



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 5, 2024 – 10:05 AM EDT

PDB ID : 8U1A
Title : De novo Design of Near Infrared Fluorescent Proteins
Authors : Liu, Y.; Xu, C.; Bera, A.K.; Kang, A.; Baker, D.
Deposited on : 2023-08-31
Resolution : 3.28 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.20.1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.002 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.38.3

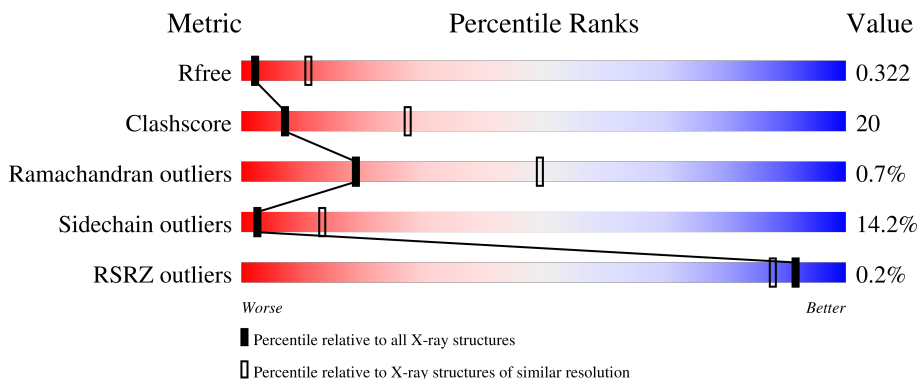
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.28 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}	164625	1214 (3.30-3.26)
Clashscore	180529	1265 (3.30-3.26)
Ramachandran outliers	177936	1264 (3.30-3.26)
Sidechain outliers	177891	1263 (3.30-3.26)
RSRZ outliers	164620	1215 (3.30-3.26)

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	379	
1	B	379	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5509 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 Designed Near Infrared Fluorescent Protein MC7BP34.

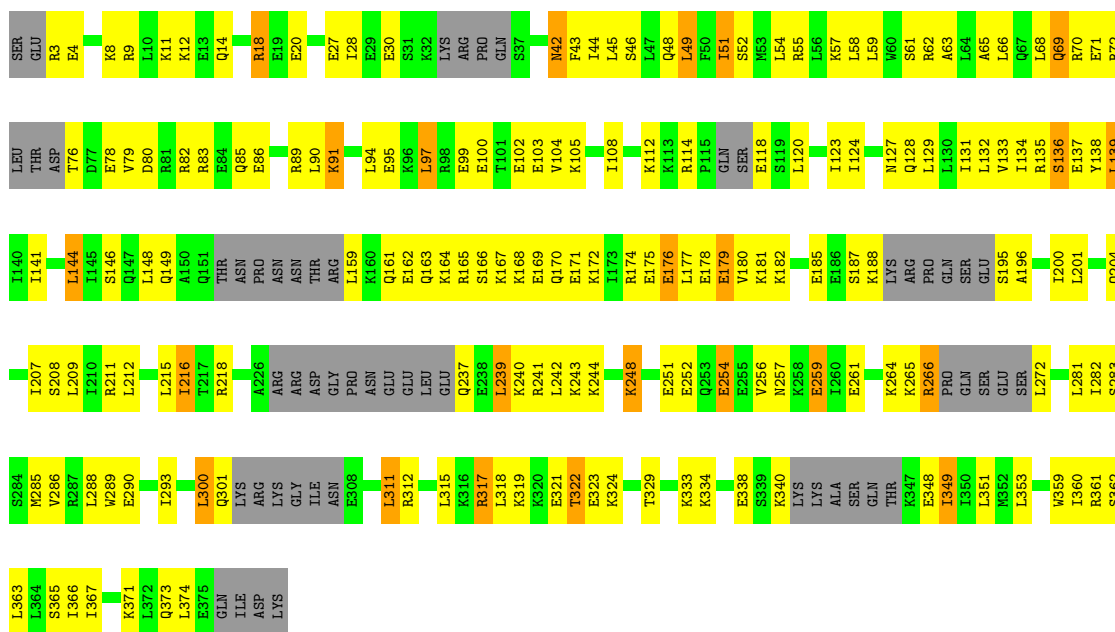
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	324	Total 2759	C 1746	N 490	O 519	S 4	0	0	0
1	B	323	Total 2750	C 1741	N 490	O 515	S 4	0	0	0

