



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 10:07 AM GMT

PDB ID : 3C29
Title : Cre-loxP Synaptic structure
Authors : Ghosh, K.; Van Duyne, G.D.
Deposited on : 2008-01-24
Resolution : 2.20 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

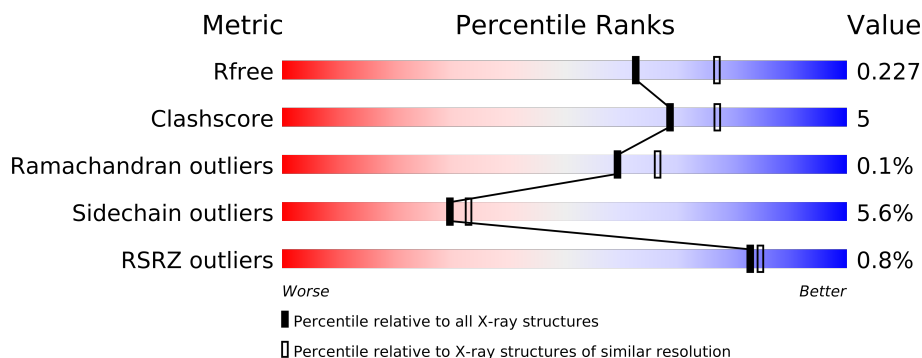
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.20 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}	66092	2938 (2.20-2.20)
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)
RSRZ outliers	66119	2939 (2.20-2.20)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	322	
1	B	322	
1	G	322	
1	H	322	
2	C	35	
3	D	34	
3	F	34	
4	E	34	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13461 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Recombinase cre.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	322	Total	C	N	O	S	0	0	0
			2547	1581	485	466	15			
1	B	322	Total	C	N	O	S	0	0	0
			2547	1581	485	466	15			
1	G	322	Total	C	N	O	S	0	0	0
			2547	1581	485	466	15			
1	H	322	Total	C	N	O	S	0	0	0
			2547	1581	485	466	15			

- Molecule 2 is a DNA chain called LoxP DNA, chain C,.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	35	Total	C	N	O	P	0	0	0
			716	346	126	210	34			

- Molecule 3 is a DNA chain called LoxP DNA, chain D,F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	34	Total	C	N	O	P	0	0	0
			696	335	124	203	34			
3	F	34	Total	C	N	O	P	0	0	0
			696	335	124	203	34			

- Molecule 4 is a DNA chain called LoxP DNA, chain E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	34	Total	C	N	O	P	0	0	0
			699	336	124	205	34			

- Molecule 5 is water.

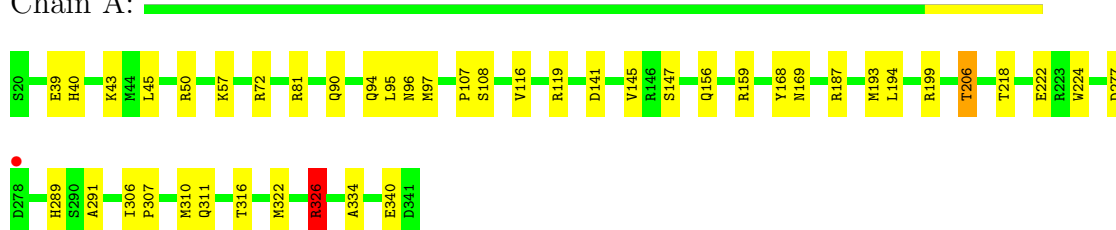
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	30	Total 30	O 30	0	0
5	D	28	Total 28	O 28	0	0
5	A	86	Total 86	O 86	0	0
5	B	104	Total 104	O 104	0	0
5	G	73	Total 73	O 73	0	0
5	H	96	Total 96	O 96	0	0
5	E	27	Total 27	O 27	0	0
5	F	22	Total 22	O 22	0	0

3 Residue-property plots

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.

