



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 04:41 PM GMT

PDB ID : 3C9C
Title : Structural Basis of Histone H4 Recognition by p55
Authors : Song, J.J.; Garlick, J.D.; Kingston, R.E.
Deposited on : 2008-02-15
Resolution : 3.20 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>

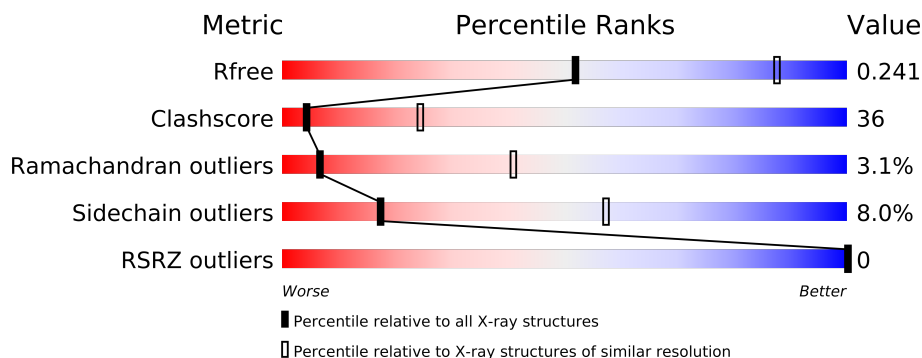
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.20 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	1824 (3.30-3.10)
Clashscore	79885	1078 (3.26-3.14)
Ramachandran outliers	78287	1059 (3.26-3.14)
Sidechain outliers	78261	1058 (3.26-3.14)
RSRZ outliers	66119	1825 (3.30-3.10)

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	432	<div><div></div><div></div><div></div><div></div><div></div></div>
2	B	27	<div><div></div><div></div><div></div><div></div><div></div></div>

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	CD	A	437	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3152 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 Chromatin assembly factor 1 p55 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	380	Total	C	N	O	S	0	0	0
			3054	1927	522	594	11			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP Q24572
A	0	ALA	-	EXPRESSION TAG	UNP Q24572

- Molecule 2 is a protein called Histone H4, 27-residue peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	11	Total	C	N	O	0	0	0
			91	55	24	12			

- Molecule 3 is CADMIUM ION (three-letter code: CD) (formula: Cd).

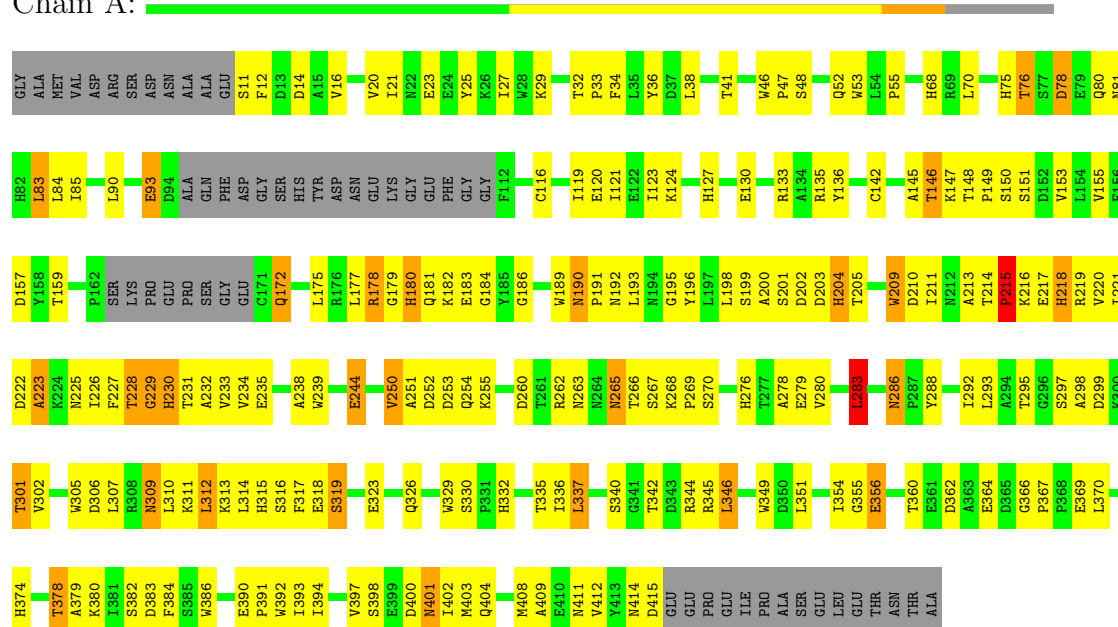
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	7	Total	Cd	0	0
			7	7		

