



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:59 PM UTC

PDB ID : 3C9C / pdb_00003c9c
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 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

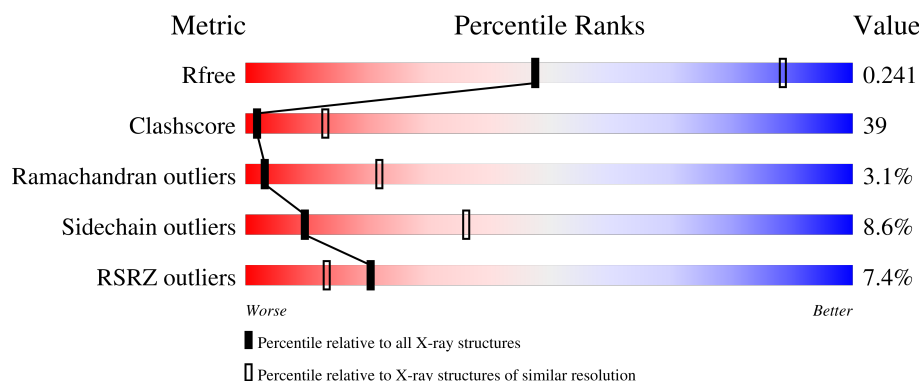
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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 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 $\leq 5\%$. 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	A	432	
2	B	27	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3152 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 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			

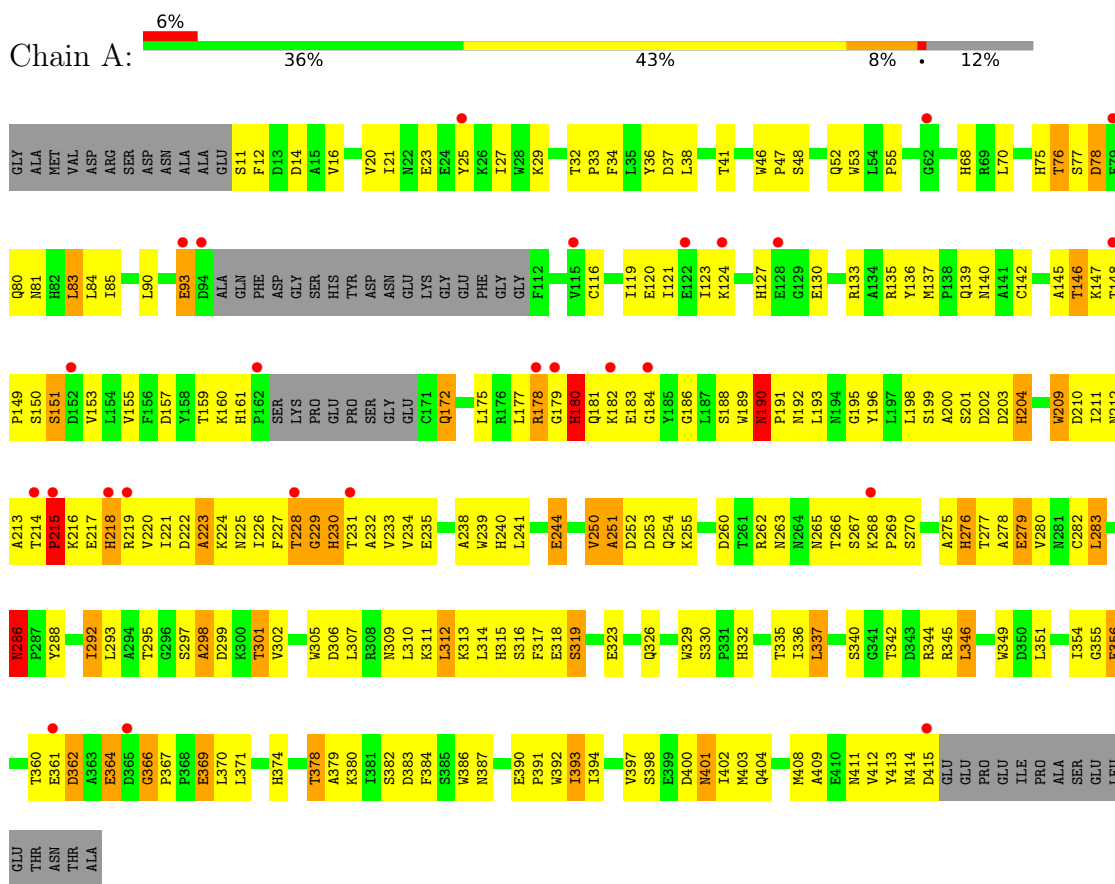
- Molecule 3 is CADMIUM ION (CCD ID: CD) (formula: Cd).