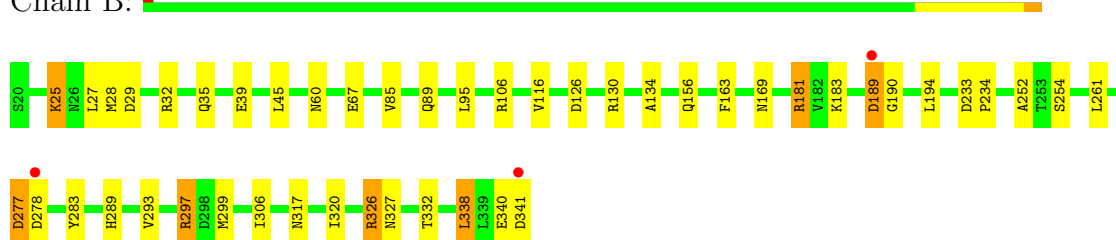
- Molecule 1: Recombinase cre

Chain A:



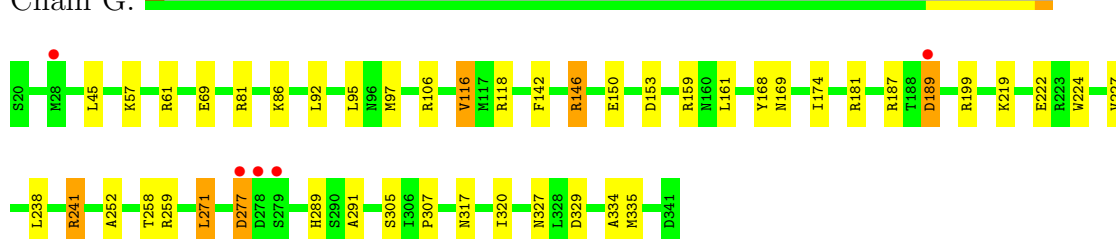
- Molecule 1: Recombinase cre

Chain B:



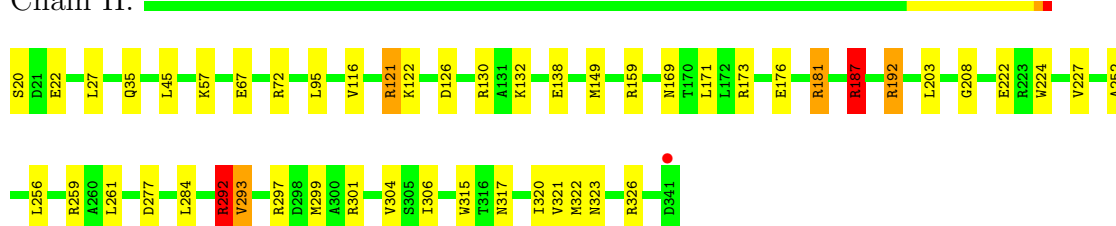
- Molecule 1: Recombinase cre

Chain G:



- Molecule 1: Recombinase cre

Chain H:



- Molecule 2: LoxP DNA, chain C,

Chain C: 



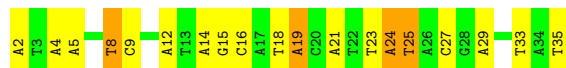
- Molecule 3: LoxP DNA, chain D,F

Chain D: 



- Molecule 3: LoxP DNA, chain D,F

Chain F: 



- Molecule 4: LoxP DNA, chain E

Chain E: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	136.41Å 136.41Å 218.83Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.13 – 2.20 38.76 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (40.13-2.20) 99.9 (38.76-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.30 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.192 , 0.228 0.192 , 0.227	Depositor DCC
R_{free} test set	6018 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	32.5	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 22.9	EDS
Estimated twinning fraction	0.016 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 119629 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13461	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.15% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: 1AP

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	0.64	0/2588	0.73	3/3489 (0.1%)
1	B	0.62	0/2588	0.76	6/3489 (0.2%)
1	G	0.64	0/2588	0.71	3/3489 (0.1%)
1	H	0.67	0/2588	0.81	10/3489 (0.3%)
2	C	1.03	0/776	1.75	16/1194 (1.3%)
3	D	1.02	0/780	1.76	17/1201 (1.4%)
3	F	1.03	0/780	1.73	20/1201 (1.7%)
4	E	1.08	0/757	1.76	20/1164 (1.7%)
All	All	0.75	0/13445	1.10	95/18716 (0.5%)

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	B	0	1

There are no bond length outliers.

