



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:42 PM UTC

PDB ID : 4JPO / pdb_00004jpo
Title : 5A resolution structure of Proteasome Assembly Chaperone Hsm3 in complex with a C-terminal fragment of Rpt1
Authors : Lovell, S.; Battaile, K.P.; Singh, R.; Roelofs, J.
Deposited on : 2013-03-19
Resolution : 5.00 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

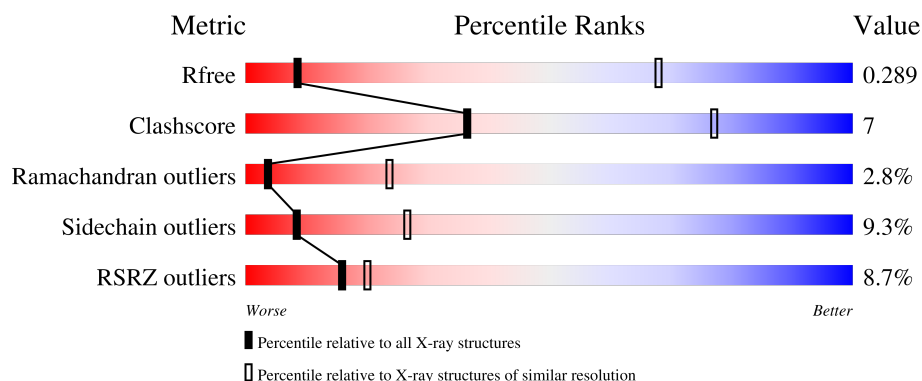
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 5.00 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	1009 (6.02-3.98)
Clashscore	190562	1040 (6.00-4.00)
Ramachandran outliers	187476	1015 (6.06-3.92)
Sidechain outliers	187428	1136 (6.10-3.90)
RSRZ outliers	180081	1004 (6.02-3.98)

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	491	 8% 69% 21% • 8%
1	B	491	 7% 65% 22% • • 9%
2	C	100	 9% 50% 21% • 26%
2	D	100	 7% 55% 16% • 26%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8391 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 DNA mismatch repair protein HSM3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	452	Total	C	N	O	S	0	0	0
			3629	2346	578	693	12			
1	B	447	Total	C	N	O	S	0	0	0
			3600	2327	573	688	12			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP P38348
A	2	PRO	-	expression tag	UNP P38348
A	3	LEU	-	expression tag	UNP P38348
A	4	THR	-	expression tag	UNP P38348
A	5	ARG	-	expression tag	UNP P38348
A	6	ARG	-	expression tag	UNP P38348
A	7	ALA	-	expression tag	UNP P38348
A	8	SER	-	expression tag	UNP P38348
A	9	VAL	-	expression tag	UNP P38348
A	10	GLY	-	expression tag	UNP P38348
A	11	SER	-	expression tag	UNP P38348
B	1	GLY	-	expression tag	UNP P38348
B	2	PRO	-	expression tag	UNP P38348
B	3	LEU	-	expression tag	UNP P38348
B	4	THR	-	expression tag	UNP P38348
B	5	ARG	-	expression tag	UNP P38348
B	6	ARG	-	expression tag	UNP P38348
B	7	ALA	-	expression tag	UNP P38348
B	8	SER	-	expression tag	UNP P38348
B	9	VAL	-	expression tag	UNP P38348
B	10	GLY	-	expression tag	UNP P38348
B	11	SER	-	expression tag	UNP P38348

- Molecule 2 is a protein called 26S protease regulatory subunit 7 homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	74	Total 584	C 365	N 112	O 103	S 4	0	0	0
2	D	74	Total 578	C 359	N 111	O 104	S 4	0	0	0

