



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 11:28 pm GMT

PDB ID : 2Y4T
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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

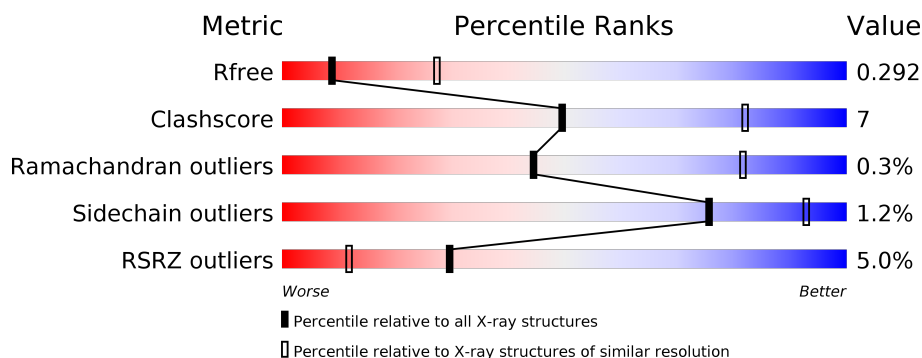
1 Overall quality at a glance

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}	100719	1692 (3.00-3.00)
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>73%</div> <div>20%</div> <div>6%</div> </div>
1	B	450	<div> <div>7%</div> <div>80%</div> <div>14%</div> <div>6%</div> </div>
1	C	450	<div> <div>7%</div> <div>82%</div> <div>12%</div> <div>6%</div> </div>

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

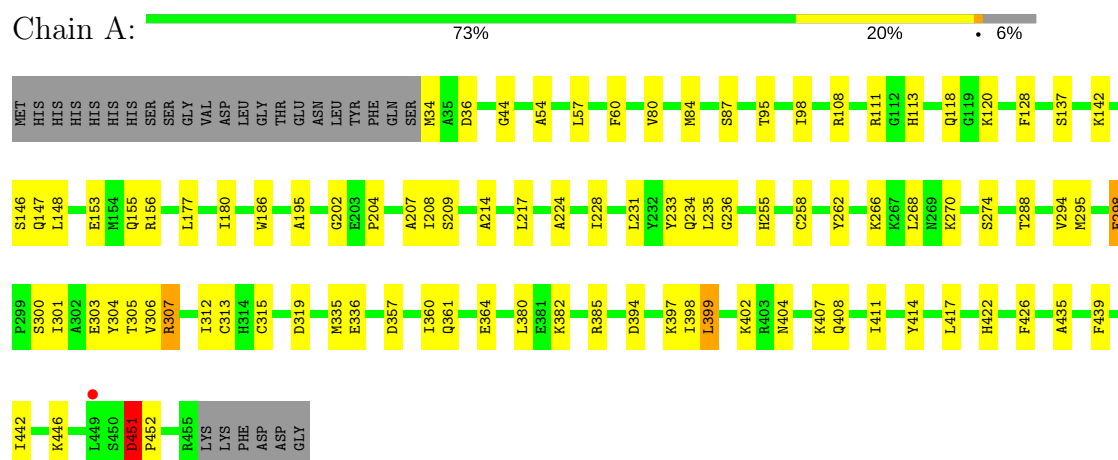
- Molecule 2 is water.

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

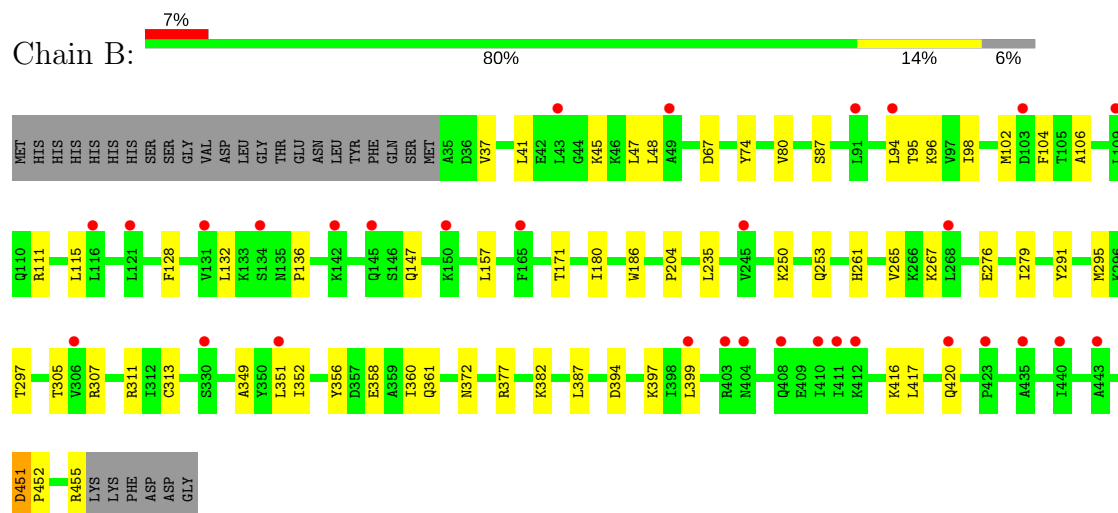
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