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

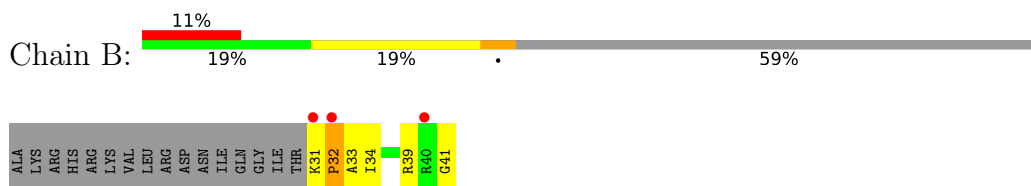
3 Residue-property plots [i](#)

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

- Molecule 1: Chromatin assembly factor 1 p55 subunit



- Molecule 2: Histone H4, 27-residue peptide



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 50.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	95.0 (50.00-3.20) 94.9 (50.00-3.20)	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	Depositor
R, R_{free}	0.203 , 0.242 0.203 , 0.241	Depositor DCC
R_{free} test set	1036 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	78.0	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 70.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.025 for -h,-k,l	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.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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:
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	0.45	0/3135	1.06	26/4271 (0.6%)
2	B	0.45	0/91	1.70	2/117 (1.7%)
All	All	0.45	0/3226	1.08	28/4388 (0.6%)

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	32	PRO	N-CA-C	-11.34	102.88	114.68
1	A	180	HIS	N-CA-C	7.96	119.72	108.74
1	A	77	SER	N-CA-C	-7.57	104.94	112.97
1	A	83	LEU	N-CA-C	-7.20	97.50	109.24
2	B	34	ILE	N-CA-C	-7.14	103.22	111.00
1	A	387	ASN	CA-C-N	7.07	126.70	119.56
1	A	387	ASN	C-N-CA	7.07	126.70	119.56
1	A	364	GLU	N-CA-C	-6.82	99.19	109.96
1	A	241	LEU	N-CA-C	6.42	119.09	111.71
1	A	275	ALA	N-CA-C	6.07	118.39	111.11
1	A	37	ASP	N-CA-C	-6.05	105.71	114.12
1	A	212	ASN	N-CA-C	-6.02	106.28	113.21
1	A	160	LYS	N-CA-C	-5.93	106.02	113.20
1	A	292	ILE	N-CA-C	5.75	116.48	108.89
1	A	282	CYS	N-CA-C	5.73	117.56	108.79
1	A	362	ASP	N-CA-C	-5.71	106.96	114.04
1	A	188	SER	N-CA-C	5.47	116.95	107.93
1	A	366	GLY	CA-C-N	5.43	125.98	120.38
1	A	366	GLY	C-N-CA	5.43	125.98	120.38
1	A	190	ASN	CA-C-N	5.37	124.88	119.19
1	A	190	ASN	C-N-CA	5.37	124.88	119.19
1	A	240	HIS	N-CA-C	-5.28	102.46	110.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	276	HIS	N-CA-C	5.28	117.01	109.14
1	A	298	ALA	N-CA-C	-5.27	106.68	113.01
1	A	151	SER	N-CA-C	-5.22	106.82	114.39
1	A	251	ALA	N-CA-C	5.22	115.94	108.74
1	A	286	ASN	CA-C-N	5.01	125.28	119.47
1	A	286	ASN	C-N-CA	5.01	125.28	119.47

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	A	3054	0	2897	239	0
2	B	91	0	106	4	0
3	A	7	0	0	0	0
All	All	3152	0	3003	242	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 39.