3 Residue-property plots

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

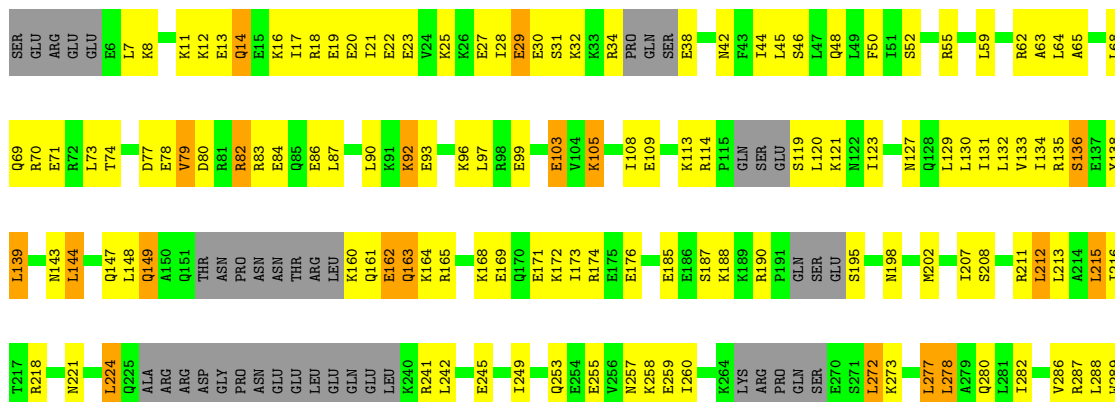
- Molecule 1: Designed Near Infrared Fluorescent Protein MC7BP34

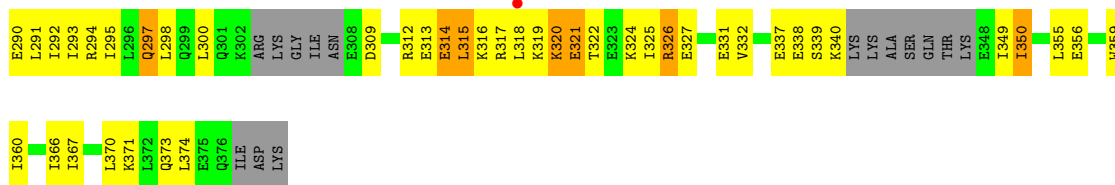
Chain A: 



- Molecule 1: Designed Near Infrared Fluorescent Protein MC7BP34

Chain B: 





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.19Å 80.44Å 72.63Å 90.00° 94.26° 90.00°	Depositor
Resolution (Å)	72.43 – 3.28 72.43 – 3.29	Depositor EDS
% Data completeness (in resolution range)	98.5 (72.43-3.28) 98.6 (72.43-3.29)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 3.26Å)	Xtrriage
Refinement program	PHENIX dev_4761	Depositor
R, R_{free}	0.261 , 0.318 0.265 , 0.322	Depositor DCC
R_{free} test set	625 reflections (5.55%)	wwPDB-VP
Wilson B-factor (Å ²)	137.7	Xtrriage
Anisotropy	0.398	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 142.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5509	wwPDB-VP
Average B, all atoms (Å ²)	147.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.61% 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	A	0.30	0/2761	0.51	0/3653
1	B	0.29	0/2754	0.52	0/3646
All	All	0.30	0/5515	0.52	0/7299

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	A	2759	0	2993	118	0
1	B	2750	0	2991	120	0
All	All	5509	0	5984	234	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 20.

