



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 2, 2023 – 10:56 PM EDT

PDB ID : 1HR7  
Title : Yeast Mitochondrial Processing Peptidase beta-E73Q Mutant  
Authors : Taylor, A.B.; Smith, B.S.; Kitada, S.; Kojima, K.; Miyaura, H.; Otwinowski, Z.; Ito, A.; Deisenhofer, J.  
Deposited on : 2000-12-21  
Resolution : 2.55 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](mailto: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>.

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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 : 2.34  
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) : 2.34

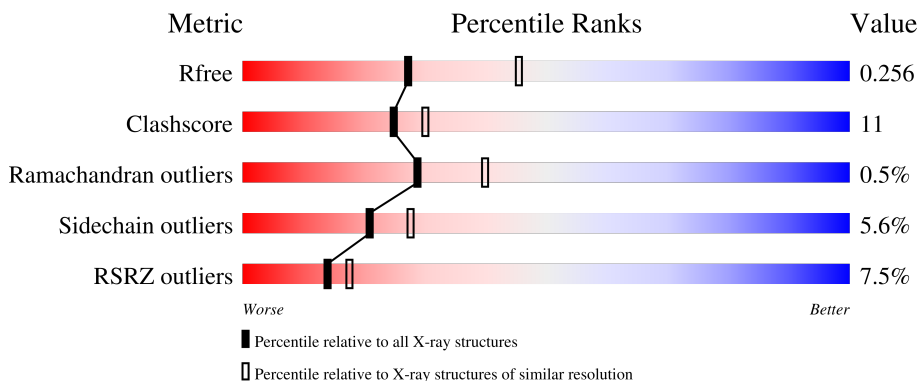
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.55 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.



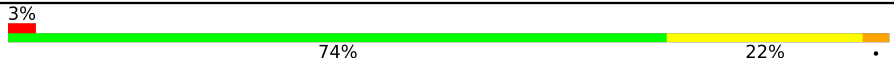

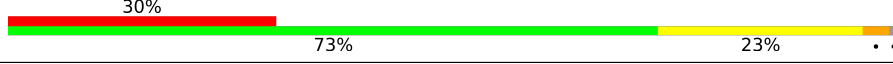
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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  $\geq 3$ , 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	475	 5% 74% 20% . .
1	C	475	 3% 74% 17% 7%
1	E	475	 5% 72% 20% 6%
1	G	475	 4% 71% 20% 5%
2	B	443	 2% 75% 21% . .

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Mol	Chain	Length	Quality of chain
2	D	443	
2	F	443	
2	H	443	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 27725 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 MITOCHONDRIAL PROCESSING PEPTIDASE ALPHA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	457	3531	2233	599	680	19	0	0	0
1	C	444	3447	2183	582	663	19	0	0	0
1	E	448	3478	2201	590	668	19	0	0	0
1	G	450	3485	2206	592	668	19	0	0	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	177	GLY	GLU	SEE REMARK 999	UNP P11914
A	217	GLY	GLU	SEE REMARK 999	UNP P11914
A	483	HIS	-	expression tag	UNP P11914
A	484	HIS	-	expression tag	UNP P11914
A	485	HIS	-	expression tag	UNP P11914
A	486	HIS	-	expression tag	UNP P11914
A	487	HIS	-	expression tag	UNP P11914
A	488	HIS	-	expression tag	UNP P11914
C	177	GLY	GLU	SEE REMARK 999	UNP P11914
C	217	GLY	GLU	SEE REMARK 999	UNP P11914
C	483	HIS	-	expression tag	UNP P11914
C	484	HIS	-	expression tag	UNP P11914
C	485	HIS	-	expression tag	UNP P11914
C	486	HIS	-	expression tag	UNP P11914
C	487	HIS	-	expression tag	UNP P11914
C	488	HIS	-	expression tag	UNP P11914
E	177	GLY	GLU	SEE REMARK 999	UNP P11914
E	217	GLY	GLU	SEE REMARK 999	UNP P11914
E	483	HIS	-	expression tag	UNP P11914
E	484	HIS	-	expression tag	UNP P11914

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Chain	Residue	Modelled	Actual	Comment	Reference
E	485	HIS	-	expression tag	UNP P11914
E	486	HIS	-	expression tag	UNP P11914
E	487	HIS	-	expression tag	UNP P11914
E	488	HIS	-	expression tag	UNP P11914
G	177	GLY	GLU	SEE REMARK 999	UNP P11914
G	217	GLY	GLU	SEE REMARK 999	UNP P11914
G	483	HIS	-	expression tag	UNP P11914
G	484	HIS	-	expression tag	UNP P11914
G	485	HIS	-	expression tag	UNP P11914
G	486	HIS	-	expression tag	UNP P11914
G	487	HIS	-	expression tag	UNP P11914
G	488	HIS	-	expression tag	UNP P11914