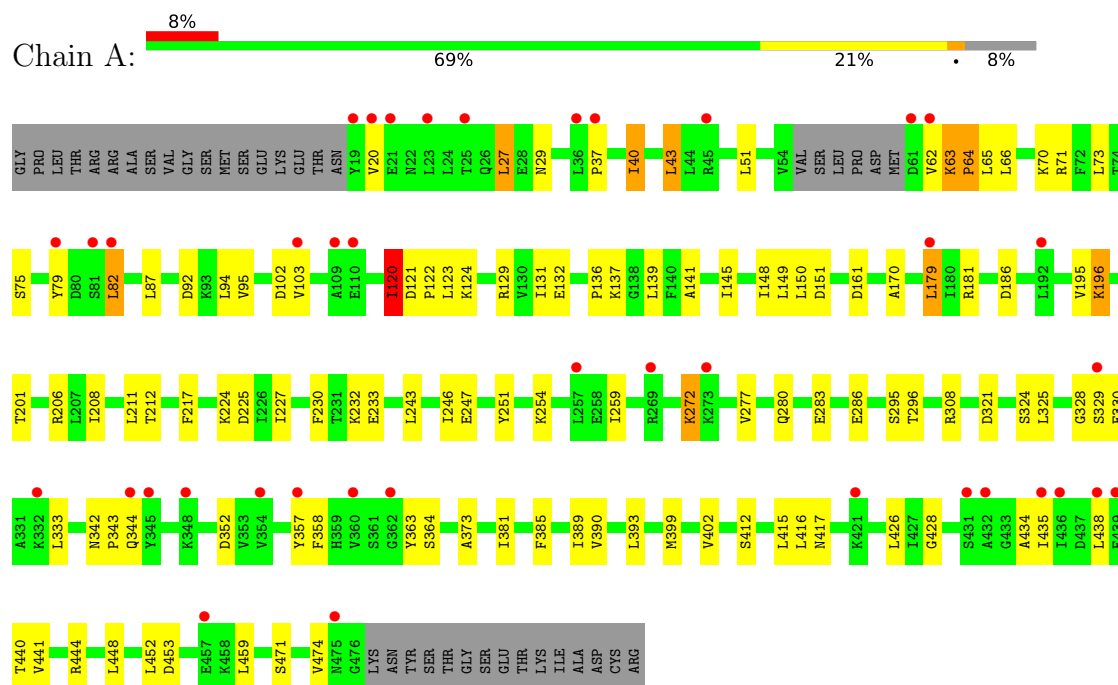
There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	368	MET	-	expression tag	UNP P33299
C	369	HIS	-	expression tag	UNP P33299
C	370	HIS	-	expression tag	UNP P33299
C	371	HIS	-	expression tag	UNP P33299
C	372	HIS	-	expression tag	UNP P33299
C	373	HIS	-	expression tag	UNP P33299
C	374	HIS	-	expression tag	UNP P33299
C	375	SER	-	expression tag	UNP P33299
C	376	GLN	-	expression tag	UNP P33299
C	377	HIS	-	expression tag	UNP P33299
C	378	MET	-	expression tag	UNP P33299
D	368	MET	-	expression tag	UNP P33299
D	369	HIS	-	expression tag	UNP P33299
D	370	HIS	-	expression tag	UNP P33299
D	371	HIS	-	expression tag	UNP P33299
D	372	HIS	-	expression tag	UNP P33299
D	373	HIS	-	expression tag	UNP P33299
D	374	HIS	-	expression tag	UNP P33299
D	375	SER	-	expression tag	UNP P33299
D	376	GLN	-	expression tag	UNP P33299
D	377	HIS	-	expression tag	UNP P33299
D	378	MET	-	expression tag	UNP P33299

