



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:37 PM UTC

PDB ID : 2Y4T / pdb_00002y4t
Title : Crystal structure of the human co-chaperone P58(IPK)
Authors : Svard, M.; Biterova, E.I.; Bourhis, J.-M.; Guy, J.E.
Deposited on : 2011-01-10
Resolution : 3.00 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

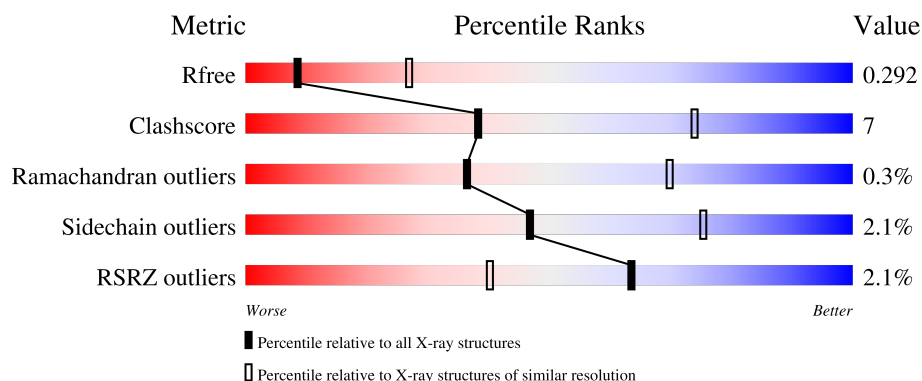
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	450	0% 71% 21% 6%
1	B	450	2% 80% 13% 6%
1	C	450	3% 81% 13% 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10259 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 DNAJ HOMOLOG SUBFAMILY C MEMBER 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	422	Total	C	N	O	S	0	0	0
			3414	2140	596	663	15			
1	B	421	Total	C	N	O	S	0	0	0
			3406	2135	595	662	14			
1	C	422	Total	C	N	O	S	0	0	0
			3414	2140	596	663	15			

There are 69 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	MET	-	expression tag	UNP Q13217
A	13	HIS	-	expression tag	UNP Q13217
A	14	HIS	-	expression tag	UNP Q13217
A	15	HIS	-	expression tag	UNP Q13217
A	16	HIS	-	expression tag	UNP Q13217
A	17	HIS	-	expression tag	UNP Q13217
A	18	HIS	-	expression tag	UNP Q13217
A	19	SER	-	expression tag	UNP Q13217
A	20	SER	-	expression tag	UNP Q13217
A	21	GLY	-	expression tag	UNP Q13217
A	22	VAL	-	expression tag	UNP Q13217
A	23	ASP	-	expression tag	UNP Q13217
A	24	LEU	-	expression tag	UNP Q13217
A	25	GLY	-	expression tag	UNP Q13217
A	26	THR	-	expression tag	UNP Q13217
A	27	GLU	-	expression tag	UNP Q13217
A	28	ASN	-	expression tag	UNP Q13217
A	29	LEU	-	expression tag	UNP Q13217
A	30	TYR	-	expression tag	UNP Q13217
A	31	PHE	-	expression tag	UNP Q13217
A	32	GLN	-	expression tag	UNP Q13217
A	33	SER	-	expression tag	UNP Q13217
A	34	MET	-	expression tag	UNP Q13217