All (242) 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: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:401:ASN:C	1:A:401:ASN:HD22	1.75	0.94
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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:364:GLU:C	1:A:366:GLY:H	1.91	0.77
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:408:MET:HE2	1:A:413:TYR:HD2	1.50	0.76
1:A:148:THR:HG22	1:A:150:SER:H	1.50	0.76
1:A:137:MET:HE3	1:A:139:GLN:HB2	1.69	0.75
1:A:307:LEU:HA	1:A:310:LEU:CD2	2.17	0.73
1:A:286:ASN:HD22	1:A:286:ASN:C	1.96	0.72
1:A:93:GLU:CD	1:A:93:GLU:H	1.98	0.72
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:225:ASN:C	1:A:226:ILE:HD12	2.18	0.69
1:A:312:LEU:HD22	1:A:313:LYS:N	2.07	0.69
1:A:408:MET:HE3	1:A:412:VAL:HB	1.74	0.69
1:A:155:VAL:HB	1:A:175:LEU:HB2	1.75	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:209:TRP:CD1	1:A:209:TRP:H	2.13	0.67
1:A:204:HIS:CD2	1:A:232:ALA:HA	2.31	0.66
1:A:298:ALA:HA	1:A:323:GLU:HG2	1.78	0.66
1:A:190:ASN:HD22	1:A:190:ASN:C	2.04	0.65
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: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:123:ILE:HG22	1:A:124:LYS:N	2.13	0.64
1:A:254:GLN:HG2	1:A:278:ALA:O	1.98	0.64
1:A:55:PRO:HG3	1:A:136:TYR:OH	1.97	0.64
1:A:222:ASP:O	1:A:223:ALA:HB2	1.97	0.64
1:A:116:CYS:HB3	1:A:120:GLU:OE2	1.97	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:PHE:HZ	1:A:351:LEU:CD2	2.11	0.63
1:A:401:ASN:C	1:A:401:ASN:ND2	2.48	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:202:ASP:HA	1:A:233:VAL:HG13	1.82	0.61
1:A:137:MET:HE2	1:A:140:ASN:HB3	1.83	0.60
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:119:ILE:HD13	1:A:403:MET:HE2	1.84	0.59
1:A:84:LEU:O	1:A:85:ILE:HD12	2.03	0.59
1:A:233:VAL:O	1:A:251:ALA:HB1	2.03	0.59
1:A:133:ARG:HG3	1:A:133:ARG:HH11	1.67	0.58
1:A:400:ASP:O	1:A:401:ASN:ND2	2.36	0.58
1:A:286:ASN:ND2	1:A:286:ASN:C	2.62	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:371:LEU:HD21	1:A:408:MET:HE1	1.86	0.58
1:A:364:GLU:C	1:A:366:GLY:N	2.58	0.58
1:A:312:LEU:HD22	1:A:312:LEU:C	2.29	0.57
1:A:120:GLU:C	1:A:121:ILE:HD12	2.30	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:292:ILE:HD12	1:A:292:ILE:N	2.20	0.56
1:A:332:HIS:CD2	1:A:391:PRO:HA	2.41	0.56
1:A:364:GLU:O	1:A:366:GLY:N	2.38	0.56
1:A:80:GLN:HE21	1:A:81:ASN:H	1.52	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:215:PRO:C	1:A:216:LYS:HG3	2.30	0.56
2:B:31:LYS:C	2:B:33:ALA:H	2.12	0.56
1:A:214:THR:O	1:A:215:PRO:O	2.22	0.56
1:A:142:CYS:SG	1:A:157:ASP:OD1	2.63	0.56
1:A:180:HIS:CE1	1:A:201:SER:HB2	2.41	0.56
1:A:355:GLY:O	1:A:356:GLU:C	2.49	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: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:408:MET:HE2	1:A:413:TYR:CD2	2.39	0.53
1:A:182:LYS:HG2	1:A:203:ASP:HB3	1.91	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
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
2:B:31:LYS:N	2:B:32:PRO:CD	2.74	0.51
1:A:211:ILE:C	1:A:213:ALA:H	2.19	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:HG3	1:A:133:ARG:NH1	2.26	0.50
1:A:238:ALA:HB3	1:A:283:LEU:HD21	1.94	0.50
1:A:84:LEU:C	1:A:85:ILE:HD12	2.35	0.50
1:A:25:TYR:OH	1:A:29:LYS:HE3	2.11	0.50
1:A:190:ASN:HD22	1:A:191:PRO:CD	2.25	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
1:A:222:ASP:O	1:A:223:ALA:CB	2.60	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:THR:C	1:A:78:ASP:H	2.19	0.50
1:A:378:THR:O	1:A:378:THR:CG2	2.59	0.49
1:A:52:GLN:OE1	1:A:135:ARG:HA	2.13	0.49
1:A:286:ASN:HD21	1:A:288:TYR:H	1.53	0.49