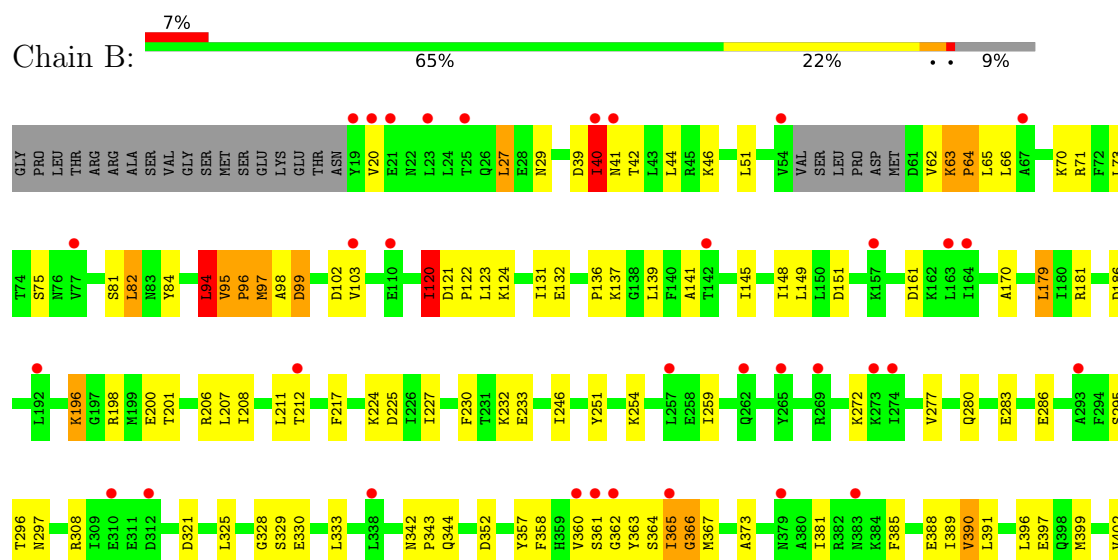
3 Residue-property plots

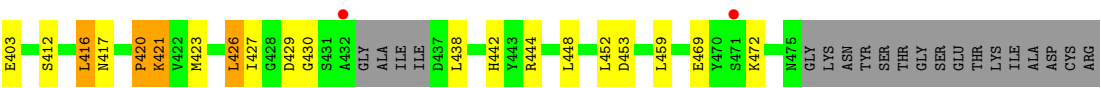
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: DNA mismatch repair protein HSM3



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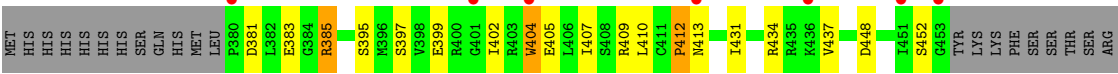




• Molecule 2: 26S protease regulatory subunit 7 homolog



• Molecule 2: 26S protease regulatory subunit 7 homolog



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	185.30Å 185.30Å 357.38Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.87 – 5.00 46.87 – 5.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.87-5.00) 99.7 (46.87-5.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.05 (at 5.10Å)	Xtriage
Refinement program	BUSTER-TNT, BUSTER 2.10.0	Depositor
R, R_{free}	0.253 , 0.273 0.267 , 0.289	Depositor DCC
R_{free} test set	829 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	300.2	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 269.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	8391	wwPDB-VP
Average B, all atoms (Å ²)	273.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% 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

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	0.78	0/3693	1.41	12/5012 (0.2%)
1	B	0.80	0/3663	1.44	22/4970 (0.4%)
2	C	0.68	0/591	1.40	0/788
2	D	0.76	0/585	1.39	1/781 (0.1%)
All	All	0.78	0/8532	1.42	35/11551 (0.3%)

There are no bond length outliers.