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Chain	Residue	Modelled	Actual	Comment	Reference
B	12	MET	-	expression tag	UNP Q13217
B	13	HIS	-	expression tag	UNP Q13217
B	14	HIS	-	expression tag	UNP Q13217
B	15	HIS	-	expression tag	UNP Q13217
B	16	HIS	-	expression tag	UNP Q13217
B	17	HIS	-	expression tag	UNP Q13217
B	18	HIS	-	expression tag	UNP Q13217
B	19	SER	-	expression tag	UNP Q13217
B	20	SER	-	expression tag	UNP Q13217
B	21	GLY	-	expression tag	UNP Q13217
B	22	VAL	-	expression tag	UNP Q13217
B	23	ASP	-	expression tag	UNP Q13217
B	24	LEU	-	expression tag	UNP Q13217
B	25	GLY	-	expression tag	UNP Q13217
B	26	THR	-	expression tag	UNP Q13217
B	27	GLU	-	expression tag	UNP Q13217
B	28	ASN	-	expression tag	UNP Q13217
B	29	LEU	-	expression tag	UNP Q13217
B	30	TYR	-	expression tag	UNP Q13217
B	31	PHE	-	expression tag	UNP Q13217
B	32	GLN	-	expression tag	UNP Q13217
B	33	SER	-	expression tag	UNP Q13217
B	34	MET	-	expression tag	UNP Q13217
C	12	MET	-	expression tag	UNP Q13217
C	13	HIS	-	expression tag	UNP Q13217
C	14	HIS	-	expression tag	UNP Q13217
C	15	HIS	-	expression tag	UNP Q13217
C	16	HIS	-	expression tag	UNP Q13217
C	17	HIS	-	expression tag	UNP Q13217
C	18	HIS	-	expression tag	UNP Q13217
C	19	SER	-	expression tag	UNP Q13217
C	20	SER	-	expression tag	UNP Q13217
C	21	GLY	-	expression tag	UNP Q13217
C	22	VAL	-	expression tag	UNP Q13217
C	23	ASP	-	expression tag	UNP Q13217
C	24	LEU	-	expression tag	UNP Q13217
C	25	GLY	-	expression tag	UNP Q13217
C	26	THR	-	expression tag	UNP Q13217
C	27	GLU	-	expression tag	UNP Q13217
C	28	ASN	-	expression tag	UNP Q13217
C	29	LEU	-	expression tag	UNP Q13217
C	30	TYR	-	expression tag	UNP Q13217

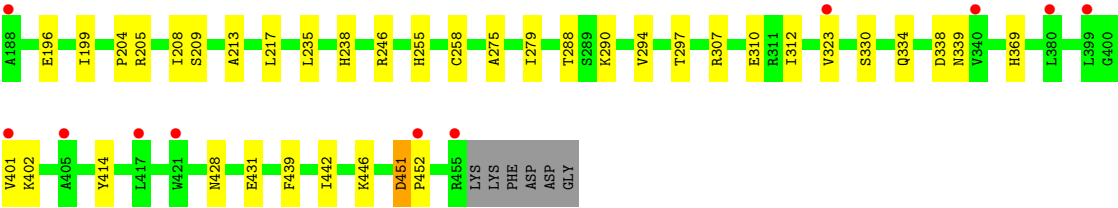
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Chain	Residue	Modelled	Actual	Comment	Reference
C	31	PHE	-	expression tag	UNP Q13217
C	32	GLN	-	expression tag	UNP Q13217
C	33	SER	-	expression tag	UNP Q13217
C	34	MET	-	expression tag	UNP Q13217

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	10	Total	O	0	0
			10	10		
2	B	8	Total	O	0	0
			8	8		
2	C	7	Total	O	0	0
			7	7		



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	212.25Å 212.25Å 283.46Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 3.00 25.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	96.5 (25.00-3.00) 84.5 (25.00-3.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.6.0081	Depositor
R, R_{free}	0.243 , 0.291 0.244 , 0.292	Depositor DCC
R_{free} test set	2119 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	73.9	Xtriage
Anisotropy	0.192	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 78.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10259	wwPDB-VP
Average B, all atoms (Å ²)	107.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 52.06 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.1367e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.63	0/3464	0.98	5/4644 (0.1%)
1	B	0.47	0/3456	0.91	0/4634
1	C	0.48	0/3464	0.91	0/4644
All	All	0.53	0/10384	0.93	5/13922 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	284	TYR	N-CA-C	6.13	118.04	111.36
1	A	321	LYS	CA-C-N	5.23	124.41	118.97
1	A	321	LYS	C-N-CA	5.23	124.41	118.97
1	A	203	GLU	CA-C-N	5.00	125.02	119.32
1	A	203	GLU	C-N-CA	5.00	125.02	119.32

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	3414	0	3419	70	0
1	B	3406	0	3410	39	0
1	C	3414	0	3419	34	0
2	A	10	0	0	0	0
2	B	8	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	7	0	0	0	0
All	All	10259	0	10248	141	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 7.

