Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:31 PM GMT

PDB ID	:	1U0C
Title	:	Y33C Mutant of Homing endonuclease I-CreI
Authors	:	Sussman, D.; Chadsey, M.; Fauce, S.; Engel, A.; Bruett, A.; Monnat, R.; Stoddard, B.L.; Seligman, L.M.
Deposited on	:	2004-07-13
Resolution	:	2.50 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
http://wwpdb.org/validation/2016/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:

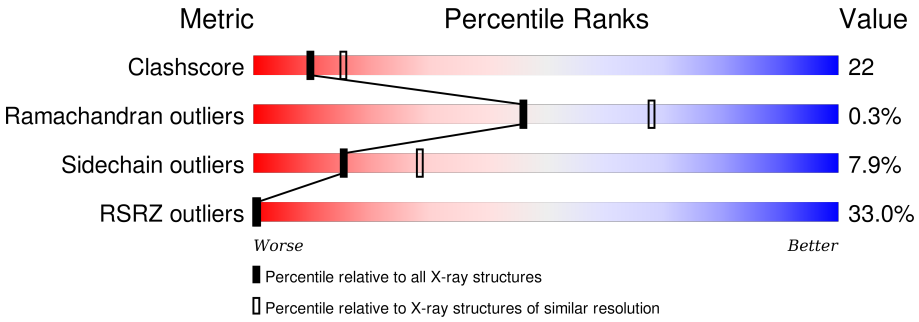
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.50 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))
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	1-C	24	100%: 46%, 50%, ·
1	2-C	24	100%: 38%, 54%, 8%
2	1-D	24	100%: 25%, 67%, 8%
2	2-D	24	100%: 33%, 63%, ·
3	1-A	163	21%: 62%, 27%, ·, 7%
3	1-B	163	20%: 49%, 39%, 5%, 7%
3	2-A	163	21%: 63%, 26%, 5%, 7%

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Mol	Chain	Length	Quality of chain
3	2-B	163	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7062 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(*GP*CP*TP*AP*AP*AP*CP*GP*TP*CP*GP*TP*GP*AP*GP*AP*CP*AP*GP*TP*TP*AP*CP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1-C	24	Total	C	N	O	P	0	0	0
			493	235	95	140	23			
1	2-C	24	Total	C	N	O	P	0	0	0
			493	235	95	140	23			

- Molecule 2 is a DNA chain called 5'-D(*CP*GP*TP*AP*AP*CP*TP*GP*TP*CP*TP*CP*AP*CP*GP*AP*CP*GP*TP*TP*TP*AP*GP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1-D	24	Total	C	N	O	P	0	0	0
			485	233	85	144	23			
2	2-D	24	Total	C	N	O	P	0	0	0
			485	233	85	144	23			

- Molecule 3 is a protein called DNA endonuclease I-CreI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	1-A	152	Total	C	N	O	S	0	0	0
			1230	790	209	229	2			
3	2-A	152	Total	C	N	O	S	0	0	0
			1230	790	209	229	2			
3	1-B	152	Total	C	N	O	S	0	0	0
			1230	790	209	229	2			
3	2-B	152	Total	C	N	O	S	0	0	0
			1230	790	209	229	2			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	33	CYS	TYR	ENGINEERED MUTATION	UNP P05725
A	42	THR	ALA	ENGINEERED MUTATION	UNP P05725

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Chain	Residue	Modelled	Actual	Comment	Reference
A	47	GLU	GLN	ENGINEERED MUTATION	UNP P05725
A	110	GLU	TRP	ENGINEERED MUTATION	UNP P05725
A	111	GLN	ARG	ENGINEERED MUTATION	UNP P05725
B	333	CYS	TYR	ENGINEERED MUTATION	UNP P05725
B	342	THR	ALA	ENGINEERED MUTATION	UNP P05725
B	347	GLU	GLN	ENGINEERED MUTATION	UNP P05725
B	410	GLU	TRP	ENGINEERED MUTATION	UNP P05725
B	411	GLN	ARG	ENGINEERED MUTATION	UNP P05725

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	1-B	1	Total Mg 1 1	0	0
4	1-C	1	Total Mg 1 1	0	0
4	2-C	1	Total Mg 1 1	0	0
4	1-A	1	Total Mg 1 1	0	0
4	2-B	1	Total Mg 1 1	0	0
4	2-A	1	Total Mg 1 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	1-A	34	Total O 34 34	0	0
5	2-A	32	Total O 32 32	0	0
5	1-B	28	Total O 28 28	0	0
5	2-B	28	Total O 28 28	0	0
5	1-C	11	Total O 11 11	0	0
5	2-C	12	Total O 12 12	0	0
5	1-D	17	Total O 17 17	0	0

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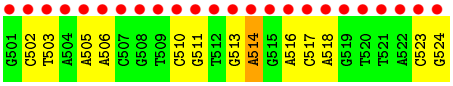
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	2-D	18	Total	O	0	0
			18	18		

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.

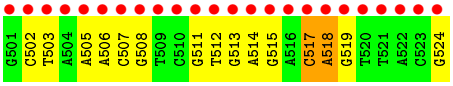
• Molecule 1: 5'-D(*GP*CP*TP*AP*AP*AP*CP*GP*TP*CP*GP*TP*GP*AP*GP*AP*CP*AP*GP*TP*TP*AP*CP*G)-3'

Chain 1-C:



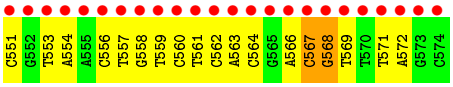
• Molecule 1: 5'-D(*GP*CP*TP*AP*AP*AP*CP*GP*TP*CP*GP*TP*GP*AP*GP*AP*CP*AP*GP*TP*TP*AP*CP*G)-3'

Chain 2-C:



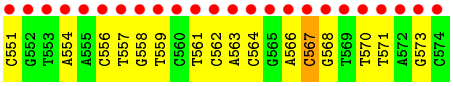
• Molecule 2: 5'-D(*CP*GP*TP*AP*AP*CP*TP*GP*TP*CP*TP*CP*AP*CP*GP*AP*CP*GP*TP*TP*TP*AP*GP*C)-3'

Chain 1-D:



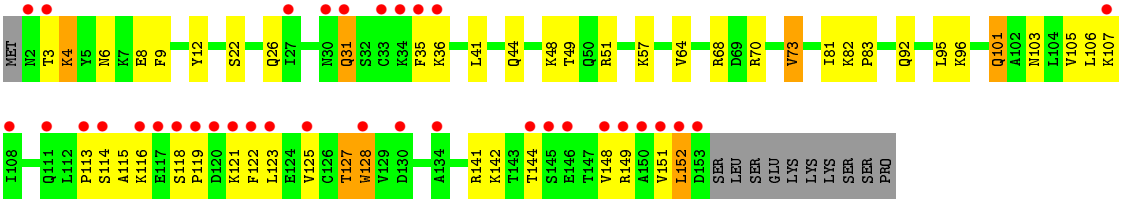
• Molecule 2: 5'-D(*CP*GP*TP*AP*AP*CP*TP*GP*TP*CP*TP*CP*AP*CP*GP*AP*CP*GP*TP*TP*TP*AP*GP*C)-3'

Chain 2-D:



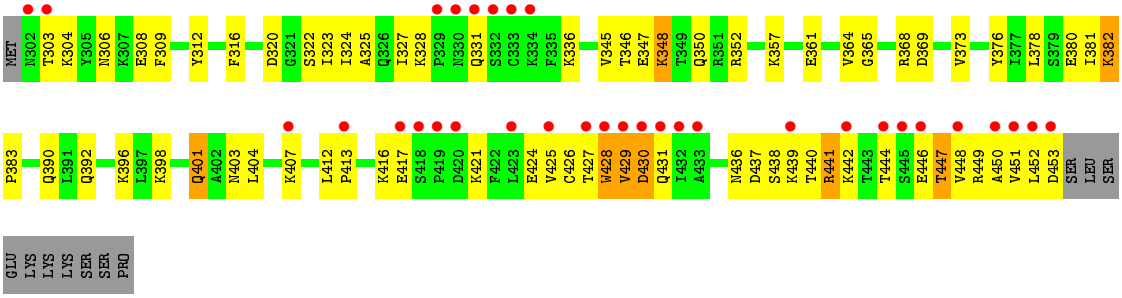
• Molecule 3: DNA endonuclease I-CreI

Chain 1-A:



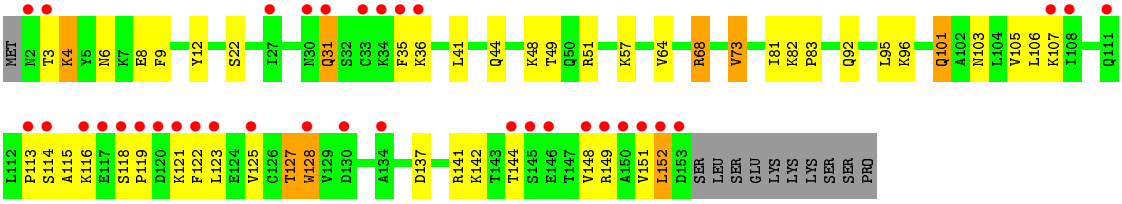
• Molecule 3: DNA endonuclease I-CreI

Chain 1-B:



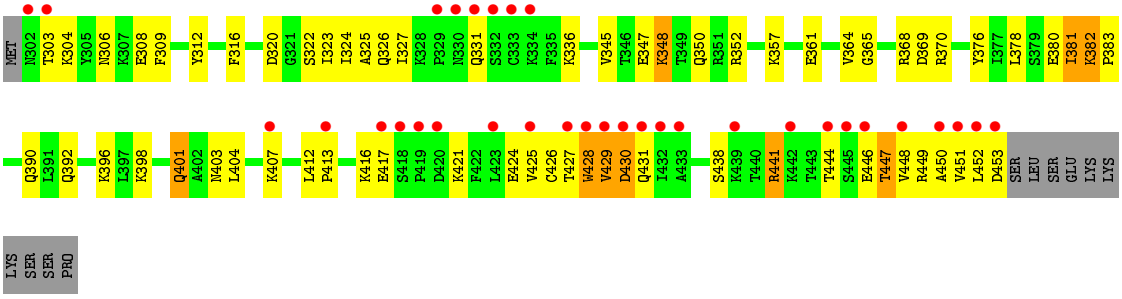
• Molecule 3: DNA endonuclease I-CreI

Chain 2-A:



• Molecule 3: DNA endonuclease I-CreI

Chain 2-B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	43.09Å 68.02Å 87.18Å 90.00° 92.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 43.56 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.50) 96.1 (43.56-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.26 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.214 , 0.277 0.275 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	38.7	Xtriage
Anisotropy	0.232	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.50 , 44.6	EDS
Estimated twinning fraction	0.042 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 17529 reflections	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	7062	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.02% 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, 0.375 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: MG

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	1-C	0.30	0/554	0.71	0/854
1	2-C	0.29	0/554	0.67	0/854
2	1-D	0.29	0/542	0.75	0/834
2	2-D	0.29	0/542	0.71	0/834
3	1-A	0.43	0/1252	0.67	0/1690
3	1-B	0.42	0/1252	0.68	1/1690 (0.1%)
3	2-A	0.43	0/1252	0.67	0/1690
3	2-B	0.42	0/1252	0.68	1/1690 (0.1%)
All	All	0.39	0/7200	0.69	2/10136 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1-C	0	1
1	2-C	0	2
2	1-D	0	2
2	2-D	0	1
All	All	0	6

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	1-B	376	TYR	N-CA-C	-5.33	96.61	111.00
3	2-B	376	TYR	N-CA-C	-5.33	96.61	111.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1-C	514	DA	Sidechain
2	1-D	567	DC	Sidechain
2	1-D	568	DG	Sidechain
1	2-C	517	DC	Sidechain
1	2-C	518	DA	Sidechain
2	2-D	567	DC	Sidechain

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	1-C	493	0	271	26	0
1	2-C	493	0	271	26	0
2	1-D	485	0	273	24	0
2	2-D	485	0	273	17	0
3	1-A	1230	0	1264	62	0
3	1-B	1230	0	1264	64	0
3	2-A	1230	0	1264	61	0
3	2-B	1230	0	1264	55	0
4	1-A	1	0	0	0	0
4	1-B	1	0	0	0	0
4	1-C	1	0	0	0	0
4	2-A	1	0	0	0	0
4	2-B	1	0	0	0	0
4	2-C	1	0	0	0	0
5	1-A	34	0	0	2	0
5	1-B	28	0	0	2	0
5	1-C	11	0	0	2	0
5	1-D	17	0	0	0	0
5	2-A	32	0	0	2	0
5	2-B	28	0	0	2	0
5	2-C	12	0	0	0	0
5	2-D	18	0	0	1	0
All	All	7062	0	6144	291	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 22.