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	27	LEU	CA-C-N	6.45	129.25	120.54
1	B	27	LEU	C-N-CA	6.45	129.25	120.54
1	A	27	LEU	CA-C-N	6.41	129.20	120.54
1	A	27	LEU	C-N-CA	6.41	129.20	120.54
1	B	40	ILE	N-CA-C	-6.16	104.69	113.07
1	A	120	ILE	CA-C-N	5.63	127.13	120.09
1	A	120	ILE	C-N-CA	5.63	127.13	120.09
1	B	120	ILE	CA-C-N	5.61	127.11	120.09
1	B	120	ILE	C-N-CA	5.61	127.11	120.09
1	A	412	SER	CA-C-N	5.51	127.66	120.28
1	A	412	SER	C-N-CA	5.51	127.66	120.28
1	B	232	LYS	CA-C-N	5.43	127.49	120.44
1	B	232	LYS	C-N-CA	5.43	127.49	120.44
1	B	84	TYR	CA-C-N	5.38	127.81	120.54
1	B	84	TYR	C-N-CA	5.38	127.81	120.54
1	A	232	LYS	CA-C-N	5.36	127.46	120.28
1	A	232	LYS	C-N-CA	5.36	127.46	120.28
1	B	412	SER	CA-C-N	5.35	127.45	120.28
1	B	412	SER	C-N-CA	5.35	127.45	120.28
1	B	420	PRO	CA-C-N	5.28	127.36	120.28
1	B	420	PRO	C-N-CA	5.28	127.36	120.28
1	A	195	VAL	CA-C-N	5.26	127.27	120.44
1	A	195	VAL	C-N-CA	5.26	127.27	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	352	ASP	CA-C-N	5.25	127.18	120.56
1	A	352	ASP	C-N-CA	5.25	127.18	120.56
1	B	42	THR	CA-C-N	5.22	127.53	120.38
1	B	42	THR	C-N-CA	5.22	127.53	120.38
1	B	95	VAL	N-CA-CB	5.13	113.95	110.52
1	B	46	LYS	CA-C-N	5.09	127.35	120.38
1	B	46	LYS	C-N-CA	5.09	127.35	120.38
1	B	352	ASP	CA-C-N	5.06	126.93	120.56
1	B	352	ASP	C-N-CA	5.06	126.93	120.56
1	B	94	LEU	CA-C-N	5.05	125.28	120.43
1	B	94	LEU	C-N-CA	5.05	125.28	120.43
2	D	383	GLU	N-CA-C	-5.03	105.99	111.82