All (234) 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:120:LEU:HA	1:A:123:ILE:HD12	1.64	0.80
1:A:177:LEU:HD11	1:A:207:ILE:HG23	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:LYS:HG2	1:B:23:GLU:HB2	1.66	0.78
1:A:333:LYS:HB2	1:A:360:ILE:HG21	1.68	0.76
1:A:66:LEU:HD11	1:A:86:GLU:HG2	1.66	0.76
1:A:49:LEU:HD21	1:A:131:ILE:HG13	1.67	0.76
1:B:123:ILE:O	1:B:127:ASN:ND2	2.20	0.73
1:B:87:LEU:HD21	1:B:148:LEU:HD12	1.70	0.72
1:B:42:ASN:HA	1:B:45:LEU:HB2	1.71	0.70
1:A:254:GLU:HA	1:A:257:ASN:HB2	1.76	0.68
1:B:147:GLN:HG2	1:B:224:LEU:HD11	1.75	0.67
1:B:298:LEU:HD11	1:B:314:GLU:HG3	1.77	0.66
1:B:139:LEU:O	1:B:143:ASN:ND2	2.25	0.66
1:B:162:GLU:OE2	1:B:165:ARG:NH1	2.29	0.66
1:A:86:GLU:HA	1:A:89:ARG:HE	1.60	0.65
1:A:188:LYS:HG2	1:B:82:ARG:HD3	1.79	0.64
1:B:160:LYS:HG2	1:B:163:GLN:HG3	1.78	0.64
1:A:164:LYS:O	1:A:168:LYS:N	2.31	0.64
1:A:329:THR:HG22	1:A:360:ILE:HG23	1.79	0.64
1:A:135:ARG:HH22	1:A:172:LYS:HG2	1.62	0.63
1:B:213:LEU:HD23	1:B:216:ILE:HD12	1.79	0.63
1:A:340:LYS:HE3	1:A:353:LEU:HD13	1.80	0.63
1:A:76:THR:HG22	1:A:78:GLU:H	1.64	0.62
1:A:204:GLN:OE1	1:A:211:ARG:NH2	2.33	0.62
1:B:113:LYS:O	1:B:114:ARG:NH1	2.31	0.62
1:A:43:PHE:HE1	1:A:123:ILE:HD13	1.63	0.62
1:A:371:LYS:HA	1:A:374:LEU:HD12	1.82	0.62
1:A:4:GLU:O	1:A:8:LYS:N	2.33	0.62
1:A:69:GLN:HA	1:A:72:ARG:HB3	1.81	0.62
1:B:59:LEU:HD11	1:B:93:GLU:HB3	1.82	0.61
1:B:202:MET:HE1	1:B:278:LEU:HB3	1.81	0.61
1:B:119:SER:OG	1:B:120:LEU:N	2.34	0.61
1:B:120:LEU:HD13	1:B:123:ILE:HD12	1.83	0.61
1:B:139:LEU:HD11	1:B:173:ILE:HD11	1.83	0.61
1:A:102:GLU:HA	1:A:105:LYS:HE2	1.83	0.60
1:A:28:ILE:HG21	1:A:48:GLN:HG2	1.83	0.60
1:A:132:LEU:O	1:A:136:SER:OG	2.20	0.60
1:A:201:LEU:HD21	1:A:259:GLU:HB3	1.82	0.60
1:A:319:LYS:HG3	1:A:374:LEU:HD13	1.83	0.59
1:A:209:LEU:HD11	1:A:289:TRP:HD1	1.67	0.59
1:B:77:ASP:HB2	1:B:80:ASP:HB2	1.84	0.59
1:B:195:SER:O	1:B:198:ASN:ND2	2.32	0.59
1:B:8:LYS:HD2	1:B:11:LYS:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:LYS:NZ	1:B:109:GLU:OE2	2.30	0.58
1:B:78:GLU:OE1	1:B:82:ARG:NH2	2.37	0.58
1:B:84:GLU:HA	1:B:87:LEU:HD12	1.85	0.58
1:B:338:GLU:O	1:B:340:LYS:N	2.37	0.57
1:B:64:LEU:HD22	1:B:373:GLN:HE22	1.70	0.57
1:B:143:ASN:O	1:B:147:GLN:HG3	2.04	0.57
1:B:70:ARG:HB2	1:B:83:ARG:HH12	1.68	0.57
1:B:21:ILE:O	1:B:25:LYS:HB2	2.05	0.56
1:B:287:ARG:HD3	1:B:325:ILE:HG12	1.88	0.56
1:A:288:LEU:HD22	1:A:363:LEU:HD11	1.88	0.56
1:B:317:ARG:O	1:B:321:GLU:HG2	2.05	0.56
1:B:207:ILE:HG22	1:B:211:ARG:HE	1.70	0.56
1:A:28:ILE:HG23	1:A:44:ILE:HG23	1.87	0.55
1:B:139:LEU:HB3	1:B:165:ARG:HH22	1.72	0.55
1:B:16:LYS:HA	1:B:19:GLU:HG3	1.89	0.54