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	21	DG	O4'-C1'-N9	-10.42	100.70	108.00
3	F	16	DC	O4'-C4'-C3'	-9.98	100.01	106.00
1	A	72	ARG	NE-CZ-NH2	-8.59	116.01	120.30
4	E	26	DA	O4'-C1'-N9	-8.47	102.07	108.00
3	D	16	DC	O4'-C4'-C3'	-8.45	100.93	106.00
1	H	326	ARG	NE-CZ-NH2	-8.40	116.10	120.30
1	B	326	ARG	NE-CZ-NH2	-8.37	116.12	120.30
3	D	8	DT	O4'-C1'-N1	-8.09	102.34	108.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	13	DT	P-O3'-C3'	8.08	129.40	119.70
2	C	5	DA	O4'-C1'-N9	7.78	113.44	108.00
3	D	24	DA	O4'-C4'-C3'	-7.77	101.34	106.00
1	H	181	ARG	NE-CZ-NH2	-7.77	116.42	120.30
3	D	26	DA	O4'-C1'-N9	-7.70	102.61	108.00
1	H	181	ARG	NE-CZ-NH1	7.64	124.12	120.30
4	E	8	DT	O4'-C1'-N1	-7.62	102.67	108.00
4	E	12	DA	O4'-C1'-N9	7.61	113.33	108.00
2	C	18	DT	C6-C5-C7	-7.39	118.47	122.90
3	F	21	DA	O4'-C1'-N9	7.36	113.15	108.00
1	B	326	ARG	NE-CZ-NH1	7.30	123.95	120.30
3	D	11	DT	O4'-C1'-N1	7.28	113.09	108.00
4	E	17	DG	N3-C4-N9	-7.25	121.65	126.00
3	F	2	DA	P-O3'-C3'	7.21	128.35	119.70
3	D	5	DA	O4'-C1'-N9	7.20	113.04	108.00
3	F	4	DA	O4'-C1'-N9	-7.17	102.98	108.00
4	E	5	DA	O4'-C1'-N9	7.16	113.01	108.00
4	E	21	DG	O4'-C1'-N9	-7.16	102.99	108.00
3	D	21	DA	O4'-C1'-N9	7.15	113.00	108.00
4	E	24	DA	O5'-P-OP2	-7.07	99.34	105.70
1	B	106	ARG	NE-CZ-NH2	-6.79	116.90	120.30
1	B	181	ARG	NE-CZ-NH2	-6.73	116.94	120.30
2	C	8	DT	O4'-C1'-N1	-6.71	103.30	108.00
4	E	17	DG	N3-C2-N2	-6.49	115.36	119.90
4	E	26	DA	N1-C2-N3	-6.40	126.10	129.30
1	H	326	ARG	NE-CZ-NH1	6.38	123.49	120.30
3	F	5	DA	C1'-O4'-C4'	-6.30	103.80	110.10
3	D	24	DA	C4'-C3'-C2'	-6.29	97.44	103.10
4	E	6	DC	O4'-C4'-C3'	-6.21	102.02	104.50
4	E	23	DT	C4-C5-C7	6.20	122.72	119.00
2	C	18	DT	C4-C5-C7	6.15	122.69	119.00
3	F	27	DC	O4'-C1'-N1	6.14	112.30	108.00
3	D	13	DT	O4'-C1'-N1	6.12	112.28	108.00
3	D	3	DT	O4'-C1'-N1	6.09	112.26	108.00
1	H	187	ARG	NE-CZ-NH2	-6.07	117.27	120.30
1	B	106	ARG	NE-CZ-NH1	6.06	123.33	120.30
4	E	29	DA	O4'-C1'-N9	6.06	112.24	108.00
1	H	192	ARG	NE-CZ-NH1	6.01	123.31	120.30
4	E	3	DT	P-O3'-C3'	6.01	126.91	119.70
3	D	7	DT	O4'-C1'-N1	-6.00	103.80	108.00
3	F	24	DA	O5'-P-OP2	-6.00	100.30	105.70
1	H	121	ARG	NE-CZ-NH2	-5.97	117.31	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	4	DA	O4'-C1'-N9	-5.94	103.84	108.00
3	F	23	DT	C4-C5-C7	5.93	122.56	119.00