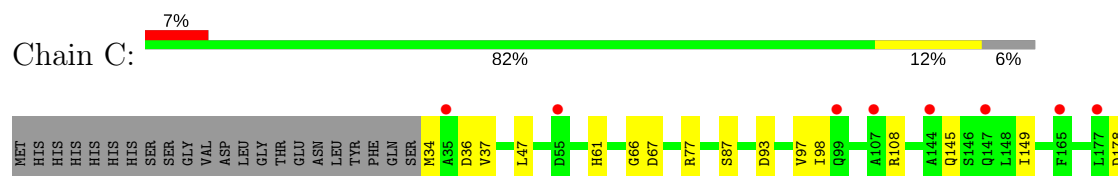
• Molecule 1: DNAJ HOMOLOG SUBFAMILY C MEMBER 3

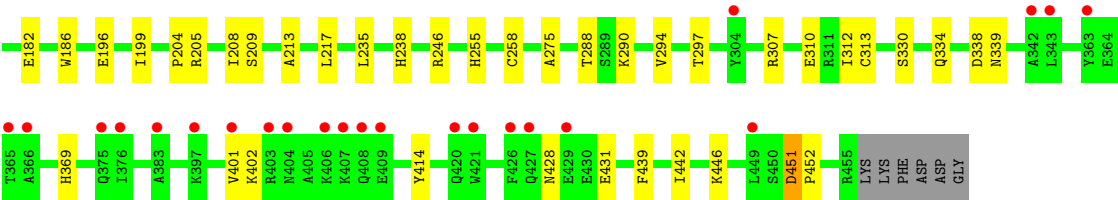


• Molecule 1: DNAJ HOMOLOG SUBFAMILY C MEMBER 3



• Molecule 1: DNAJ HOMOLOG SUBFAMILY C MEMBER 3





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 56.12 – 3.00	Depositor EDS
% Data completeness (in resolution range)	96.5 (25.00-3.00) 84.7 (56.12-3.00)	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	2118 reflections (5.35%)	DCC
Wilson B-factor (Å ²)	73.9	Xtriage
Anisotropy	0.192	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 74.0	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	0.52	0/3464	0.62	0/4644
1	B	0.36	0/3456	0.49	0/4634
1	C	0.36	0/3464	0.49	0/4644
All	All	0.42	0/10384	0.54	0/13922

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	3414	0	3419	67	0
1	B	3406	0	3410	39	0
1	C	3414	0	3419	33	0
2	A	10	0	0	0	0
2	B	8	0	0	1	0
2	C	7	0	0	0	0
All	All	10259	0	10248	137	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 (137) 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: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:A:233:TYR:HH	1:A:298:GLU:HG2	1.61	0.65
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
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:H	1:B:455:ARG:HH11	1.49	0.59
1:A:208:ILE:HD11	1:A:235:LEU:CD1	2.33	0.59
1:A:54:ALA:HA	1:A:84:MET:HE1	1.85	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:307:ARG:HH22	1:A:336:GLU:CD	2.11	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:178:ASP:O	1:C:182:GLU:HG2	2.08	0.53
1:C:87:SER:HB2	1:C:186:TRP:CE3	2.43	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:HG22	1:A:398:ILE:O	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
1:A:306:VAL:HG13	1:A:335:MET:CE	2.42	0.49
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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:394:ASP:OD2	1:B:397:LYS:HG3	2.16	0.46
1:B:41:LEU:O	1:B:45:LYS:HG3	2.16	0.46
1:A:268:LEU:HD11	1:A:294:VAL:HG13	1.98	0.46
1:A:306:VAL:HG13	1:A:335:MET:HE3	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: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:B:74:TYR:CE1	1:B:96:LYS:HG2	2.53	0.43
1:A:270:LYS:O	1:A:274:SER:HB3	2.18	0.43
1:A:402:LYS:C	1:A:404:ASN:N	2.72	0.43
1:C:451:ASP:CB	1:C:452:PRO:CD	2.90	0.43
1:A:306:VAL:HA	1:A:335:MET:HE1	2.01	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:202:GLY:C	1:A:204:PRO:HD3	2.42	0.40
1:A:180:ILE:H	1:A:180:ILE:HG13	1.69	0.40
1:B:307:ARG:HA	1:B:307:ARG:HD3	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%)	32	74
1	B	419/450 (93%)	397 (95%)	21 (5%)	1 (0%)	51	86
1	C	420/450 (93%)	408 (97%)	11 (3%)	1 (0%)	51	86
All	All	1259/1350 (93%)	1203 (96%)	52 (4%)	4 (0%)	44	81