All (141) 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:B:451:ASP:HB3	1:B:452:PRO:HD2	1.30	1.09
1:A:451:ASP:HB2	1:A:452:PRO:CD	1.82	1.06
1:A:451:ASP:HB2	1:A:452:PRO:HD3	1.15	1.06
1:C:451:ASP:HB3	1:C:452:PRO:HD2	1.41	0.99
1:B:451:ASP:HB3	1:B:452:PRO:CD	1.99	0.93
1:A:118:GLN:OE1	1:A:120:LYS:NZ	2.09	0.86
1:A:451:ASP:CB	1:A:452:PRO:HD3	2.07	0.83
1:A:233:TYR:OH	1:A:298:GLU:HG2	1.78	0.83
1:B:267:LYS:HE2	1:B:297:THR:HG21	1.62	0.82
1:A:87:SER:HB2	1:A:186:TRP:CE3	2.15	0.82
1:A:451:ASP:CB	1:A:452:PRO:CD	2.58	0.82
1:A:306:VAL:HG13	1:A:335:MET:HE3	1.63	0.79
1:B:37:VAL:HG21	1:B:67:ASP:HB2	1.65	0.79
1:B:95:THR:HG22	1:B:111:ARG:HH11	1.47	0.78
1:C:451:ASP:HB3	1:C:452:PRO:CD	2.13	0.78
1:A:95:THR:HG22	1:A:111:ARG:HD2	1.64	0.77
1:C:307:ARG:NH1	1:C:310:GLU:OE1	2.17	0.76
1:A:98:ILE:HD11	1:A:108:ARG:HA	1.67	0.75
1:C:255:HIS:HD2	1:C:258:CYS:H	1.31	0.75
1:C:255:HIS:CD2	1:C:258:CYS:H	2.11	0.68
1:A:414:TYR:CG	1:A:446:LYS:HG3	2.30	0.67
1:A:233:TYR:OH	1:A:298:GLU:CG	2.44	0.66
1:A:113:HIS:HD2	1:A:147:GLN:OE1	1.79	0.66
1:C:93:ASP:O	1:C:97:VAL:HG23	1.96	0.65
1:B:267:LYS:HE2	1:B:297:THR:CG2	2.27	0.64
1:A:414:TYR:CD1	1:A:446:LYS:HG3	2.33	0.64
1:A:224:ALA:O	1:A:228:ILE:HG22	1.99	0.61
1:A:382:LYS:HG2	1:A:385:ARG:HH12	1.65	0.61
1:B:307:ARG:O	1:B:311:ARG:HG2	2.01	0.60
1:A:417:LEU:HB3	1:A:442:ILE:HD13	1.84	0.60
1:A:236:GLY:HA2	1:A:304:TYR:CZ	2.36	0.60
1:A:177:LEU:HD23	1:A:180:ILE:HD12	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:399:LEU:HD12	1:B:417:LEU:HD11	1.84	0.59
1:B:111:ARG:HG2	1:B:115:LEU:HD12	1.84	0.59
1:B:455:ARG:HH11	1:B:455:ARG:H	1.49	0.59
1:A:208:ILE:HD11	1:A:235:LEU:CD1	2.33	0.59
1:A:307:ARG:HH22	1:A:336:GLU:CD	2.11	0.59
1:A:407:LYS:HG3	1:A:408:GLN:H	1.68	0.58
1:C:330:SER:O	1:C:334:GLN:HG2	2.04	0.58
1:A:398:ILE:O	1:A:399:LEU:HB2	2.04	0.58
1:A:303:GLU:OE2	1:A:307:ARG:HD2	2.02	0.58
1:C:98:ILE:HD11	1:C:108:ARG:HA	1.86	0.57
1:A:255:HIS:CE1	1:A:258:CYS:SG	2.98	0.56
1:C:414:TYR:HB2	1:C:446:LYS:HD3	1.87	0.55
1:B:204:PRO:HB2	1:B:235:LEU:HD21	1.89	0.55
1:A:288:THR:HG23	1:A:312:ILE:HG12	1.89	0.54
1:B:250:LYS:HG2	2:B:2007:HOH:O	2.08	0.54
1:A:315:CYS:O	1:A:319:ASP:HB2	2.08	0.54
