



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:42 PM UTC

PDB ID : 4A3V / pdb_00004a3v
Title : yeast regulatory particle proteasome assembly chaperone Hsm3 in complex with Rpt1 C-terminal fragment
Authors : Richet, N.; Barrault, M.B.; Godart, C.; Murciano, B.; Le Tallec, B.; Rousseau, E.; Ledu, M.H.; Charbonnier, J.B.; Legrand, P.; Guerois, R.; Peyroche, A.; Ochsenbein, F.
Deposited on : 2011-10-04
Resolution : 3.80 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

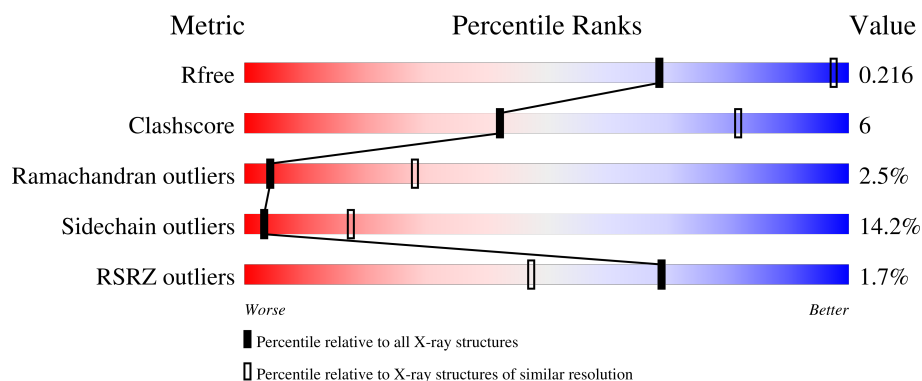
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)

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	496	4% 61% 25% 5% 8%
1	C	496	61% 26% .. 8%
2	B	95	64% 17% .. 17%
2	D	95	4% 62% 16% .. 19%
3	E	10	100%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 8722 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	455	Total	C	N	O	S	0	0	0
			3716	2396	594	713	13			
1	C	458	Total	C	N	O	S	0	0	0
			3735	2409	596	717	13			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP P38348
A	-3	ALA	-	expression tag	UNP P38348
A	-2	MET	-	expression tag	UNP P38348
A	-1	ALA	-	expression tag	UNP P38348
A	0	ASP	-	expression tag	UNP P38348
A	1	PRO	-	expression tag	UNP P38348
A	481	SER	-	expression tag	UNP P38348
A	482	GLY	-	expression tag	UNP P38348
A	483	SER	-	expression tag	UNP P38348
A	484	GLY	-	expression tag	UNP P38348
A	485	GLY	-	expression tag	UNP P38348
A	486	LEU	-	expression tag	UNP P38348
A	487	GLU	-	expression tag	UNP P38348
A	488	VAL	-	expression tag	UNP P38348
A	489	LEU	-	expression tag	UNP P38348
A	490	PHE	-	expression tag	UNP P38348
A	491	GLN	-	expression tag	UNP P38348
C	-4	GLY	-	expression tag	UNP P38348
C	-3	ALA	-	expression tag	UNP P38348
C	-2	MET	-	expression tag	UNP P38348
C	-1	ALA	-	expression tag	UNP P38348
C	0	ASP	-	expression tag	UNP P38348
C	1	PRO	-	expression tag	UNP P38348
C	481	SER	-	expression tag	UNP P38348
C	482	GLY	-	expression tag	UNP P38348

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Chain	Residue	Modelled	Actual	Comment	Reference
C	483	SER	-	expression tag	UNP P38348
C	484	GLY	-	expression tag	UNP P38348
C	485	GLY	-	expression tag	UNP P38348
C	486	LEU	-	expression tag	UNP P38348
C	487	GLU	-	expression tag	UNP P38348
C	488	VAL	-	expression tag	UNP P38348
C	489	LEU	-	expression tag	UNP P38348
C	490	PHE	-	expression tag	UNP P38348
C	491	GLN	-	expression tag	UNP P38348

