



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:40 PM UTC

PDB ID : 7PB8 / pdb_00007pb8
Title : Crystal structure of the CENP-OPQUR complex
Authors : Bellini, D.; Yatskevich, S.; Muir, K.W.; Barford, D.
Deposited on : 2021-07-31
Resolution : 3.68 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

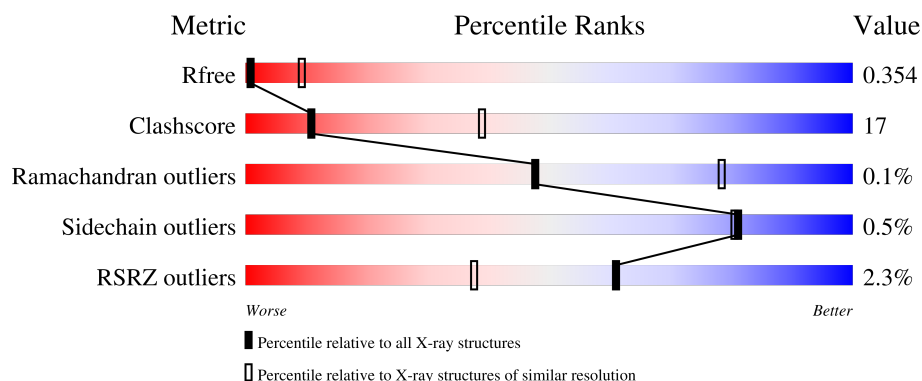
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.68 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	1263 (3.80-3.56)
Clashscore	190562	1305 (3.80-3.56)
Ramachandran outliers	187476	1259 (3.80-3.56)
Sidechain outliers	187428	1256 (3.80-3.56)
RSRZ outliers	180081	1262 (3.80-3.56)

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	O	300	% 46% 20% 34%
2	Q	137	3% 55% 27% 18%
3	U	418	% 17% 7% 75%
4	P	294	% 44% 32% 24%
5	R	177	% 24% 15% 61%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5706 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 Centromere protein O.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	O	198	Total	C	N	O	S	0	0	0
			1586	1020	265	294	7			

- Molecule 2 is a protein called Centromere protein Q.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Q	112	Total	C	N	O	S	0	0	0
			886	555	145	181	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	132	MET	-	initiating methionine	UNP Q7L2Z9

- Molecule 3 is a protein called Centromere protein U.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	U	103	Total	C	N	O	S	0	0	0
			858	538	154	165	1			

- Molecule 4 is a protein called Centromere protein P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	P	224	Total	C	N	O	S	0	0	0
			1818	1158	316	336	8			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	289	GLU	-	expression tag	UNP Q6IPU0
P	290	ASN	-	expression tag	UNP Q6IPU0
P	291	LEU	-	expression tag	UNP Q6IPU0

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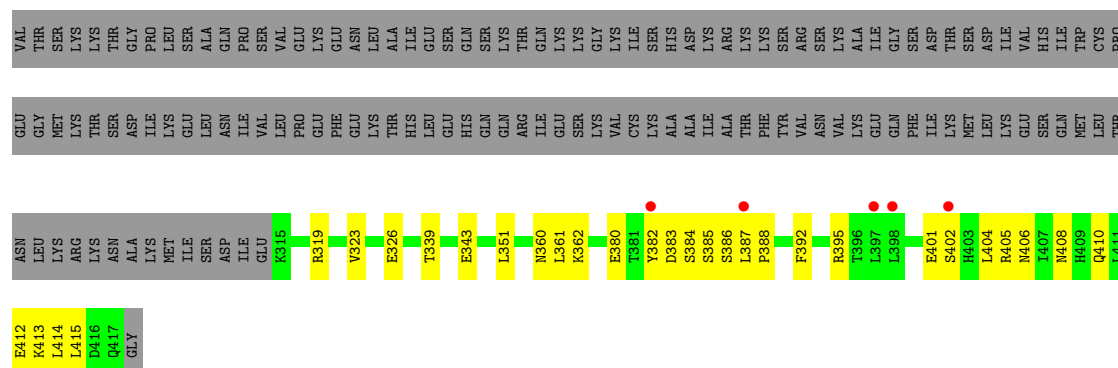
Chain	Residue	Modelled	Actual	Comment	Reference
P	292	TYR	-	expression tag	UNP Q6IPU0
P	293	PHE	-	expression tag	UNP Q6IPU0
P	294	GLN	-	expression tag	UNP Q6IPU0

- Molecule 5 is a protein called Centromere protein R.