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	3629	0	3610	51	0
1	B	3600	0	3576	59	0
2	C	584	0	610	10	0
2	D	578	0	600	7	0
All	All	8391	0	8396	121	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 (121) 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:40:ILE:O	1:B:41:ASN:HB2	1.62	0.97
1:B:363:TYR:N	1:B:364:SER:HA	1.93	0.81
1:A:63:LYS:HD3	1:A:102:ASP:O	1.79	0.80
1:B:63:LYS:HD3	1:B:102:ASP:O	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:382:LEU:HA	2:C:385:ARG:HD3	1.67	0.74
1:B:399:MET:HE1	1:B:426:LEU:HA	1.77	0.67
1:B:211:LEU:HD21	1:B:227:ILE:HG13	1.84	0.60
1:B:388:GLU:HA	1:B:391:LEU:HD12	1.84	0.59
1:B:416:LEU:HA	1:B:423:MET:HG3	1.84	0.59
1:A:211:LEU:HD21	1:A:227:ILE:HG13	1.85	0.58
1:A:79:TYR:HB3	1:A:82:LEU:HB3	1.86	0.58
1:B:469:GLU:HA	1:B:472:LYS:HD3	1.85	0.57
1:B:308:ARG:HG3	1:B:342:ASN:HB2	1.86	0.56
1:A:308:ARG:HG3	1:A:342:ASN:HB2	1.87	0.56
1:B:198:ARG:HE	1:B:200:GLU:HB2	1.72	0.55
1:A:63:LYS:CG	1:A:102:ASP:HB3	2.37	0.55
2:D:385:ARG:HH11	2:D:412:PRO:HA	1.73	0.54
1:A:390:VAL:HA	1:A:393:LEU:HD12	1.88	0.54
1:B:208:ILE:HG23	1:B:251:TYR:HB2	1.88	0.54
1:A:206:ARG:HG2	2:C:409:ARG:HH11	1.72	0.54
1:A:208:ILE:HG23	1:A:251:TYR:HB2	1.88	0.54
1:A:399:MET:HE1	1:A:426:LEU:HA	1.89	0.54
1:A:444:ARG:O	1:A:448:LEU:HG	2.08	0.53
1:A:212:THR:HG21	1:A:254:LYS:HD3	1.91	0.53
1:A:321:ASP:HA	1:A:325:LEU:HB2	1.91	0.52
1:B:63:LYS:CG	1:B:102:ASP:HB3	2.39	0.52
1:A:92:ASP:HA	1:A:129:ARG:HD2	1.92	0.51
1:B:62:VAL:C	1:B:64:PRO:HD2	2.35	0.51
1:A:70:LYS:HA	1:A:73:LEU:HD12	1.93	0.51
1:B:63:LYS:N	1:B:64:PRO:CD	2.73	0.51
1:B:358:PHE:HD1	1:B:367:MET:HE3	1.75	0.51
1:B:206:ARG:HG2	2:D:409:ARG:HH11	1.74	0.51
1:A:63:LYS:N	1:A:64:PRO:CD	2.74	0.50
1:A:95:VAL:HG13	1:A:103:VAL:HG11	1.93	0.50
1:B:70:LYS:HA	1:B:73:LEU:HD12	1.93	0.50
1:B:364:SER:C	1:B:366:GLY:H	2.20	0.50
1:B:95:VAL:HG13	1:B:103:VAL:HG11	1.94	0.50
1:B:196:LYS:HG3	1:B:230:PHE:HE1	1.77	0.50
1:A:62:VAL:C	1:A:64:PRO:HD2	2.35	0.49
1:B:94:LEU:HA	1:B:97:MET:HE2	1.94	0.49
1:B:27:LEU:HD23	1:B:65:LEU:HD21	1.94	0.49
1:B:362:GLY:C	1:B:364:SER:HA	2.37	0.49
1:B:212:THR:HG21	1:B:254:LYS:HD3	1.93	0.49
1:A:27:LEU:HD23	1:A:65:LEU:HD21	1.94	0.49
1:A:145:ILE:HA	1:A:148:ILE:HD12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:PRO:HG2	1:B:65:LEU:H	1.79	0.48
1:B:321:ASP:HA	1:B:325:LEU:HB2	1.96	0.48
1:B:145:ILE:HA	1:B:148:ILE:HD12	1.96	0.48
1:A:64:PRO:HG2	1:A:65:LEU:H	1.79	0.47
1:B:444:ARG:O	1:B:448:LEU:HG	2.14	0.47
1:B:44:LEU:HB2	1:B:82:LEU:HD11	1.95	0.47
1:B:328:GLY:O	1:B:330:GLU:N	2.48	0.47
1:B:63:LYS:HA	1:B:66:LEU:HD12	1.96	0.47
1:B:40:ILE:O	1:B:41:ASN:CB	2.45	0.47
2:C:384:GLY:HA2	2:C:387:ASN:HB2	1.97	0.47
1:A:471:SER:HA	1:A:474:VAL:HG22	1.97	0.46
1:A:328:GLY:O	1:A:330:GLU:N	2.48	0.46
1:A:342:ASN:HD21	1:A:344:GLN:HB3	1.81	0.46
1:B:360:VAL:HG11	1:B:390:VAL:HG22	1.97	0.46
1:A:63:LYS:HA	1:A:66:LEU:HD12	1.98	0.46
1:B:402:VAL:HG11	1:B:426:LEU:HD13	1.98	0.46