1:B:157:LEU:HB3	1:B:180:ILE:HG12	1.88	0.54
1:A:95:THR:HG22	1:A:111:ARG:CD	2.37	0.53
1:C:87:SER:HB2	1:C:186:TRP:CE3	2.43	0.53
1:C:178:ASP:O	1:C:182:GLU:HG2	2.08	0.53
1:C:204:PRO:HB2	1:C:235:LEU:HD21	1.89	0.53
1:A:307:ARG:NH2	1:A:336:GLU:OE1	2.32	0.53
1:B:356:TYR:HB2	1:B:387:LEU:HD23	1.91	0.53
1:B:261:HIS:O	1:B:265:VAL:HG23	2.09	0.53
1:A:398:ILE:O	1:A:398:ILE:HG22	2.09	0.53
1:A:394:ASP:HB3	1:A:397:LYS:HB2	1.91	0.52
1:C:428:ASN:HB3	1:C:431:GLU:HB2	1.91	0.52
1:A:231:LEU:O	1:A:235:LEU:HG	2.08	0.52
1:A:426:PHE:CE2	1:A:435:ALA:HB2	2.44	0.52
1:C:288:THR:HG23	1:C:312:ILE:HG12	1.92	0.52
1:A:177:LEU:HA	1:A:180:ILE:HD12	1.93	0.51
1:B:47:LEU:HD11	1:C:47:LEU:HD11	1.92	0.51
1:C:61:HIS:HA	1:C:77:ARG:HH11	1.76	0.51
1:C:439:PHE:O	1:C:442:ILE:HG13	2.12	0.50
1:A:57:LEU:HB2	1:A:80:VAL:HG11	1.93	0.50
1:A:364:GLU:HG3	1:A:380:LEU:HD11	1.94	0.50
1:A:208:ILE:HD11	1:A:235:LEU:HD12	1.94	0.49
1:A:128:PHE:CE2	1:A:147:GLN:HB3	2.47	0.49
1:A:360:ILE:HG13	1:A:361:GLN:N	2.28	0.49
1:B:128:PHE:CZ	1:B:147:GLN:HB3	2.48	0.49
1:C:294:VAL:O	1:C:297:THR:HG22	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:ILE:O	1:A:399:LEU:CB	2.60	0.49
1:B:276:GLU:O	1:B:279:ILE:HG13	2.13	0.49
1:A:34:MET:HG3	1:A:36:ASP:HB2	1.95	0.48
1:A:332:VAL:HA	1:A:335:MET:HE2	1.95	0.48
1:B:48:LEU:HD13	1:B:80:VAL:HG22	1.95	0.48
1:B:87:SER:HB2	1:B:186:TRP:CE3	2.49	0.48
1:A:426:PHE:CE2	1:A:435:ALA:CB	2.96	0.48
1:B:128:PHE:CE2	1:B:147:GLN:HB3	2.49	0.48
1:A:214:ALA:HA	1:A:217:LEU:HD12	1.96	0.48
1:A:402:LYS:C	1:A:404:ASN:N	2.72	0.48
1:A:295:MET:HG2	1:A:305:THR:HA	1.96	0.47
1:B:132:LEU:HA	1:B:136:PRO:HG3	1.95	0.47
1:A:195:ALA:HB1	1:A:207:ALA:HB1	1.96	0.47
1:A:357:ASP:O	1:A:360:ILE:HG13	2.15	0.47
1:B:94:LEU:HD13	1:B:111:ARG:HA	1.96	0.46
1:A:451:ASP:OD2	1:A:452:PRO:HD2	2.16	0.46
1:C:37:VAL:HG21	1:C:67:ASP:HB2	1.96	0.46
1:A:450:SER:C	1:A:451:ASP:CG	2.83	0.46
1:B:41:LEU:O	1:B:45:LYS:HG3	2.16	0.46
1:B:394:ASP:OD2	1:B:397:LYS:HG3	2.16	0.46
1:A:268:LEU:HD11	1:A:294:VAL:HG13	1.98	0.46
1:C:145:GLN:O	1:C:149:ILE:HG12	2.15	0.46
1:A:44:GLY:HA3	1:A:60:PHE:CE1	2.51	0.45
1:B:291:TYR:CZ	1:B:311:ARG:HG3	2.51	0.45
