Full wwPDB X-ray Structure Validation Report ⓘ

Aug 19, 2023 – 06:48 PM EDT

PDB ID	:	2HOF
Title	:	Crystal structure of the pre-cleavage synaptic complex in the cre-loxp site-specific recombination
Authors	:	Ghosh, K.; Van Duyne, G.D.
Deposited on	:	2006-07-14
Resolution	:	2.40 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:

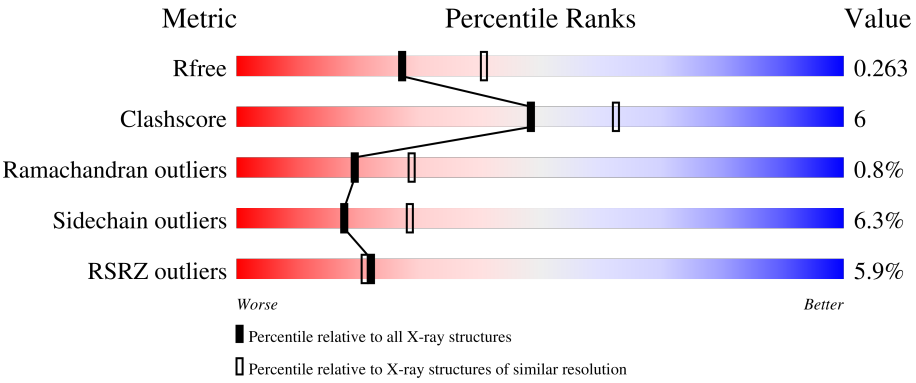
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	C	35	9%, 66%, 31%, .
2	D	35	77%, 20%, .
3	A	343	7%, 71%, 17%, ., 10%
3	B	343	4%, 77%, 13%, .., 8%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6858 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 LoxP DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	34	Total	C	N	O	P	0	0	0
			693	334	122	203	34			

- Molecule 2 is a DNA chain called LoxP DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	34	Total	C	N	O	P	0	0	0
			701	337	125	205	34			

- Molecule 3 is a protein called Recombinase cre.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	309	Total	C	N	O	S	0	0	0
			2459	1529	469	446	15			
3	B	316	Total	C	N	O	S	0	0	0
			2504	1557	479	453	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	201	ALA	LYS	engineered mutation	UNP P06956
B	201	ALA	LYS	engineered mutation	UNP P06956

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	64	Total	O	0	0
			64	64		
4	D	62	Total	O	0	0
			62	62		
4	A	158	Total	O	0	0
			158	158		

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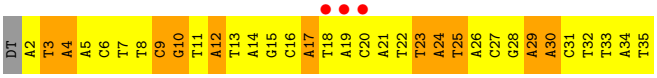
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	217	Total O 217 217	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

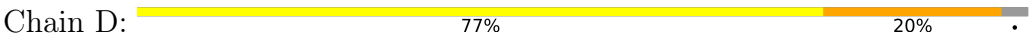
• Molecule 1: LoxP DNA

Chain C:



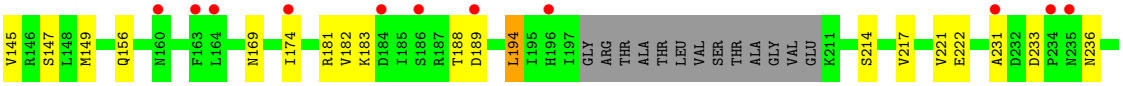
• Molecule 2: LoxP DNA

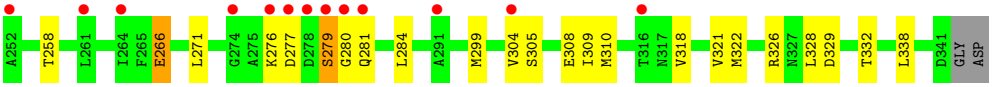
Chain D:



• Molecule 3: Recombinase cre

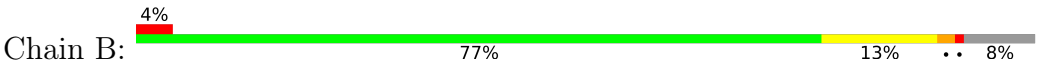
Chain A:

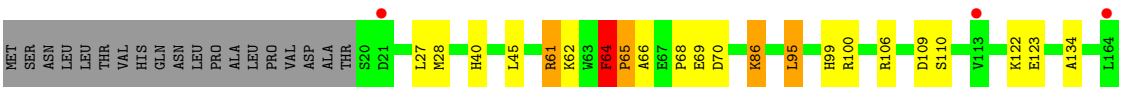


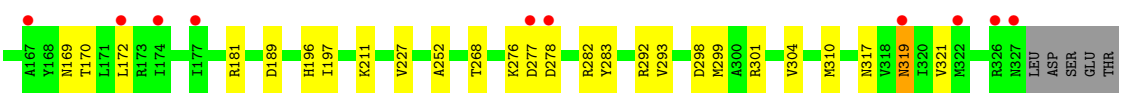


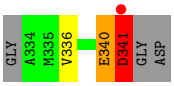
• Molecule 3: Recombinase cre

Chain B:








GLY
A334
M335
V336
E340
D341
GLY
ASP

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	107.62Å 122.13Å 178.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.96 – 2.40 29.96 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.8 (29.96-2.40) 98.8 (29.96-2.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	4.41 (at 2.42Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.209 , 0.263 0.211 , 0.263	Depositor DCC
R_{free} test set	2309 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	49.5	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 51.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6858	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% 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	C	1.18	1/776 (0.1%)	2.05	62/1194 (5.2%)
2	D	1.15	2/786 (0.3%)	2.04	57/1212 (4.7%)
3	A	0.41	0/2499	0.65	0/3367
3	B	0.46	0/2544	0.77	5/3429 (0.1%)
All	All	0.68	3/6605 (0.0%)	1.21	124/9202 (1.3%)

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
3	A	0	1
3	B	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	9	DC	N1-C2	-6.38	1.33	1.40
1	C	16	DC	N1-C2	-5.70	1.34	1.40
2	D	27	DC	N1-C2	-5.54	1.34	1.40