4	E	17	DG	N9-C4-C5	5.92	107.77	105.40
3	F	33	DT	N3-C2-O2	-5.88	118.77	122.30
4	E	25	DT	C4-C5-C7	5.88	122.53	119.00
2	C	24	DA	O5'-P-OP2	-5.87	100.42	105.70
3	F	24	DA	C4'-C3'-C2'	-5.81	97.87	103.10
3	D	7	DT	C4-C5-C7	5.78	122.47	119.00
1	G	116	VAL	CB-CA-C	-5.75	100.48	111.40
1	G	61	ARG	NE-CZ-NH2	-5.69	117.45	120.30
2	C	26	DA	O4'-C1'-N9	-5.68	104.02	108.00
1	A	50	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	H	72	ARG	NE-CZ-NH2	-5.60	117.50	120.30
3	F	8	DT	O4'-C1'-N1	-5.58	104.09	108.00
2	C	11	DT	C6-C5-C7	-5.57	119.56	122.90
3	F	2	DA	O4'-C4'-C3'	-5.55	102.28	104.50
2	C	17	DG	N3-C2-N2	-5.49	116.06	119.90
4	E	13	DT	O4'-C1'-N1	5.46	111.83	108.00
4	E	24	DA	O4'-C1'-C2'	5.45	110.26	105.90
3	F	35	DT	C4-C5-C7	5.41	122.25	119.00
2	C	12	DA	N1-C2-N3	-5.41	126.60	129.30
1	H	292	ARG	NE-CZ-NH2	-5.40	117.60	120.30
3	F	25	DT	P-O3'-C3'	5.38	126.16	119.70
3	F	5	DA	O4'-C1'-N9	5.37	111.76	108.00
2	C	23	DT	C5-C4-O4	-5.35	121.16	124.90
2	C	11	DT	O4'-C1'-N1	5.35	111.74	108.00
4	E	19	DA	O4'-C1'-N9	5.31	111.72	108.00
3	F	16	DC	C4'-C3'-C2'	-5.27	98.36	103.10
3	D	4	DA	P-O3'-C3'	5.25	126.00	119.70
2	C	13	DT	O4'-C1'-N1	5.25	111.67	108.00
2	C	17	DG	N9-C4-C5	5.23	107.49	105.40
3	D	24	DA	C1'-O4'-C4'	-5.22	104.88	110.10
1	G	271	LEU	CA-CB-CG	5.22	127.30	115.30
3	F	29	DA	O4'-C1'-N9	5.21	111.64	108.00
3	F	9	DC	O4'-C1'-N1	-5.16	104.39	108.00
4	E	23	DT	C6-C5-C7	-5.16	119.81	122.90
1	B	297	ARG	NE-CZ-NH2	-5.15	117.73	120.30
3	D	19	DA	N1-C2-N3	-5.14	126.73	129.30
4	E	13	DT	P-O3'-C3'	5.13	125.86	119.70
1	H	192	ARG	NE-CZ-NH2	-5.13	117.73	120.30
3	F	25	DT	C5-C4-O4	-5.09	121.33	124.90
2	C	9	DC	O4'-C1'-N1	5.08	111.55	108.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	23	DT	C6-N1-C2	5.02	123.81	121.30
1	A	326	ARG	NE-CZ-NH1	5.01	122.81	120.30
3	F	19	DA	O4'-C1'-N9	-5.01	104.50	108.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	340	GLU	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2547	0	2560	28	0
1	B	2547	0	2560	28	0
1	G	2547	0	2560	29	1
1	H	2547	0	2560	37	0
2	C	716	0	402	9	0
3	D	696	0	387	3	0
3	F	696	0	387	9	0
4	E	699	0	389	11	0
5	A	86	0	0	0	0
5	B	104	0	0	4	0
5	C	30	0	0	1	0
5	D	28	0	0	0	0
5	E	27	0	0	7	0
5	F	22	0	0	2	0
5	G	73	0	0	1	0
5	H	96	0	0	2	0
All	All	13461	0	11805	119	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