All (291) 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:505:DA:H2"	1:C:506:DA:H5"	1.50	0.91
3:A:4:LYS:H	3:A:4:LYS:HE2	1.38	0.87
3:A:4:LYS:H	3:A:4:LYS:HE2	1.38	0.87
3:B:322:SER:OG	3:B:324:ILE:HD11	1.75	0.87
3:B:322:SER:OG	3:B:324:ILE:HD11	1.75	0.87
3:A:92:GLN:HG3	3:A:103:ASN:ND2	1.92	0.84
3:A:92:GLN:HG3	3:A:103:ASN:ND2	1.92	0.84
3:B:348:LYS:HE2	3:B:350:GLN:HE21	1.41	0.84
3:B:348:LYS:HE2	3:B:350:GLN:HE21	1.41	0.84
1:C:523:DC:H2"	1:C:524:DG:N7	1.93	0.83
3:A:31:GLN:HE22	3:A:36:LYS:HE3	1.44	0.80
3:A:31:GLN:HE22	3:A:36:LYS:HE3	1.44	0.80
1:C:517:DC:OP1	1:C:517:DC:H4'	1.81	0.80
1:C:502:DC:H1'	1:C:503:DT:H5'	1.63	0.79
1:C:502:DC:H42	2:D:573:DG:H1	1.29	0.78
3:A:82:LYS:HB3	3:A:83:PRO:HD3	1.65	0.78
3:A:82:LYS:HB3	3:A:83:PRO:HD3	1.65	0.78
1:C:519:DG:H1	2:D:556:DC:H42	1.30	0.78
3:A:115:ALA:HA	3:A:121:LYS:HB2	1.63	0.78
3:A:115:ALA:HA	3:A:121:LYS:HB2	1.63	0.78
3:A:149:ARG:O	3:A:152:LEU:HD22	1.83	0.76
3:A:149:ARG:O	3:A:152:LEU:HD22	1.83	0.76
3:A:142:LYS:HD3	5:A:629:HOH:O	1.86	0.74
1:C:505:DA:H2"	1:C:506:DA:C5'	2.16	0.74
5:C:71:HOH:O	3:A:142:LYS:HD3	1.86	0.74
3:A:114:SER:OG	3:A:121:LYS:HD3	1.84	0.74
3:A:114:SER:OG	3:A:121:LYS:HD3	1.84	0.74
3:B:331:GLN:HE22	3:B:336:LYS:HD2	1.52	0.74
3:B:331:GLN:HE22	3:B:336:LYS:HD2	1.52	0.74
1:C:524:DG:H1	2:D:551:DC:H42	1.35	0.74
2:D:569:DT:O4	3:B:328:LYS:HE3	1.87	0.74
3:A:35:PHE:HE1	3:A:119:PRO:HG3	1.54	0.73
3:A:35:PHE:HE1	3:A:119:PRO:HG3	1.54	0.73
1:C:517:DC:H2'	3:A:26:GLN:OE1	1.87	0.73
1:C:513:DG:OP2	3:A:48:LYS:HE3	1.88	0.73
3:A:92:GLN:HG3	3:A:103:ASN:HD21	1.51	0.72
3:A:92:GLN:HG3	3:A:103:ASN:HD21	1.51	0.72
1:C:505:DA:C2'	1:C:506:DA:H5"	2.21	0.71
2:D:566:DA:H2"	2:D:567:DC:O5'	1.90	0.70
3:A:35:PHE:CE1	3:A:119:PRO:HG3	2.26	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:35:PHE:CE1	3:A:119:PRO:HG3	2.26	0.70
1:C:511:DG:H4'	3:B:439:LYS:HD2	1.72	0.70
3:B:382:LYS:HE3	3:B:382:LYS:HA	1.77	0.67
3:B:382:LYS:HE3	3:B:382:LYS:HA	1.77	0.67
3:B:424:GLU:O	3:B:427:THR:HB	1.95	0.66
3:B:449:ARG:O	3:B:452:LEU:HG	1.96	0.66
3:B:424:GLU:O	3:B:427:THR:HB	1.95	0.66
3:B:449:ARG:O	3:B:452:LEU:HG	1.96	0.66
1:C:513:DG:OP1	3:A:137:ASP:HB3	1.95	0.66
3:A:101:GLN:O	3:A:105:VAL:HG23	1.95	0.66
3:A:101:GLN:O	3:A:105:VAL:HG23	1.95	0.66
2:D:566:DA:H2"	2:D:567:DC:O5'	1.96	0.65
1:C:505:DA:H2"	1:C:506:DA:H5'	1.77	0.65
3:B:348:LYS:CE	3:B:350:GLN:HE21	2.09	0.65
3:B:348:LYS:CE	3:B:350:GLN:HE21	2.09	0.65
3:A:149:ARG:HG2	3:A:152:LEU:HD13	1.78	0.65
3:A:149:ARG:HG2	3:A:152:LEU:HD13	1.78	0.65
2:D:557:DT:H2"	2:D:558:DG:OP2	1.96	0.65
3:A:148:VAL:O	3:A:151:VAL:HB	1.99	0.62
3:A:148:VAL:O	3:A:151:VAL:HB	1.99	0.62
3:B:323:ILE:C	3:B:324:ILE:HD13	2.21	0.61
3:B:327:ILE:HD11	3:B:429:VAL:HG11	1.83	0.61
3:B:323:ILE:C	3:B:324:ILE:HD13	2.21	0.61
3:B:327:ILE:HD11	3:B:429:VAL:HG11	1.83	0.61
3:A:31:GLN:NE2	3:A:36:LYS:HE3	2.15	0.61
3:A:31:GLN:NE2	3:A:36:LYS:HE3	2.15	0.61
2:D:567:DC:H2"	2:D:568:DG:H5'	1.83	0.60
3:B:449:ARG:C	3:B:451:VAL:H	2.04	0.60
3:B:449:ARG:C	3:B:451:VAL:H	2.04	0.60
2:D:566:DA:H5"	3:B:437:ASP:H	1.68	0.59
3:A:114:SER:O	3:A:121:LYS:HD2	2.02	0.58
3:A:114:SER:O	3:A:121:LYS:HD2	2.02	0.58
2:D:554:DA:OP1	3:B:381:ILE:HB	2.04	0.58
2:D:566:DA:H5"	3:B:437:ASP:N	2.18	0.58
1:C:523:DC:H2"	1:C:524:DG:C8	2.38	0.58
3:B:304:LYS:HA	3:B:390:GLN:HE22	1.67	0.58
3:B:304:LYS:HA	3:B:390:GLN:HE22	1.67	0.58
3:B:331:GLN:NE2	3:B:336:LYS:HD2	2.17	0.57
1:C:517:DC:H2"	1:C:518:DA:H8	1.69	0.57
3:B:331:GLN:NE2	3:B:336:LYS:HD2	2.17	0.57
3:A:141:ARG:NH2	3:A:144:THR:HG22	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:141:ARG:NH2	3:A:144:THR:HG22	2.18	0.57
3:B:364:VAL:HG22	3:B:365:GLY:N	2.19	0.57
3:B:364:VAL:HG22	3:B:365:GLY:N	2.19	0.57
2:D:568:DG:OP1	3:A:142:LYS:N	2.37	0.57
3:B:438:SER:HB3	5:B:48:HOH:O	2.04	0.57
3:B:438:SER:HB3	5:B:48:HOH:O	2.04	0.57
2:D:564:DC:H5'	3:B:346:THR:O	2.05	0.56
3:A:31:GLN:HE22	3:A:36:LYS:CE	2.15	0.56
3:A:31:GLN:HE22	3:A:36:LYS:CE	2.15	0.56
3:A:64:VAL:HG11	3:A:83:PRO:HB3	1.87	0.56
3:A:127:THR:HG22	3:A:128:TRP:CE3	2.41	0.56
3:A:64:VAL:HG11	3:A:83:PRO:HB3	1.87	0.56
3:A:127:THR:HG22	3:A:128:TRP:CE3	2.41	0.56
3:B:316:PHE:HE2	3:B:345:VAL:CG1	2.19	0.55
3:B:316:PHE:HE2	3:B:345:VAL:CG1	2.19	0.55
3:A:115:ALA:HB2	3:A:125:VAL:HG21	1.87	0.55
3:A:115:ALA:HB2	3:A:125:VAL:HG21	1.87	0.55
2:D:561:DT:H1'	2:D:562:DC:O4'	2.06	0.55
3:A:3:THR:HA	3:A:4:LYS:NZ	2.21	0.55
3:A:3:THR:HA	3:A:4:LYS:NZ	2.21	0.55
2:D:568:DG:H2'	2:D:569:DT:H72	1.88	0.55
1:C:517:DC:H2"	1:C:518:DA:C8	2.42	0.55
3:B:392:GLN:HG3	3:B:403:ASN:OD1	2.07	0.54
3:B:392:GLN:HG3	3:B:403:ASN:OD1	2.07	0.54
3:B:357:LYS:HE2	3:B:361:GLU:OE1	2.07	0.54
3:B:357:LYS:HE2	3:B:361:GLU:OE1	2.07	0.54
1:C:515:DG:O6	3:B:370:ARG:NH1	2.32	0.54
3:A:57:LYS:HE2	3:B:396:LYS:HE3	1.89	0.54
3:A:57:LYS:HE2	3:B:396:LYS:HE3	1.89	0.54
1:C:517:DC:H2'	3:B:326:GLN:OE1	2.07	0.53
1:C:517:DC:H2"	1:C:518:DA:O5'	2.07	0.53
2:D:563:DA:H1'	2:D:564:DC:O4'	2.08	0.53
2:D:567:DC:H4'	2:D:567:DC:OP1	2.09	0.53
1:C:506:DA:H2"	1:C:507:DC:O5'	2.09	0.53
2:D:567:DC:H2'	2:D:568:DG:C8	2.44	0.52
3:B:412:LEU:N	3:B:413:PRO:HD2	2.24	0.52
3:A:48:LYS:HA	3:A:73:VAL:HG23	1.91	0.52
2:D:553:DT:H2"	2:D:554:DA:OP2	2.08	0.52
3:A:48:LYS:HA	3:A:73:VAL:HG23	1.91	0.52
3:B:412:LEU:N	3:B:413:PRO:HD2	2.24	0.52
1:C:505:DA:H2"	1:C:506:DA:C5'	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:511:DG:H1'	1:C:512:DT:O4'	2.10	0.52
2:D:563:DA:H1'	2:D:564:DC:O4'	2.10	0.52
1:C:502:DC:C6	1:C:503:DT:H72	2.45	0.52
1:C:510:DC:H1'	3:B:440:THR:HG21	1.91	0.52
3:B:352:ARG:O	3:B:352:ARG:HG3	2.10	0.52
3:B:352:ARG:O	3:B:352:ARG:HG3	2.10	0.52
1:C:524:DG:H1	2:D:551:DC:N4	2.04	0.52
1:C:502:DC:H1'	1:C:503:DT:C5'	2.39	0.52
1:C:502:DC:N4	2:D:573:DG:H1	2.04	0.52
1:C:524:DG:H1	2:D:551:DC:H42	1.58	0.51
2:D:564:DC:C5	3:B:373:VAL:HG21	2.45	0.51
3:A:6:ASN:ND2	3:A:9:PHE:H	2.09	0.51
3:A:6:ASN:ND2	3:A:9:PHE:H	2.09	0.51
3:A:49:THR:C	3:A:51:ARG:H	2.13	0.51
2:D:554:DA:OP1	3:A:81:ILE:HG12	2.11	0.51
3:A:49:THR:C	3:A:51:ARG:H	2.13	0.51
3:A:4:LYS:CE	3:A:4:LYS:H	2.16	0.51
3:A:4:LYS:H	3:A:4:LYS:CE	2.16	0.51
3:B:380:GLU:HB3	3:B:383:PRO:HD2	1.92	0.50
3:B:380:GLU:HB3	3:B:383:PRO:HD2	1.92	0.50
3:B:364:VAL:HG22	3:B:365:GLY:H	1.74	0.50
3:B:364:VAL:HG22	3:B:365:GLY:H	1.74	0.50
3:A:103:ASN:HA	3:A:106:LEU:HD23	1.94	0.50
3:A:103:ASN:HA	3:A:106:LEU:HD23	1.94	0.50
3:A:6:ASN:HD21	3:A:8:GLU:HB2	1.77	0.50
1:C:511:DG:C4'	3:B:439:LYS:HD2	2.40	0.50
3:A:6:ASN:HD21	3:A:8:GLU:HB2	1.77	0.50