All (124) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	341	ASP	CA-C-O	19.48	161.02	120.10
2	D	6	DG	O4'-C4'-C3'	-13.45	97.93	106.00
1	C	13	DT	O4'-C1'-N1	10.22	115.16	108.00
2	D	16	DT	O4'-C4'-C3'	-10.04	99.98	106.00
1	C	6	DC	O4'-C4'-C3'	-9.61	100.23	106.00
2	D	3	DT	O4'-C1'-N1	8.29	113.80	108.00
1	C	29	DA	O4'-C1'-N9	7.64	113.35	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	18	DT	C4-C5-C7	7.42	123.45	119.00
3	B	64	PHE	CB-CA-C	7.19	124.79	110.40
2	D	4	DA	O4'-C4'-C3'	-7.17	101.63	104.50
2	D	14	DA	OP1-P-OP2	-7.09	108.97	119.60
1	C	20	DC	OP1-P-OP2	-6.97	109.15	119.60
1	C	13	DT	O4'-C4'-C3'	-6.94	101.72	104.50
1	C	17	DA	OP1-P-OP2	-6.93	109.20	119.60
2	D	26	DA	OP1-P-OP2	-6.93	109.20	119.60
1	C	28	DG	OP1-P-OP2	-6.91	109.24	119.60
1	C	26	DA	OP1-P-OP2	-6.88	109.27	119.60
3	B	64	PHE	CB-CG-CD2	-6.88	115.99	120.80
3	B	64	PHE	CB-CG-CD1	6.86	125.60	120.80
2	D	27	DC	OP1-P-OP2	-6.86	109.31	119.60
2	D	10	DG	OP1-P-OP2	-6.85	109.33	119.60
1	C	21	DA	O4'-C4'-C3'	-6.80	101.78	104.50
1	C	4	DA	O4'-C4'-C3'	-6.75	101.80	104.50
1	C	16	DC	OP1-P-OP2	-6.74	109.49	119.60
2	D	15	DA	OP1-P-OP2	-6.71	109.53	119.60
2	D	12	DA	OP1-P-OP2	-6.71	109.54	119.60
2	D	32	DT	OP1-P-OP2	-6.67	109.60	119.60
2	D	5	DA	OP1-P-OP2	-6.65	109.62	119.60
2	D	18	DT	OP1-P-OP2	-6.64	109.64	119.60
2	D	22	DC	OP1-P-OP2	-6.62	109.67	119.60
2	D	19	DA	OP1-P-OP2	-6.61	109.68	119.60
1	C	9	DC	OP1-P-OP2	-6.61	109.69	119.60
1	C	24	DA	OP1-P-OP2	-6.57	109.75	119.60
1	C	18	DT	OP1-P-OP2	-6.56	109.76	119.60
1	C	22	DT	OP1-P-OP2	-6.56	109.76	119.60
1	C	7	DT	OP1-P-OP2	-6.55	109.78	119.60
1	C	19	DA	OP1-P-OP2	-6.53	109.81	119.60
2	D	25	DT	C4-C5-C7	6.51	122.91	119.00
1	C	12	DA	OP1-P-OP2	-6.51	109.84	119.60
2	D	16	DT	C6-C5-C7	-6.50	119.00	122.90
2	D	25	DT	OP1-P-OP2	-6.49	109.87	119.60
2	D	29	DA	OP1-P-OP2	-6.47	109.89	119.60
1	C	2	DA	OP1-P-OP2	-6.46	109.91	119.60
2	D	3	DT	OP1-P-OP2	-6.45	109.92	119.60
1	C	34	DA	OP1-P-OP2	-6.45	109.93	119.60
2	D	31	DG	OP1-P-OP2	-6.44	109.94	119.60
2	D	21	DG	OP1-P-OP2	-6.42	109.97	119.60
1	C	4	DA	OP1-P-OP2	-6.42	109.98	119.60
2	D	16	DT	C4-C5-C7	6.40	122.84	119.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	15	DG	OP1-P-OP2	-6.40	110.00	119.60
1	C	13	DT	OP1-P-OP2	-6.39	110.01	119.60
1	C	21	DA	C3'-C2'-C1'	-6.38	94.84	102.50
2	D	17	DG	OP1-P-OP2	-6.38	110.03	119.60
1	C	30	DA	OP1-P-OP2	-6.36	110.06	119.60
2	D	13	DT	OP1-P-OP2	-6.36	110.06	119.60
1	C	21	DA	OP1-P-OP2	-6.36	110.06	119.60
2	D	18	DT	C6-C5-C7	-6.35	119.09	122.90
2	D	11	DT	OP1-P-OP2	-6.34	110.09	119.60
1	C	8	DT	OP1-P-OP2	-6.33	110.11	119.60
1	C	25	DT	OP1-P-OP2	-6.31	110.14	119.60
1	C	17	DA	O4'-C1'-N9	6.29	112.40	108.00