1:B:98:ILE:O	1:B:102:MET:HG3	2.17	0.45
1:B:253:GLN:NE2	1:C:246:ARG:HD3	2.32	0.45
1:A:202:GLY:C	1:A:204:PRO:HD3	2.42	0.45
1:C:338:ASP:HA	1:C:369:HIS:CE1	2.51	0.45
1:C:205:ARG:O	1:C:208:ILE:HG12	2.17	0.45
1:C:208:ILE:HG13	1:C:209:SER:N	2.31	0.45
1:B:372:ASN:HA	1:B:377:ARG:HH22	1.81	0.45
1:C:401:VAL:HG13	1:C:402:LYS:HG2	1.98	0.45
1:C:37:VAL:HG22	1:C:66:GLY:HA3	1.98	0.45
1:B:267:LYS:CE	1:B:297:THR:HG21	2.39	0.44
1:C:34:MET:HB3	1:C:36:ASP:OD1	2.17	0.44
1:B:360:ILE:HG13	1:B:361:GLN:N	2.32	0.44
1:A:262:TYR:CZ	1:A:266:LYS:HE2	2.52	0.44
1:A:422:HIS:HD2	1:A:439:PHE:CE2	2.36	0.44
1:A:54:ALA:HA	1:A:84:MET:HE1	1.99	0.43
1:B:74:TYR:CE1	1:B:96:LYS:HG2	2.53	0.43
1:A:292:GLU:HA	1:A:295:MET:HE3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:LYS:O	1:A:274:SER:HB3	2.18	0.43
1:C:451:ASP:CB	1:C:452:PRO:CD	2.90	0.43
1:B:358:GLU:OE1	1:B:358:GLU:N	2.52	0.43
1:B:349:ALA:HA	1:B:352:ILE:HD12	2.01	0.42
1:A:142:LYS:HD3	1:A:142:LYS:HA	1.89	0.42
1:B:351:LEU:HD13	1:B:382:LYS:HE3	2.01	0.42
1:A:306:VAL:HG13	1:A:335:MET:CE	2.42	0.42
1:B:295:MET:HG2	1:B:305:THR:HA	2.00	0.42
1:C:213:ALA:O	1:C:217:LEU:HG	2.19	0.42
1:C:275:ALA:HB2	1:C:290:LYS:HB3	2.02	0.42
1:C:238:HIS:CD2	1:C:238:HIS:H	2.38	0.41
1:A:360:ILE:HG13	1:A:361:GLN:H	1.85	0.41
1:A:402:LYS:C	1:A:404:ASN:H	2.27	0.41
1:C:196:GLU:O	1:C:199:ILE:HG13	2.20	0.41
1:A:153:GLU:HG3	1:A:156:ARG:HH21	1.85	0.41
1:A:255:HIS:ND1	1:A:258:CYS:HB2	2.35	0.41
1:A:234:GLN:HA	1:A:301:ILE:HD12	2.03	0.41
1:A:153:GLU:CG	1:A:156:ARG:NH2	2.84	0.41
1:C:307:ARG:HH12	1:C:339:ASN:ND2	2.19	0.41
1:A:303:GLU:OE2	1:A:307:ARG:CD	2.69	0.41
1:B:104:PHE:CE1	1:B:106:ALA:HB3	2.56	0.41
1:C:67:ASP:C	1:C:69:ASP:H	2.29	0.41
1:A:54:ALA:HA	1:A:84:MET:CE	2.50	0.40
1:A:180:ILE:H	1:A:180:ILE:HG13	1.69	0.40
1:B:307:ARG:HD3	1:B:307:ARG:HA	1.75	0.40
1:B:416:LYS:O	1:B:420:GLN:HB2	2.21	0.40
1:A:408:GLN:HA	1:A:411:ILE:HD13	2.04	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	420/450 (93%)	398 (95%)	20 (5%)	2 (0%)	24	60
1	B	419/450 (93%)	397 (95%)	21 (5%)	1 (0%)	43	76
1	C	420/450 (93%)	408 (97%)	11 (3%)	1 (0%)	43	76
All	All	1259/1350 (93%)	1203 (96%)	52 (4%)	4 (0%)	36	70

