Full wwPDB X-ray Structure Validation Report (i)

Oct 23, 2021 – 09:50 AM EDT

PDB ID	:	1DRG
Title	:	CRYSTAL STRUCTURE OF TRIMERIC CRE RECOMBINASE-LOX COMPLEX
Authors	:	Woods, K.C.; Baldwin, E.P.
Deposited on	:	2000-01-06
Resolution	:	2.55 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

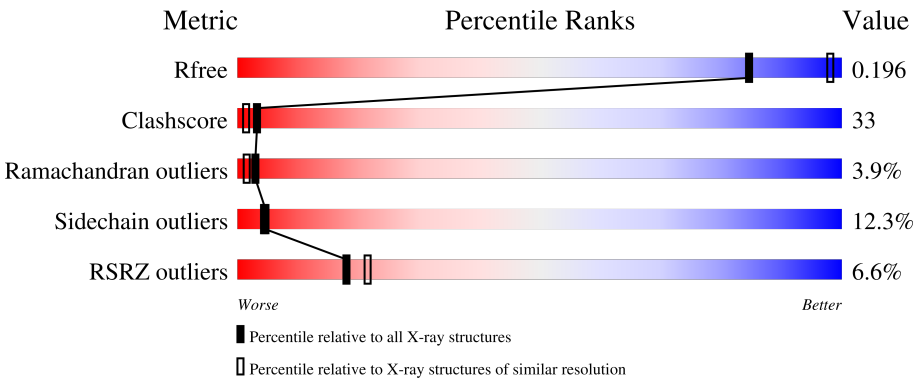
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.55 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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	B	16	12% 62% 25%
2	C	19	26% 63% 11%
3	A	323	7% 47% 40% 9% • •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3310 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 DNA chain called 5'-D(*TP*AP*TP*AP*AP*CP*TP*TP*CP*GP*TP*AP*TP*AP*GP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	B	16	323	157	56	95	15	0	0	0

- Molecule 2 is a DNA chain called 5'-D(*AP*TP*AP*TP*GP*CP*TP*AP*TP*AP*CP*GP*AP*AP*GP*TP*TP*AP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	C	19	388	188	70	112	18	0	0	0

- Molecule 3 is a protein called CRE RECOMBINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	313	2485	1544	473	453	15	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	324	PHE	TYR	engineered mutation	UNP P06956

- Molecule 4 is water.

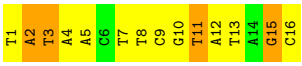
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	B	12	12	12	0	0
4	C	10	10	10	0	0
4	A	92	92	92	0	0

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.

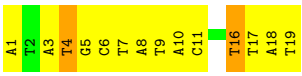
• Molecule 1: 5'-D(*TP*AP*TP*AP*AP*CP*TP*TP*CP*GP*TP*AP*TP*AP*GP*C)-3'

Chain B: 12% 62% 25%



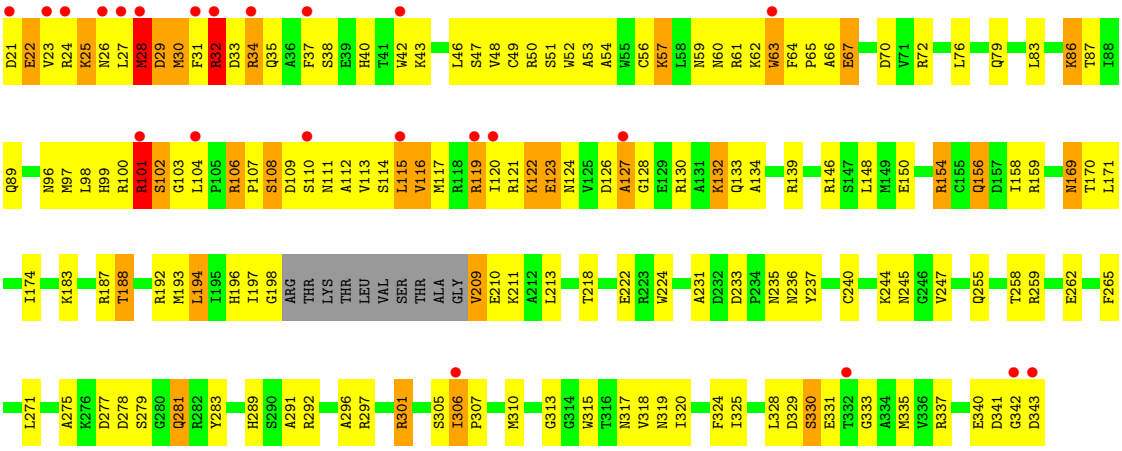
• Molecule 2: 5'-D(*AP*TP*AP*TP*GP*CP*TP*AP*TP*AP*CP*GP*AP*AP*GP*TP*TP*AP*T)-3'