2	D	6	DG	OP1-P-OP2	-6.28	110.18	119.60
2	D	2	DA	OP1-P-OP2	-6.27	110.19	119.60
2	D	9	DC	OP1-P-OP2	-6.27	110.20	119.60
2	D	28	DG	OP1-P-OP2	-6.27	110.19	119.60
1	C	33	DT	OP1-P-OP2	-6.25	110.22	119.60
1	C	27	DC	O4'-C1'-N1	6.21	112.35	108.00
2	D	7	DT	OP1-P-OP2	-6.20	110.31	119.60
2	D	30	DA	OP1-P-OP2	-6.19	110.31	119.60
1	C	29	DA	OP1-P-OP2	-6.18	110.32	119.60
2	D	20	DT	OP1-P-OP2	-6.18	110.32	119.60
2	D	4	DA	OP1-P-OP2	-6.17	110.34	119.60
1	C	22	DT	C6-C5-C7	-6.17	119.20	122.90
2	D	25	DT	C6-C5-C7	-6.17	119.20	122.90
1	C	6	DC	OP1-P-OP2	-6.16	110.36	119.60
1	C	27	DC	OP1-P-OP2	-6.15	110.37	119.60
2	D	35	DT	OP1-P-OP2	-6.15	110.38	119.60
1	C	35	DT	OP1-P-OP2	-6.12	110.41	119.60
1	C	23	DT	OP1-P-OP2	-6.10	110.45	119.60
1	C	14	DA	OP1-P-OP2	-6.08	110.48	119.60
2	D	8	DT	C4-C5-C7	6.07	122.64	119.00
1	C	16	DC	N1-C1'-C2'	6.06	124.12	112.60
2	D	8	DT	OP1-P-OP2	-6.06	110.51	119.60
2	D	8	DT	C6-C5-C7	-6.04	119.28	122.90
1	C	10	DG	OP1-P-OP2	-6.01	110.58	119.60
2	D	33	DT	OP1-P-OP2	-6.01	110.59	119.60
1	C	31	DC	OP1-P-OP2	-6.00	110.59	119.60
2	D	23	DT	C4-C5-C7	5.95	122.57	119.00
1	C	30	DA	O4'-C4'-C3'	-5.90	102.14	104.50
2	D	23	DT	OP1-P-OP2	-5.89	110.76	119.60
1	C	5	DA	OP1-P-OP2	-5.89	110.77	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	292	ARG	NE-CZ-NH2	-5.89	117.36	120.30
2	D	35	DT	C4-C5-C7	5.88	122.53	119.00
2	D	24	DA	OP1-P-OP2	-5.87	110.79	119.60
1	C	11	DT	OP1-P-OP2	-5.87	110.80	119.60
1	C	35	DT	O4'-C1'-N1	5.87	112.11	108.00
1	C	8	DT	C4-C5-C7	5.86	122.52	119.00
1	C	3	DT	OP1-P-OP2	-5.79	110.92	119.60
2	D	16	DT	OP1-P-OP2	-5.76	110.96	119.60
1	C	32	DT	OP1-P-OP2	-5.71	111.04	119.60
1	C	23	DT	C4-C5-C7	5.68	122.41	119.00
2	D	11	DT	O4'-C1'-N1	5.67	111.97	108.00
2	D	34	DA	OP1-P-OP2	-5.60	111.20	119.60
1	C	23	DT	O4'-C4'-C3'	-5.59	102.27	104.50
1	C	22	DT	C4-C5-C7	5.58	122.35	119.00
1	C	11	DT	C4-C5-C7	5.51	122.31	119.00
1	C	23	DT	C3'-C2'-C1'	-5.48	95.92	102.50
1	C	11	DT	C6-C5-C7	-5.42	119.65	122.90
1	C	15	DG	O4'-C1'-N9	-5.38	104.23	108.00
1	C	23	DT	O4'-C1'-N1	5.34	111.74	108.00
2	D	13	DT	O4'-C1'-N1	5.33	111.73	108.00
2	D	33	DT	C6-C5-C7	-5.29	119.72	122.90
2	D	29	DA	C3'-C2'-C1'	-5.28	96.16	102.50
2	D	7	DT	C4-C5-C7	5.28	122.17	119.00
2	D	29	DA	O4'-C1'-N9	5.26	111.68	108.00
2	D	15	DA	C3'-C2'-C1'	-5.25	96.20	102.50
1	C	35	DT	C4-C5-C7	5.19	122.11	119.00
1	C	5	DA	O4'-C1'-N9	5.15	111.61	108.00
1	C	23	DT	C6-C5-C7	-5.14	119.82	122.90
1	C	4	DA	O4'-C1'-N9	-5.13	104.41	108.00
2	D	23	DT	C6-C5-C7	-5.07	119.86	122.90
1	C	8	DT	C6-C5-C7	-5.03	119.88	122.90
2	D	27	DC	O4'-C1'-N1	5.03	111.52	108.00
1	C	10	DG	O4'-C4'-C3'	5.01	109.01	106.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	64	PHE	Peptide
3	B	64	PHE	Peptide