3:A:118:SER:HB3	3:A:121:LYS:HE2	1.94	0.50
3:B:446:GLU:O	3:B:449:ARG:HB2	2.12	0.50
3:A:118:SER:HB3	3:A:121:LYS:HE2	1.94	0.50
3:B:446:GLU:O	3:B:449:ARG:HB2	2.12	0.50
1:C:516:DA:H2"	1:C:517:DC:O5'	2.12	0.49
1:C:502:DC:H2"	1:C:503:DT:OP2	2.12	0.49
3:B:444:THR:O	3:B:447:THR:HG23	2.12	0.49
3:B:444:THR:O	3:B:447:THR:HG23	2.12	0.49
3:B:331:GLN:NE2	3:B:331:GLN:HA	2.27	0.49
3:B:331:GLN:HA	3:B:331:GLN:NE2	2.27	0.49
1:C:514:DA:N6	2:D:560:DC:N4	2.61	0.49
3:A:115:ALA:HB1	3:A:122:PHE:HA	1.94	0.49
3:A:115:ALA:HB1	3:A:122:PHE:HA	1.94	0.49
3:A:118:SER:HB3	3:A:121:LYS:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:452:LEU:O	3:B:453:ASP:OD1	2.31	0.48
3:A:118:SER:HB3	3:A:121:LYS:HG3	1.95	0.48
3:B:452:LEU:O	3:B:453:ASP:OD1	2.31	0.48
3:B:444:THR:H	3:B:447:THR:CG2	2.27	0.48
3:A:116:LYS:HG2	3:A:116:LYS:O	2.14	0.48
3:B:444:THR:H	3:B:447:THR:CG2	2.27	0.48
3:A:116:LYS:HG2	3:A:116:LYS:O	2.14	0.48
3:B:320:ASP:OD2	3:B:347:GLU:OE1	2.32	0.48
2:D:566:DA:H5"	3:B:436:ASN:HB3	1.96	0.48
3:B:320:ASP:OD2	3:B:347:GLU:OE1	2.32	0.48
3:A:6:ASN:HD22	3:A:9:PHE:H	1.62	0.48
3:A:6:ASN:HD22	3:A:9:PHE:H	1.62	0.48
1:C:517:DC:OP1	1:C:517:DC:H4'	2.14	0.48
3:A:92:GLN:HA	3:A:95:LEU:HD12	1.95	0.48
1:C:513:DG:OP2	3:B:348:LYS:NZ	2.42	0.48
3:A:96:LYS:HD2	3:B:312:TYR:CZ	2.49	0.48
3:A:92:GLN:HA	3:A:95:LEU:HD12	1.95	0.48
1:C:513:DG:H5"	3:B:437:ASP:OD2	2.13	0.48
3:A:96:LYS:HD2	3:B:312:TYR:CZ	2.49	0.48
2:D:571:DT:H2"	2:D:572:DA:OP2	2.14	0.47
3:B:306:ASN:OD1	3:B:308:GLU:N	2.48	0.47
3:B:306:ASN:OD1	3:B:308:GLU:N	2.48	0.47
3:A:41:LEU:HD23	3:A:81:ILE:HD11	1.95	0.47
1:C:506:DA:H1'	1:C:507:DC:H5'	1.97	0.47
3:A:41:LEU:HD23	3:A:81:ILE:HD11	1.95	0.47
2:D:566:DA:H4'	3:B:438:SER:HA	1.95	0.47
1:C:505:DA:H3'	5:C:69:HOH:O	2.13	0.47
3:A:141:ARG:CZ	3:A:144:THR:HG22	2.44	0.47
3:A:141:ARG:CZ	3:A:144:THR:HG22	2.44	0.47
3:A:31:GLN:HG2	5:A:624:HOH:O	2.14	0.46
3:A:31:GLN:HG2	5:A:627:HOH:O	2.14	0.46
3:A:36:LYS:HD2	3:A:36:LYS:N	2.29	0.46
3:A:36:LYS:HD2	3:A:36:LYS:N	2.29	0.46
3:A:107:LYS:HE3	3:A:128:TRP:CE2	2.51	0.46
3:A:107:LYS:HE3	3:A:128:TRP:CE2	2.51	0.46
2:D:561:DT:H1'	2:D:562:DC:O4'	2.16	0.46
2:D:559:DT:H2'	5:D:87:HOH:O	2.16	0.45
3:B:324:ILE:HD13	3:B:324:ILE:N	2.30	0.45
3:B:324:ILE:N	3:B:324:ILE:HD13	2.30	0.45
3:B:348:LYS:HE2	3:B:350:GLN:NE2	2.20	0.45
3:B:348:LYS:HE2	3:B:350:GLN:NE2	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:31:GLN:NE2	3:A:36:LYS:HG3	2.32	0.45
3:B:382:LYS:HB3	3:B:383:PRO:HD3	1.98	0.45
3:A:31:GLN:NE2	3:A:36:LYS:HG3	2.32	0.45
3:B:382:LYS:HB3	3:B:383:PRO:HD3	1.98	0.45
3:B:413:PRO:O	3:B:416:LYS:HB2	2.17	0.45
3:B:413:PRO:O	3:B:416:LYS:HB2	2.17	0.45
1:C:513:DG:C2	1:C:514:DA:C4	3.05	0.45
3:B:448:VAL:O	3:B:451:VAL:HB	2.17	0.45
3:B:448:VAL:O	3:B:451:VAL:HB	2.17	0.45
3:B:316:PHE:HE2	3:B:345:VAL:HG11	1.82	0.45
3:B:316:PHE:HE2	3:B:345:VAL:HG11	1.82	0.45
3:B:325:ALA:HB1	3:B:429:VAL:HB	1.99	0.44
3:B:325:ALA:HB1	3:B:429:VAL:HB	1.99	0.44
2:D:554:DA:H5"	3:B:380:GLU:HA	2.00	0.44
1:C:518:DA:O3'	3:A:142:LYS:HD2	2.17	0.44
3:A:81:ILE:HA	3:A:81:ILE:HD13	1.80	0.44
3:A:81:ILE:HD13	3:A:81:ILE:HA	1.80	0.44
1:C:514:DA:H61	2:D:560:DC:N4	2.15	0.44
1:C:517:DC:C4'	1:C:517:DC:OP1	2.60	0.44
2:D:570:DT:H2"	2:D:571:DT:OP2	2.17	0.44
1:C:524:DG:H1	2:D:551:DC:N4	2.16	0.44
3:A:4:LYS:N	3:A:4:LYS:HE2	2.20	0.43
3:B:427:THR:O	3:B:431:GLN:HG3	2.18	0.43
3:A:4:LYS:HE2	3:A:4:LYS:N	2.20	0.43
3:B:427:THR:O	3:B:431:GLN:HG3	2.18	0.43
1:C:519:DG:H1	2:D:556:DC:N4	2.08	0.43
1:C:513:DG:H2"	1:C:514:DA:O5'	2.17	0.43
3:A:121:LYS:O	3:A:125:VAL:HG23	2.17	0.43
3:B:426:CYS:O	3:B:429:VAL:HG13	2.19	0.43
3:A:121:LYS:O	3:A:125:VAL:HG23	2.17	0.43
3:B:426:CYS:O	3:B:429:VAL:HG13	2.19	0.43
3:A:118:SER:CB	3:A:121:LYS:HE2	2.49	0.43
3:B:451:VAL:HG13	3:B:451:VAL:O	2.19	0.43
3:B:398:LYS:HA	3:B:401:GLN:OE1	2.18	0.43
3:A:118:SER:CB	3:A:121:LYS:HE2	2.49	0.43
3:B:451:VAL:HG13	3:B:451:VAL:O	2.19	0.43
1:C:510:DC:C1'	3:B:440:THR:HG21	2.48	0.43
3:B:398:LYS:HA	3:B:401:GLN:OE1	2.18	0.43
3:B:407:LYS:HE2	3:B:428:TRP:CE2	2.53	0.43
3:B:407:LYS:HE2	3:B:428:TRP:CE2	2.53	0.43
3:B:421:LYS:O	3:B:425:VAL:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:421:LYS:O	3:B:425:VAL:HG23	2.19	0.43
3:B:306:ASN:O	3:B:309:PHE:HB3	2.19	0.42
3:B:306:ASN:O	3:B:309:PHE:HB3	2.19	0.42
3:B:306:ASN:C	3:B:306:ASN:OD1	2.57	0.42
2:D:568:DG:H5"	3:B:442:LYS:HB2	2.02	0.42
3:B:306:ASN:OD1	3:B:306:ASN:C	2.57	0.42
3:B:449:ARG:C	3:B:451:VAL:N	2.72	0.42
3:B:449:ARG:C	3:B:451:VAL:N	2.72	0.42
3:A:123:LEU:HD11	3:A:149:ARG:NH2	2.35	0.42
3:A:149:ARG:O	3:A:151:VAL:N	2.46	0.42
3:A:123:LEU:HD11	3:A:149:ARG:NH2	2.35	0.42
3:A:149:ARG:O	3:A:151:VAL:N	2.46	0.42
1:C:516:DA:H4'	5:A:616:HOH:O	2.19	0.42
1:C:513:DG:H1'	1:C:514:DA:O4'	2.19	0.42
3:A:81:ILE:HG22	3:A:82:LYS:N	2.33	0.42
3:A:81:ILE:HG22	3:A:82:LYS:N	2.33	0.42
1:C:507:DC:C5	3:A:68:ARG:NH1	2.88	0.42
3:B:404:LEU:HA	3:B:404:LEU:HD23	1.84	0.42
3:B:404:LEU:HA	3:B:404:LEU:HD23	1.84	0.42
3:B:304:LYS:HB2	5:B:89:HOH:O	2.20	0.41
3:B:304:LYS:HB2	5:B:89:HOH:O	2.20	0.41
3:A:3:THR:HA	3:A:4:LYS:HZ1	1.86	0.41
3:A:96:LYS:HD2	3:B:312:TYR:CE1	2.55	0.41
2:D:557:DT:H2"	2:D:558:DG:OP2	2.20	0.41
3:A:3:THR:HA	3:A:4:LYS:HZ1	1.86	0.41
3:A:96:LYS:HD2	3:B:312:TYR:CE1	2.55	0.41
3:A:82:LYS:HB3	3:A:83:PRO:CD	2.42	0.41
1:C:515:DG:C4'	1:C:515:DG:OP1	2.68	0.41
3:A:12:TYR:CD1	3:A:12:TYR:C	2.92	0.41
3:A:82:LYS:HB3	3:A:83:PRO:CD	2.42	0.41
3:A:12:TYR:CD1	3:A:12:TYR:C	2.92	0.41
3:A:31:GLN:HE21	3:A:31:GLN:CA	2.33	0.41
3:A:31:GLN:HE21	3:A:31:GLN:CA	2.33	0.41
3:A:22:SER:HB3	3:A:44:GLN:CG	2.51	0.41
3:A:22:SER:HB3	3:A:44:GLN:CG	2.51	0.41
2:D:559:DT:O4	3:A:70:ARG:HD2	2.20	0.41
3:B:430:ASP:HA	3:B:441:ARG:NH2	2.36	0.40
3:B:430:ASP:HA	3:B:441:ARG:NH2	2.36	0.40
3:A:125:VAL:O	3:A:128:TRP:HB2	2.21	0.40
3:A:113:PRO:O	3:A:116:LYS:HB3	2.21	0.40
3:A:125:VAL:O	3:A:128:TRP:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:113:PRO:O	3:A:116:LYS:HB3	2.21	0.40
1:C:518:DA:H2"	1:C:519:DG:C8	2.56	0.40
2:D:569:DT:O4	3:B:328:LYS:CE	2.64	0.40
1:C:508:DG:N7	3:A:68:ARG:NH1	2.62	0.40
2:D:556:DC:C5	2:D:557:DT:H72	2.57	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	1-A	150/163 (92%)	139 (93%)	11 (7%)	0	100	100
3	1-B	150/163 (92%)	138 (92%)	11 (7%)	1 (1%)	26	46
3	2-A	150/163 (92%)	139 (93%)	11 (7%)	0	100	100
3	2-B	150/163 (92%)	138 (92%)	11 (7%)	1 (1%)	26	46
All	All	600/652 (92%)	554 (92%)	44 (7%)	2 (0%)	46	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	1-B	450	ALA
3	2-B	450	ALA