Chain C: 26% 63% 11%



• Molecule 3: CRE RECOMBINASE

Chain A: 7% 47% 40% 9%



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α, β, γ	160.99Å 160.99Å 160.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	5.00 – 2.55 80.50 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.7 (5.00-2.55) 97.3 (80.50-2.55)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.96 (at 2.55Å)	Xtriage
Refinement program	TNT 5E	Depositor
R, R_{free}	0.186 , 0.268 0.197 , 0.196	Depositor DCC
R_{free} test set	1139 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	43.0	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 88.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.026 for -l,-k,-h	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	3310	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% 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 (i)

5.1 Standard geometry (i)

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	B	0.72	0/361	1.52	8/555 (1.4%)
2	C	0.72	0/435	1.38	5/670 (0.7%)
3	A	0.64	0/2525	0.75	0/3400
All	All	0.66	0/3321	0.98	13/4625 (0.3%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	15	DG	P-O3'-C3'	7.40	128.58	119.70
1	B	11	DT	P-O3'-C3'	7.14	128.27	119.70
2	C	7	DT	P-O3'-C3'	6.46	127.46	119.70
1	B	5	DA	P-O5'-C5'	-5.85	111.54	120.90
2	C	10	DA	O4'-C1'-N9	-5.67	104.03	108.00
1	B	13	DT	P-O3'-C3'	5.54	126.34	119.70
1	B	2	DA	O4'-C4'-C3'	-5.47	102.31	104.50
2	C	16	DT	O4'-C1'-C2'	-5.46	101.54	105.90
1	B	12	DA	O4'-C1'-C2'	-5.33	101.64	105.90
2	C	4	DT	C6-N1-C1'	5.18	128.17	120.40
1	B	12	DA	P-O3'-C3'	5.15	125.88	119.70
2	C	11	DC	O4'-C1'-C2'	-5.02	101.89	105.90
1	B	3	DT	P-O3'-C3'	5.00	125.70	119.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	323	0	184	17	0
2	C	388	0	218	19	0
3	A	2485	0	2492	179	0
4	A	92	0	0	12	0
4	B	12	0	0	2	0
4	C	10	0	0	2	0
All	All	3310	0	2894	200	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 33.