All (119) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:227:VAL:HB	5:H:394:HOH:O	1.54	1.06
1:A:306:ILE:HG22	1:A:310:MET:HE2	1.41	1.02
1:H:187:ARG:NH2	1:H:222:GLU:OE2	2.02	0.92
1:A:306:ILE:HG22	1:A:310:MET:CE	2.00	0.91
1:B:299:MET:HE2	1:G:334:ALA:HB3	1.52	0.91
1:H:121:ARG:HD2	5:H:390:HOH:O	1.75	0.86
1:G:81:ARG:NH2	3:F:12:DA:OP1	2.11	0.83
1:H:171:LEU:O	1:H:292:ARG:HD2	1.79	0.82
1:A:334:ALA:HB3	1:H:299:MET:CE	2.08	0.81
1:B:67:GLU:HG3	5:B:390:HOH:O	1.80	0.81
1:A:81:ARG:NH2	3:D:12:DA:OP1	2.17	0.78
1:A:334:ALA:HB3	1:H:299:MET:HE3	1.66	0.78
1:H:181:ARG:NH2	1:H:252:ALA:O	2.18	0.76
2:C:10:DG:H2''	2:C:11:DT:H5'	1.68	0.76
1:G:187:ARG:NH2	1:G:222:GLU:OE2	2.14	0.75
1:B:299:MET:CE	1:G:334:ALA:HB3	2.17	0.74
1:H:320:ILE:HD12	1:H:321:VAL:N	2.03	0.73
1:A:96:ASN:HD21	1:A:108:SER:H	1.36	0.71
4:E:11:DT:H5'	5:E:47:HOH:O	1.92	0.69
1:H:320:ILE:HG21	4:E:16:DT:H3'	1.76	0.68
1:A:119:ARG:HG3	1:H:35:GLN:HB2	1.76	0.68
1:H:293:VAL:O	1:H:297:ARG:HG3	1.95	0.66
1:H:122:LYS:HE2	4:E:23:DT:OP1	1.97	0.65
1:G:305:SER:HB3	1:G:307:PRO:HD2	1.79	0.65
1:H:121:ARG:NH2	3:F:18:DT:OP1	2.32	0.62
1:B:299:MET:HE1	1:G:335:MET:HG2	1.81	0.62
1:B:332:THR:HG22	1:B:332:THR:O	2.00	0.61
1:B:326:ARG:NH2	2:C:15:1AP:OP2	2.33	0.61
1:G:146:ARG:O	1:G:150:GLU:HB2	2.01	0.61
1:G:159:ARG:HB2	1:G:224:TRP:CZ3	2.36	0.60
1:B:181:ARG:NH2	1:B:252:ALA:O	2.34	0.60
1:H:277:ASP:HB2	1:H:284:LEU:HD13	1.85	0.59
1:A:334:ALA:HB3	1:H:299:MET:HE2	1.86	0.58
1:A:96:ASN:HD22	1:A:107:PRO:HD2	1.69	0.57
1:H:159:ARG:HB2	1:H:224:TRP:CZ3	2.40	0.56
1:G:181:ARG:NH2	1:G:252:ALA:O	2.37	0.56
1:A:39:GLU:O	1:A:43:LYS:HD3	2.05	0.56
1:H:20:SER:N	1:H:22:GLU:OE2	2.39	0.56
1:G:277:ASP:N	1:G:277:ASP:OD2	2.38	0.56
1:G:81:ARG:CZ	3:F:12:DA:OP1	2.54	0.56