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	1-A	139/150 (93%)	131 (94%)	8 (6%)	25 45
3	1-B	139/150 (93%)	125 (90%)	14 (10%)	9 17
3	2-A	139/150 (93%)	131 (94%)	8 (6%)	25 45
3	2-B	139/150 (93%)	125 (90%)	14 (10%)	9 17
All	All	556/600 (93%)	512 (92%)	44 (8%)	15 28

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1-A	4	LYS
3	1-A	31	GLN
3	1-A	68	ARG
3	1-A	73	VAL
3	1-A	101	GLN
3	1-A	127	THR
3	1-A	128	TRP
3	1-A	152	LEU
3	1-B	303	THR
3	1-B	348	LYS
3	1-B	368	ARG
3	1-B	369	ASP
3	1-B	378	LEU
3	1-B	381	ILE
3	1-B	382	LYS
3	1-B	401	GLN
3	1-B	417	GLU
3	1-B	428	TRP
3	1-B	429	VAL
3	1-B	430	ASP
3	1-B	441	ARG
3	1-B	447	THR
3	2-A	4	LYS
3	2-A	31	GLN
3	2-A	68	ARG
3	2-A	73	VAL
3	2-A	101	GLN
3	2-A	127	THR
3	2-A	128	TRP
3	2-A	152	LEU
3	2-B	303	THR

