



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 09:50 pm BST

PDB ID : 4A3V
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

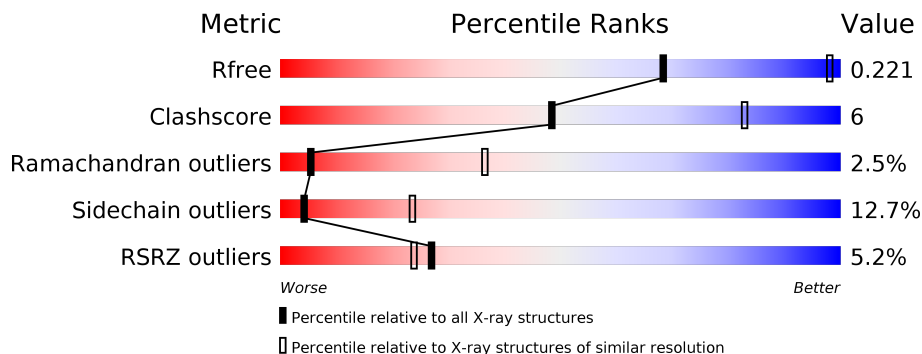
1 Overall quality at a glance

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}	130704	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)

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 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% 65% 23% 8%
1	C	496	 6% 65% 24% 8%
2	B	95	 3% 66% 16% 17%
2	D	95	 2% 66% 13% 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
			Total	C	N	O	S			
1	A	455	3716	2396	594	713	13	0	0	0
1	C	458	3735	2409	596	717	13	0	0	0

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

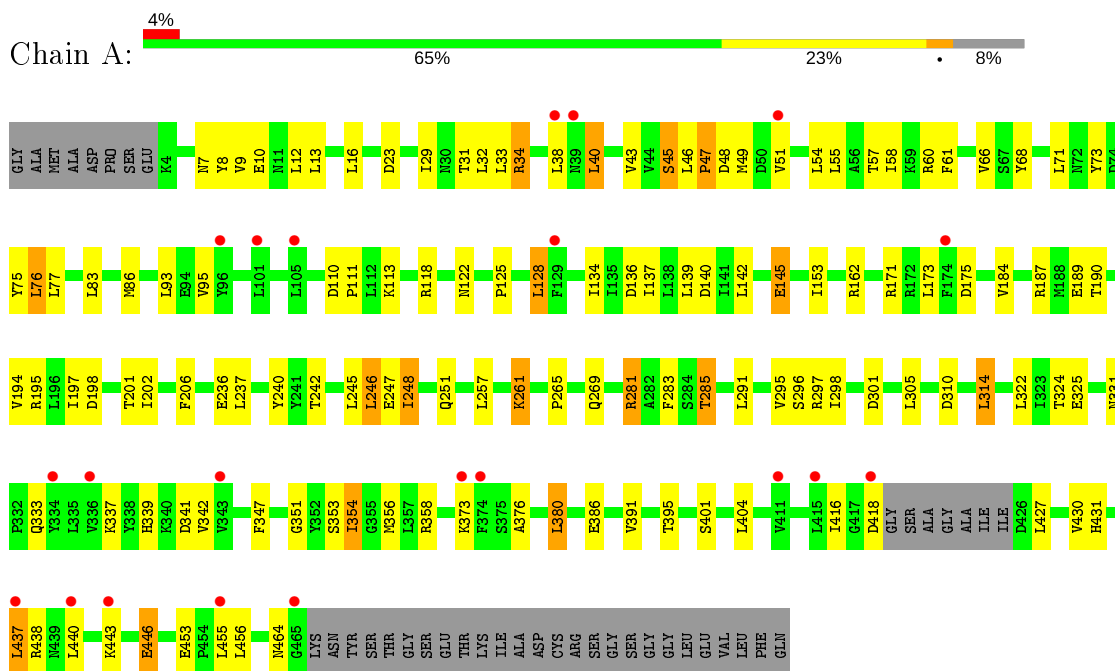
- Molecule 3 is a protein called LINKER.