1:A:12:PHE:O	1:A:16:VAL:HG23	2.13	0.49
1:A:362:ASP:C	1:A:364:GLU:H	2.19	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:HA	1:A:235:GLU:OE1	2.14	0.48
1:A:252:ASP:C	1:A:254:GLN:H	2.21	0.48
1:A:216:LYS:O	1:A:217:GLU:HG3	2.13	0.48
1:A:123:ILE:CG2	1:A:124:LYS:N	2.76	0.48
1:A:216:LYS:O	1:A:220:VAL:O	2.30	0.48
1:A:400:ASP:OD1	1:A:402:ILE:HB	2.12	0.48
1:A:33:PRO:HG2	1:A:34:PHE:HD1	1.77	0.48
1:A:391:PRO:O	1:A:392:TRP:HB2	2.14	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
2:B:31:LYS:C	2:B:33:ALA:N	2.73	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:203:ASP:C	1:A:203:ASP:OD1	2.58	0.47
1:A:228:THR:O	1:A:229:GLY:C	2.58	0.47
1:A:46:TRP:CE2	1:A:76:THR:HG21	2.50	0.46
1:A:55:PRO:HG3	1:A:136:TYR:CZ	2.49	0.46
1:A:190:ASN:HB2	1:A:239:TRP:CE2	2.51	0.46
1:A:266:THR:HG23	1:A:266:THR:O	2.14	0.46
1:A:250:VAL:HG11	1:A:280:VAL:HG12	1.98	0.46
1:A:153:VAL:CG1	1:A:177:LEU:HD12	2.45	0.46
1:A:195:GLY:CA	1:A:211:ILE:HG22	2.44	0.46
1:A:345:ARG:NH1	2:B:41:GLY:C	2.74	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:181:GLN:CD	1:A:181:GLN:N	2.74	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:177:LEU:HB3	1:A:209:TRP:CD2	2.52	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
1:A:227:PHE:N	1:A:227:PHE:CD1	2.84	0.45
1:A:329:TRP:CE3	1:A:337:LEU:HB3	2.52	0.45
1:A:148:THR:C	1:A:150:SER:H	2.25	0.45
1:A:213:ALA:O	1:A:214:THR:C	2.60	0.44
1:A:23:GLU:O	1:A:27:ILE:HG12	2.17	0.44
1:A:46:TRP:CZ2	1:A:76:THR:HG21	2.52	0.44
1:A:265:ASN:HD22	1:A:265:ASN:C	2.24	0.44
1:A:148:THR:CG2	1:A:149:PRO:CD	2.95	0.44
1:A:153:VAL:HB	1:A:177:LEU:HB2	1.98	0.44
1:A:318:GLU:O	1:A:319:SER:CB	2.65	0.44
1:A:336:ILE:O	1:A:336:ILE:HG13	2.18	0.44
1:A:354:ILE:HA	1:A:369:GLU:HG3	1.99	0.44
1:A:147:LYS:HE3	1:A:186:GLY:O	2.17	0.44
1:A:335:THR:HG23	1:A:336:ILE:HG23	1.99	0.44
1:A:93:GLU:CD	1:A:93:GLU:N	2.72	0.44
1:A:172:GLN:N	1:A:172:GLN:CD	2.76	0.44
1:A:204:HIS:NE2	1:A:232:ALA:HA	2.32	0.44
1:A:190:ASN:C	1:A:190:ASN:ND2	2.74	0.43
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:224:LYS:O	1:A:225:ASN:CG	2.61	0.43
1:A:159:THR:C	1:A:161:HIS:H	2.25	0.43
1:A:32:THR:N	1:A:33:PRO:HD2	2.34	0.43
1:A:25:TYR:CZ	1:A:29:LYS:HE3	2.53	0.43
1:A:260:ASP:HB3	1:A:263:ASN:ND2	2.34	0.43
1:A:309:ASN:ND2	1:A:309:ASN:C	2.77	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:254:GLN:HG2	1:A:278:ALA:C	2.43	0.42
1:A:336:ILE:HD13	1:A:392:TRP:CH2	2.54	0.42
1:A:190:ASN:HA	1:A:191:PRO:HD3	1.83	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:LEU:HD21	1:A:244:GLU:OE2	2.19	0.42
1:A:195:GLY:HA2	1:A:211:ILE:CG2	2.48	0.42
1:A:68:HIS:CD2	1:A:90:LEU:HD12	2.54	0.42
1:A:267:SER:O	1:A:269:PRO:HD3	2.19	0.42
1:A:214:THR:O	1:A:215:PRO:C	2.63	0.42
1:A:53:TRP:CE2	1:A:70:LEU:HD21	2.55	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:386:TRP:CZ3	1:A:394:ILE:HD11	2.55	0.42
1:A:180:HIS:CB	1:A:203:ASP:OD2	2.55	0.41
1:A:342:THR:O	1:A:342:THR:HG22	2.19	0.41
1:A:400:ASP:O	1:A:401:ASN:CG	2.63	0.41
1:A:254:GLN:CD	1:A:277:THR:O	2.63	0.41
1:A:299:ASP:OD1	1:A:299:ASP:C	2.63	0.41
1:A:231:THR:HB	1:A:253:ASP:HB2	2.00	0.41
1:A:276:HIS:CE1	1:A:301:THR:HG22	2.55	0.41
1:A:309:ASN:C	1:A:309:ASN:HD22	2.28	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
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:369:GLU:CD	1:A:369:GLU:H	2.28	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 [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	
1	A	374/432 (87%)	306 (82%)	56 (15%)	12 (3%)	3	21
2	B	9/27 (33%)	9 (100%)	0	0	100	100
All	All	383/459 (83%)	315 (82%)	56 (15%)	12 (3%)	3	22