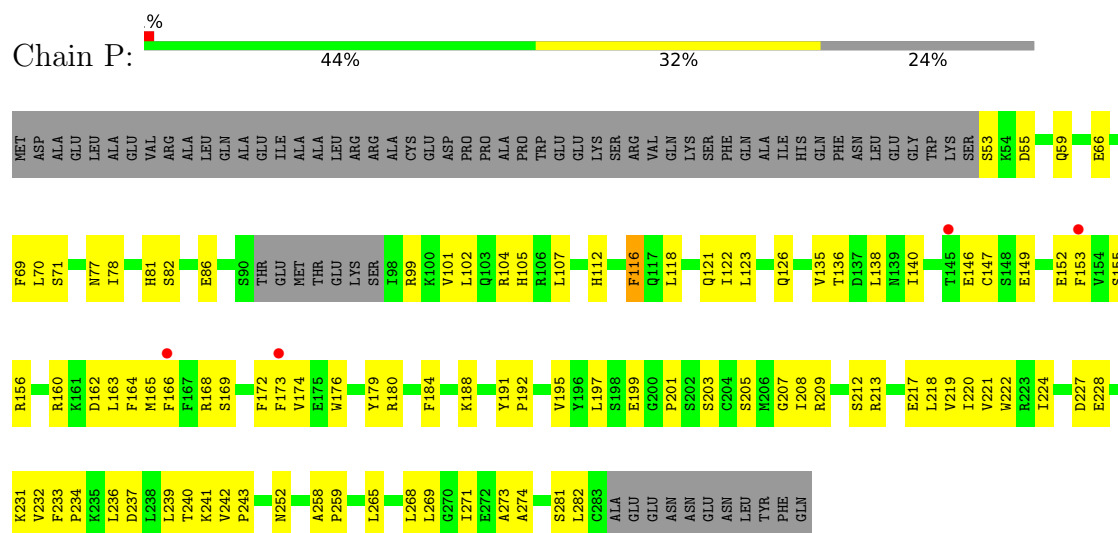
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	R	69	Total	C	N	O	S	0	0	0
			557	351	92	107	7			

- Molecule 6 is water.

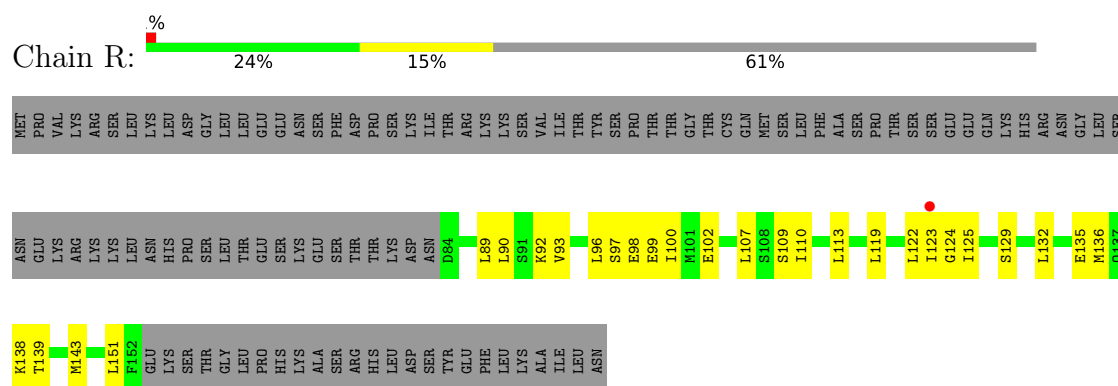
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	U	1	Total	O	0	0
			1	1		