- Molecule 2 is a protein called 26S PROTEASE REGULATORY SUBUNIT 7 HOMOLOG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	79	Total	C	N	O	S	0	0	0
			618	386	117	111	4			
2	D	77	Total	C	N	O	S	0	0	0
			603	377	114	108	4			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	373	GLY	-	expression tag	UNP P33299
B	374	PRO	-	expression tag	UNP P33299
B	375	GLY	-	expression tag	UNP P33299
B	376	GLY	-	expression tag	UNP P33299
B	377	SER	-	expression tag	UNP P33299
D	373	GLY	-	expression tag	UNP P33299
D	374	PRO	-	expression tag	UNP P33299
D	375	GLY	-	expression tag	UNP P33299
D	376	GLY	-	expression tag	UNP P33299
D	377	SER	-	expression tag	UNP P33299

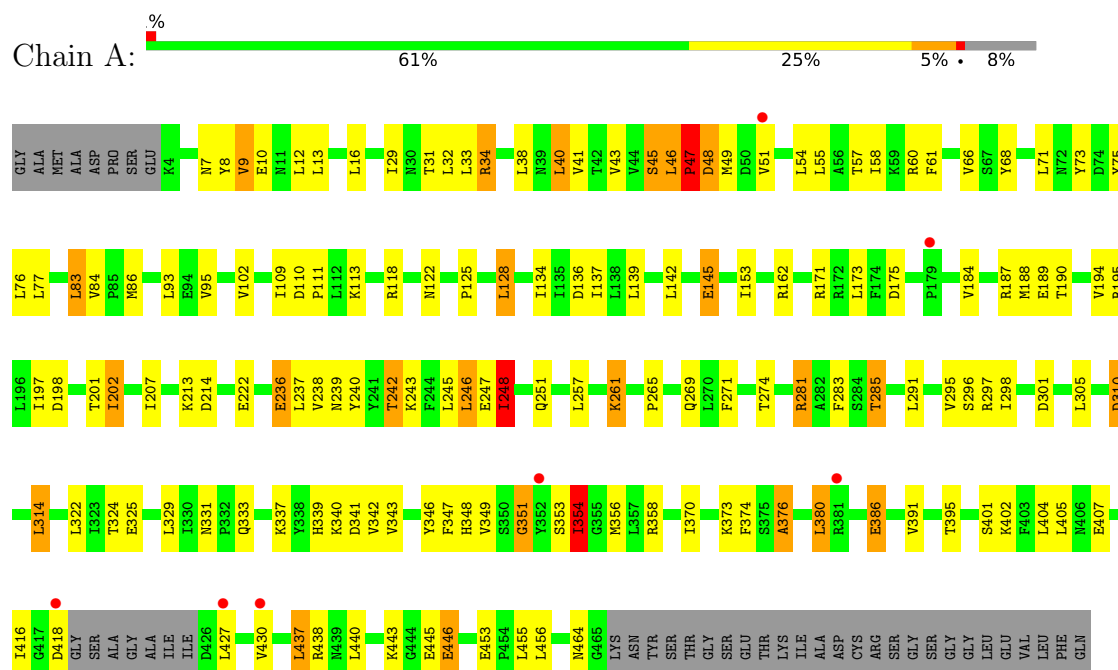
- Molecule 3 is a protein called LINKER.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	10	Total	C	N	O	0	0	0
			50	30	10	10			