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Mol	Chain	Res	Type
3	2-B	348	LYS
3	2-B	368	ARG
3	2-B	369	ASP
3	2-B	378	LEU
3	2-B	381	ILE
3	2-B	382	LYS
3	2-B	401	GLN
3	2-B	417	GLU
3	2-B	428	TRP
3	2-B	429	VAL
3	2-B	430	ASP
3	2-B	441	ARG
3	2-B	447	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
3	1-A	6	ASN
3	1-A	31	GLN
3	1-A	50	GLN
3	1-A	103	ASN
3	1-B	331	GLN
3	1-B	350	GLN
3	2-A	6	ASN
3	2-A	26	GLN
3	2-A	31	GLN
3	2-A	50	GLN
3	2-A	103	ASN
3	2-B	331	GLN
3	2-B	350	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	1-C	24/24 (100%)	4.09	24 (100%)	0	0	16, 35, 46, 49	24 (100%)
1	2-C	24/24 (100%)	4.09	24 (100%)	0	0	16, 35, 46, 49	24 (100%)
2	1-D	24/24 (100%)	4.01	24 (100%)	0	0	19, 34, 38, 43	24 (100%)
2	2-D	24/24 (100%)	4.01	24 (100%)	0	0	19, 34, 38, 43	24 (100%)
3	1-A	152/163 (93%)	1.02	35 (23%)	1	1	13, 31, 58, 70	0
3	1-B	152/163 (93%)	1.04	33 (21%)	1	1	17, 33, 61, 71	0
3	2-A	152/163 (93%)	1.02	35 (23%)	1	1	13, 31, 58, 70	0
3	2-B	152/163 (93%)	1.04	33 (21%)	1	1	17, 33, 61, 71	0
All	All	704/748 (94%)	1.44	232 (32%)	0	0	13, 32, 59, 71	96 (13%)