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%)	354 (97%)	10 (3%)	50	82
1	B	363/389 (93%)	361 (99%)	2 (1%)	89	96
1	C	364/389 (94%)	363 (100%)	1 (0%)	94	98
All	All	1091/1167 (94%)	1078 (99%)	13 (1%)	75	93

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	137	SER
1	A	146	SER
1	A	148	LEU
1	A	155	GLN
1	A	209	SER
1	A	298	GLU
1	A	300	SER
1	A	307	ARG
1	A	313	CYS
1	A	451	ASP
1	B	171	THR
1	B	313	CYS
1	C	313	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	113	HIS
1	A	155	GLN
1	A	163	ASN
1	A	408	GLN
1	A	425	ASN
1	B	59	GLN
1	B	113	HIS
1	B	253	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	269	ASN
1	B	367	GLN
1	C	145	GLN
1	C	147	GLN
1	C	255	HIS
1	C	369	HIS

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 carbohydrates 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%)	0.30	1 (0%) 94 85	29, 60, 126, 180	0
1	B	421/450 (93%)	0.44	31 (7%) 15 6	84, 118, 169, 222	0
1	C	422/450 (93%)	0.46	31 (7%) 16 6	81, 120, 181, 220	0
All	All	1265/1350 (93%)	0.40	63 (4%) 30 12	29, 108, 169, 222	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	404	ASN	6.7
1	C	406	LYS	6.2
1	C	421	TRP	6.2
1	C	426	PHE	6.2
1	C	401	VAL	5.2
1	B	103	ASP	4.7
1	C	407	LYS	4.3
1	C	409	GLU	4.0
1	C	375	GLN	3.9
1	C	147	GLN	3.7
1	B	109	LEU	3.7
1	C	376	ILE	3.6
1	C	449	LEU	3.6
1	B	91	LEU	3.5
1	C	427	GLN	3.4
1	C	403	ARG	3.4
1	C	397	LYS	3.3
1	C	35	ALA	3.2
1	B	49	ALA	3.2
1	B	440	ILE	3.2
1	B	116	LEU	3.1
1	B	142	LYS	3.1
1	B	134	SER	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	429	GLU	3.0
1	C	343	LEU	3.0
1	C	366	ALA	2.9
1	C	408	GLN	2.9
1	B	43	LEU	2.8
1	B	412	LYS	2.8
1	B	435	ALA	2.8
1	C	107	ALA	2.8
1	B	268	LEU	2.8
1	B	408	GLN	2.7
1	C	304	TYR	2.7
1	B	423	PRO	2.7
1	A	449	LEU	2.7
1	B	145	GLN	2.7
1	C	420	GLN	2.6
1	C	99	GLN	2.6
1	B	403	ARG	2.6
1	C	177	LEU	2.6
1	B	94	LEU	2.5
1	B	399	LEU	2.5
1	C	144	ALA	2.5
1	B	131	VAL	2.4
1	B	411	ILE	2.4
1	B	306	VAL	2.4
1	C	363	TYR	2.4
1	C	342	ALA	2.4
1	B	330	SER	2.3
1	C	404	ASN	2.3
1	C	383	ALA	2.3
1	B	245	VAL	2.3
1	B	410	ILE	2.2
1	C	165	PHE	2.2
1	B	443	ALA	2.2
1	B	420	GLN	2.2
1	B	121	LEU	2.1
1	B	150	LYS	2.1
1	C	365	THR	2.1
1	B	165	PHE	2.1
1	C	55	ASP	2.0
1	B	351	LEU	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 carbohydrates 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.