• Molecule 4: Centromere protein P



• Molecule 5: Centromere protein R



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	199.61Å 51.30Å 110.00Å 90.00° 117.49° 90.00°	Depositor
Resolution (Å)	25.65 – 3.68 25.65 – 3.68	Depositor EDS
% Data completeness (in resolution range)	55.4 (25.65-3.68) 55.3 (25.65-3.68)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 3.64Å)	Xtriage
Refinement program	REFMAC 1.17.1 _3660, PHENIX 1.17.1 _3660	Depositor
R, R_{free}	0.256 , 0.352 0.259 , 0.354	Depositor DCC
R_{free} test set	295 reflections (2.67%)	wwPDB-VP
Wilson B-factor (Å ²)	79.9	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 53.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	5706	wwPDB-VP
Average B, all atoms (Å ²)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.52% 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 [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	O	0.22	0/1622	0.44	0/2202
2	Q	0.19	0/891	0.38	0/1195
3	U	0.20	0/869	0.40	0/1166
4	P	0.23	0/1850	0.47	0/2487
5	R	0.21	0/560	0.49	0/741
All	All	0.22	0/5792	0.44	0/7791

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	O	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	O	221	THR	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	O	1586	0	1572	54	0
2	Q	886	0	918	29	0
3	U	858	0	875	36	0
4	P	1818	0	1845	87	0
5	R	557	0	584	30	0
6	U	1	0	0	0	0
All	All	5706	0	5794	191	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 17.