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
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%)	312 (92%)	29 (8%)	10	37
2	B	8/22 (36%)	7 (88%)	1 (12%)	4	21
All	All	349/403 (87%)	319 (91%)	30 (9%)	10	36

All (30) 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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	279	GLU
1	A	283	LEU
1	A	286	ASN
1	A	293	LEU
1	A	301	THR
1	A	312	LEU
1	A	337	LEU
1	A	346	LEU
1	A	360	THR
1	A	361	GLU
1	A	369	GLU
1	A	370	LEU
1	A	378	THR
1	A	393	ILE
1	A	401	ASN
1	A	411	ASN
2	B	39	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	60	GLN
1	A	68	HIS
1	A	75	HIS
1	A	80	GLN
1	A	181	GLN
1	A	190	ASN
1	A	204	HIS
1	A	263	ASN
1	A	265	ASN
1	A	271	HIS
1	A	286	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	309	ASN
1	A	332	HIS
1	A	374	HIS
1	A	389	ASN
1	A	401	ASN
1	A	407	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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.

No monomer is involved in short contacts.

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, 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%)	0.24	26 (6%) 23 15	45, 75, 122, 181	0
2	B	11/27 (40%)	1.34	3 (27%) 1 1	78, 99, 137, 143	0
All	All	391/459 (85%)	0.27	29 (7%) 20 13	45, 76, 124, 181	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	268	LYS	5.0
1	A	415	ASP	4.8
1	A	218	HIS	4.7
2	B	31	LYS	4.3
2	B	32	PRO	3.9
1	A	361	GLU	3.8
1	A	228	THR	3.7
1	A	179	GLY	3.6
1	A	162	PRO	3.3
1	A	215	PRO	3.1
2	B	40	ARG	3.1
1	A	231	THR	3.0
1	A	79	GLU	2.8
1	A	214	THR	2.8
1	A	94	ASP	2.7
1	A	219	ARG	2.5
1	A	184	GLY	2.5
1	A	62	GLY	2.4
1	A	365	ASP	2.3
1	A	122	GLU	2.3
1	A	93	GLU	2.2
1	A	182	LYS	2.2
1	A	128	GLU	2.2
1	A	178	ARG	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	115	VAL	2.1
1	A	148	THR	2.1
1	A	25	TYR	2.1
1	A	152	ASP	2.0
1	A	124	LYS	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 oligosaccharides 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. 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	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	CD	A	434	1/1	0.94	0.08	140,140,140,140	0
3	CD	A	436	1/1	0.95	0.17	185,185,185,185	0
3	CD	A	435	1/1	0.98	0.11	117,117,117,117	0
3	CD	A	433	1/1	0.98	0.08	141,141,141,141	0
3	CD	A	431	1/1	1.00	0.02	105,105,105,105	0
3	CD	A	432	1/1	1.00	0.02	79,79,79,79	0
3	CD	A	437	1/1	1.00	0.02	99,99,99,99	0

6.5 Other polymers [i](#)

There are no such residues in this entry.