- Molecule 2 is a protein called MITOCHONDRIAL PROCESSING PEPTIDASE BETA SUB-UNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	439	Total 3414	C 2148	N 591	O 668	S 7	0	0	0
2	D	441	Total 3431	C 2159	N 594	O 671	S 7	0	0	0
2	F	440	Total 3422	C 2154	N 592	O 669	S 7	0	0	0
2	H	440	Total 3422	C 2154	N 592	O 669	S 7	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	20	ALA	-	cloning artifact	UNP P10507
B	73	GLN	GLU	engineered mutation	UNP P10507
B	84	PRO	SER	SEE REMARK 999	UNP P10507
B	350	ARG	GLN	SEE REMARK 999	UNP P10507
D	20	ALA	-	cloning artifact	UNP P10507
D	73	GLN	GLU	engineered mutation	UNP P10507
D	84	PRO	SER	SEE REMARK 999	UNP P10507
D	350	ARG	GLN	SEE REMARK 999	UNP P10507
F	20	ALA	-	cloning artifact	UNP P10507
F	73	GLN	GLU	engineered mutation	UNP P10507
F	84	PRO	SER	SEE REMARK 999	UNP P10507
F	350	ARG	GLN	SEE REMARK 999	UNP P10507
H	20	ALA	-	cloning artifact	UNP P10507

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Chain	Residue	Modelled	Actual	Comment	Reference
H	73	GLN	GLU	engineered mutation	UNP P10507
H	84	PRO	SER	SEE REMARK 999	UNP P10507
H	350	ARG	GLN	SEE REMARK 999	UNP P10507

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Zn 1 1	0	0
3	D	1	Total Zn 1 1	0	0
3	F	1	Total Zn 1 1	0	0
3	H	1	Total Zn 1 1	0	0

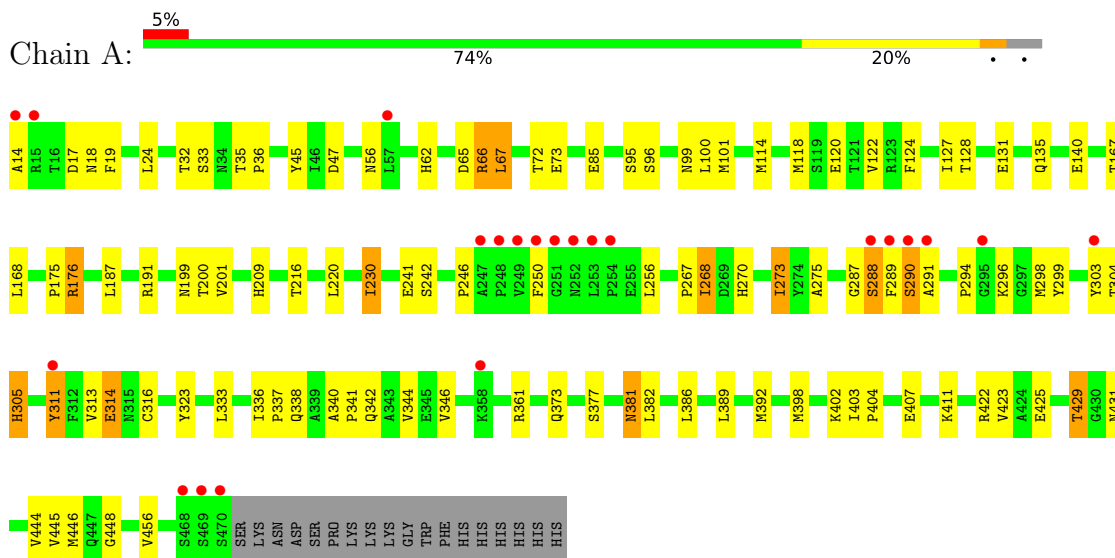
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	20	Total O 20 20	0	0
4	B	27	Total O 27 27	0	0
4	C	13	Total O 13 13	0	0
4	D	10	Total O 10 10	0	0
4	E	9	Total O 9 9	0	0
4	F	4	Total O 4 4	0	0
4	G	7	Total O 7 7	0	0
4	H	1	Total O 1 1	0	0