All (191) 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:P:86:GLU:OE2	4:P:104:ARG:NH1	2.11	0.83
3:U:412:GLU:HA	3:U:415:LEU:HB2	1.61	0.83
4:P:160:ARG:HE	4:P:165:MET:HE1	1.44	0.82
1:O:223:LYS:HG2	1:O:232:PRO:HA	1.64	0.79
4:P:217:GLU:HG2	4:P:241:LYS:HD3	1.64	0.77
2:Q:161:GLU:HG2	2:Q:164:LYS:HD3	1.68	0.75
4:P:123:LEU:HD13	4:P:136:THR:HB	1.66	0.75
5:R:107:LEU:HD22	5:R:110:ILE:HG12	1.69	0.75
1:O:104:ILE:HG22	4:P:81:HIS:HB3	1.72	0.72
3:U:404:LEU:HD22	5:R:139:THR:HG21	1.72	0.71
4:P:184:PHE:HB3	4:P:197:LEU:HD21	1.73	0.70
5:R:96:LEU:O	5:R:100:ILE:N	2.20	0.70
1:O:107:ALA:HA	1:O:110:PHE:HD2	1.55	0.69
2:Q:232:ILE:HG21	2:Q:238:LEU:HD11	1.72	0.69
4:P:188:LYS:HD2	4:P:197:LEU:HD13	1.73	0.69
5:R:93:VAL:O	5:R:97:SER:N	2.24	0.68
4:P:122:ILE:HG22	4:P:135:VAL:HG12	1.74	0.68
3:U:395:ARG:NH2	5:R:124:GLY:O	2.28	0.67
4:P:224:ILE:HA	4:P:234:PRO:HA	1.77	0.66
5:R:92:LYS:HG2	5:R:96:LEU:HD13	1.77	0.65
4:P:176:TRP:HA	4:P:179:TYR:HD2	1.62	0.65
4:P:78:ILE:HG23	4:P:107:LEU:HD11	1.78	0.65
4:P:152:GLU:HA	4:P:155:SER:HB2	1.79	0.65
3:U:395:ARG:HB2	5:R:125:ILE:HG21	1.79	0.64
3:U:401:GLU:HG3	5:R:135:GLU:HG2	1.81	0.63
5:R:90:LEU:HD13	5:R:143:MET:HB3	1.78	0.63
1:O:243:THR:OG1	4:P:231:LYS:NZ	2.33	0.62
4:P:224:ILE:HG22	4:P:234:PRO:HB3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:404:LEU:HB3	5:R:139:THR:OG1	2.00	0.61
4:P:180:ARG:HE	4:P:222:TRP:CD1	2.19	0.61
1:O:212:ASN:HB3	1:O:216:ASN:H	1.64	0.61
2:Q:229:LEU:HD11	2:Q:235:GLN:HG3	1.82	0.60
1:O:212:ASN:HD22	1:O:216:ASN:HB3	1.66	0.60
1:O:156:PRO:HB3	1:O:158:PHE:HD2	1.65	0.60
3:U:339:THR:O	3:U:343:GLU:N	2.36	0.59
4:P:209:ARG:HB3	4:P:217:GLU:HB3	1.84	0.58
3:U:351:LEU:HD23	4:P:268:LEU:HD13	1.83	0.58
4:P:99:ARG:O	4:P:126:GLN:HB2	2.03	0.58
1:O:232:PRO:HD2	1:O:264:TRP:HH2	1.67	0.58
2:Q:172:MET:HB2	2:Q:176:ILE:HD12	1.86	0.58
1:O:237:LEU:HD22	1:O:247:PRO:HG2	1.85	0.58
4:P:102:LEU:HD22	4:P:123:LEU:HA	1.85	0.57
4:P:107:LEU:HB3	4:P:118:LEU:HD11	1.86	0.57
1:O:132:GLY:H	4:P:162:ASP:HB3	1.68	0.57
1:O:135:LEU:HD21	1:O:192:TYR:HB2	1.86	0.57
4:P:147:CYS:HB3	4:P:149:GLU:HG2	1.86	0.57
1:O:112:GLY:HA2	4:P:164:PHE:HD1	1.70	0.56
2:Q:166:VAL:HA	2:Q:169:THR:HG22	1.87	0.56
4:P:265:LEU:HG	4:P:274:ALA:HB1	1.86	0.56
3:U:383:ASP:OD1	3:U:384:SER:N	2.38	0.56
4:P:180:ARG:NH2	4:P:222:TRP:O	2.39	0.55
1:O:232:PRO:O	1:O:264:TRP:HZ3	1.89	0.55
1:O:101:VAL:O	1:O:105:LEU:HD13	2.07	0.54
2:Q:224:LEU:HG	4:P:237:ASP:HB2	1.88	0.54
1:O:192:TYR:CZ	1:O:196:ARG:HD2	2.43	0.54
1:O:194:ALA:HB1	1:O:209:LEU:HD21	1.88	0.54
1:O:205:LEU:HA	1:O:222:TYR:HA	1.89	0.54
4:P:104:ARG:HB3	4:P:121:GLN:HG2	1.90	0.54
1:O:122:VAL:HG11	4:P:69:PHE:CE2	2.43	0.54
1:O:240:LYS:HB2	1:O:248:THR:HG21	1.89	0.53
3:U:392:PHE:O	3:U:395:ARG:HG2	2.08	0.53
4:P:205:SER:HB2	4:P:220:ILE:O	2.08	0.53
4:P:86:GLU:O	4:P:101:VAL:HG13	2.08	0.53
4:P:269:LEU:HB3	4:P:273:ALA:HB3	1.91	0.53
2:Q:250:GLN:HB3	5:R:100:ILE:HG22	1.91	0.52
4:P:156:ARG:HD2	4:P:160:ARG:HH12	1.75	0.52