5:G:351:HOH:O	1:H:322:MET:HE3	2.05	0.55
1:G:174:ILE:HD12	1:G:258:THR:HB	1.87	0.55
2:C:10:DG:H2''	2:C:11:DT:C5'	2.35	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:97:MET:HG3	4:E:22:DC:OP2	2.07	0.55
4:E:11:DT:C5'	5:E:47:HOH:O	2.52	0.54
1:A:159:ARG:HB2	1:A:224:TRP:CZ3	2.43	0.54
2:C:24:DA:H2'	2:C:25:DT:C6	2.43	0.54
1:A:322:MET:O	1:A:326:ARG:HB3	2.09	0.53
1:B:25:LYS:HE3	1:B:29:ASP:OD2	2.08	0.53
1:H:299:MET:HE2	1:H:304:VAL:HG11	1.91	0.52
2:C:34:DA:H2''	2:C:35:DT:O5'	2.09	0.52
1:H:320:ILE:HG22	5:E:53:HOH:O	2.10	0.51
1:G:307:PRO:HG3	1:H:306:ILE:HD11	1.91	0.51
1:H:292:ARG:NH2	4:E:16:DT:OP1	2.44	0.51
1:G:81:ARG:NH1	3:F:12:DA:OP1	2.44	0.50
1:B:277:ASP:OD1	1:B:277:ASP:C	2.49	0.50
1:H:173:ARG:HD2	1:H:176:GLU:OE2	2.12	0.50
1:A:306:ILE:HG22	1:A:310:MET:HE1	1.88	0.50
1:G:86:LYS:HD2	5:F:40:HOH:O	2.10	0.50
1:A:334:ALA:CB	1:H:299:MET:HE2	2.43	0.49
1:A:40:HIS:HE1	5:C:40:HOH:O	1.95	0.49
1:G:241:ARG:HD3	5:F:41:HOH:O	2.13	0.48
1:G:97:MET:HG3	4:E:22:DC:P	2.54	0.48
1:G:259:ARG:HG2	3:F:8:DT:O4	2.12	0.48
1:B:134:ALA:HA	1:B:283:TYR:CD2	2.49	0.48
1:H:259:ARG:HG2	4:E:8:DT:O4	2.14	0.48
1:A:206:THR:HG21	1:A:316:THR:HG23	1.97	0.47
1:A:90:GLN:HE22	1:A:94:GLN:HE21	1.62	0.47
1:B:189:ASP:N	1:B:189:ASP:OD1	2.43	0.47
1:B:85:VAL:O	1:B:89:GLN:HG3	2.15	0.47
1:B:341:ASP:HA	5:B:386:HOH:O	2.13	0.47
4:E:33:DT:H2''	4:E:34:DA:C8	2.50	0.46
1:G:142:PHE:O	1:G:146:ARG:HB2	2.16	0.46
1:G:86:LYS:HE3	3:F:15:DG:N7	2.31	0.46
1:A:156:GLN:NE2	3:D:6:DC:OP2	2.47	0.46
1:H:320:ILE:CG2	5:E:53:HOH:O	2.63	0.46
2:C:10:DG:H2'	2:C:11:DT:C6	2.51	0.46
1:B:32:ARG:NH1	1:G:69:GLU:OE1	2.31	0.45
1:B:332:THR:O	1:B:332:THR:CG2	2.63	0.45
1:G:168:TYR:HA	1:G:291:ALA:HB1	1.98	0.45
1:A:206:THR:HG21	1:A:316:THR:CG2	2.46	0.45