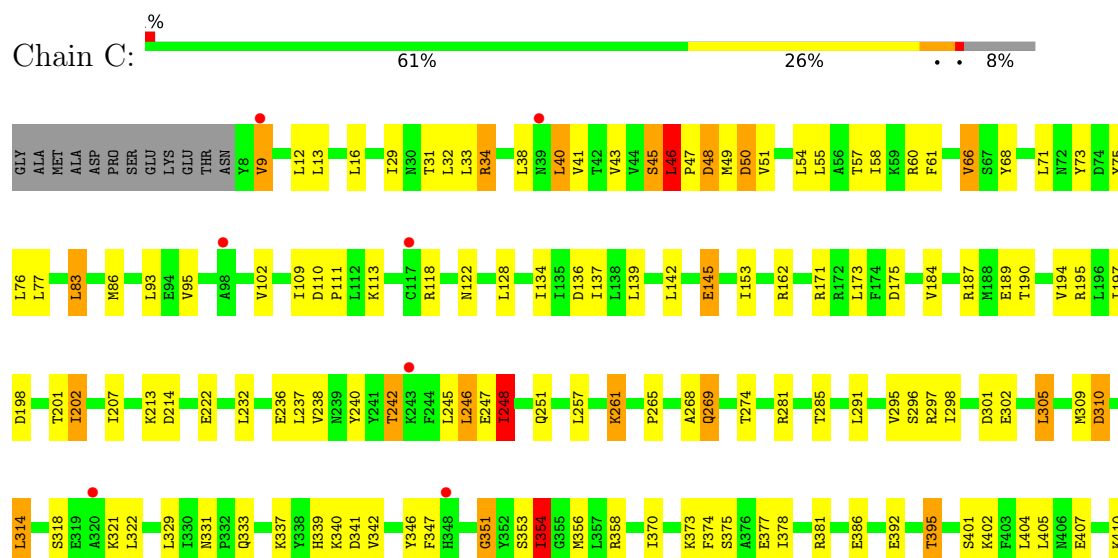
3 Residue-property plots [i](#)

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



• Molecule 1: DNA MISMATCH REPAIR PROTEIN HSM3





• Molecule 2: 26S PROTEASE REGULATORY SUBUNIT 7 HOMOLOG

Chain B: 64% 17% 17%



• Molecule 2: 26S PROTEASE REGULATORY SUBUNIT 7 HOMOLOG

Chain D: 4% 62% 16% 19%



• Molecule 3: LINKER

Chain E: 100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	186.66Å 186.66Å 373.77Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	58.35 – 3.80 58.35 – 3.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (58.35-3.80) 99.9 (58.35-3.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 3.77Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.190 , 0.208 (Not available) , 0.216	Depositor DCC
R_{free} test set	1933 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	179.6	Xtriage
Anisotropy	0.237	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 244.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8722	wwPDB-VP
Average B, all atoms (Å ²)	225.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% 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	0.82	1/3782 (0.0%)	1.54	37/5125 (0.7%)
1	C	0.82	1/3802 (0.0%)	1.55	31/5152 (0.6%)
2	B	0.82	0/626	1.48	3/837 (0.4%)
2	D	0.82	1/611 (0.2%)	1.43	2/818 (0.2%)
All	All	0.82	3/8821 (0.0%)	1.53	73/11932 (0.6%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	46	LEU	CA-C	6.02	1.60	1.52
2	D	428	MET	SD-CE	-5.91	1.64	1.79
1	A	84	VAL	CA-CB	5.60	1.56	1.54