2:Q:242:LEU:HD12	2:Q:245:LEU:HD12	1.91	0.52
1:O:194:ALA:HB2	1:O:218:LEU:HD21	1.92	0.52
2:Q:266:ASP:CG	4:P:201:PRO:HG2	2.35	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:91:GLN:NE2	4:P:53:SER:OG	2.40	0.52
3:U:360:ASN:HD21	4:P:252:ASN:ND2	2.07	0.52
4:P:227:ASP:HB2	4:P:233:PHE:CD2	2.45	0.52
3:U:386:SER:HA	4:P:240:THR:O	2.10	0.51
4:P:138:LEU:HD21	4:P:140:ILE:HD11	1.92	0.51
4:P:169:SER:O	4:P:173:PHE:N	2.39	0.51
1:O:98:LEU:HA	1:O:101:VAL:HG12	1.91	0.51
3:U:395:ARG:NH1	5:R:123:ILE:O	2.44	0.51
4:P:219:VAL:HG23	4:P:239:LEU:HB2	1.92	0.51
5:R:113:LEU:O	5:R:119:LEU:HD12	2.11	0.51
3:U:383:ASP:C	3:U:385:SER:H	2.19	0.50
4:P:188:LYS:O	4:P:192:PRO:HB3	2.12	0.50
4:P:81:HIS:HB2	4:P:107:LEU:HD13	1.93	0.50
4:P:81:HIS:HE1	4:P:105:HIS:CD2	2.29	0.50
4:P:107:LEU:HB3	4:P:118:LEU:CD1	2.42	0.50
1:O:107:ALA:HA	1:O:110:PHE:CD2	2.43	0.50
3:U:388:PRO:HB2	4:P:239:LEU:HD22	1.93	0.50
3:U:414:LEU:HD13	5:R:151:LEU:HD21	1.94	0.50
4:P:258:ALA:H	4:P:259:PRO:HD2	1.76	0.50
2:Q:231:LEU:HD22	5:R:122:LEU:HD12	1.94	0.50
4:P:208:ILE:HG22	4:P:282:LEU:HD13	1.93	0.49
5:R:129:SER:HA	5:R:132:LEU:HD13	1.95	0.49
4:P:112:HIS:HB3	4:P:174:VAL:HG21	1.94	0.49
2:Q:165:MET:HB3	3:U:323:VAL:HG22	1.94	0.49
4:P:55:ASP:O	4:P:59:GLN:HG2	2.12	0.49
4:P:180:ARG:HE	4:P:222:TRP:HD1	1.60	0.49
5:R:93:VAL:HA	5:R:96:LEU:HB2	1.93	0.49
1:O:212:ASN:OD1	1:O:213:PRO:HD2	2.12	0.49
3:U:380:GLU:HB3	4:P:243:PRO:HB3	1.94	0.49
4:P:107:LEU:HD23	4:P:118:LEU:HD21	1.93	0.49
2:Q:198:LYS:HD3	2:Q:201:HIS:CE1	2.48	0.49
5:R:135:GLU:OE1	5:R:138:LYS:HD2	2.13	0.49
4:P:149:GLU:O	4:P:153:PHE:N	2.45	0.48
1:O:112:GLY:HA2	4:P:164:PHE:CD1	2.48	0.48
2:Q:201:HIS:ND1	2:Q:202:GLN:O	2.47	0.48
1:O:133:ASN:ND2	1:O:192:TYR:OH	2.46	0.48
1:O:206:THR:HG21	1:O:223:LYS:HE3	1.95	0.48
1:O:117:LEU:HG	4:P:66:GLU:HG2	1.95	0.47
3:U:402:SER:HB3	5:R:125:ILE:HD11	1.97	0.47
1:O:126:ILE:N	1:O:138:TYR:O	2.47	0.47
1:O:250:VAL:HG12	1:O:272:GLU:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:197:LEU:HD23	4:P:201:PRO:HA	1.96	0.47
2:Q:231:LEU:HG	5:R:119:LEU:HD22	1.97	0.47
4:P:212:SER:HB3	4:P:213:ARG:HH11	1.80	0.47
1:O:168:TYR:O	1:O:176:PHE:HB2	2.15	0.46
3:U:402:SER:O	3:U:406:ASN:N	2.43	0.46
1:O:91:GLN:O	1:O:95:GLU:HG3	2.15	0.46
3:U:410:GLN:HA	3:U:413:LYS:HD3	1.96	0.46
1:O:158:PHE:C	1:O:214:LEU:HD21	2.41	0.46
4:P:116:PHE:HE2	4:P:166:PHE:CE2	2.34	0.46
5:R:89:LEU:O	5:R:93:VAL:HG23	2.15	0.46
1:O:220:PHE:CD1	1:O:220:PHE:N	2.84	0.46
4:P:207:GLY:HA2	4:P:219:VAL:HG12	1.97	0.46
4:P:212:SER:HB3	4:P:213:ARG:NH1	2.30	0.46
2:Q:155:LEU:O	2:Q:159:GLN:N	2.47	0.46
2:Q:239:LEU:HB2	3:U:387:LEU:HD12	1.96	0.46
1:O:185:ASN:HD22	4:P:168:ARG:HE	1.62	0.45
4:P:163:LEU:H	4:P:163:LEU:HD23	1.82	0.45
3:U:360:ASN:ND2	4:P:252:ASN:HD22	2.14	0.45
1:O:261:SER:O	1:O:264:TRP:HD1	2.00	0.45
4:P:209:ARG:HB3	4:P:217:GLU:CB	2.47	0.45
2:Q:214:LEU:HB3	2:Q:218:THR:OG1	2.17	0.45
4:P:191:TYR:O	4:P:195:VAL:HG22	2.17	0.45