1:A:11:LYS:HE3	1:A:65:ALA:HB3	1.88	0.54
1:A:45:LEU:HD22	1:A:104:VAL:HG13	1.89	0.53
1:A:318:LEU:O	1:A:322:THR:OG1	2.23	0.53
1:A:216:ILE:HG12	1:A:293:ILE:HD11	1.90	0.53
1:A:209:LEU:HD11	1:A:289:TRP:CD1	2.44	0.53
1:A:51:ILE:O	1:A:55:ARG:HG3	2.08	0.53
1:B:132:LEU:O	1:B:136:SER:OG	2.27	0.53
1:A:185:GLU:HA	1:A:188:LYS:HE3	1.91	0.52
1:B:29:GLU:HA	1:B:32:LYS:HB3	1.90	0.52
1:B:319:LYS:HG3	1:B:374:LEU:HD13	1.92	0.52
1:A:49:LEU:HD23	1:A:134:ILE:HD12	1.90	0.52
1:A:171:GLU:CD	1:A:174:ARG:HH21	2.13	0.52
1:B:28:ILE:HD13	1:B:48:GLN:HG2	1.92	0.52
1:A:112:LYS:HG2	1:A:124:ILE:HG21	1.91	0.52
1:A:86:GLU:HB2	1:A:89:ARG:HH21	1.75	0.52
1:B:7:LEU:HD11	1:B:68:LEU:HD23	1.91	0.51
1:B:70:ARG:O	1:B:74:THR:OG1	2.27	0.51
1:B:18:ARG:O	1:B:22:GLU:HG2	2.10	0.51
1:A:159:LEU:HA	1:A:162:GLU:HG3	1.92	0.51
1:B:171:GLU:HA	1:B:174:ARG:HG2	1.92	0.51
1:B:108:ILE:HD12	1:B:131:ILE:HD11	1.93	0.50
1:A:139:LEU:HD12	1:A:170:GLN:OE1	2.12	0.50
1:A:239:LEU:HD13	1:A:300:LEU:HD13	1.92	0.50
1:B:312:ARG:HA	1:B:315:LEU:HB2	1.93	0.50
1:B:132:LEU:HD21	1:B:176:GLU:HB3	1.94	0.50
1:B:277:LEU:HD21	1:B:332:VAL:HG13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:LYS:HE2	1:A:218:ARG:HE	1.76	0.50
1:B:38:GLU:N	1:B:38:GLU:OE1	2.45	0.50
1:B:326:ARG:HB2	1:B:367:ILE:HG21	1.94	0.50
1:B:80:ASP:O	1:B:84:GLU:HG2	2.12	0.49
1:B:132:LEU:HA	1:B:135:ARG:HD3	1.92	0.49
1:A:212:LEU:HD12	1:A:215:LEU:HD12	1.94	0.49
1:B:65:ALA:HB1	1:B:69:GLN:HE22	1.77	0.49
1:B:185:GLU:HA	1:B:188:LYS:HB3	1.94	0.49
1:A:54:LEU:HD21	1:A:359:TRP:HB2	1.95	0.49
1:B:169:GLU:O	1:B:173:ILE:HG13	2.13	0.49
1:B:212:LEU:HD21	1:B:289:TRP:HB2	1.95	0.49
1:A:201:LEU:HD23	1:A:256:VAL:HG22	1.94	0.48
1:A:135:ARG:HH22	1:A:172:LYS:CG	2.24	0.48
1:A:103:GLU:N	1:A:103:GLU:OE1	2.46	0.48
1:A:146:SER:HA	1:A:149:GLN:HG3	1.94	0.48
1:B:93:GLU:O	1:B:97:LEU:HG	2.14	0.48
1:B:255:GLU:HA	1:B:258:LYS:HE2	1.96	0.48
1:B:288:LEU:O	1:B:292:ILE:HG12	2.14	0.48
1:A:178:GLU:HA	1:A:181:LYS:HB3	1.96	0.48
1:B:62:ARG:HD2	1:B:90:LEU:HD22	1.95	0.47
1:A:128:GLN:O	1:A:132:LEU:HG	2.14	0.47
1:A:212:LEU:HA	1:A:215:LEU:HD12	1.96	0.47
1:B:70:ARG:NH2	1:B:71:GLU:HB2	2.29	0.47
1:B:28:ILE:HG23	1:B:44:ILE:HG23	1.95	0.47
1:B:65:ALA:O	1:B:69:GLN:NE2	2.48	0.47
1:B:245:GLU:O	1:B:249:ILE:HG12	2.15	0.47
1:B:294:ARG:HB3	1:B:318:LEU:HD21	1.96	0.47
1:A:44:ILE:O	1:A:48:GLN:HG3	2.14	0.47
1:A:131:ILE:O	1:A:135:ARG:HG3	2.14	0.47
1:A:178:GLU:O	1:A:182:LYS:HG3	2.14	0.47
1:A:248:LYS:NZ	1:B:19:GLU:HA	2.30	0.47
1:B:366:ILE:O	1:B:370:LEU:N	2.47	0.47
1:B:169:GLU:HA	1:B:172:LYS:HG2	1.97	0.47
1:A:18:ARG:HH11	1:A:55:ARG:NH2	2.12	0.47