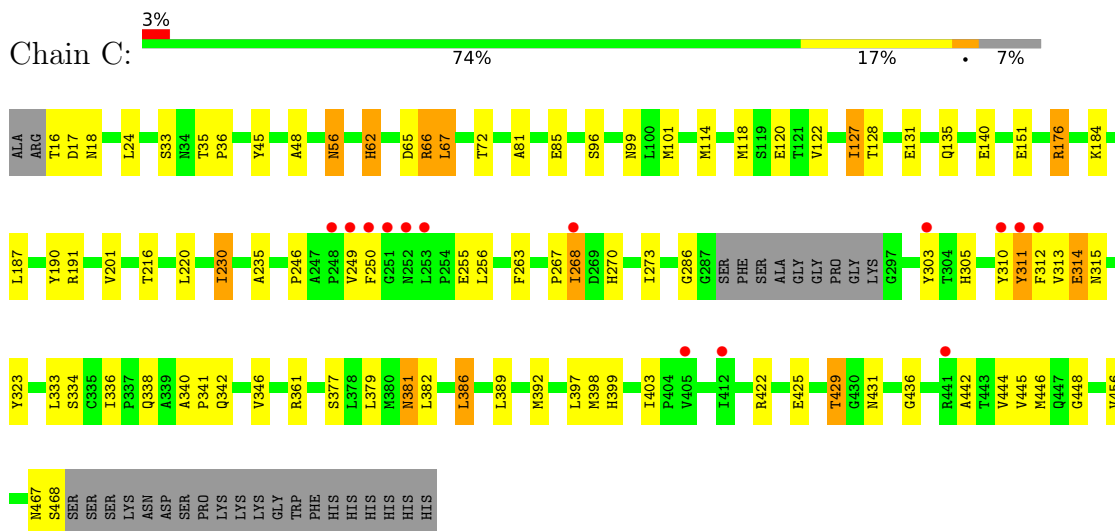
### 3 Residue-property plots [i](#)