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	48	ASP	CA-CB-CG	7.99	120.59	112.60
1	C	351	GLY	CA-C-N	7.93	130.75	120.44
1	C	351	GLY	C-N-CA	7.93	130.75	120.44
1	A	41	VAL	N-CA-C	-7.39	103.59	110.53
1	C	41	VAL	N-CA-C	-7.32	103.65	110.53
1	A	7	ASN	CA-C-N	7.08	135.06	121.54
1	A	7	ASN	C-N-CA	7.08	135.06	121.54
1	C	248	ILE	N-CA-C	-7.08	105.72	111.81
1	C	47	PRO	N-CA-C	7.04	122.99	113.84
1	A	7	ASN	N-CA-C	-6.75	102.54	111.24
2	B	440	GLU	N-CA-C	-6.60	104.16	111.82
1	C	310	ASP	CA-CB-CG	6.26	118.86	112.60
1	A	351	GLY	CA-C-N	6.22	128.53	120.44
1	A	351	GLY	C-N-CA	6.22	128.53	120.44
2	B	404	TRP	N-CA-C	6.17	118.81	111.71
1	A	213	LYS	CA-C-N	6.11	128.78	120.54
1	A	213	LYS	C-N-CA	6.11	128.78	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	242	THR	CA-C-N	6.07	128.32	120.44
1	A	242	THR	C-N-CA	6.07	128.32	120.44
1	C	214	ASP	CA-C-N	6.00	128.34	120.60
1	C	214	ASP	C-N-CA	6.00	128.34	120.60
1	A	248	ILE	N-CA-C	-5.96	106.01	111.67
1	C	213	LYS	CA-C-N	5.92	128.53	120.54
1	C	213	LYS	C-N-CA	5.92	128.53	120.54
1	A	310	ASP	CA-CB-CG	5.82	118.42	112.60
1	A	271	PHE	CA-C-N	5.81	128.00	120.44
1	A	271	PHE	C-N-CA	5.81	128.00	120.44
2	D	450	VAL	N-CA-C	5.80	116.45	110.82
1	C	269	GLN	CA-C-N	5.75	128.56	120.28
1	C	269	GLN	C-N-CA	5.75	128.56	120.28
2	D	440	GLU	N-CA-C	-5.70	105.21	111.82
1	C	274	THR	N-CA-C	-5.68	106.99	114.04
1	A	83	LEU	CA-C-N	5.67	125.87	120.43
1	A	83	LEU	C-N-CA	5.67	125.87	120.43
1	C	48	ASP	N-CA-C	5.58	122.69	110.80
1	A	47	PRO	N-CA-C	5.57	123.94	112.47
1	A	48	ASP	N-CA-C	5.56	122.63	110.80
1	A	329	LEU	N-CA-C	5.48	120.22	112.93
1	C	374	PHE	N-CA-C	5.44	118.13	107.57
1	C	83	LEU	CA-C-N	5.42	125.63	120.43
1	C	83	LEU	C-N-CA	5.42	125.63	120.43
1	A	46	LEU	N-CA-C	5.41	121.77	109.81
1	C	346	TYR	N-CA-C	5.35	120.08	113.50
1	C	242	THR	CA-C-N	5.33	127.43	120.28
1	C	242	THR	C-N-CA	5.33	127.43	120.28
2	B	450	VAL	N-CA-C	5.31	115.97	110.82
1	C	102	VAL	CA-C-N	5.27	127.29	120.44
1	C	102	VAL	C-N-CA	5.27	127.29	120.44
1	A	407	GLU	N-CA-C	5.19	119.70	112.90
1	A	340	LYS	CA-C-N	5.19	127.50	120.65
1	A	340	LYS	C-N-CA	5.19	127.50	120.65
1	A	274	THR	N-CA-C	-5.18	107.62	114.04
1	A	102	VAL	CA-C-N	5.17	127.16	120.44
1	A	102	VAL	C-N-CA	5.17	127.16	120.44
1	A	445	GLU	CA-C-N	5.17	127.65	120.63
1	A	445	GLU	C-N-CA	5.17	127.65	120.63
1	C	445	GLU	CA-C-N	5.13	127.61	120.63
1	C	445	GLU	C-N-CA	5.13	127.61	120.63
1	A	346	TYR	N-CA-C	5.10	119.77	113.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	349	VAL	N-CA-C	5.09	114.52	106.32
1	C	340	LYS	CA-C-N	5.08	127.36	120.65
1	C	340	LYS	C-N-CA	5.08	127.36	120.65
1	C	318	SER	N-CA-C	-5.08	105.82	111.36
1	C	407	GLU	N-CA-C	5.08	119.55	112.90
1	A	376	ALA	N-CA-C	-5.06	105.95	111.82
1	A	238	VAL	N-CA-C	-5.05	105.05	110.36
1	C	329	LEU	N-CA-C	5.05	119.65	112.93
1	A	214	ASP	CA-C-N	5.03	127.62	120.53
1	A	214	ASP	C-N-CA	5.03	127.62	120.53
1	C	238	VAL	N-CA-C	-5.02	105.08	110.36
1	A	348	HIS	CA-C-N	-5.02	117.07	122.59
1	A	348	HIS	C-N-CA	-5.02	117.07	122.59
1	A	374	PHE	N-CA-C	5.00	117.28	107.57

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3716	0	3730	53	0
1	C	3735	0	3761	50	0
2	B	618	0	639	7	0
2	D	603	0	621	8	0
3	E	50	0	12	0	0
All	All	8722	0	8763	110	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 6.