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.

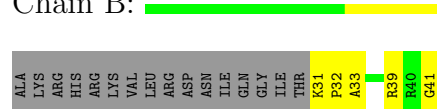
- Molecule 1: Chromatin assembly factor 1 p55 subunit

Chain A:



- Molecule 2: Histone H4, 27-residue peptide

Chain B:



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	150.12Å 150.12Å 97.82Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.20 43.91 – 3.19	Depositor EDS
% Data completeness (in resolution range)	95.0 (50.00-3.20) 94.7 (43.91-3.19)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.02 (at 3.19Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.203 , 0.242 0.203 , 0.241	Depositor DCC
R_{free} test set	990 reflections (4.90%)	DCC
Wilson B-factor (Å ²)	78.0	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 55.0	EDS
Estimated twinning fraction	0.025 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 21395 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3152	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

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	0.38	0/3135	0.69	2/4271 (0.0%)
2	B	0.34	0/91	0.75	0/117
All	All	0.37	0/3226	0.69	2/4388 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	283	LEU	CA-CB-CG	5.95	128.98	115.30
1	A	83	LEU	N-CA-C	-5.00	97.50	111.00

There are no chirality outliers.

There are no planarity outliers.

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	3054	0	2897	218	0
2	B	91	0	106	4	0
3	A	7	0	0	0	0
All	All	3152	0	3003	221	0

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 36.