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	451	ASP
1	B	451	ASP
1	A	399	LEU
1	C	451	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	364/389 (94%)	349 (96%)	15 (4%)	27	61
1	B	363/389 (93%)	358 (99%)	5 (1%)	59	80
1	C	364/389 (94%)	361 (99%)	3 (1%)	73	86
All	All	1091/1167 (94%)	1068 (98%)	23 (2%)	47	75

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	95	THR
1	A	137	SER
1	A	148	LEU
1	A	155	GLN
1	A	209	SER
1	A	217	LEU
1	A	227	LYS
1	A	298	GLU
1	A	300	SER

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Mol	Chain	Res	Type
1	A	301	ILE
1	A	307	ARG
1	A	313	CYS
1	A	318	LYS
1	A	387	LEU
1	A	451	ASP
1	B	171	THR
1	B	265	VAL
1	B	307	ARG
1	B	313	CYS
1	B	398	ILE
1	C	48	LEU
1	C	279	ILE
1	C	323	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	113	HIS
1	A	147	GLN
1	A	155	GLN
1	A	408	GLN
1	B	147	GLN
1	B	160	GLN
1	B	221	ASN
1	B	253	GLN
1	B	367	GLN
1	C	147	GLN
1	C	160	GLN
1	C	238	HIS
1	C	255	HIS
1	C	269	ASN
1	C	369	HIS
1	C	384	GLN
1	C	404	ASN

5.3.3 RNA ⓘ

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

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	422/450 (93%)	-0.20	6 (1%) 73 51	29, 60, 126, 180	0
1	B	421/450 (93%)	0.14	9 (2%) 63 40	84, 118, 169, 222	0
1	C	422/450 (93%)	0.12	12 (2%) 55 32	81, 120, 181, 220	0
All	All	1265/1350 (93%)	0.02	27 (2%) 63 40	29, 108, 169, 222	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	49	ALA	4.2
1	C	455	ARG	3.1
1	A	401	VAL	3.0
1	C	401	VAL	2.9
1	C	405	ALA	2.8
1	C	399	LEU	2.7
1	B	109	LEU	2.7
1	B	248	CYS	2.6
1	A	454	MET	2.6
1	C	421	TRP	2.5
1	B	401	VAL	2.4
1	C	452	PRO	2.4
1	A	380	LEU	2.3
1	B	399	LEU	2.3
1	B	149	ILE	2.2
1	A	452	PRO	2.2
1	C	147	GLN	2.2
1	C	323	VAL	2.2
1	C	188	ALA	2.1
1	C	340	VAL	2.1
1	B	398	ILE	2.1
1	A	367	GLN	2.1
1	C	380	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	144	ALA	2.1
1	A	71	TYR	2.0
1	C	417	LEU	2.0
1	B	279	ILE	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.