All (110) 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:C:395:THR:HG21	1:C:436:ALA:HA	1.37	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:SER:O	1:A:331:ASN:HB2	1.71	0.91
1:C:296:SER:O	1:C:331:ASN:HB2	1.71	0.91
1:A:456:LEU:HG	2:D:428:MET:CE	2.03	0.89
1:A:376:ALA:O	1:A:380:LEU:HD22	1.83	0.78
1:A:10:GLU:HB2	1:A:47:PRO:HB3	1.68	0.75
2:B:402:ILE:HG23	2:B:440:GLU:HG3	1.69	0.74
2:D:402:ILE:HG23	2:D:440:GLU:HG3	1.68	0.74
1:C:417:GLY:HA3	1:C:421:ALA:HB3	1.69	0.73
1:C:194:VAL:HG13	1:C:236:GLU:HG2	1.75	0.68
1:C:392:GLU:O	1:C:395:THR:HG22	1.94	0.67
1:A:145:GLU:HG2	1:A:189:GLU:OE1	1.95	0.66
1:C:145:GLU:HG2	1:C:189:GLU:OE1	1.96	0.65
1:A:34:ARG:HD2	1:A:75:TYR:HE1	1.63	0.64
1:C:34:ARG:HD2	1:C:75:TYR:HE1	1.62	0.63
1:A:194:VAL:HG13	1:A:236:GLU:HG2	1.81	0.62
1:A:354:ILE:O	1:A:358:ARG:HG2	2.00	0.62
1:A:446:GLU:H	1:A:446:GLU:CD	2.08	0.60
1:C:354:ILE:O	1:C:358:ARG:HG2	2.01	0.60
1:C:446:GLU:H	1:C:446:GLU:CD	2.08	0.60
1:A:283:PHE:CE2	2:B:441:LYS:HB3	2.37	0.60
1:A:391:VAL:O	1:A:395:THR:HG23	2.02	0.59
1:C:401:SER:HB2	1:C:443:LYS:HE2	1.84	0.58
1:C:395:THR:HG23	1:C:439:ASN:HD22	1.69	0.58
1:C:310:ASP:HA	1:C:314:LEU:HB2	1.89	0.55
1:A:325:GLU:HG3	2:B:454:TYR:OH	2.08	0.54
1:A:261:LYS:HG2	1:A:305:LEU:HD22	1.89	0.54
1:A:401:SER:HB2	1:A:443:LYS:HE2	1.88	0.54
1:A:310:ASP:HA	1:A:314:LEU:HB2	1.90	0.53
1:C:347:PHE:O	1:C:373:LYS:HD2	2.09	0.53
1:C:245:LEU:HD22	1:C:298:ILE:HG21	1.91	0.53
1:C:68:TYR:HB2	1:C:71:LEU:HB3	1.91	0.52
1:A:110:ASP:HA	1:A:113:LYS:HD2	1.92	0.52
1:A:242:THR:HG23	1:A:291:LEU:HA	1.91	0.51
1:C:197:ILE:HG23	1:C:240:TYR:HB2	1.93	0.51
1:C:110:ASP:HA	1:C:113:LYS:HD2	1.92	0.51
1:A:68:TYR:HB2	1:A:71:LEU:HB3	1.92	0.51
1:A:351:GLY:HA2	1:A:386:GLU:HG2	1.91	0.50
1:C:242:THR:HG23	1:C:291:LEU:HA	1.93	0.50
1:A:353:SER:HA	1:A:356:MET:HE3	1.92	0.50
1:C:351:GLY:HA2	1:C:386:GLU:HG2	1.93	0.50
1:A:347:PHE:O	1:A:373:LYS:HD2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:134:ILE:HA	1:C:137:ILE:HD12	1.94	0.50
1:A:134:ILE:HA	1:A:137:ILE:HD12	1.94	0.49
1:C:291:LEU:O	1:C:295:VAL:HG23	2.13	0.49
1:A:456:LEU:HG	2:D:428:MET:HE2	1.92	0.49
1:C:265:PRO:O	1:C:269:GLN:HG3	2.12	0.49
1:A:281:ARG:HD2	1:A:285:THR:HG23	1.95	0.48
1:A:291:LEU:O	1:A:295:VAL:HG23	2.13	0.48
1:C:401:SER:CB	1:C:443:LYS:HE2	2.42	0.48
1:A:283:PHE:HE2	2:B:441:LYS:HB3	1.76	0.48
2:D:385:ARG:HA	2:D:388:ILE:HD12	1.96	0.48
1:A:9:VAL:HG13	1:A:47:PRO:HG3	1.96	0.48
1:A:245:LEU:HD22	1:A:298:ILE:HG21	1.94	0.48
1:A:339:HIS:HB3	1:A:342:VAL:HB	1.95	0.48
1:C:392:GLU:HA	1:C:395:THR:HG22	1.96	0.47
1:A:139:LEU:HD11	1:A:173:LEU:HD23	1.97	0.47