All (221) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:127:HIS:NE2	1:A:146:THR:HG21	1.68	1.06
1:A:213:ALA:HB3	1:A:221:ILE:HD12	1.43	0.99
1:A:286:ASN:ND2	1:A:288:TYR:H	1.62	0.96
1:A:309:ASN:HD21	1:A:311:LYS:HB2	1.34	0.92
1:A:307:LEU:HA	1:A:310:LEU:HD21	1.53	0.91
1:A:180:HIS:HB2	1:A:203:ASP:OD2	1.71	0.90
1:A:401:ASN:HD22	1:A:401:ASN:C	1.75	0.90
1:A:390:GLU:HB3	1:A:393:ILE:HD13	1.53	0.89
1:A:155:VAL:HG21	1:A:211:ILE:HD11	1.54	0.87
1:A:172:GLN:HB3	1:A:219:ARG:HH12	1.39	0.87
1:A:75:HIS:CD2	1:A:130:GLU:HG2	2.10	0.86
1:A:48:SER:HB3	1:A:397:VAL:HG11	1.57	0.86
1:A:250:VAL:HG13	1:A:280:VAL:HB	1.60	0.84
1:A:340:SER:HB3	1:A:346:LEU:HD22	1.60	0.83
1:A:148:THR:HG23	1:A:149:PRO:HD2	1.64	0.80
1:A:214:THR:OG1	1:A:215:PRO:HD2	1.82	0.80
1:A:47:PRO:HG3	1:A:401:ASN:HB3	1.63	0.79
1:A:354:ILE:HG12	1:A:369:GLU:HG2	1.63	0.79
1:A:286:ASN:HD22	1:A:288:TYR:H	1.29	0.77
1:A:299:ASP:OD1	1:A:301:THR:HB	1.83	0.77
1:A:148:THR:HG22	1:A:150:SER:H	1.50	0.76
1:A:364:GLU:C	1:A:366:GLY:H	1.91	0.73
1:A:307:LEU:HA	1:A:310:LEU:CD2	2.17	0.73
1:A:213:ALA:CB	1:A:221:ILE:HD12	2.18	0.71
1:A:234:VAL:HA	1:A:251:ALA:HB2	1.72	0.70
1:A:312:LEU:HD22	1:A:313:LYS:N	2.07	0.69
1:A:155:VAL:HB	1:A:175:LEU:HB2	1.75	0.68
1:A:286:ASN:HD22	1:A:286:ASN:C	1.96	0.68
1:A:190:ASN:HD22	1:A:191:PRO:N	1.93	0.67
1:A:148:THR:CG2	1:A:149:PRO:HD2	2.24	0.67
1:A:80:GLN:HE21	1:A:81:ASN:N	1.93	0.67
1:A:177:LEU:HB3	1:A:209:TRP:CE3	2.30	0.67
1:A:11:SER:HB3	1:A:14:ASP:OD2	1.95	0.67
1:A:204:HIS:CD2	1:A:232:ALA:HA	2.31	0.66
1:A:93:GLU:H	1:A:93:GLU:CD	1.98	0.66
1:A:298:ALA:HA	1:A:323:GLU:HG2	1.78	0.66
1:A:190:ASN:ND2	1:A:192:ASN:H	1.94	0.65
1:A:192:ASN:O	1:A:193:LEU:HD23	1.96	0.65
1:A:225:ASN:C	1:A:226:ILE:HD12	2.18	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:157:ASP:OD1	1:A:159:THR:HB	1.97	0.64
1:A:342:THR:HA	1:A:380:LYS:HG3	1.79	0.64
1:A:145:ALA:HB2	1:A:189:TRP:CZ2	2.33	0.64
1:A:254:GLN:HG2	1:A:278:ALA:O	1.98	0.64
1:A:123:ILE:HG22	1:A:124:LYS:N	2.13	0.64
1:A:222:ASP:O	1:A:223:ALA:HB2	1.97	0.64
1:A:55:PRO:HG3	1:A:136:TYR:OH	1.97	0.64
1:A:317:PHE:HZ	1:A:351:LEU:CD2	2.11	0.63
1:A:116:CYS:HB3	1:A:120:GLU:OE2	1.97	0.63
1:A:209:TRP:CD1	1:A:209:TRP:N	2.65	0.62
1:A:16:VAL:O	1:A:20:VAL:HG23	1.99	0.62
1:A:172:GLN:HB3	1:A:219:ARG:NH1	2.14	0.62
1:A:286:ASN:ND2	1:A:288:TYR:N	2.43	0.62
1:A:306:ASP:HB2	1:A:314:LEU:HD11	1.82	0.62
1:A:193:LEU:HB3	1:A:196:TYR:CD1	2.36	0.61