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	C	693	0	387	8	0
2	D	701	0	388	4	0
3	A	2459	0	2472	35	0
3	B	2504	0	2526	29	0
4	A	158	0	0	6	0
4	B	217	0	0	4	0
4	C	64	0	0	3	0
4	D	62	0	0	2	0
All	All	6858	0	5773	71	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 6.

All (71) 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)
4:C:39:HOH:O	3:B:86:LYS:HD2	1.76	0.85
3:A:169:ASN:HD21	3:A:214:SER:H	1.29	0.79
3:B:66:ALA:H	3:B:99:HIS:HE1	1.33	0.75
3:B:268:THR:HG22	4:B:495:HOH:O	1.89	0.71
3:A:277:ASP:HB3	3:A:284:LEU:HD13	1.71	0.71
1:C:17:DA:H2'	4:C:94:HOH:O	1.92	0.69
4:D:40:HOH:O	3:A:156:GLN:HG3	1.96	0.64
3:B:95:LEU:O	3:B:99:HIS:HD2	1.81	0.63
4:D:55:HOH:O	3:B:40:HIS:HE1	1.80	0.63
3:A:30:MET:HG2	4:A:463:HOH:O	1.99	0.61
3:A:66:ALA:H	3:A:99:HIS:HE1	1.46	0.61
3:B:62:LYS:HD2	3:B:64:PHE:O	2.03	0.59
3:A:39:GLU:HG2	4:A:415:HOH:O	2.04	0.58
3:A:318:VAL:HG22	3:A:322:MET:HG2	1.87	0.55
3:B:298:ASP:OD1	3:B:301:ARG:NH2	2.34	0.55
3:A:66:ALA:H	3:A:99:HIS:CE1	2.23	0.55
3:A:169:ASN:ND2	3:A:214:SER:H	2.01	0.55
3:A:305:SER:O	3:A:308:GLU:HG2	2.07	0.53
3:B:181:ARG:NH2	3:B:252:ALA:O	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:24:DA:H2'	1:C:25:DT:C6	2.44	0.53
1:C:3:DT:H2"	1:C:4:DA:C8	2.45	0.51
3:B:340:GLU:HA	3:B:341:ASP:C	2.31	0.51
2:D:11:DT:OP2	3:A:50:ARG:NH1	2.43	0.51
3:B:196:HIS:HE1	4:B:499:HOH:O	1.94	0.50
3:A:174:ILE:HD12	3:A:258:THR:HB	1.94	0.49
3:B:310:MET:HG2	3:B:321:VAL:HG21	1.94	0.49
3:B:66:ALA:H	3:B:99:HIS:CE1	2.22	0.48
1:C:17:DA:H8	4:C:94:HOH:O	1.95	0.48
3:B:69:GLU:HB2	4:B:389:HOH:O	2.14	0.48
3:B:64:PHE:O	3:B:65:PRO:O	2.31	0.48
1:C:9:DC:H2"	1:C:10:DG:C8	2.50	0.47
3:A:182:VAL:HG11	3:A:231:ALA:HA	1.96	0.47
3:A:156:GLN:HB2	4:A:462:HOH:O	2.15	0.47
3:B:317:ASN:OD1	3:B:319:ASN:ND2	2.49	0.46
3:B:172:LEU:HD21	3:B:197:ILE:HG13	1.98	0.46
3:B:134:ALA:HA	3:B:283:TYR:CD2	2.50	0.45
3:A:100:ARG:HG3	3:A:106:ARG:HD2	1.99	0.45
3:A:25:LYS:HE3	3:A:29:ASP:OD1	2.17	0.45
3:B:227:VAL:HG11	4:B:560:HOH:O	2.17	0.45
3:A:181:ARG:HD2	3:A:183:LYS:HE2	1.98	0.44
3:A:188:THR:HB	3:A:189:ASP:H	1.65	0.44
1:C:29:DA:H2"	1:C:30:DA:C8	2.53	0.44
3:B:95:LEU:O	3:B:99:HIS:CD2	2.68	0.44
3:A:233:ASP:HB3	3:A:236:ASN:ND2	2.33	0.43
3:A:149:MET:HE1	4:A:350:HOH:O	2.18	0.43
3:A:35:GLN:NE2	3:B:123:GLU:OE1	2.51	0.43
3:B:170:THR:HB	3:B:211:LYS:HD3	2.00	0.43
2:D:18:DT:H2"	2:D:19:DA:C8	2.53	0.43
3:A:329:ASP:HA	3:A:332:THR:HG23	2.00	0.43
3:A:141:ASP:O	3:A:145:VAL:HG23	2.18	0.43
1:C:23:DT:OP1	3:B:122:LYS:CE	2.67	0.42
3:A:279:SER:O	3:A:281:GLN:N	2.53	0.42
1:C:12:DA:H1'	3:B:282:ARG:HH22	1.85	0.42
3:A:188:THR:HG23	3:A:194:LEU:HD12	2.01	0.42
3:A:217:VAL:O	3:A:221:VAL:HG23	2.20	0.41
3:A:72:ARG:NH2	4:A:425:HOH:O	2.50	0.41
3:B:68:PRO:HB3	3:B:110:SER:OG	2.20	0.41
2:D:15:DA:C8	2:D:16:DT:H72	2.55	0.41
3:A:214:SER:HA	3:B:336:VAL:HG13	2.02	0.41
3:B:64:PHE:CD2	3:B:65:PRO:HD3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:106:ARG:NH1	3:B:109:ASP:OD2	2.54	0.41
3:A:72:ARG:HG3	3:A:116:VAL:HG11	2.03	0.41
3:A:95:LEU:HD12	3:A:95:LEU:HA	1.93	0.41
3:A:304:VAL:HG12	3:A:309:ILE:HG13	2.02	0.41
3:A:266:GLU:HG2	4:A:395:HOH:O	2.21	0.41
3:A:299:MET:O	3:A:304:VAL:HB	2.21	0.41
3:B:61:ARG:HD3	3:B:70:ASP:OD2	2.20	0.41
3:A:310:MET:HG2	3:A:321:VAL:HG21	2.01	0.40
2:D:24:DA:H2'	2:D:25:DT:C6	2.56	0.40
3:A:104:LEU:HB3	3:A:105:PRO:HD2	2.03	0.40
3:B:299:MET:HG2	3:B:304:VAL:HG21	2.04	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	305/343 (89%)	293 (96%)	9 (3%)	3 (1%)	15	23
3	B	312/343 (91%)	304 (97%)	6 (2%)	2 (1%)	25	36
All	All	617/686 (90%)	597 (97%)	15 (2%)	5 (1%)	19	29