1:A:283:PHE:CZ	2:B:441:LYS:HD2	2.50	0.47
1:A:401:SER:CB	1:A:443:LYS:HE2	2.44	0.47
2:B:385:ARG:HA	2:B:388:ILE:HD12	1.97	0.47
1:C:261:LYS:HG2	1:C:305:LEU:HD22	1.95	0.47
1:C:353:SER:HA	1:C:356:MET:HE3	1.96	0.47
1:A:55:LEU:HB3	1:A:95:VAL:HG11	1.97	0.46
1:A:265:PRO:O	1:A:269:GLN:HG3	2.15	0.46
1:C:198:ASP:O	1:C:202:ILE:HD12	2.14	0.46
1:A:198:ASP:O	1:A:202:ILE:HD12	2.15	0.46
1:A:246:LEU:C	1:A:248:ILE:H	2.24	0.46
1:A:456:LEU:HG	2:D:428:MET:HE3	1.90	0.46
1:C:139:LEU:HD11	1:C:173:LEU:HD23	1.96	0.46
1:C:55:LEU:HB3	1:C:95:VAL:HG11	1.96	0.46
1:C:246:LEU:C	1:C:248:ILE:H	2.24	0.45
1:C:142:LEU:O	1:C:195:ARG:HD3	2.17	0.45
1:C:33:LEU:HD22	1:C:76:LEU:HA	1.98	0.45
1:C:268:ALA:HB2	1:C:309:MET:HE3	1.98	0.44
1:A:142:LEU:O	1:A:195:ARG:HD3	2.17	0.44
1:C:122:ASN:HD22	1:C:162:ARG:HH12	1.65	0.44
1:A:353:SER:HA	1:A:356:MET:CE	2.48	0.44
1:C:339:HIS:HB3	1:C:342:VAL:HB	1.99	0.44
1:A:33:LEU:HD22	1:A:76:LEU:HA	1.98	0.44
1:A:16:LEU:HD23	1:A:54:LEU:HD21	1.99	0.44
1:A:197:ILE:HG23	1:A:240:TYR:HB2	2.00	0.43
1:A:437:LEU:HD13	1:A:455:LEU:HD23	2.01	0.43
1:C:9:VAL:HG13	1:C:46:LEU:HD22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:THR:HG23	1:C:60:ARG:HH21	1.83	0.43
1:A:16:LEU:HA	1:A:32:LEU:HD21	2.01	0.43
1:C:16:LEU:HA	1:C:32:LEU:HD21	2.01	0.43
1:C:425:ILE:HG23	1:C:426:ASP:H	1.84	0.43
1:A:122:ASN:HD22	1:A:162:ARG:HH12	1.67	0.42
1:A:77:LEU:HD11	1:A:111:PRO:HB3	2.01	0.42
1:C:232:LEU:HD12	2:D:444:LEU:HD21	2.01	0.42
1:C:353:SER:HA	1:C:356:MET:CE	2.49	0.42
1:A:171:ARG:O	1:A:175:ASP:HB3	2.19	0.42
1:C:16:LEU:HD23	1:C:54:LEU:HD21	2.00	0.42
1:C:77:LEU:HD11	1:C:111:PRO:HB3	2.01	0.42
1:A:29:ILE:HD12	1:A:32:LEU:HD23	2.02	0.42
1:C:29:ILE:HD12	1:C:32:LEU:HD23	2.01	0.42
1:A:34:ARG:HD2	1:A:75:TYR:CE1	2.50	0.42
1:A:57:THR:HG23	1:A:60:ARG:HH21	1.84	0.41
2:B:446:ALA:O	2:B:450:VAL:HG13	2.21	0.41
1:C:375:SER:H	1:C:378:ILE:HG22	1.86	0.41
1:A:13:LEU:HD21	1:A:40:LEU:HD11	2.02	0.41
1:C:171:ARG:O	1:C:175:ASP:HB3	2.19	0.41
1:C:13:LEU:HD21	1:C:40:LEU:HD11	2.01	0.41
1:C:377:GLU:O	1:C:381:ARG:HG2	2.21	0.41
1:A:239:ASN:C	1:A:243:LYS:HE3	2.46	0.41
1:A:125:PRO:HD2	1:A:128:LEU:HD12	2.03	0.41
1:C:417:GLY:HA3	1:C:421:ALA:CB	2.45	0.40
1:C:437:LEU:HD13	1:C:455:LEU:HD23	2.01	0.40
2:D:446:ALA:O	2:D:450:VAL:HG13	2.22	0.40
2:D:410:LEU:C	2:D:412:PRO:HD3	2.46	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	451/496 (91%)	413 (92%)	25 (6%)	13 (3%)	3	25
1	C	456/496 (92%)	418 (92%)	26 (6%)	12 (3%)	4	27
2	B	77/95 (81%)	68 (88%)	8 (10%)	1 (1%)	9	38
2	D	75/95 (79%)	67 (89%)	7 (9%)	1 (1%)	9	38
All	All	1059/1182 (90%)	966 (91%)	66 (6%)	27 (2%)	4	28