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

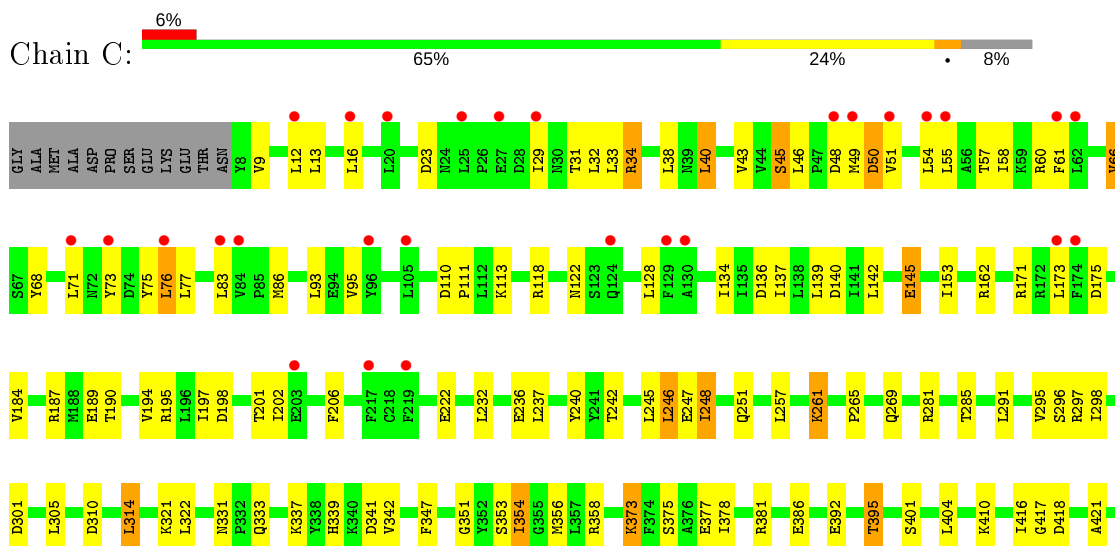
3 Residue-property plots

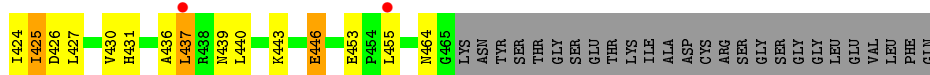
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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



- Molecule 1: DNA MISMATCH REPAIR PROTEIN HSM3





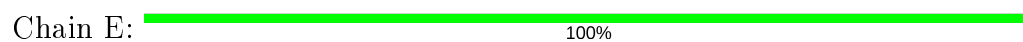
- Molecule 2: 26S PROTEASE REGULATORY SUBUNIT 7 HOMOLOG



- Molecule 2: 26S PROTEASE REGULATORY SUBUNIT 7 HOMOLOG



- Molecule 3: LINKER



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) 100.0 (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)	Xtrriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.190 , 0.208 0.205 , 0.221	Depositor DCC
R_{free} test set	1933 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	179.6	Xtrriage
Anisotropy	0.237	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 239.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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 [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	0.51	0/3782	0.75	1/5125 (0.0%)
1	C	0.50	0/3802	0.75	0/5152
2	B	0.52	0/626	0.75	0/837
2	D	0.48	0/611	0.71	0/818
All	All	0.51	0/8821	0.75	1/11932 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	7	ASN	C-N-CA	5.34	135.06	121.70

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	3716	0	3730	51	0
1	C	3735	0	3761	48	0
2	B	618	0	639	7	0
2	D	603	0	621	7	0
3	E	50	0	12	0	0
All	All	8722	0	8763	105	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 (105) 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
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:C:354:ILE:O	1:C:358:ARG:HG2	2.01	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:446:GLU:CD	1:C:446:GLU:H	2.08	0.56
1:A:446:GLU:H	1:A:446:GLU:CD	2.08	0.55
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:456:LEU:HG	2:D:428:MET:HE2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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:245:LEU:HD22	1:A:298:ILE:HG21	1.94	0.48
1:A:9:VAL:HG13	1:A:47:PRO:HG3	1.96	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:401:SER:CB	1:A:443:LYS:HE2	2.44	0.47
1:C:261:LYS:HG2	1:C:305:LEU:HD22	1.95	0.47
1:A:283:PHE:CZ	2:B:441:LYS:HD2	2.50	0.47
2:B:385:ARG:HA	2:B:388:ILE:HD12	1.97	0.47
1:A:265:PRO:O	1:A:269:GLN:HG3	2.15	0.46
1:A:55:LEU:HB3	1:A:95:VAL:HG11	1.97	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:456:LEU:HG	2:D:428:MET:HE3	1.91	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: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: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:57:THR:HG23	1:C:60:ARG:HH21	1.83	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: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:353:SER:HA	1:C:356:MET:CE	2.49	0.42
1:C:232:LEU:HD12	2:D:444:LEU:HD21	2.01	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:246:LEU:C	1:A:248:ILE:H	2.24	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:125:PRO:HD2	1:A:128:LEU:HD12	2.03	0.41
1:C:246:LEU:C	1:C:248:ILE:H	2.24	0.40
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

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	451/496 (91%)	413 (92%)	25 (6%)	13 (3%)	4	34
1	C	456/496 (92%)	418 (92%)	26 (6%)	12 (3%)	5	36
2	B	77/95 (81%)	68 (88%)	8 (10%)	1 (1%)	12	48
2	D	75/95 (79%)	67 (89%)	7 (9%)	1 (1%)	12	48
All	All	1059/1182 (90%)	966 (91%)	66 (6%)	27 (2%)	5	36