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	65	PRO
3	A	280	GLY
3	B	65	PRO
3	B	277	ASP
3	A	279	SER

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	259/286 (91%)	241 (93%)	18 (7%)	15 25
3	B	263/286 (92%)	248 (94%)	15 (6%)	20 33
All	All	522/572 (91%)	489 (94%)	33 (6%)	18 28

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	25	LYS
3	A	39	GLU
3	A	45	LEU
3	A	51	SER
3	A	95	LEU
3	A	97	MET
3	A	100	ARG
3	A	122	LYS
3	A	133	GLN
3	A	147	SER
3	A	194	LEU
3	A	222	GLU
3	A	266	GLU
3	A	271	LEU
3	A	276	LYS
3	A	326	ARG
3	A	328	LEU
3	A	338	LEU
3	B	27	LEU
3	B	28	MET
3	B	45	LEU
3	B	61	ARG
3	B	86	LYS
3	B	95	LEU
3	B	100	ARG
3	B	169	ASN
3	B	189	ASP

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Mol	Chain	Res	Type
3	B	276	LYS
3	B	278	ASP
3	B	293	VAL
3	B	319	ASN
3	B	340	GLU
3	B	341	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	99	HIS
3	A	133	GLN
3	A	169	ASN
3	A	289	HIS
3	A	317	ASN
3	A	319	ASN
3	A	323	ASN
3	B	40	HIS
3	B	99	HIS
3	B	311	GLN
3	B	327	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)

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

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	C	34/35 (97%)	-0.15	3 (8%) 10 9	29, 45, 71, 79	0
2	D	34/35 (97%)	-0.43	0 100 100	29, 44, 62, 74	0
3	A	309/343 (90%)	0.35	24 (7%) 13 11	36, 58, 84, 95	0
3	B	316/343 (92%)	0.14	14 (4%) 34 33	28, 45, 83, 98	0
All	All	693/756 (91%)	0.19	41 (5%) 22 21	28, 51, 83, 98	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	279	SER	6.3
3	A	277	ASP	4.7
3	A	278	ASP	4.5
3	A	280	GLY	4.4
3	B	319	ASN	4.2
3	A	235	ASN	4.0
3	A	186	SER	3.7
3	A	189	ASP	3.7
3	B	341	ASP	3.6
3	A	163	PHE	3.5
3	A	231	ALA	3.5
3	B	327	ASN	3.3
3	A	264	ILE	3.3
3	B	278	ASP	3.3
3	A	316	THR	3.0
3	A	164	LEU	2.9
3	A	291	ALA	2.8
3	A	234	PRO	2.8
3	A	304	VAL	2.7
3	A	174	ILE	2.6
3	A	276	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
3	B	21	ASP	2.6
3	A	160	ASN	2.5
3	A	252	ALA	2.5
3	A	281	GLN	2.5
3	B	164	LEU	2.4
1	C	19	DA	2.4
1	C	18	DT	2.4
3	B	174	ILE	2.4
3	B	322	MET	2.4
3	A	184	ASP	2.4
3	A	274	GLY	2.3
3	B	326	ARG	2.3
3	B	277	ASP	2.2
3	B	172	LEU	2.2
3	B	167	ALA	2.1
3	A	261	LEU	2.1
3	B	113	VAL	2.1
3	B	177	ILE	2.1
1	C	20	DC	2.1
3	A	196	HIS	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.