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	TYR
1	A	45	SER
1	A	48	ASP
1	A	51	VAL
1	A	66	VAL
1	A	301	ASP
1	A	354	ILE
2	B	400	ARG
1	C	45	SER
1	C	48	ASP
1	C	51	VAL
1	C	66	VAL
1	C	301	ASP
1	C	354	ILE
2	D	400	ARG
1	A	43	VAL
1	A	47	PRO
1	C	43	VAL
1	A	261	LYS
1	C	261	LYS
1	C	425	ILE
1	A	46	LEU
1	A	190	THR
1	C	73	TYR
1	C	190	THR
1	A	73	TYR
1	C	50	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	422/455 (93%)	362 (86%)	60 (14%)	3	17
1	C	424/455 (93%)	362 (85%)	62 (15%)	3	17
2	B	66/80 (82%)	57 (86%)	9 (14%)	3	18
2	D	64/80 (80%)	56 (88%)	8 (12%)	4	21
All	All	976/1070 (91%)	837 (86%)	139 (14%)	3	17

All (139) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	VAL
1	A	12	LEU
1	A	31	THR
1	A	34	ARG
1	A	38	LEU
1	A	40	LEU
1	A	45	SER
1	A	49	MET
1	A	58	ILE
1	A	61	PHE
1	A	83	LEU
1	A	86	MET
1	A	93	LEU
1	A	109	ILE
1	A	118	ARG
1	A	128	LEU
1	A	136	ASP
1	A	145	GLU
1	A	153	ILE
1	A	184	VAL
1	A	187	ARG
1	A	188	MET
1	A	201	THR
1	A	202	ILE
1	A	207	ILE
1	A	222	GLU
1	A	236	GLU
1	A	237	LEU