All (200) 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)
3:A:124:ASN:HA	3:A:127:ALA:HB3	1.48	0.96
3:A:66:ALA:H	3:A:99:HIS:HE1	1.12	0.93
3:A:47:SER:HA	3:A:50:ARG:NH1	1.84	0.92
3:A:340:GLU:C	3:A:342:GLY:H	1.73	0.91
1:B:2:DA:H5"	1:B:2:DA:C8	2.06	0.91
2:C:16:DT:H2"	2:C:17:DT:H5"	1.53	0.90
3:A:28:MET:HE3	3:A:46:LEU:HD23	1.54	0.90
3:A:28:MET:CE	3:A:46:LEU:HD23	2.03	0.88
3:A:66:ALA:H	3:A:99:HIS:CE1	1.93	0.86
3:A:96:ASN:HD21	3:A:108:SER:HB2	1.42	0.82
2:C:18:DA:H2	3:A:244:LYS:HE2	1.44	0.82
3:A:30:MET:HG3	3:A:31:PHE:H	1.43	0.82
1:B:1:DT:H2"	1:B:2:DA:H5"	1.64	0.79
3:A:47:SER:HA	3:A:50:ARG:HH12	1.46	0.78
3:A:197:ILE:HB	3:A:209:VAL:HG12	1.65	0.76
3:A:28:MET:O	3:A:29:ASP:C	2.24	0.76
3:A:34:ARG:HH11	3:A:34:ARG:HG2	1.49	0.76
3:A:193:MET:CE	3:A:222:GLU:HG3	2.17	0.75
1:B:8:DT:H2"	1:B:9:DC:H5'	1.69	0.74
2:C:3:DA:H1'	2:C:4:DT:H5'	1.68	0.74
3:A:117:MET:O	3:A:121:ARG:HG3	1.88	0.74
2:C:17:DT:H2"	2:C:18:DA:C8	2.24	0.73
3:A:96:ASN:HD21	3:A:108:SER:CB	2.00	0.73
3:A:96:ASN:ND2	3:A:108:SER:HB2	2.03	0.73
3:A:119:ARG:O	3:A:123:GLU:HG3	1.89	0.72
3:A:30:MET:HG3	3:A:31:PHE:N	2.05	0.71
2:C:8:DA:H2'	2:C:9:DT:H71	1.75	0.69
3:A:64:PHE:HE1	3:A:99:HIS:CD2	2.11	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:101:ARG:HG2	3:A:101:ARG:HH11	1.57	0.69
3:A:25:LYS:HD3	3:A:26:ASN:OD1	1.92	0.69
3:A:148:LEU:HD23	3:A:271:LEU:HD21	1.73	0.68
3:A:102:SER:O	3:A:104:LEU:HG	1.94	0.68
1:B:3:DT:H2"	1:B:4:DA:C8	2.29	0.68
3:A:340:GLU:O	3:A:342:GLY:N	2.26	0.68
2:C:18:DA:C2	3:A:244:LYS:HE2	2.28	0.68
3:A:134:ALA:HA	3:A:283:TYR:CD2	2.29	0.68
3:A:28:MET:O	3:A:30:MET:HG2	1.94	0.67
3:A:119:ARG:NH1	4:A:411:HOH:O	2.28	0.67
3:A:340:GLU:C	3:A:342:GLY:N	2.42	0.67
3:A:64:PHE:CZ	3:A:104:LEU:HD12	2.30	0.67
3:A:245:ASN:HB3	3:A:247:VAL:HG23	1.77	0.67
1:B:1:DT:H2"	1:B:2:DA:C5'	2.26	0.66
3:A:34:ARG:HG2	3:A:34:ARG:NH1	2.10	0.66
3:A:194:LEU:HD22	3:A:210:GLU:HB3	1.75	0.66
2:C:5:DG:OP1	3:A:106:ARG:NH1	2.28	0.66
1:B:16:DC:H2'	3:A:320:ILE:HD13	1.78	0.66
3:A:279:SER:OG	3:A:281:GLN:NE2	2.29	0.66
3:A:48:VAL:O	3:A:51:SER:HB3	1.96	0.65
3:A:301:ARG:NH2	3:A:329:ASP:OD1	2.29	0.65
3:A:197:ILE:O	3:A:198:GLY:C	2.35	0.64
3:A:101:ARG:O	3:A:103:GLY:N	2.29	0.64
3:A:25:LYS:NZ	3:A:29:ASP:OD2	2.30	0.64
3:A:124:ASN:HA	3:A:127:ALA:CB	2.27	0.64
3:A:337:ARG:HG2	3:A:343:ASP:HA	1.80	0.64
3:A:34:ARG:O	3:A:42:TRP:NE1	2.30	0.64
3:A:187:ARG:NH1	3:A:222:GLU:OE2	2.27	0.63
3:A:64:PHE:HZ	3:A:104:LEU:HD12	1.63	0.63
3:A:38:SER:HB2	4:A:365:HOH:O	1.98	0.63
3:A:128:GLY:HA2	3:A:130:ARG:NH1	2.14	0.62
3:A:292:ARG:NH2	3:A:313:GLY:O	2.28	0.61
3:A:31:PHE:CE2	3:A:101:ARG:HG3	2.35	0.61
3:A:193:MET:HE3	3:A:222:GLU:HG3	1.83	0.61
1:B:11:DT:OP2	3:A:50:ARG:NH1	2.34	0.61
3:A:66:ALA:N	3:A:99:HIS:HE1	1.94	0.60
3:A:25:LYS:NZ	3:A:26:ASN:ND2	2.50	0.60
2:C:18:DA:H2"	2:C:19:DT:O5'	2.02	0.60
1:B:7:DT:H5"	4:B:19:HOH:O	2.02	0.59