1:A:176:GLU:HA	1:A:179:GLU:HB2	1.97	0.47
1:B:29:GLU:H	1:B:29:GLU:HG2	1.43	0.46
1:B:356:GLU:O	1:B:360:ILE:HG12	2.15	0.46
1:A:66:LEU:HD21	1:A:86:GLU:HG2	1.96	0.46
1:B:272:LEU:HD23	1:B:272:LEU:H	1.81	0.46
1:A:91:LYS:O	1:A:95:GLU:HG2	2.16	0.46
1:B:63:ALA:HB1	1:B:144:LEU:HD21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:LYS:CE	1:B:19:GLU:HA	2.46	0.46
1:B:92:LYS:O	1:B:96:LYS:HG3	2.16	0.46
1:A:171:GLU:HB3	1:A:174:ARG:NH2	2.31	0.46
1:B:80:ASP:HA	1:B:83:ARG:HE	1.81	0.45
1:B:314:GLU:HA	1:B:317:ARG:HD3	1.98	0.45
1:B:321:GLU:HA	1:B:324:LYS:HG2	1.98	0.45
1:B:215:LEU:HD22	1:B:242:LEU:HD12	1.98	0.45
1:A:128:GLN:HE21	1:A:180:VAL:HG22	1.82	0.45
1:B:73:LEU:O	1:B:79:VAL:HG11	2.16	0.45
1:A:311:LEU:O	1:A:315:LEU:HB2	2.17	0.45
1:B:316:LYS:HB3	1:B:320:LYS:NZ	2.32	0.45
1:A:321:GLU:HA	1:A:324:LYS:HD2	1.99	0.45
1:B:282:ILE:O	1:B:286:VAL:HG23	2.16	0.45
1:A:97:LEU:HB3	1:A:138:TYR:OH	2.17	0.45
1:A:240:LYS:O	1:A:244:LYS:HG3	2.16	0.45
1:B:187:SER:HA	1:B:190:ARG:HD3	1.98	0.45
1:B:68:LEU:HD13	1:B:373:GLN:HG2	1.98	0.45
1:B:165:ARG:HA	1:B:168:LYS:HE3	1.98	0.45
1:B:216:ILE:HG12	1:B:293:ILE:HD11	1.98	0.45
1:A:265:LYS:HB2	1:A:266:ARG:HH21	1.82	0.45
1:B:298:LEU:HD13	1:B:298:LEU:HA	1.81	0.44
1:B:30:GLU:OE2	1:B:34:ARG:NH2	2.50	0.44
1:B:293:ILE:H	1:B:293:ILE:HG13	1.60	0.44
1:B:257:ASN:HA	1:B:260:ILE:HB	2.00	0.44
1:A:349:ILE:O	1:A:353:LEU:HG	2.16	0.44
1:B:160:LYS:O	1:B:164:LYS:NZ	2.40	0.44
1:A:14:GLN:OE1	1:A:61:SER:OG	2.34	0.44
1:A:300:LEU:HB3	1:A:301:GLN:OE1	2.18	0.44
1:A:165:ARG:O	1:A:169:GLU:HG2	2.18	0.43
1:B:216:ILE:HG12	1:B:293:ILE:CD1	2.47	0.43
1:B:327:GLU:O	1:B:331:GLU:HG2	2.18	0.43
1:A:76:THR:HG22	1:A:78:GLU:N	2.30	0.43
1:A:78:GLU:O	1:A:82:ARG:HB2	2.17	0.43
1:B:21:ILE:HG21	1:B:55:ARG:HH11	1.84	0.43
1:B:160:LYS:N	1:B:161:GLN:OE1	2.52	0.43
1:B:260:ILE:HG21	1:B:280:GLN:HG2	2.00	0.43
1:A:239:LEU:HA	1:A:242:LEU:HD12	2.01	0.43
1:A:257:ASN:OD1	1:A:283:SER:OG	2.18	0.43
1:B:291:LEU:O	1:B:295:ILE:HG13	2.19	0.43
1:A:80:ASP:OD1	1:A:83:ARG:NH1	2.52	0.43
1:A:124:ILE:O	1:A:128:GLN:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:ASP:O	1:B:312:ARG:HG2	2.19	0.43
1:B:350:ILE:H	1:B:350:ILE:HG12	1.52	0.43
1:A:63:ALA:HA	1:A:66:LEU:HD12	2.00	0.42
1:B:295:ILE:HG13	1:B:295:ILE:H	1.66	0.42
1:A:204:GLN:HA	1:A:207:ILE:HD12	2.01	0.42
1:B:297:GLN:HE21	1:B:297:GLN:HB2	1.70	0.42
1:A:68:LEU:HD11	1:A:373:GLN:HA	2.01	0.42
1:A:359:TRP:CZ2	1:A:363:LEU:HD13	2.54	0.42
1:B:208:SER:OG	1:B:253:GLN:OE1	2.32	0.42
1:B:99:GLU:O	1:B:103:GLU:HG2	2.20	0.42
1:B:202:MET:HE3	1:B:202:MET:HB2	1.88	0.42