1:A:286:ASN:HD22	1:A:288:TYR:N	1.96	0.61
1:A:190:ASN:HD22	1:A:190:ASN:C	2.04	0.61
1:A:202:ASP:HA	1:A:233:VAL:HG13	1.82	0.61
1:A:265:ASN:HD22	1:A:266:THR:N	1.99	0.60
1:A:182:LYS:HB3	1:A:202:ASP:HB2	1.84	0.60
1:A:309:ASN:ND2	1:A:311:LYS:HB2	2.12	0.60
1:A:217:GLU:O	1:A:218:HIS:HB3	2.02	0.60
1:A:307:LEU:HD23	1:A:310:LEU:HD21	1.83	0.59
1:A:47:PRO:HA	1:A:401:ASN:HA	1.85	0.59
1:A:315:HIS:ND1	1:A:316:SER:N	2.50	0.59
1:A:231:THR:HB	1:A:253:ASP:CB	2.32	0.59
1:A:233:VAL:O	1:A:251:ALA:HB1	2.03	0.59
1:A:401:ASN:ND2	1:A:401:ASN:C	2.48	0.59
1:A:84:LEU:O	1:A:85:ILE:HD12	2.03	0.59
1:A:400:ASP:O	1:A:401:ASN:ND2	2.36	0.58
1:A:133:ARG:HH11	1:A:133:ARG:HG3	1.67	0.58
1:A:409:ALA:HB3	1:A:412:VAL:HG23	1.86	0.58
1:A:21:ILE:HG12	1:A:344:ARG:NH2	2.19	0.58
1:A:364:GLU:C	1:A:366:GLY:N	2.58	0.57
1:A:151:SER:HB3	1:A:181:GLN:O	2.04	0.57
1:A:312:LEU:CD1	1:A:314:LEU:HD23	2.35	0.57
1:A:85:ILE:HB	1:A:123:ILE:HB	1.87	0.57
1:A:177:LEU:HB3	1:A:209:TRP:CZ3	2.39	0.56
1:A:231:THR:HB	1:A:253:ASP:HB3	1.87	0.56
1:A:195:GLY:HA2	1:A:211:ILE:HG22	1.86	0.56
1:A:364:GLU:O	1:A:366:GLY:N	2.38	0.56
1:A:332:HIS:CD2	1:A:391:PRO:HA	2.41	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:292:ILE:HD12	1:A:292:ILE:N	2.20	0.56
1:A:80:GLN:HE21	1:A:81:ASN:H	1.52	0.56
1:A:81:ASN:HB2	1:A:127:HIS:O	2.04	0.56
1:A:155:VAL:HG21	1:A:211:ILE:CD1	2.29	0.56
1:A:214:THR:O	1:A:215:PRO:O	2.22	0.56
1:A:180:HIS:CE1	1:A:201:SER:HB2	2.41	0.56
1:A:142:CYS:SG	1:A:157:ASP:OD1	2.63	0.56
1:A:354:ILE:HG12	1:A:369:GLU:CG	2.33	0.56
1:A:233:VAL:HB	1:A:252:ASP:OD2	2.06	0.55
1:A:250:VAL:HG13	1:A:280:VAL:CB	2.34	0.55
1:A:147:LYS:HE2	1:A:199:SER:HB2	1.88	0.55
1:A:217:GLU:O	1:A:218:HIS:CB	2.55	0.54
1:A:309:ASN:ND2	1:A:311:LYS:H	2.05	0.54
1:A:153:VAL:HG12	1:A:177:LEU:HD12	1.90	0.54
1:A:75:HIS:HD2	1:A:130:GLU:HG2	1.68	0.54
1:A:145:ALA:HB2	1:A:189:TRP:HZ2	1.71	0.54
1:A:286:ASN:C	1:A:286:ASN:ND2	2.62	0.53
1:A:80:GLN:NE2	1:A:81:ASN:H	2.06	0.53
1:A:76:THR:HG22	1:A:78:ASP:OD2	2.08	0.53
1:A:119:ILE:HD13	1:A:403:MET:CE	2.38	0.53
1:A:182:LYS:HG2	1:A:203:ASP:HB3	1.91	0.52
1:A:312:LEU:C	1:A:312:LEU:HD22	2.29	0.52
1:A:120:GLU:C	1:A:121:ILE:HD12	2.30	0.52
1:A:228:THR:O	1:A:230:HIS:N	2.43	0.52
1:A:151:SER:HB2	1:A:180:HIS:O	2.09	0.52
1:A:382:SER:O	1:A:383:ASP:HB2	2.09	0.52
2:B:31:LYS:C	2:B:33:ALA:H	2.12	0.52
1:A:234:VAL:HA	1:A:251:ALA:CB	2.40	0.52
1:A:186:GLY:HA3	1:A:200:ALA:HB3	1.91	0.52