2:C:405:GLU:O	2:C:409:ARG:HB2	2.16	0.46
1:A:243:LEU:HD12	2:C:444:LEU:HD11	1.98	0.46
1:A:452:LEU:HA	1:A:459:LEU:HD11	1.97	0.45
1:B:71:ARG:O	1:B:75:SER:HB2	2.16	0.45
1:B:73:LEU:HB3	1:B:123:LEU:HA	1.98	0.45
1:B:96:PRO:O	1:B:98:ALA:N	2.49	0.45
1:B:429:ASP:N	1:B:430:GLY:HA2	2.32	0.45
1:A:82:LEU:HD21	1:A:87:LEU:HD22	1.98	0.45
1:A:121:ASP:HA	1:A:124:LYS:HD3	1.97	0.45
1:B:136:PRO:HD2	1:B:139:LEU:HD13	1.98	0.45
1:A:73:LEU:HB3	1:A:123:LEU:HA	1.98	0.45
1:A:343:PRO:HG3	1:A:373:ALA:HB3	1.98	0.45
1:B:420:PRO:HD2	1:B:421:LYS:HD2	1.99	0.45
1:B:121:ASP:HA	1:B:124:LYS:HD3	1.98	0.45
1:B:63:LYS:HG2	1:B:102:ASP:HB3	1.98	0.45
2:D:405:GLU:O	2:D:409:ARG:HB2	2.16	0.45
1:A:37:PRO:O	1:A:40:ILE:HB	2.17	0.44
1:B:358:PHE:HD2	1:B:381:ILE:HG21	1.82	0.44
1:A:358:PHE:HE2	1:A:381:ILE:HD13	1.82	0.44
1:A:358:PHE:HD2	1:A:381:ILE:HG21	1.83	0.44
1:B:343:PRO:HG3	1:B:373:ALA:HB3	1.98	0.44
1:B:391:LEU:HD21	1:B:421:LYS:HB3	2.00	0.44
1:A:196:LYS:HG3	1:A:230:PHE:HE1	1.83	0.44
1:B:120:ILE:HG22	1:B:122:PRO:HD2	2.00	0.44
1:B:277:VAL:HA	1:B:280:GLN:HE21	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:ASN:HD21	1:B:344:GLN:HB3	1.82	0.44
2:C:397:SER:HB2	2:C:437:VAL:HG12	1.99	0.44
1:A:141:ALA:CB	1:A:179:LEU:HB3	2.48	0.44
1:A:277:VAL:HA	1:A:280:GLN:HE21	1.83	0.44
2:D:397:SER:HB2	2:D:437:VAL:HG12	1.98	0.44
1:A:181:ARG:HD3	1:A:217:PHE:HB2	2.00	0.43
1:B:131:ILE:HG21	1:B:149:LEU:HD11	1.99	0.43
1:A:40:ILE:HA	1:A:43:LEU:HD23	2.00	0.43
1:B:132:GLU:HA	1:B:170:ALA:HA	2.00	0.43
2:C:402:ILE:HG23	2:C:404:TRP:H	1.83	0.43
2:C:448:ASP:HA	2:C:452:SER:HB3	1.98	0.43
2:D:402:ILE:HG23	2:D:404:TRP:H	1.83	0.43
2:D:412:PRO:HB2	2:D:413:ASN:H	1.65	0.43
1:A:247:GLU:HG2	2:C:410:LEU:HG	2.00	0.43
1:B:181:ARG:HD3	1:B:217:PHE:HB2	2.00	0.43
1:A:120:ILE:HG22	1:A:122:PRO:HD2	1.99	0.43
1:A:132:GLU:HA	1:A:170:ALA:HA	2.00	0.43
1:B:246:ILE:HG12	1:B:295:SER:HB3	2.00	0.43
1:A:233:GLU:H	1:A:233:GLU:CD	2.27	0.43
1:A:246:ILE:HG12	1:A:295:SER:HB3	2.01	0.43
1:B:452:LEU:HA	1:B:459:LEU:HD11	2.00	0.43
1:B:358:PHE:HE2	1:B:381:ILE:HD13	1.82	0.43
1:A:136:PRO:HD2	1:A:139:LEU:HD13	1.99	0.43
1:A:71:ARG:O	1:A:75:SER:HB2	2.18	0.42
1:B:96:PRO:HB2	1:B:97:MET:H	1.74	0.42
1:B:41:ASN:O	1:B:82:LEU:HD23	2.19	0.42
1:B:233:GLU:H	1:B:233:GLU:CD	2.27	0.42
1:A:131:ILE:HG21	1:A:149:LEU:HD11	2.00	0.42
1:A:201:THR:HG21	2:C:403:ARG:HH22	1.85	0.41
1:B:141:ALA:CB	1:B:179:LEU:HB3	2.49	0.41
1:B:297:ASN:HB3	2:D:452:SER:HB2	2.01	0.41
1:A:131:ILE:HD13	1:A:149:LEU:HD11	2.03	0.41
1:A:358:PHE:HD1	1:A:364:SER:HB2	1.86	0.41
1:A:63:LYS:HG2	1:A:102:ASP:HB3	2.03	0.40
1:A:402:VAL:HG13	1:A:415:LEU:HD21	2.03	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	A	448/491 (91%)	395 (88%)	41 (9%)	12 (3%)	4	24
1	B	441/491 (90%)	395 (90%)	32 (7%)	14 (3%)	3	20
2	C	72/100 (72%)	64 (89%)	6 (8%)	2 (3%)	4	24
2	D	72/100 (72%)	63 (88%)	8 (11%)	1 (1%)	9	38
All	All	1033/1182 (87%)	917 (89%)	87 (8%)	29 (3%)	4	24