3:A:31:PHE:O	3:A:33:ASP:N	2.35	0.59
3:A:192:ARG:HB3	3:A:213:LEU:O	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:154:ARG:NH2	3:A:156:GLN:OE1	2.35	0.58
2:C:5:DG:N7	4:C:24:HOH:O	2.32	0.57
3:A:292:ARG:HG2	3:A:324:PHE:CZ	2.39	0.57
3:A:28:MET:HE2	3:A:46:LEU:HD23	1.83	0.57
3:A:193:MET:HE1	3:A:222:GLU:HG3	1.85	0.57
3:A:30:MET:O	3:A:31:PHE:C	2.43	0.57
3:A:306:ILE:O	3:A:310:MET:HG3	2.04	0.57
3:A:240:CYS:HB3	4:A:402:HOH:O	2.04	0.57
3:A:27:LEU:CD2	3:A:63:TRP:HZ2	2.19	0.56
3:A:194:LEU:CD2	3:A:210:GLU:HB3	2.35	0.56
3:A:139:ARG:HD3	4:A:425:HOH:O	2.05	0.56
3:A:64:PHE:CG	3:A:65:PRO:HA	2.40	0.56
3:A:24:ARG:N	3:A:24:ARG:HD2	2.21	0.56
3:A:112:ALA:O	3:A:116:VAL:HG22	2.07	0.55
3:A:330:SER:O	3:A:331:GLU:HB3	2.07	0.55
3:A:115:LEU:HD12	3:A:115:LEU:O	2.06	0.55
3:A:49:CYS:SG	3:A:98:LEU:HD11	2.47	0.55
3:A:79:GLN:NE2	3:A:123:GLU:OE1	2.39	0.55
2:C:6:DC:OP1	3:A:100:ARG:NH2	2.40	0.55
2:C:8:DA:H2'	2:C:9:DT:C6	2.43	0.54
3:A:196:HIS:ND1	3:A:210:GLU:OE2	2.34	0.54
3:A:333:GLY:HA2	4:A:427:HOH:O	2.07	0.54
2:C:3:DA:H3'	3:A:121:ARG:HH12	1.72	0.54
3:A:24:ARG:H	3:A:24:ARG:CD	2.20	0.54
3:A:106:ARG:O	3:A:107:PRO:C	2.46	0.54
3:A:159:ARG:HB2	3:A:224:TRP:CZ3	2.43	0.54
2:C:16:DT:C2'	2:C:17:DT:H5"	2.34	0.53
3:A:37:PHE:HB2	3:A:42:TRP:CZ2	2.42	0.53
3:A:97:MET:O	3:A:98:LEU:C	2.47	0.53
3:A:30:MET:CG	3:A:31:PHE:H	2.11	0.53
3:A:317:ASN:OD1	3:A:319:ASN:N	2.42	0.53
3:A:325:ILE:O	3:A:325:ILE:HG22	2.10	0.52
3:A:123:GLU:O	3:A:127:ALA:HB2	2.10	0.52
3:A:233:ASP:O	3:A:236:ASN:HB2	2.09	0.52
3:A:64:PHE:HA	3:A:65:PRO:C	2.30	0.52
3:A:106:ARG:O	3:A:109:ASP:N	2.40	0.52
3:A:158:ILE:HD12	4:A:412:HOH:O	2.10	0.52
3:A:21:ASP:N	3:A:24:ARG:HD3	2.24	0.52
3:A:24:ARG:HD2	3:A:24:ARG:H	1.74	0.52
3:A:126:ASP:O	3:A:128:GLY:N	2.43	0.52
3:A:24:ARG:HG2	3:A:50:ARG:HA	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:24:ARG:NE	3:A:53:ALA:HB1	2.26	0.51
1:B:2:DA:H2	2:C:19:DT:O2	1.94	0.51
1:B:15:DG:N7	3:A:86:LYS:HE3	2.26	0.51
3:A:25:LYS:HZ2	3:A:26:ASN:CG	2.13	0.51
3:A:28:MET:O	3:A:29:ASP:O	2.29	0.50
3:A:24:ARG:HE	3:A:53:ALA:HB1	1.75	0.50
3:A:148:LEU:CD2	3:A:271:LEU:HD21	2.39	0.50
2:C:4:DT:OP2	3:A:121:ARG:NH2	2.27	0.50
3:A:237:TYR:CZ	3:A:255:GLN:HG2	2.47	0.50
3:A:22:GLU:O	3:A:26:ASN:OD1	2.30	0.50
3:A:315:TRP:CZ2	3:A:324:PHE:CD2	2.99	0.50
3:A:193:MET:HG3	3:A:218:THR:HG23	1.94	0.50
3:A:315:TRP:HZ2	3:A:324:PHE:CD2	2.30	0.50
3:A:278:ASP:O	3:A:278:ASP:OD1	2.29	0.49
1:B:8:DT:O4	3:A:259:ARG:HG2	2.12	0.49
3:A:119:ARG:HH11	3:A:119:ARG:CG	2.26	0.49
3:A:121:ARG:O	3:A:122:LYS:C	2.50	0.49
2:C:19:DT:H1'	3:A:244:LYS:HE3	1.93	0.49
3:A:25:LYS:HZ2	3:A:26:ASN:ND2	2.10	0.49
3:A:231:ALA:HB3	4:A:374:HOH:O	2.13	0.49
3:A:101:ARG:C	3:A:103:GLY:H	2.13	0.48
3:A:120:ILE:O	3:A:123:GLU:HB2	2.14	0.48
3:A:54:ALA:O	3:A:57:LYS:HB3	2.13	0.48
3:A:59:ASN:O	3:A:61:ARG:NE	2.45	0.48
3:A:34:ARG:NH1	3:A:42:TRP:CD1	2.82	0.48