1:A:326:ARG:NH2	1:H:208:GLY:O	2.50	0.45
1:H:320:ILE:HG23	5:E:48:HOH:O	2.16	0.45
1:G:159:ARG:HB2	1:G:224:TRP:CE3	2.51	0.45
4:E:15:1AP:H4	4:E:16:DT:OP1	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:181:ARG:HD3	1:B:183:LYS:HE2	1.98	0.45
1:A:307:PRO:HG3	1:B:306:ILE:HD11	1.98	0.45
1:H:320:ILE:HB	5:E:53:HOH:O	2.17	0.44
1:B:233:ASP:HA	1:B:234:PRO:HD2	1.85	0.44
1:H:320:ILE:HD12	1:H:321:VAL:H	1.82	0.44
1:B:194:LEU:CD1	1:G:327:ASN:HB2	2.48	0.44
1:A:97:MET:HG3	2:C:22:DC:OP2	2.18	0.44
1:A:199:ARG:HD2	1:B:126:ASP:HA	2.00	0.44
1:B:297:ARG:NH2	1:B:327:ASN:O	2.51	0.43
1:H:315:TRP:CD2	1:H:320:ILE:HD13	2.53	0.43
1:A:193:MET:HG3	1:A:218:THR:HG23	2.00	0.43
1:A:168:TYR:HA	1:A:291:ALA:HB1	1.99	0.43
1:B:163:PHE:CE1	1:B:261:LEU:HD22	2.54	0.43
2:C:1:DT:H2''	2:C:2:DA:OP2	2.19	0.42
4:E:24:DA:H2'	4:E:25:DT:C6	2.54	0.42
1:B:35:GLN:HG3	5:B:348:HOH:O	2.19	0.42
1:B:338:LEU:O	1:B:341:ASP:HB2	2.19	0.42
1:A:187:ARG:NH2	1:A:222:GLU:OE2	2.53	0.42
1:B:60:ASN:ND2	5:B:425:HOH:O	2.53	0.41
2:C:24:DA:C2	3:D:14:DA:C2	3.09	0.41
1:G:86:LYS:HD3	3:F:14:DA:N7	2.36	0.41
1:H:256:LEU:HD23	1:H:261:LEU:HD21	2.02	0.41
1:H:317:ASN:HB3	5:E:48:HOH:O	2.21	0.41
1:B:289:HIS:CD2	1:B:293:VAL:HG12	2.55	0.41
1:H:138:GLU:OE2	1:H:301:ARG:NH2	2.53	0.41
1:A:141:ASP:O	1:A:145:VAL:HG23	2.21	0.41
3:F:18:DT:H2''	3:F:19:DA:C8	2.56	0.41
1:H:299:MET:CE	1:H:304:VAL:HG11	2.51	0.40
1:B:317:ASN:O	1:B:320:ILE:HG22	2.21	0.40
3:F:24:DA:H2'	3:F:25:DT:C6	2.57	0.40
1:A:340:GLU:OE2	1:H:192:ARG:HD3	2.21	0.40
1:G:317:ASN:HD22	1:G:320:ILE:HG13	1.87	0.40
1:G:199:ARG:HD2	1:H:126:ASP:HA	2.03	0.40
1:B:190:GLY:N	1:G:329:ASP:OD1	2.50	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:153:ASP:O	1:G:153:ASP:CB[5_675]	2.08	0.12