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	272	LYS
1	A	329	SER
1	B	97	MET
1	B	272	LYS
1	B	329	SER
1	B	365	ILE
1	A	64	PRO
1	A	357	TYR
1	A	440	THR
1	B	64	PRO
1	B	96	PRO
1	B	357	TYR
2	C	383	GLU
2	C	412	PRO
2	D	412	PRO
1	A	20	VAL
1	B	20	VAL
1	B	81	SER
1	B	99	ASP
1	A	438	LEU
1	B	201	THR
1	A	186	ASP

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Mol	Chain	Res	Type
1	A	225	ASP
1	A	363	TYR
1	A	434	ALA
1	B	186	ASP
1	B	225	ASP
1	B	366	GLY
1	A	428	GLY

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	402/453 (89%)	373 (93%)	29 (7%)	13	35
1	B	400/453 (88%)	363 (91%)	37 (9%)	8	26
2	C	62/88 (70%)	52 (84%)	10 (16%)	2	12
2	D	62/88 (70%)	52 (84%)	10 (16%)	2	12
All	All	926/1082 (86%)	840 (91%)	86 (9%)	8	26

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	A	40	ILE
1	A	43	LEU
1	A	51	LEU
1	A	63	LYS
1	A	82	LEU
1	A	94	LEU
1	A	120	ILE
1	A	137	LYS
1	A	150	LEU
1	A	151	ASP
1	A	161	ASP
1	A	179	LEU
1	A	196	LYS

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Mol	Chain	Res	Type
1	A	224	LYS
1	A	259	ILE
1	A	272	LYS
1	A	283	GLU
1	A	286	GLU
1	A	296	THR
1	A	324	SER
1	A	333	LEU
1	A	385	PHE
1	A	389	ILE
1	A	416	LEU
1	A	417	ASN
1	A	435	ILE
1	A	441	VAL
1	A	453	ASP
1	B	29	ASN
1	B	39	ASP
1	B	40	ILE
1	B	51	LEU
1	B	63	LYS
1	B	82	LEU
1	B	94	LEU
1	B	99	ASP
1	B	120	ILE
1	B	137	LYS
1	B	151	ASP
1	B	161	ASP
1	B	179	LEU
1	B	196	LYS
1	B	207	LEU
1	B	224	LYS
1	B	259	ILE
1	B	283	GLU
1	B	286	GLU
1	B	296	THR
1	B	333	LEU
1	B	361	SER
1	B	365	ILE
1	B	385	PHE
1	B	389	ILE
1	B	390	VAL
1	B	396	LEU

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Mol	Chain	Res	Type
1	B	397	GLU
1	B	403	GLU
1	B	416	LEU
1	B	417	ASN
1	B	421	LYS
1	B	426	LEU
1	B	427	ILE
1	B	438	LEU
1	B	442	HIS
1	B	453	ASP
2	C	395	SER
2	C	399	GLU
2	C	404	TRP
2	C	407	ILE
2	C	410	LEU
2	C	424	THR
2	C	428	MET
2	C	431	ILE
2	C	434	ARG
2	C	448	ASP
2	D	381	ASP
2	D	385	ARG
2	D	395	SER
2	D	399	GLU
2	D	404	TRP
2	D	407	ILE
2	D	410	LEU
2	D	431	ILE
2	D	434	ARG
2	D	448	ASP

