CYS:HB3	2.02	0.41
1:D:386:VAL:HA	1:D:409:ILE:HB	2.02	0.41
3:Y:423:DG:H2'	3:Y:424:DG:C8	2.55	0.41
1:A:19:LYS:HA	1:A:20:PRO:HD3	1.88	0.41
1:A:456:LEU:HA	1:B:262:ARG:HG2	2.02	0.41
1:B:209:ALA:HB1	1:B:260:ARG:HG2	2.01	0.41
1:B:282:GLU:HG3	1:B:419:ARG:HH11	1.85	0.41
1:B:289:LEU:HD22	1:B:293:TYR:HE2	1.86	0.41
1:A:394:GLN:NE2	1:A:398:GLU:OE1	2.53	0.41
1:D:39:ASP:OD1	1:D:39:ASP:N	2.53	0.41
1:A:157:PHE:HD2	1:A:178:PHE:HE1	1.68	0.41
1:C:148:GLU:HA	1:C:151:LEU:HD12	2.02	0.41
1:A:344:LEU:HD22	1:B:104:GLU:HB3	2.03	0.41
1:B:119:LYS:HA	1:B:120:PRO:HD3	1.94	0.41
1:B:435:ALA:HA	1:B:438:VAL:HG22	2.03	0.41
1:C:184:ILE:HA	1:C:208:LEU:HD23	2.02	0.41
1:A:399:ILE:HG23	1:A:404:TYR:HB2	2.02	0.41
1:D:96:HIS:HA	1:D:97:GLU:HA	1.67	0.41
1:D:229:ASN:HB3	1:D:232:LEU:HB2	2.02	0.41
1:D:118:HIS:HB2	1:D:132:ASN:HD21	1.86	0.41
1:D:351:VAL:HB	1:D:381:TRP:CD1	2.56	0.41
2:X:401:DA:H2"	2:X:402:DG:C8	2.56	0.41
1:A:84:LEU:HD23	1:A:155:PRO:HD2	2.02	0.40
1:C:373:VAL:HG21	1:C:385:TYR:HD2	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:302:LEU:HD23	1:D:437:THR:HA	2.02	0.40
1:A:185:GLU:OE1	1:A:260:ARG:NH1	2.52	0.40
1:A:304:ALA:HB1	1:A:386:VAL:HB	2.03	0.40
1:D:325:SER:OG	1:D:326:ARG:N	2.54	0.40
1:D:360:GLN:HA	1:D:361:PRO:HD3	1.93	0.40
1:C:70:ALA:HA	1:C:71:PRO:HD3	1.91	0.40
1:C:111:HIS:HE1	1:C:207:ASP:HB3	1.85	0.40
1:C:162:VAL:HG12	1:C:177:GLU:HB2	2.04	0.40
1:D:271:SER:OG	1:D:275:GLN:NE2	2.54	0.40
2:X:408:DG:H2'	2:X:409:DA:C8	2.56	0.40
1:A:194:ASP:HA	1:A:195:PRO:HD3	1.87	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	447/456 (98%)	437 (98%)	10 (2%)	0	100	100
1	B	445/456 (98%)	428 (96%)	16 (4%)	1 (0%)	47	77
1	C	447/456 (98%)	427 (96%)	19 (4%)	1 (0%)	47	77
1	D	447/456 (98%)	431 (96%)	16 (4%)	0	100	100
All	All	1786/1824 (98%)	1723 (96%)	61 (3%)	2 (0%)	51	81

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	164	VAL
1	B	164	VAL

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	305/358 (85%)	295 (97%)	10 (3%)	38	67
1	B	308/358 (86%)	306 (99%)	2 (1%)	86	93
1	C	316/358 (88%)	307 (97%)	9 (3%)	43	71
1	D	317/358 (88%)	307 (97%)	10 (3%)	39	68
All	All	1246/1432 (87%)	1215 (98%)	31 (2%)	47	74

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	VAL
1	A	62	VAL
1	A	78	ASP
1	A	103	ASP
1	A	129	THR
1	A	172	VAL
1	A	207	ASP
1	A	271	SER
1	A	328	SER
1	A	441	TYR
1	B	321	GLU
1	B	440	GLU
1	C	81	ARG
1	C	206	LEU
1	C	221	PHE
1	C	226	ASP
1	C	238	LEU
1	C	324	LEU
1	C	330	ASP
1	C	343	SER
1	C	430	LEU
1	D	75	VAL
1	D	97	GLU
1	D	101	TRP

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Mol	Chain	Res	Type
1	D	146	THR
1	D	216	ILE
1	D	298	HIS
1	D	321	GLU
1	D	330	ASP
1	D	426	TYR
1	D	430	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	274	GLN
1	C	396	GLN
1	D	192	GLN
1	D	275	GLN
1	D	355	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	5CM	X	405	2	17,21,22	1.00	2 (11%)	24,30,33	1.32	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
2	5CM	X	405	2	-	0/7/21/22	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	405	5CM	C6-C5	2.72	1.39	1.34
2	X	405	5CM	C6-N1	-2.21	1.34	1.38

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	X	405	5CM	C5-C6-N1	-3.33	119.91	123.34
2	X	405	5CM	C5-C4-N3	-2.64	118.82	121.67
2	X	405	5CM	O2-C2-N3	-2.06	118.98	122.33

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	449/456 (98%)	-0.22	10 (2%) 62 38	47, 91, 154, 281	0
1	B	447/456 (98%)	-0.27	10 (2%) 62 38	43, 92, 147, 189	0
1	C	449/456 (98%)	-0.23	10 (2%) 62 38	58, 93, 148, 243	0
1	D	449/456 (98%)	-0.29	6 (1%) 77 56	58, 92, 135, 200	0
2	X	24/27 (88%)	-0.74	0 100 100	77, 95, 112, 127	0
3	Y	26/27 (96%)	-0.79	0 100 100	72, 94, 123, 140	0
All	All	1844/1878 (98%)	-0.27	36 (1%) 65 41	43, 92, 149, 281	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	168	GLY	8.7
1	A	93	LYS	6.9
1	A	96	HIS	6.8
1	A	168	GLY	6.1
1	A	95	GLY	6.0
1	B	165	HIS	5.6
1	C	170	ALA	4.7
1	A	94	ALA	4.2
1	B	171	VAL	4.2
1	B	169	ARG	3.8
1	A	236	GLU	3.5
1	A	55	GLY	3.4
1	C	164	VAL	3.4
1	B	167	ALA	3.2
1	C	167	ALA	3.2
1	D	59	LEU	3.1
1	D	390	SER	3.0
1	D	327	SER	2.9
1	B	170	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	96	HIS	2.9
1	A	234	ALA	2.8
1	B	166	ARG	2.7
1	C	212	SER	2.7
1	B	203	ASN	2.6
1	C	445	VAL	2.5
1	D	274	GLN	2.3
1	D	318	ARG	2.3
1	B	191	VAL	2.2
1	C	19	LYS	2.2
1	C	98	THR	2.2
1	C	163	THR	2.2
1	B	119	LYS	2.1
1	C	96	HIS	2.1
1	A	165	HIS	2.0
1	A	235	GLY	2.0
1	B	121	SER	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	5CM	X	405	20/21	0.96	0.14	69,83,87,88	0

6.3 Carbohydrates (i)

There are no monosaccharides 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.