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Mol	Chain	Res	Type
1	A	246	LEU
1	A	247	GLU
1	A	248	ILE
1	A	251	GLN
1	A	257	LEU
1	A	281	ARG
1	A	285	THR
1	A	297	ARG
1	A	314	LEU
1	A	322	LEU
1	A	324	THR
1	A	333	GLN
1	A	337	LYS
1	A	341	ASP
1	A	343	VAL
1	A	354	ILE
1	A	370	ILE
1	A	380	LEU
1	A	386	GLU
1	A	402	LYS
1	A	404	LEU
1	A	405	LEU
1	A	416	ILE
1	A	418	ASP
1	A	427	LEU
1	A	430	VAL
1	A	437	LEU
1	A	438	ARG
1	A	440	LEU
1	A	446	GLU
1	A	453	GLU
1	A	464	ASN
2	B	378	SER
2	B	382	LEU
2	B	391	ILE
2	B	398	VAL
2	B	406	LEU
2	B	413	ASN
2	B	415	THR
2	B	436	LYS
2	B	450	VAL
1	C	9	VAL

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Mol	Chain	Res	Type
1	C	12	LEU
1	C	31	THR
1	C	34	ARG
1	C	38	LEU
1	C	40	LEU
1	C	45	SER
1	C	46	LEU
1	C	49	MET
1	C	50	ASP
1	C	58	ILE
1	C	61	PHE
1	C	66	VAL
1	C	83	LEU
1	C	86	MET
1	C	93	LEU
1	C	109	ILE
1	C	118	ARG
1	C	128	LEU
1	C	136	ASP
1	C	145	GLU
1	C	153	ILE
1	C	184	VAL
1	C	187	ARG
1	C	201	THR
1	C	202	ILE
1	C	207	ILE
1	C	222	GLU
1	C	237	LEU
1	C	246	LEU
1	C	247	GLU
1	C	248	ILE
1	C	251	GLN
1	C	257	LEU
1	C	281	ARG
1	C	285	THR
1	C	297	ARG
1	C	302	GLU
1	C	305	LEU
1	C	314	LEU
1	C	321	LYS
1	C	322	LEU
1	C	333	GLN

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Mol	Chain	Res	Type
1	C	337	LYS
1	C	341	ASP
1	C	354	ILE
1	C	370	ILE
1	C	395	THR
1	C	402	LYS
1	C	404	LEU
1	C	405	LEU
1	C	410	LYS
1	C	416	ILE
1	C	418	ASP
1	C	424	ILE
1	C	427	LEU
1	C	430	VAL
1	C	437	LEU
1	C	440	LEU
1	C	446	GLU
1	C	453	GLU
1	C	464	ASN
2	D	382	LEU
2	D	391	ILE
2	D	398	VAL
2	D	406	LEU
2	D	413	ASN
2	D	415	THR
2	D	439	THR
2	D	450	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	18	ASN
1	A	72	ASN
1	A	122	ASN
1	A	176	ASN
1	A	205	GLN
1	A	259	HIS
1	A	276	ASN
2	B	413	ASN
1	C	15	GLN
1	C	18	ASN
1	C	72	ASN

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Mol	Chain	Res	Type
1	C	122	ASN
1	C	176	ASN
1	C	205	GLN
1	C	259	HIS
1	C	276	ASN
1	C	439	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	455/496 (91%)	-0.24	7 (1%) 72 50	142, 211, 286, 300	0
1	C	458/496 (92%)	-0.09	7 (1%) 72 50	146, 235, 300, 300	0
2	B	79/95 (83%)	-0.07	0 100 100	149, 198, 283, 290	0
2	D	77/95 (81%)	0.04	4 (5%) 33 25	163, 219, 285, 293	0
3	E	0/10	-	-	-	-
All	All	1069/1192 (89%)	-0.14	18 (1%) 69 47	142, 219, 298, 300	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	320	ALA	3.9
1	A	381	ARG	3.8
2	D	391	ILE	3.6
1	C	348	HIS	3.1
1	C	9	VAL	3.0
1	C	39	ASN	2.9
1	A	179	PRO	2.8
1	C	98	ALA	2.7
1	A	51	VAL	2.6
1	A	418	ASP	2.5
1	A	427	LEU	2.5
1	A	430	VAL	2.5
1	C	243	LYS	2.4
1	C	117	CYS	2.3
1	A	352	TYR	2.2
2	D	454	TYR	2.1
2	D	413	ASN	2.1
2	D	380	PRO	2.1

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.