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

Mol	Chain	Res	Type
1	A	50	ASN
1	A	135	GLN
1	A	216	GLN
1	A	261	ASN
1	A	280	GLN
1	A	301	GLN
1	A	342	ASN
1	A	344	GLN

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Mol	Chain	Res	Type
1	A	475	ASN
1	B	133	ASN
1	B	216	GLN
1	B	261	ASN
1	B	280	GLN
1	B	342	ASN

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 ⓘ

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	452/491 (92%)	0.64	39 (8%)	16 20	273, 273, 273, 273	0
1	B	447/491 (91%)	0.71	36 (8%)	18 22	273, 273, 273, 273	0
2	C	74/100 (74%)	0.76	9 (12%)	8 14	273, 273, 273, 273	0
2	D	74/100 (74%)	0.55	7 (9%)	14 19	273, 273, 273, 273	0
All	All	1047/1182 (88%)	0.67	91 (8%)	16 20	273, 273, 273, 273	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	21	GLU	4.7
1	A	20	VAL	4.5
1	B	21	GLU	4.3
1	A	19	TYR	4.2
2	C	450	VAL	4.1
1	B	273	LYS	4.0
1	B	310	GLU	3.9
2	D	380	PRO	3.9
1	B	432	ALA	3.9
1	B	40	ILE	3.9
1	A	438	LEU	3.8
1	A	81	SER	3.7
1	A	273	LYS	3.7
1	B	20	VAL	3.7
1	A	475	ASN	3.6
1	A	360	VAL	3.6
1	A	436	ILE	3.5
1	A	357	TYR	3.5
1	A	435	ILE	3.5
1	A	457	GLU	3.4
1	B	19	TYR	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	312	ASP	3.3
1	A	179	LEU	3.3
1	B	361	SER	3.1
1	B	338	LEU	3.1
2	D	436	LYS	3.1
1	A	25	THR	3.0
1	B	157	LYS	3.0
1	B	192	LEU	2.9
1	A	37	PRO	2.9
1	A	61	ASP	2.9
1	A	62	VAL	2.9
1	A	82	LEU	2.9
2	D	453	GLY	2.9
1	A	344	GLN	2.9
1	A	45	ARG	2.8
1	A	192	LEU	2.8
2	C	415	THR	2.8
2	C	441	LYS	2.8
2	C	455	LYS	2.8
1	A	36	LEU	2.8
1	B	360	VAL	2.7
2	C	425	GLU	2.7
1	A	362	GLY	2.7
2	C	404	TRP	2.6
1	A	109	ALA	2.6
1	B	212	THR	2.6
1	B	269	ARG	2.6
1	B	41	ASN	2.6
1	B	103	VAL	2.5
1	A	103	VAL	2.5
1	A	329	SER	2.4
1	A	23	LEU	2.4
1	B	23	LEU	2.4
1	B	293	ALA	2.4
1	B	471	SER	2.4
2	D	413	ASN	2.4
1	B	77	VAL	2.4
1	A	345	TYR	2.4
1	A	354	VAL	2.3
1	A	432	ALA	2.3
1	A	269	ARG	2.3
2	C	449	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	110	GLU	2.3
1	B	362	GLY	2.3
1	B	379	ASN	2.2
1	B	67	ALA	2.2
1	A	79	TYR	2.2
2	D	401	GLY	2.2
1	B	163	LEU	2.2
1	B	383	ASN	2.2
1	B	262	GLN	2.2
1	A	348	LYS	2.2
1	B	164	ILE	2.2
1	B	365	ILE	2.2
1	B	110	GLU	2.2
1	B	274	ILE	2.1
1	B	25	THR	2.1
1	B	265	TYR	2.1
1	B	257	LEU	2.1
1	A	257	LEU	2.1
1	A	431	SER	2.1
1	B	142	THR	2.1
2	C	386	ALA	2.1
2	C	424	THR	2.1
2	D	404	TRP	2.1
1	B	54	VAL	2.1
1	A	332	LYS	2.1
1	A	421	LYS	2.0
1	A	439	GLU	2.0
2	D	451	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.