3:A:67:GLU:O	3:A:70:ASP:HB2	2.13	0.48
4:B:20:HOH:O	3:A:156:GLN:HG3	2.13	0.48
3:A:64:PHE:CZ	3:A:104:LEU:CD1	2.96	0.48
3:A:317:ASN:OD1	3:A:319:ASN:HB2	2.14	0.47
3:A:64:PHE:CD1	3:A:65:PRO:HA	2.50	0.47
3:A:83:LEU:HD13	3:A:87:THR:HG21	1.97	0.47
3:A:100:ARG:O	3:A:101:ARG:C	2.51	0.47
3:A:279:SER:CB	3:A:281:GLN:NE2	2.77	0.47
3:A:27:LEU:HD22	3:A:63:TRP:HZ2	1.79	0.47
3:A:119:ARG:NH1	3:A:119:ARG:HG2	2.30	0.47
3:A:170:THR:O	3:A:171:LEU:HB2	2.14	0.47
3:A:64:PHE:CE1	3:A:99:HIS:CD2	2.98	0.46
3:A:183:LYS:HE2	3:A:235:ASN:OD1	2.15	0.46
2:C:1:DA:N3	4:C:29:HOH:O	2.36	0.46
3:A:259:ARG:NH1	4:A:419:HOH:O	2.38	0.46
3:A:337:ARG:CG	3:A:343:ASP:HA	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:27:LEU:CD2	3:A:63:TRP:CZ2	2.99	0.45
3:A:174:ILE:HD12	3:A:258:THR:HB	1.98	0.45
3:A:72:ARG:HG3	3:A:116:VAL:CG2	2.47	0.44
1:B:1:DT:H2"	1:B:2:DA:C8	2.52	0.44
3:A:86:LYS:HB2	4:A:383:HOH:O	2.16	0.44
1:B:9:DC:H2"	1:B:10:DG:C8	2.52	0.44
3:A:24:ARG:NE	3:A:53:ALA:CB	2.80	0.44
2:C:3:DA:H3'	3:A:121:ARG:NH1	2.33	0.44
3:A:31:PHE:O	3:A:32:ARG:C	2.56	0.44
3:A:24:ARG:N	3:A:24:ARG:CD	2.80	0.44
3:A:30:MET:HG3	3:A:31:PHE:HD1	1.83	0.44
1:B:16:DC:OP1	3:A:292:ARG:NH1	2.51	0.43
3:A:76:LEU:HD23	3:A:76:LEU:HA	1.89	0.43
3:A:128:GLY:O	3:A:130:ARG:HD3	2.18	0.43
3:A:113:VAL:O	3:A:114:SER:C	2.57	0.43
3:A:33:ASP:N	3:A:33:ASP:OD1	2.46	0.43
3:A:27:LEU:HD23	3:A:63:TRP:HZ2	1.83	0.43
2:C:8:DA:H2"	2:C:9:DT:O5'	2.19	0.43
3:A:52:TRP:CZ2	3:A:56:CYS:SG	3.12	0.43
3:A:188:THR:OG1	3:A:194:LEU:HD12	2.19	0.42
3:A:279:SER:HB2	3:A:281:GLN:NE2	2.34	0.42
3:A:291:ALA:HB3	4:A:358:HOH:O	2.19	0.42
3:A:297:ARG:NH2	4:A:421:HOH:O	2.20	0.42
3:A:120:ILE:O	3:A:124:ASN:ND2	2.52	0.42
3:A:262:GLU:O	3:A:265:PHE:HB2	2.19	0.42
3:A:305:SER:OG	3:A:307:PRO:HD2	2.19	0.42
1:B:15:DG:OP1	3:A:133:GLN:HG3	2.18	0.42
3:A:62:LYS:HA	3:A:62:LYS:HD2	1.60	0.42
3:A:335:MET:HB2	4:A:376:HOH:O	2.19	0.42
3:A:23:VAL:O	3:A:27:LEU:HB2	2.20	0.42
3:A:169:ASN:OD1	3:A:213:LEU:HA	2.20	0.42
1:B:7:DT:H2'	1:B:8:DT:H71	2.01	0.42
3:A:30:MET:HG3	3:A:31:PHE:CD1	2.54	0.42
3:A:31:PHE:CD2	3:A:101:ARG:HG3	2.55	0.41
3:A:296:ALA:HB1	3:A:325:ILE:HD11	2.02	0.41
3:A:40:HIS:ND1	3:A:43:LYS:NZ	2.66	0.41
3:A:29:ASP:O	3:A:30:MET:HB3	2.20	0.41
3:A:318:VAL:H	3:A:318:VAL:HG23	1.65	0.41
3:A:337:ARG:HA	3:A:342:GLY:O	2.21	0.41
3:A:27:LEU:HD22	3:A:63:TRP:CZ2	2.55	0.41
3:A:64:PHE:CE1	3:A:99:HIS:NE2	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:132:LYS:HZ2	3:A:132:LYS:HG2	1.60	0.41
3:A:146:ARG:HB3	3:A:150:GLU:HG3	2.03	0.41
3:A:101:ARG:NH1	3:A:101:ARG:CG	2.83	0.41
3:A:25:LYS:HG2	3:A:26:ASN:N	2.32	0.40
3:A:28:MET:HE3	3:A:46:LEU:CD2	2.38	0.40
3:A:277:ASP:OD1	3:A:279:SER:OG	2.29	0.40
1:B:8:DT:C2'	1:B:9:DC:H5'	2.46	0.40
3:A:107:PRO:O	3:A:110:SER:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	A	309/323 (96%)	280 (91%)	17 (6%)	12 (4%)	3 1