1:B:355:LEU:O	1:B:359:TRP:N	2.44	0.42
1:A:57:LYS:HD3	1:A:57:LYS:HA	1.72	0.42
1:B:13:GLU:O	1:B:17:ILE:N	2.40	0.42
1:B:202:MET:HG3	1:B:282:ILE:HD13	2.01	0.42
1:B:12:LYS:O	1:B:16:LYS:HG2	2.18	0.42
1:B:322:THR:HG21	1:B:371:LYS:HB3	2.01	0.42
1:A:363:LEU:O	1:A:367:ILE:HG12	2.20	0.42
1:B:86:GLU:O	1:B:90:LEU:HG	2.19	0.42
1:A:166:SER:O	1:A:170:GLN:HB2	2.20	0.42
1:A:215:LEU:HB3	1:A:242:LEU:HD23	2.01	0.42
1:B:7:LEU:O	1:B:11:LYS:HG2	2.20	0.42
1:A:4:GLU:HB2	1:A:8:LYS:HE3	2.02	0.42
1:A:272:LEU:O	1:A:272:LEU:HD13	2.19	0.42
1:A:362:SER:O	1:A:365:SER:OG	2.35	0.42
1:B:316:LYS:HA	1:B:319:LYS:HZ2	1.83	0.42
1:A:257:ASN:O	1:A:261:GLU:HG3	2.19	0.42
1:A:42:ASN:HA	1:A:45:LEU:HD12	2.01	0.41
1:B:139:LEU:H	1:B:139:LEU:HG	1.47	0.41
1:A:196:ALA:O	1:A:200:ILE:HG12	2.20	0.41
1:A:248:LYS:HE2	1:A:248:LYS:HB2	1.40	0.41
1:A:361:ARG:H	1:A:361:ARG:HG3	1.70	0.41
1:B:11:LYS:HA	1:B:11:LYS:HD3	1.89	0.41
1:A:252:GLU:H	1:A:252:GLU:HG3	1.73	0.41
1:A:282:ILE:O	1:A:286:VAL:HG23	2.20	0.41
1:A:285:MET:HG2	1:A:359:TRP:HZ2	1.85	0.41
1:B:171:GLU:O	1:B:174:ARG:HG2	2.20	0.41
1:A:208:SER:HA	1:A:211:ARG:HE	1.85	0.41
1:A:86:GLU:HG3	1:A:90:LEU:HG	2.02	0.41
1:B:143:ASN:OD1	1:B:221:ASN:ND2	2.54	0.41
1:B:149:GLN:H	1:B:149:GLN:HG2	1.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:LEU:O	1:A:133:VAL:HG23	2.21	0.41
1:A:338:GLU:O	1:A:340:LYS:N	2.40	0.41
1:A:46:SER:OG	1:A:127:ASN:ND2	2.49	0.41
1:A:323:GLU:OE2	1:A:371:LYS:HE3	2.21	0.41
1:A:366:ILE:H	1:A:366:ILE:HG13	1.70	0.41
1:A:144:LEU:O	1:A:148:LEU:HG	2.21	0.41
1:A:165:ARG:HG3	1:A:169:GLU:HG2	2.02	0.41
1:A:239:LEU:HD12	1:A:243:LYS:HE2	2.02	0.41
1:B:129:LEU:O	1:B:133:VAL:HG23	2.19	0.41
1:B:132:LEU:HA	1:B:132:LEU:HD23	1.90	0.41
1:B:314:GLU:H	1:B:314:GLU:HG2	1.42	0.41
1:A:94:LEU:HD23	1:A:94:LEU:HA	1.91	0.41
1:A:108:ILE:HD13	1:A:127:ASN:HB3	2.03	0.41
1:A:171:GLU:O	1:A:175:GLU:HG2	2.21	0.41
1:A:285:MET:HE3	1:A:285:MET:HB3	2.00	0.41
1:A:317:ARG:O	1:A:321:GLU:N	2.49	0.41
1:B:23:GLU:O	1:B:27:GLU:N	2.40	0.41
1:B:14:GLN:H	1:B:14:GLN:HG2	1.49	0.40
1:A:8:LYS:HB3	1:A:12:LYS:NZ	2.36	0.40
1:A:137:GLU:O	1:A:141:ILE:HG12	2.21	0.40
1:B:130:LEU:O	1:B:134:ILE:HG13	2.22	0.40
1:A:58:LEU:HB2	1:A:62:ARG:HH2	1.86	0.40
1:A:82:ARG:HA	1:A:85:GLN:CD	2.42	0.40
1:B:103:GLU:HG2	1:B:103:GLU:H	1.52	0.40
1:A:80:ASP:O	1:A:83:ARG:HB2	2.21	0.40
1:A:212:LEU:HD12	1:A:212:LEU:HA	1.91	0.40
1:A:281:LEU:HD22	1:A:359:TRP:CZ3	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	304/379 (80%)	288 (95%)	14 (5%)	2 (1%)	19	49
1	B	305/379 (80%)	284 (93%)	19 (6%)	2 (1%)	19	49
All	All	609/758 (80%)	572 (94%)	33 (5%)	4 (1%)	19	49