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	320/322 (99%)	317 (99%)	3 (1%)	0	100	100
1	B	320/322 (99%)	318 (99%)	2 (1%)	0	100	100
1	G	320/322 (99%)	315 (98%)	4 (1%)	1 (0%)	50	53
1	H	320/322 (99%)	315 (98%)	5 (2%)	0	100	100
All	All	1280/1288 (99%)	1265 (99%)	14 (1%)	1 (0%)	59	66

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	189	ASP

5.3.2 Protein sidechains ⓘ

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	268/269 (100%)	256 (96%)	12 (4%)	38	44
1	B	268/269 (100%)	253 (94%)	15 (6%)	30	33
1	G	268/269 (100%)	250 (93%)	18 (7%)	23	24
1	H	268/269 (100%)	253 (94%)	15 (6%)	30	33
All	All	1072/1076 (100%)	1012 (94%)	60 (6%)	30	33

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	LEU
1	A	57	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	95	LEU
1	A	116	VAL
1	A	147	SER
1	A	169	ASN
1	A	194	LEU
1	A	206	THR
1	A	277	ASP
1	A	289	HIS
1	A	311	GLN
1	A	326	ARG
1	B	25	LYS
1	B	27	LEU
1	B	28	MET
1	B	39	GLU
1	B	45	LEU
1	B	95	LEU
1	B	116	VAL
1	B	130	ARG
1	B	156	GLN
1	B	169	ASN
1	B	189	ASP
1	B	254	SER
1	B	277	ASP
1	B	278	ASP
1	B	338	LEU
1	G	45	LEU
1	G	57	LYS
1	G	92	LEU
1	G	95	LEU
1	G	106	ARG
1	G	116	VAL
1	G	118	ARG
1	G	146	ARG
1	G	161	LEU
1	G	169	ASN
1	G	189	ASP
1	G	219	LYS
1	G	227	VAL
1	G	238	LEU
1	G	241	ARG
1	G	271	LEU
1	G	277	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	289	HIS
1	H	27	LEU
1	H	45	LEU
1	H	57	LYS
1	H	67	GLU
1	H	95	LEU
1	H	116	VAL
1	H	130	ARG
1	H	132	LYS
1	H	149	MET
1	H	169	ASN
1	H	187	ARG
1	H	203	LEU
1	H	292	ARG
1	H	293	VAL
1	H	323	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	HIS
1	A	94	GLN
1	A	96	ASN
1	A	133	GLN
1	A	289	HIS
1	A	311	GLN
1	A	323	ASN
1	B	35	GLN
1	B	60	ASN
1	G	40	HIS
1	G	133	GLN
1	G	196	HIS
1	G	317	ASN
1	G	323	ASN
1	H	281	GLN
1	H	323	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	1AP	C	15	3,2	22,24,25	1.02	1 (4%)	32,35,38	1.74	7 (21%)
4	1AP	E	15	3,4	22,24,25	1.02	2 (9%)	32,35,38	1.96	8 (25%)

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	1AP	C	15	3,2	-	0/6/21/22	0/1/3/3
4	1AP	E	15	3,4	-	0/6/21/22	0/1/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	15	1AP	C4-N9	-3.37	1.32	1.37
4	E	15	1AP	C4-N9	-2.78	1.33	1.37
4	E	15	1AP	O4'-C4'	-2.23	1.39	1.45

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	15	1AP	N3-C2-N1	-4.98	119.67	127.54
4	E	15	1AP	C2-N3-C4	4.92	121.82	115.30
2	C	15	1AP	N3-C2-N1	-4.16	120.97	127.54
4	E	15	1AP	C5-C4-N3	-3.90	120.29	125.94
2	C	15	1AP	O4'-C1'-N9	-3.80	100.53	107.68
4	E	15	1AP	N3-C4-N9	3.70	132.34	126.91
2	C	15	1AP	N3-C4-N9	3.59	132.17	126.91
2	C	15	1AP	C5-C4-N3	-3.44	120.96	125.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	15	1AP	O4'-C1'-N9	-3.13	101.80	107.68
2	C	15	1AP	C2-N3-C4	3.10	119.41	115.30
4	E	15	1AP	C4-C5-N7	-2.87	107.06	109.52
4	E	15	1AP	N2-C2-N1	2.45	121.43	117.19
2	C	15	1AP	C8-N9-C4	2.22	108.59	106.90
4	E	15	1AP	C2'-C3'-C4'	2.15	107.55	102.73
2	C	15	1AP	C4-C5-N7	-2.13	107.70	109.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	322/322 (100%)	-0.42	1 (0%) 91 93	19, 29, 44, 58	0
1	B	322/322 (100%)	-0.50	3 (0%) 81 82	20, 30, 43, 55	0
1	G	322/322 (100%)	-0.35	5 (1%) 68 69	19, 32, 50, 64	0
1	H	322/322 (100%)	-0.49	1 (0%) 91 93	18, 27, 41, 56	0
2	C	35/35 (100%)	-0.45	1 (2%) 49 50	20, 34, 59, 90	0
3	D	34/34 (100%)	-0.70	0 100 100	20, 31, 53, 78	0
3	F	34/34 (100%)	-0.74	0 100 100	20, 33, 49, 72	0
4	E	34/34 (100%)	-0.65	0 100 100	19, 32, 58, 66	0
All	All	1425/1425 (100%)	-0.46	11 (0%) 83 85	18, 29, 47, 90	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	277	ASP	3.5
2	C	1	DT	3.4
1	G	279	SER	3.1
1	G	278	ASP	2.9
1	H	341	ASP	2.9
1	G	189	ASP	2.8
1	A	278	ASP	2.5
1	B	341	ASP	2.4
1	B	189	ASP	2.2
1	B	278	ASP	2.2
1	G	28	MET	2.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	1AP	C	15	22/23	0.10	-0.13	18,21,25,26	0
4	1AP	E	15	22/23	0.10	-0.25	19,20,23,28	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.