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	28	MET
3	A	29	ASP
3	A	30	MET
3	A	32	ARG
3	A	102	SER
3	A	127	ALA
3	A	275	ALA
3	A	341	ASP
3	A	123	GLU
3	A	35	GLN
3	A	25	LYS
3	A	101	ARG

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
3	A	261/269 (97%)	229 (88%)	32 (12%)	4 4

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	22	GLU
3	A	28	MET
3	A	32	ARG
3	A	34	ARG
3	A	57	LYS
3	A	60	ASN
3	A	63	TRP
3	A	67	GLU
3	A	86	LYS
3	A	89	GLN
3	A	101	ARG
3	A	106	ARG
3	A	108	SER
3	A	111	ASN
3	A	115	LEU
3	A	116	VAL
3	A	119	ARG
3	A	122	LYS
3	A	132	LYS
3	A	154	ARG
3	A	156	GLN
3	A	169	ASN
3	A	188	THR
3	A	194	LEU
3	A	209	VAL
3	A	211	LYS
3	A	281	GLN
3	A	289	HIS
3	A	301	ARG
3	A	306	ILE

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Mol	Chain	Res	Type
3	A	328	LEU
3	A	330	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	26	ASN
3	A	99	HIS
3	A	111	ASN
3	A	124	ASN
3	A	269	HIS
3	A	281	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)

There are no non-standard protein/DNA/RNA residues in this entry.

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 (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	B	16/16 (100%)	0.21	0	100	100	32, 43, 79, 96	0
2	C	19/19 (100%)	-0.04	0	100	100	27, 50, 67, 69	0
3	A	313/323 (96%)	0.64	23 (7%)	15	18	27, 42, 92, 99	0
All	All	348/358 (97%)	0.59	23 (6%)	18	21	27, 43, 90, 99	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	24	ARG	8.2
3	A	31	PHE	5.6
3	A	343	ASP	5.1
3	A	32	ARG	4.9
3	A	21	ASP	4.1
3	A	42	TRP	3.8
3	A	342	GLY	3.8
3	A	27	LEU	3.6
3	A	37	PHE	3.3
3	A	34	ARG	3.1
3	A	104	LEU	2.8
3	A	26	ASN	2.8
3	A	306	ILE	2.7
3	A	119	ARG	2.6
3	A	110	SER	2.5
3	A	63	TRP	2.3
3	A	115	LEU	2.2
3	A	23	VAL	2.2
3	A	127	ALA	2.2
3	A	120	ILE	2.2
3	A	101	ARG	2.1
3	A	28	MET	2.1
3	A	332	THR	2.1

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

There are no non-standard protein/DNA/RNA residues in this entry.

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.