All (232) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	1-B	428	TRP	7.6
3	2-B	428	TRP	7.6
3	1-B	427	THR	6.1
3	2-B	427	THR	6.1
1	1-C	511	DG	6.0
1	2-C	511	DG	6.0
1	1-C	513	DG	5.7
1	2-C	513	DG	5.7
3	1-B	448	VAL	5.4
3	2-B	448	VAL	5.4
1	1-C	524	DG	5.2
1	2-C	524	DG	5.2
2	1-D	562	DC	5.1
2	2-D	562	DC	5.1
2	1-D	561	DT	5.1
2	2-D	561	DT	5.1

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Mol	Chain	Res	Type	RSRZ
3	1-A	146	GLU	5.0
3	2-A	146	GLU	5.0
1	1-C	514	DA	4.9
1	2-C	514	DA	4.9
1	1-C	508	DG	4.8
1	1-C	515	DG	4.8
1	2-C	508	DG	4.8
1	2-C	515	DG	4.8
3	1-B	445	SER	4.8
3	2-B	445	SER	4.8
2	1-D	558	DG	4.7
2	2-D	558	DG	4.7
1	1-C	510	DC	4.7
1	2-C	510	DC	4.7
2	1-D	565	DG	4.7
2	2-D	565	DG	4.7
2	1-D	564	DC	4.7
2	2-D	564	DC	4.7
1	1-C	512	DT	4.6
1	2-C	512	DT	4.6
3	1-B	419	PRO	4.6
3	2-B	419	PRO	4.6
2	1-D	573	DG	4.6
2	2-D	573	DG	4.6
2	1-D	566	DA	4.6
2	2-D	566	DA	4.6
3	1-A	34	LYS	4.6
3	2-A	34	LYS	4.6
2	1-D	567	DC	4.4
2	1-D	574	DC	4.4
2	2-D	567	DC	4.4
2	2-D	574	DC	4.4
2	1-D	563	DA	4.4
2	2-D	563	DA	4.4
2	1-D	568	DG	4.3
2	2-D	568	DG	4.3
3	1-B	332	SER	4.3
3	2-B	332	SER	4.3
2	1-D	551	DC	4.3
2	1-D	560	DC	4.3
2	2-D	551	DC	4.3
2	2-D	560	DC	4.3

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Mol	Chain	Res	Type	RSRZ
3	1-B	425	VAL	4.3
3	2-B	425	VAL	4.3
3	1-A	152	LEU	4.2
3	2-A	152	LEU	4.2
3	1-A	117	GLU	4.2
3	2-A	117	GLU	4.2
1	1-C	516	DA	4.2
1	2-C	516	DA	4.2
3	1-A	128	TRP	4.2
3	2-A	128	TRP	4.2
1	1-C	501	DG	4.2
1	1-C	519	DG	4.2
1	2-C	501	DG	4.2
1	2-C	519	DG	4.2
3	1-B	450	ALA	4.1
3	2-B	450	ALA	4.1
3	1-B	444	THR	4.1
3	2-B	444	THR	4.1
2	1-D	552	DG	4.0
2	2-D	552	DG	4.0
3	1-A	33	CYS	3.9
3	2-A	33	CYS	3.9
1	1-C	517	DC	3.8
1	2-C	517	DC	3.8
1	1-C	518	DA	3.8
1	2-C	518	DA	3.8
2	1-D	572	DA	3.7
2	2-D	572	DA	3.7
2	1-D	556	DC	3.7
2	2-D	556	DC	3.7
1	1-C	502	DC	3.7
1	1-C	507	DC	3.7
1	2-C	502	DC	3.7
1	2-C	507	DC	3.7
1	1-C	509	DT	3.7
1	2-C	509	DT	3.7
3	1-A	30	ASN	3.6
3	2-A	30	ASN	3.6
3	1-B	418	SER	3.6
3	2-B	418	SER	3.6
3	1-A	121	LYS	3.6
3	2-A	121	LYS	3.6