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	300	LEU
1	B	339	SER
1	A	99	GLU
1	B	162	GLU

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	314/366 (86%)	266 (85%)	48 (15%)	2	10
1	B	314/366 (86%)	273 (87%)	41 (13%)	3	15
All	All	628/732 (86%)	539 (86%)	89 (14%)	2	13

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	9	ARG
1	A	18	ARG
1	A	20	GLU
1	A	27	GLU
1	A	30	GLU
1	A	42	ASN
1	A	49	LEU
1	A	51	ILE
1	A	52	SER
1	A	59	LEU
1	A	69	GLN

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Mol	Chain	Res	Type
1	A	70	ARG
1	A	71	GLU
1	A	79	VAL
1	A	91	LYS
1	A	97	LEU
1	A	100	GLU
1	A	114	ARG
1	A	118	GLU
1	A	136	SER
1	A	139	LEU
1	A	144	LEU
1	A	161	GLN
1	A	163	GLN
1	A	176	GLU
1	A	179	GLU
1	A	187	SER
1	A	195	SER
1	A	216	ILE
1	A	237	GLN
1	A	239	LEU
1	A	241	ARG
1	A	248	LYS
1	A	251	GLU
1	A	254	GLU
1	A	259	GLU
1	A	264	LYS
1	A	266	ARG
1	A	290	GLU
1	A	311	LEU
1	A	312	ARG
1	A	317	ARG
1	A	322	THR
1	A	334	LYS
1	A	348	GLU
1	A	349	ILE
1	A	351	LEU
1	B	14	GLN
1	B	20	GLU
1	B	29	GLU
1	B	31	SER
1	B	46	SER
1	B	50	PHE