1:A:260:ASP:OD1	1:A:262:ARG:HB2	2.09	0.52
1:A:215:PRO:C	1:A:216:LYS:HG3	2.30	0.51
1:A:355:GLY:O	1:A:356:GLU:C	2.49	0.51
1:A:408:MET:HE3	1:A:412:VAL:HB	1.93	0.51
2:B:31:LYS:N	2:B:32:PRO:CD	2.74	0.51
1:A:312:LEU:HD13	1:A:314:LEU:HD23	1.93	0.51
1:A:210:ASP:O	1:A:213:ALA:HB2	2.11	0.51
1:A:133:ARG:NH1	1:A:133:ARG:HG3	2.26	0.50
1:A:119:ILE:HD13	1:A:403:MET:HE2	1.92	0.50
1:A:238:ALA:HB3	1:A:283:LEU:HD21	1.94	0.50
1:A:230:HIS:CE1	1:A:251:ALA:HB3	2.46	0.50
1:A:252:ASP:HA	1:A:279:GLU:CB	2.41	0.50
1:A:367:PRO:HB2	1:A:369:GLU:OE2	2.10	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:190:ASN:HD22	1:A:191:PRO:CD	2.25	0.50
1:A:25:TYR:OH	1:A:29:LYS:HE3	2.11	0.50
1:A:222:ASP:O	1:A:223:ALA:CB	2.60	0.50
1:A:378:THR:O	1:A:378:THR:CG2	2.59	0.49
1:A:286:ASN:HD21	1:A:288:TYR:H	1.53	0.49
1:A:52:GLN:OE1	1:A:135:ARG:HA	2.13	0.49
1:A:12:PHE:O	1:A:16:VAL:HG23	2.13	0.49
1:A:235:GLU:HG3	1:A:280:VAL:O	2.12	0.49
1:A:123:ILE:HG22	1:A:124:LYS:H	1.78	0.49
1:A:235:GLU:OE1	1:A:235:GLU:HA	2.14	0.48
1:A:216:LYS:O	1:A:217:GLU:HG3	2.13	0.48
1:A:216:LYS:O	1:A:220:VAL:O	2.30	0.48
1:A:123:ILE:CG2	1:A:124:LYS:N	2.76	0.48
1:A:400:ASP:OD1	1:A:402:ILE:HB	2.12	0.48
1:A:391:PRO:O	1:A:392:TRP:HB2	2.14	0.48
1:A:33:PRO:HG2	1:A:34:PHE:HD1	1.77	0.48
1:A:41:THR:HG23	1:A:404:GLN:HG2	1.96	0.48
1:A:147:LYS:HD2	1:A:184:GLY:O	2.13	0.47
1:A:319:SER:HB2	1:A:349:TRP:HH2	1.79	0.47
1:A:53:TRP:CD2	1:A:70:LEU:HD21	2.49	0.47
1:A:198:LEU:HG	1:A:239:TRP:CE2	2.49	0.47
1:A:314:LEU:O	1:A:315:HIS:HB2	2.14	0.47
1:A:55:PRO:HG3	1:A:136:TYR:CZ	2.49	0.46
1:A:46:TRP:CE2	1:A:76:THR:HG21	2.50	0.46
1:A:266:THR:O	1:A:266:THR:HG23	2.14	0.46
1:A:190:ASN:HB2	1:A:239:TRP:CE2	2.51	0.46
1:A:250:VAL:HG11	1:A:280:VAL:HG12	1.98	0.46
1:A:195:GLY:CA	1:A:211:ILE:HG22	2.44	0.46
1:A:211:ILE:C	1:A:213:ALA:H	2.19	0.46
1:A:153:VAL:CG1	1:A:177:LEU:HD12	2.45	0.46
1:A:351:LEU:O	1:A:354:ILE:HG13	2.16	0.46
1:A:379:ALA:HB3	1:A:398:SER:OG	2.15	0.46
1:A:127:HIS:NE2	1:A:146:THR:CG2	2.59	0.46
1:A:121:ILE:HD12	1:A:121:ILE:N	2.31	0.46
1:A:84:LEU:C	1:A:85:ILE:HD12	2.35	0.46
1:A:238:ALA:HB3	1:A:283:LEU:CD2	2.46	0.45
1:A:295:THR:O	1:A:302:VAL:HA	2.17	0.45
1:A:204:HIS:ND1	1:A:204:HIS:N	2.64	0.45
1:A:253:ASP:O	1:A:255:LYS:HG3	2.15	0.45
1:A:414:ASN:OD1	1:A:415:ASP:N	2.46	0.45
1:A:228:THR:HG23	1:A:229:GLY:H	1.82	0.45
1:A:265:ASN:OD1	1:A:268:LYS:HG3	2.16	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:177:LEU:HB3	1:A:209:TRP:CD2	2.52	0.45