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Mol	Chain	Res	Type	RSRZ
3	1-A	118	SER	3.5
3	2-A	118	SER	3.5
2	1-D	570	DT	3.5
2	2-D	570	DT	3.5
1	1-C	504	DA	3.5
1	2-C	504	DA	3.5
3	1-A	153	ASP	3.5
3	2-A	153	ASP	3.5
2	1-D	557	DT	3.4
2	2-D	557	DT	3.4
2	1-D	554	DA	3.4
2	2-D	554	DA	3.4
1	1-C	523	DC	3.4
1	2-C	523	DC	3.4
3	1-A	125	VAL	3.4
3	2-A	125	VAL	3.4
2	1-D	559	DT	3.4
2	2-D	559	DT	3.4
1	1-C	505	DA	3.4
1	2-C	505	DA	3.4
3	1-A	120	ASP	3.3
3	2-A	120	ASP	3.3
3	1-B	433	ALA	3.3
3	2-B	433	ALA	3.3
1	1-C	521	DT	3.3
1	2-C	521	DT	3.3
1	1-C	506	DA	3.2
1	2-C	506	DA	3.2
3	1-A	145	SER	3.2
3	2-A	145	SER	3.2
1	1-C	522	DA	3.2
1	2-C	522	DA	3.2
3	1-B	302	ASN	3.2
3	2-B	302	ASN	3.2
3	1-A	35	PHE	3.2
3	2-A	35	PHE	3.2
2	1-D	555	DA	3.2
2	2-D	555	DA	3.2
1	1-C	503	DT	3.2
1	2-C	503	DT	3.2
3	1-A	2	ASN	3.1
3	2-A	2	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
3	1-B	413	PRO	3.1
3	2-B	413	PRO	3.1
1	1-C	520	DT	3.1
1	2-C	520	DT	3.1
3	1-B	420	ASP	3.0
3	2-B	420	ASP	3.0
3	1-A	107	LYS	3.0
3	2-A	107	LYS	3.0
2	1-D	569	DT	2.9
2	2-D	569	DT	2.9
3	1-A	151	VAL	2.9
3	2-A	151	VAL	2.9
3	1-A	122	PHE	2.9
3	2-A	122	PHE	2.9
3	1-B	452	LEU	2.9
3	2-B	452	LEU	2.9
3	1-A	123	LEU	2.8
3	2-A	123	LEU	2.8
2	1-D	571	DT	2.8
2	2-D	571	DT	2.8
3	1-B	423	LEU	2.8
3	2-B	423	LEU	2.8
3	1-A	116	LYS	2.8
3	2-A	116	LYS	2.8
3	1-A	148	VAL	2.7
3	1-B	429	VAL	2.7
3	2-A	148	VAL	2.7
3	2-B	429	VAL	2.7
3	1-A	111	GLN	2.7
3	2-A	111	GLN	2.7
3	1-B	407	LYS	2.7
3	2-B	407	LYS	2.7
3	1-A	119	PRO	2.7
3	2-A	119	PRO	2.7
3	1-A	149	ARG	2.7
3	2-A	149	ARG	2.7
3	1-B	442	LYS	2.6
3	2-B	442	LYS	2.6
2	1-D	553	DT	2.6
2	2-D	553	DT	2.6
3	1-A	150	ALA	2.6
3	2-A	150	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
3	1-B	334	LYS	2.6
3	2-B	334	LYS	2.6
3	1-A	108	ILE	2.5
3	2-A	108	ILE	2.5
3	1-B	451	VAL	2.5
3	2-B	451	VAL	2.5
3	1-B	417	GLU	2.5
3	2-B	417	GLU	2.5
3	1-A	3	THR	2.4
3	1-B	330	ASN	2.4
3	2-A	3	THR	2.4
3	2-B	330	ASN	2.4
3	1-A	31	GLN	2.4
3	2-A	31	GLN	2.4
3	1-A	36	LYS	2.4
3	2-A	36	LYS	2.4
3	1-B	432	ILE	2.4
3	2-B	432	ILE	2.4
3	1-B	430	ASP	2.4
3	2-B	430	ASP	2.4
3	1-A	134	ALA	2.3
3	2-A	134	ALA	2.3
3	1-A	130	ASP	2.3
3	2-A	130	ASP	2.3
3	1-A	113	PRO	2.3
3	1-B	329	PRO	2.3
3	2-A	113	PRO	2.3
3	2-B	329	PRO	2.3
3	1-A	27	ILE	2.3
3	2-A	27	ILE	2.3
3	1-B	331	GLN	2.2
3	2-B	331	GLN	2.2
3	1-B	453	ASP	2.2
3	2-B	453	ASP	2.2
3	1-B	439	LYS	2.2
3	2-B	439	LYS	2.2
3	1-B	446	GLU	2.1
3	2-B	446	GLU	2.1
3	1-B	333	CYS	2.1
3	2-B	333	CYS	2.1
3	1-B	303	THR	2.1
3	2-B	303	THR	2.1

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Mol	Chain	Res	Type	RSRZ
3	1-A	144	THR	2.1
3	2-A	144	THR	2.1
3	1-A	114	SER	2.0
3	2-A	114	SER	2.0
3	1-B	431	GLN	2.0
3	2-B	431	GLN	2.0

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 carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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, 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	LLDF	B-factors(Å^2)	Q<0.9
4	MG	2-B	601	1/1	0.91	0.11	-1.29	4,4,4,4	0
4	MG	1-B	601	1/1	0.91	0.11	-1.30	4,4,4,4	0
4	MG	1-A	602	1/1	0.93	0.12	-1.41	9,9,9,9	0
4	MG	2-A	602	1/1	0.93	0.12	-1.42	9,9,9,9	0
4	MG	1-C	603	1/1	0.92	0.09	-1.82	22,22,22,22	0
4	MG	2-C	603	1/1	0.92	0.09	-1.82	22,22,22,22	0

6.5 Other polymers (i)

There are no such residues in this entry.