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Mol	Chain	Res	Type
1	B	52	SER
1	B	79	VAL
1	B	82	ARG
1	B	92	LYS
1	B	103	GLU
1	B	105	LYS
1	B	121	LYS
1	B	136	SER
1	B	138	TYR
1	B	139	LEU
1	B	144	LEU
1	B	149	GLN
1	B	163	GLN
1	B	212	LEU
1	B	215	LEU
1	B	218	ARG
1	B	224	LEU
1	B	241	ARG
1	B	259	GLU
1	B	272	LEU
1	B	273	LYS
1	B	277	LEU
1	B	278	LEU
1	B	290	GLU
1	B	297	GLN
1	B	300	LEU
1	B	313	GLU
1	B	314	GLU
1	B	315	LEU
1	B	320	LYS
1	B	321	GLU
1	B	326	ARG
1	B	337	GLU
1	B	349	ILE
1	B	350	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	127	ASN
1	A	274	ASN
1	A	280	GLN

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Mol	Chain	Res	Type
1	B	69	GLN
1	B	297	GLN
1	B	373	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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	324/379 (85%)	-0.95	0 100 100	76, 137, 199, 255	0
1	B	323/379 (85%)	-0.96	1 (0%) 90 85	104, 153, 201, 257	0
All	All	647/758 (85%)	-0.95	1 (0%) 92 88	76, 146, 201, 257	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	318	LEU	2.6

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.