1:A:76:THR:C	1:A:78:ASP:H	2.19	0.45
1:A:329:TRP:CE3	1:A:337:LEU:HB3	2.52	0.45
1:A:227:PHE:N	1:A:227:PHE:CD1	2.84	0.45
1:A:362:ASP:C	1:A:364:GLU:H	2.19	0.45
1:A:46:TRP:CZ2	1:A:76:THR:HG21	2.52	0.44
1:A:23:GLU:O	1:A:27:ILE:HG12	2.17	0.44
1:A:148:THR:CG2	1:A:149:PRO:CD	2.95	0.44
1:A:354:ILE:HA	1:A:369:GLU:HG3	1.99	0.44
1:A:153:VAL:HB	1:A:177:LEU:HB2	1.98	0.44
1:A:336:ILE:HG13	1:A:336:ILE:O	2.18	0.44
1:A:318:GLU:O	1:A:319:SER:CB	2.65	0.44
1:A:252:ASP:C	1:A:254:GLN:H	2.21	0.44
1:A:335:THR:HG23	1:A:336:ILE:HG23	1.99	0.44
1:A:147:LYS:HE3	1:A:186:GLY:O	2.17	0.44
1:A:204:HIS:NE2	1:A:232:ALA:HA	2.32	0.44
1:A:346:LEU:HB3	1:A:374:HIS:HB3	1.99	0.43
1:A:190:ASN:HD22	1:A:192:ASN:H	1.64	0.43
1:A:326:GLN:HB3	1:A:384:PHE:CE2	2.53	0.43
1:A:172:GLN:CB	1:A:219:ARG:HH12	2.21	0.43
1:A:298:ALA:CB	1:A:323:GLU:HG2	2.48	0.43
1:A:305:TRP:CH2	1:A:313:LYS:HE2	2.54	0.43
1:A:315:HIS:CD2	1:A:354:ILE:CG2	3.02	0.43
1:A:32:THR:N	1:A:33:PRO:HD2	2.34	0.43
1:A:203:ASP:OD1	1:A:205:THR:OG1	2.22	0.43
1:A:260:ASP:HB3	1:A:263:ASN:ND2	2.34	0.43
1:A:25:TYR:CZ	1:A:29:LYS:HE3	2.53	0.43
1:A:298:ALA:CA	1:A:323:GLU:HG2	2.46	0.42
1:A:198:LEU:HG	1:A:239:TRP:CZ2	2.54	0.42
1:A:336:ILE:HD13	1:A:392:TRP:CH2	2.54	0.42
1:A:203:ASP:C	1:A:203:ASP:OD1	2.58	0.42
1:A:195:GLY:HA2	1:A:211:ILE:CG2	2.48	0.42
1:A:190:ASN:HA	1:A:191:PRO:HD3	1.83	0.42
1:A:193:LEU:HD21	1:A:244:GLU:OE2	2.19	0.42
1:A:68:HIS:CD2	1:A:90:LEU:HD12	2.54	0.42
1:A:228:THR:O	1:A:229:GLY:C	2.58	0.42
1:A:267:SER:O	1:A:269:PRO:HD3	2.19	0.42
1:A:149:PRO:HA	1:A:183:GLU:HG3	2.01	0.42
1:A:297:SER:OG	1:A:298:ALA:N	2.53	0.42
1:A:330:SER:HB2	1:A:336:ILE:HD11	2.01	0.42
1:A:53:TRP:CE2	1:A:70:LEU:HD21	2.55	0.42
1:A:386:TRP:CZ3	1:A:394:ILE:HD11	2.55	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:180:HIS:CB	1:A:203:ASP:OD2	2.55	0.41
1:A:342:THR:HG22	1:A:342:THR:O	2.19	0.41
1:A:345:ARG:NH1	2:B:41:GLY:C	2.74	0.41
1:A:276:HIS:CE1	1:A:301:THR:HG22	2.55	0.41
1:A:231:THR:HB	1:A:253:ASP:HB2	2.00	0.41
1:A:181:GLN:N	1:A:181:GLN:CD	2.74	0.41
1:A:178:ARG:HG3	1:A:222:ASP:OD1	2.21	0.41
1:A:36:TYR:OH	1:A:374:HIS:CD2	2.74	0.41
1:A:178:ARG:HG2	1:A:220:VAL:HG13	2.03	0.41
1:A:148:THR:HG22	1:A:150:SER:N	2.27	0.40
2:B:31:LYS:C	2:B:33:ALA:N	2.73	0.40
1:A:228:THR:HG22	1:A:266:THR:HG23	2.03	0.40
1:A:252:ASP:HA	1:A:279:GLU:HB3	2.03	0.40
1:A:25:TYR:CE2	1:A:29:LYS:HE3	2.56	0.40