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 [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	422/455 (93%)	370 (88%)	52 (12%)	4	24
1	C	424/455 (93%)	367 (87%)	57 (13%)	4	22
2	B	66/80 (82%)	58 (88%)	8 (12%)	5	25
2	D	64/80 (80%)	57 (89%)	7 (11%)	6	29
All	All	976/1070 (91%)	852 (87%)	124 (13%)	4	23

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LEU
1	A	23	ASP
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	76	LEU
1	A	83	LEU
1	A	86	MET
1	A	93	LEU
1	A	118	ARG
1	A	128	LEU
1	A	136	ASP
1	A	140	ASP
1	A	145	GLU
1	A	153	ILE
1	A	184	VAL
1	A	187	ARG
1	A	201	THR
1	A	206	PHE
1	A	237	LEU
1	A	246	LEU
1	A	247	GLU
1	A	248	ILE

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Mol	Chain	Res	Type
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	380	LEU
1	A	404	LEU
1	A	416	ILE
1	A	418	ASP
1	A	427	LEU
1	A	430	VAL
1	A	431	HIS
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	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	12	LEU
1	C	23	ASP
1	C	31	THR
1	C	34	ARG
1	C	38	LEU
1	C	40	LEU
1	C	45	SER
1	C	49	MET
1	C	50	ASP
1	C	58	ILE

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Mol	Chain	Res	Type
1	C	61	PHE
1	C	66	VAL
1	C	76	LEU
1	C	83	LEU
1	C	86	MET
1	C	93	LEU
1	C	118	ARG
1	C	128	LEU
1	C	136	ASP
1	C	140	ASP
1	C	145	GLU
1	C	153	ILE
1	C	184	VAL
1	C	187	ARG
1	C	201	THR
1	C	206	PHE
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	314	LEU
1	C	321	LYS
1	C	322	LEU
1	C	333	GLN
1	C	337	LYS
1	C	341	ASP
1	C	373	LYS
1	C	395	THR
1	C	404	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	431	HIS

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Mol	Chain	Res	Type
1	C	437	LEU
1	C	440	LEU
1	C	446	GLU
1	C	453	GLU
1	C	464	ASN
2	D	391	ILE
2	D	398	VAL
2	D	400	ARG
2	D	406	LEU
2	D	413	ASN
2	D	415	THR
2	D	450	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	122	ASN
1	A	176	ASN
1	A	259	HIS
1	A	333	GLN
1	C	39	ASN
1	C	122	ASN
1	C	176	ASN
1	C	259	HIS
1	C	333	GLN
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 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	455/496 (91%)	0.35	21 (4%) 32 28	142, 211, 286, 300	0
1	C	458/496 (92%)	0.50	30 (6%) 18 14	146, 235, 300, 300	0
2	B	79/95 (83%)	0.42	3 (3%) 40 33	149, 198, 283, 290	0
2	D	77/95 (81%)	0.22	2 (2%) 56 47	163, 219, 285, 293	0
3	E	0/10	-	-	-	-
All	All	1069/1192 (89%)	0.41	56 (5%) 27 24	142, 219, 298, 300	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	378	SER	5.3
2	B	377	SER	5.0
1	C	20	LEU	4.2
1	C	62	LEU	4.1
1	C	48	ASP	3.5
1	C	12	LEU	3.4
1	C	174	PHE	3.2
1	C	71	LEU	3.2
1	C	129	PHE	3.1
1	C	25	LEU	3.0
1	C	437	LEU	3.0
1	C	455	LEU	2.9
1	A	39	ASN	2.9
1	C	49	MET	2.9
1	A	174	PHE	2.9
1	A	38	LEU	2.7
1	C	217	PHE	2.7
1	C	51	VAL	2.7
1	C	61	PHE	2.6
1	A	411	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	73	TYR	2.6
1	A	440	LEU	2.5
1	C	27	GLU	2.5
1	C	76	LEU	2.5
1	C	83	LEU	2.5
1	C	124	GLN	2.5
1	A	105	LEU	2.5
1	A	465	GLY	2.5
1	A	96	TYR	2.4
1	A	129	PHE	2.4
1	A	343	VAL	2.4
2	B	389	PHE	2.4
1	C	96	TYR	2.4
1	C	84	VAL	2.4
1	C	16	LEU	2.4
1	A	334	TYR	2.3
1	A	455	LEU	2.3
1	C	54	LEU	2.3
1	C	105	LEU	2.3
1	A	415	LEU	2.2
1	A	443	LYS	2.2
1	A	437	LEU	2.2
1	C	29	ILE	2.2
1	A	374	PHE	2.2
1	A	418	ASP	2.2
1	A	373	LYS	2.1
1	A	101	LEU	2.1
1	C	173	LEU	2.1
2	B	437	VAL	2.1
2	D	454	TYR	2.1
1	C	55	LEU	2.1
1	C	130	ALA	2.1
1	A	336	VAL	2.0
1	C	219	PHE	2.0
1	C	203	GLU	2.0
1	A	51	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.