1:O:89:ASN:C	1:O:91:GLN:H	2.25	0.44
1:O:102:LYS:O	1:O:106:GLN:HG2	2.16	0.44
2:Q:158:LEU:HD23	3:U:319:ARG:NH1	2.32	0.44
3:U:362:LYS:HA	4:P:281:SER:O	2.18	0.44
3:U:412:GLU:HG2	3:U:415:LEU:HD22	1.99	0.44
3:U:404:LEU:O	3:U:408:ASN:ND2	2.50	0.44
4:P:149:GLU:O	4:P:153:PHE:HB2	2.17	0.44
1:O:132:GLY:HA3	4:P:135:VAL:HG22	1.99	0.44
4:P:163:LEU:O	4:P:166:PHE:HB3	2.18	0.44
1:O:212:ASN:O	1:O:215:CYS:N	2.33	0.44
3:U:405:ARG:HA	3:U:408:ASN:HD22	1.82	0.44
4:P:104:ARG:CB	4:P:121:GLN:HG2	2.48	0.44
5:R:107:LEU:HD23	5:R:109:SER:H	1.84	0.43
1:O:192:TYR:CE1	1:O:196:ARG:HD2	2.53	0.43
3:U:414:LEU:HD13	5:R:151:LEU:HD11	2.01	0.43
1:O:194:ALA:HB1	1:O:211:ARG:HD3	2.01	0.43
4:P:199:GLU:H	4:P:203:SER:HB2	1.83	0.43
5:R:98:GLU:O	5:R:102:GLU:HG2	2.18	0.43
1:O:125:CYS:HA	1:O:139:PHE:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:250:VAL:HG11	1:O:272:GLU:HA	1.99	0.43
2:Q:178:SER:O	2:Q:182:LYS:HG2	2.19	0.43
2:Q:231:LEU:HD22	5:R:122:LEU:CD1	2.49	0.43
1:O:165:ALA:O	1:O:169:LEU:N	2.51	0.43
4:P:82:SER:O	4:P:105:HIS:HB2	2.19	0.43
2:Q:194:GLU:O	2:Q:198:LYS:HG2	2.20	0.42
3:U:386:SER:HB2	4:P:242:VAL:H	1.84	0.42
4:P:81:HIS:CE1	4:P:105:HIS:CD2	3.07	0.42
1:O:220:PHE:N	1:O:220:PHE:HD1	2.16	0.42
4:P:271:ILE:HD12	4:P:271:ILE:H	1.85	0.42
2:Q:224:LEU:HD11	4:P:221:VAL:HG11	2.01	0.42
2:Q:257:PHE:CE1	5:R:90:LEU:HD21	2.55	0.42
3:U:401:GLU:O	3:U:405:ARG:N	2.46	0.42
4:P:221:VAL:O	4:P:236:LEU:HD12	2.19	0.42
4:P:172:PHE:HB3	4:P:232:VAL:HG11	2.01	0.42
1:O:100:ASN:O	1:O:104:ILE:HG12	2.20	0.42
1:O:239:TYR:CZ	1:O:247:PRO:HG3	2.55	0.42
3:U:360:ASN:HD21	4:P:252:ASN:HD22	1.67	0.42
1:O:115:GLY:HA3	4:P:70:LEU:HD21	2.02	0.41
1:O:233:PHE:HA	1:O:254:CYS:SG	2.61	0.41
4:P:222:TRP:HZ3	4:P:271:ILE:HG21	1.85	0.41
1:O:216:ASN:O	1:O:239:TYR:HB2	2.20	0.41
2:Q:175:ASN:O	2:Q:179:LEU:HD13	2.20	0.41
2:Q:185:ILE:O	2:Q:188:SER:OG	2.29	0.41
2:Q:235:GLN:HG2	2:Q:236:ASN:N	2.35	0.41
2:Q:224:LEU:O	2:Q:228:ILE:HG13	2.20	0.41
4:P:227:ASP:HB2	4:P:233:PHE:HD2	1.82	0.41
4:P:146:GLU:HB2	5:R:124:GLY:O	2.20	0.41
4:P:227:ASP:CG	4:P:228:GLU:H	2.29	0.41
1:O:122:VAL:HG13	1:O:144:ILE:HD11	2.02	0.41
5:R:96:LEU:HA	5:R:99:GLU:HB2	2.02	0.41
4:P:71:SER:HB2	4:P:77:ASN:HB3	2.03	0.41
5:R:100:ILE:HD11	5:R:136:MET:HE3	2.03	0.40
1:O:223:LYS:HE2	1:O:232:PRO:HB3	2.02	0.40
2:Q:169:THR:HB	3:U:326:GLU:OE2	2.21	0.40
2:Q:239:LEU:HD21	3:U:382:TYR:HB2	2.02	0.40
3:U:401:GLU:HA	5:R:135:GLU:HG2	2.02	0.40
4:P:165:MET:HG3	4:P:168:ARG:NH1	2.36	0.40
1:O:209:LEU:HD12	1:O:220:PHE:HB3	2.03	0.40
3:U:361:LEU:HD11	4:P:218:LEU:HD11	2.04	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	O	194/300 (65%)	173 (89%)	21 (11%)	0	100	100
2	Q	108/137 (79%)	103 (95%)	4 (4%)	1 (1%)	14	45
3	U	101/418 (24%)	97 (96%)	4 (4%)	0	100	100
4	P	220/294 (75%)	204 (93%)	16 (7%)	0	100	100
5	R	67/177 (38%)	63 (94%)	4 (6%)	0	100	100
All	All	690/1326 (52%)	640 (93%)	49 (7%)	1 (0%)	48	78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	Q	203	ILE