There are no symmetry-related clashes.

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	374/432 (87%)	306 (82%)	56 (15%)	12 (3%)	6	39
2	B	9/27 (33%)	9 (100%)	0	0	100	100
All	All	383/459 (83%)	315 (82%)	56 (15%)	12 (3%)	7	41

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	178	ARG
1	A	215	PRO
1	A	218	HIS
1	A	223	ALA
1	A	229	GLY
1	A	319	SER

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Mol	Chain	Res	Type
1	A	179	GLY
1	A	244	GLU
1	A	356	GLU
1	A	93	GLU
1	A	270	SER
1	A	172	GLN

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	341/381 (90%)	314 (92%)	27 (8%)	18	58
2	B	8/22 (36%)	7 (88%)	1 (12%)	7	30
All	All	349/403 (87%)	321 (92%)	28 (8%)	17	57

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	LEU
1	A	76	THR
1	A	78	ASP
1	A	83	LEU
1	A	146	THR
1	A	180	HIS
1	A	190	ASN
1	A	204	HIS
1	A	209	TRP
1	A	215	PRO
1	A	228	THR
1	A	230	HIS
1	A	250	VAL
1	A	265	ASN
1	A	283	LEU
1	A	286	ASN
1	A	293	LEU
1	A	301	THR
1	A	309	ASN

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Mol	Chain	Res	Type
1	A	312	LEU
1	A	337	LEU
1	A	346	LEU
1	A	360	THR
1	A	370	LEU
1	A	378	THR
1	A	401	ASN
1	A	411	ASN
2	B	39	ARG

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

Mol	Chain	Res	Type
1	A	31	ASN
1	A	68	HIS
1	A	75	HIS
1	A	80	GLN
1	A	181	GLN
1	A	190	ASN
1	A	265	ASN
1	A	286	ASN
1	A	309	ASN
1	A	332	HIS
1	A	374	HIS
1	A	401	ASN
1	A	407	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 7 ligands modelled in this entry, 7 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.

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	380/432 (87%)	-0.12	0 100 100	45, 75, 122, 181	0
2	B	11/27 (40%)	0.33	0 100 100	78, 99, 137, 143	0
All	All	391/459 (85%)	-0.11	0 100 100	45, 76, 124, 181	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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
3	CD	A	437	1/1	0.20	2.04	99,99,99,99	0
3	CD	A	432	1/1	0.17	0.83	79,79,79,79	0
3	CD	A	431	1/1	0.16	0.62	105,105,105,105	0
3	CD	A	434	1/1	0.23	0.42	140,140,140,140	0
3	CD	A	433	1/1	0.12	-1.56	141,141,141,141	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	CD	A	435	1/1	0.19	-1.79	117,117,117,117	0
3	CD	A	436	1/1	0.10	-3.20	185,185,185,185	0

6.5 Other polymers ⓘ

There are no such residues in this entry.