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	O	177/263 (67%)	175 (99%)	2 (1%)	65	72
2	Q	103/125 (82%)	103 (100%)	0	100	100
3	U	96/379 (25%)	96 (100%)	0	100	100
4	P	205/265 (77%)	204 (100%)	1 (0%)	81	80
5	R	65/166 (39%)	65 (100%)	0	100	100
All	All	646/1198 (54%)	643 (100%)	3 (0%)	81	80

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	220	PHE
1	O	222	TYR
4	P	116	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	O	91	GLN
1	O	109	HIS
1	O	133	ASN
1	O	185	ASN
1	O	198	GLN
2	Q	246	HIS
3	U	360	ASN
3	U	372	GLN
3	U	408	ASN
4	P	81	HIS
4	P	103	GLN
4	P	105	HIS
4	P	112	HIS
5	R	137	GLN
5	R	149	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides 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	O	198/300 (66%)	0.19	2 (1%)	79	55	43, 73, 138, 174	0
2	Q	112/137 (81%)	0.26	4 (3%)	46	29	57, 115, 170, 183	0
3	U	103/418 (24%)	0.43	5 (4%)	35	22	55, 104, 166, 173	0
4	P	224/294 (76%)	0.26	4 (1%)	67	42	49, 86, 131, 167	0
5	R	69/177 (38%)	0.14	1 (1%)	73	47	137, 160, 174, 179	0
All	All	706/1326 (53%)	0.25	16 (2%)	61	37	43, 93, 167, 183	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	Q	241	ASP	3.2
4	P	145	THR	3.1
2	Q	265	LEU	2.7
3	U	398	LEU	2.7
3	U	382	TYR	2.5
3	U	397	LEU	2.4
2	Q	254	MET	2.4
1	O	176	PHE	2.4
2	Q	190	VAL	2.3
1	O	250	VAL	2.2
5	R	123	ILE	2.2
4	P	173	PHE	2.2
4	P	153	PHE	2.1
4	P	166	PHE	2.1
3	U	387	LEU	2.1
3	U	402	SER	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.