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: MITOCHONDRIAL PROCESSING PEPTIDASE ALPHA SUBUNIT

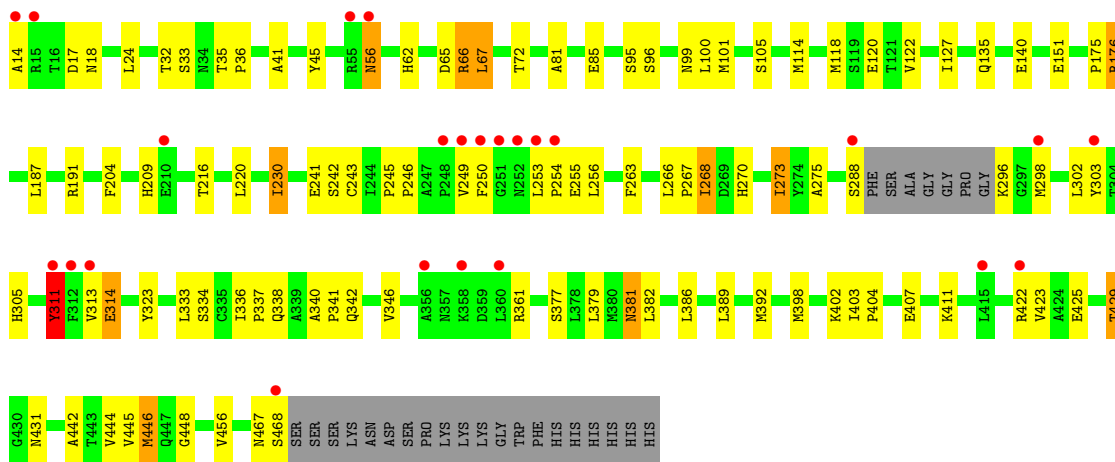


- Molecule 1: MITOCHONDRIAL PROCESSING PEPTIDASE ALPHA SUBUNIT

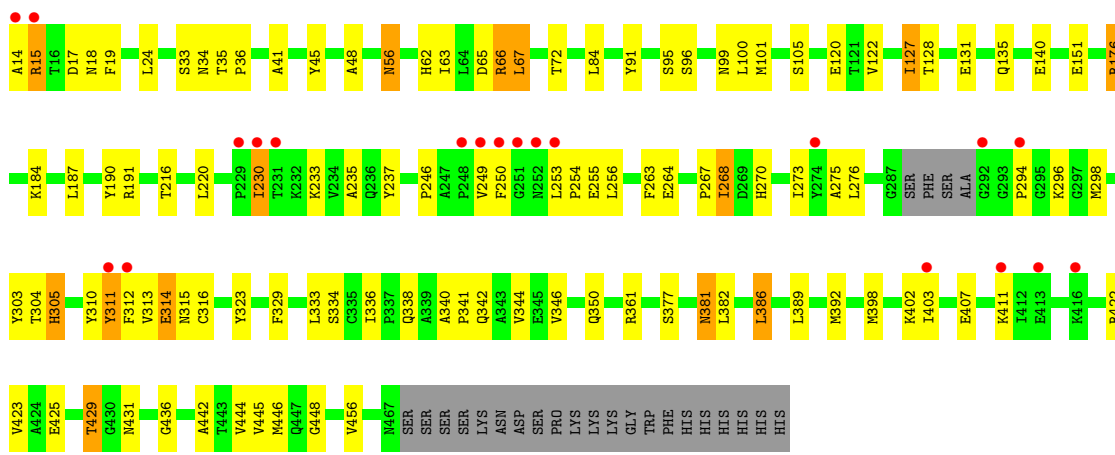


- Molecule 1: MITOCHONDRIAL PROCESSING PEPTIDASE ALPHA SUBUNIT

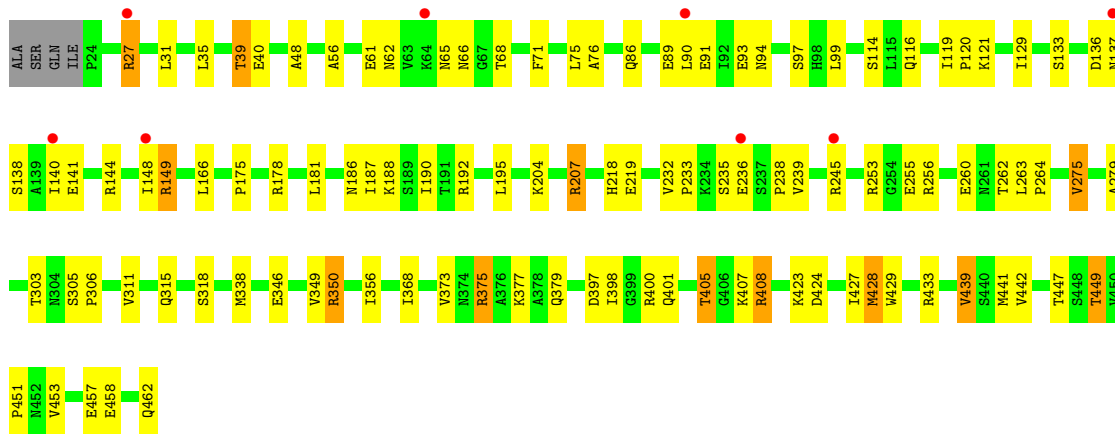
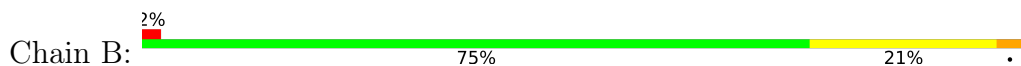




• Molecule 1: MITOCHONDRIAL PROCESSING PEPTIDASE ALPHA SUBUNIT

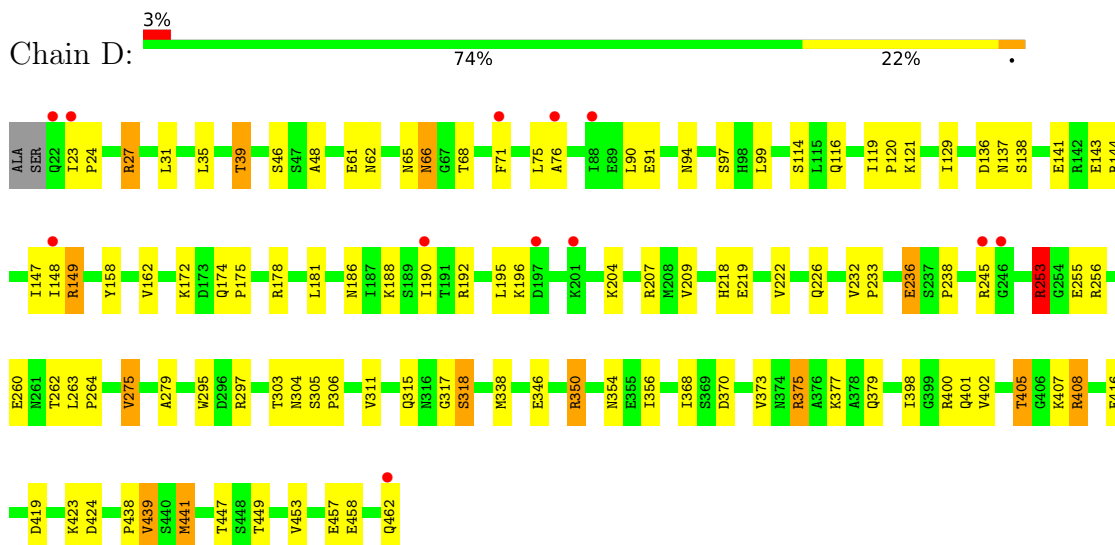


• Molecule 2: MITOCHONDRIAL PROCESSING PEPTIDASE BETA SUBUNIT

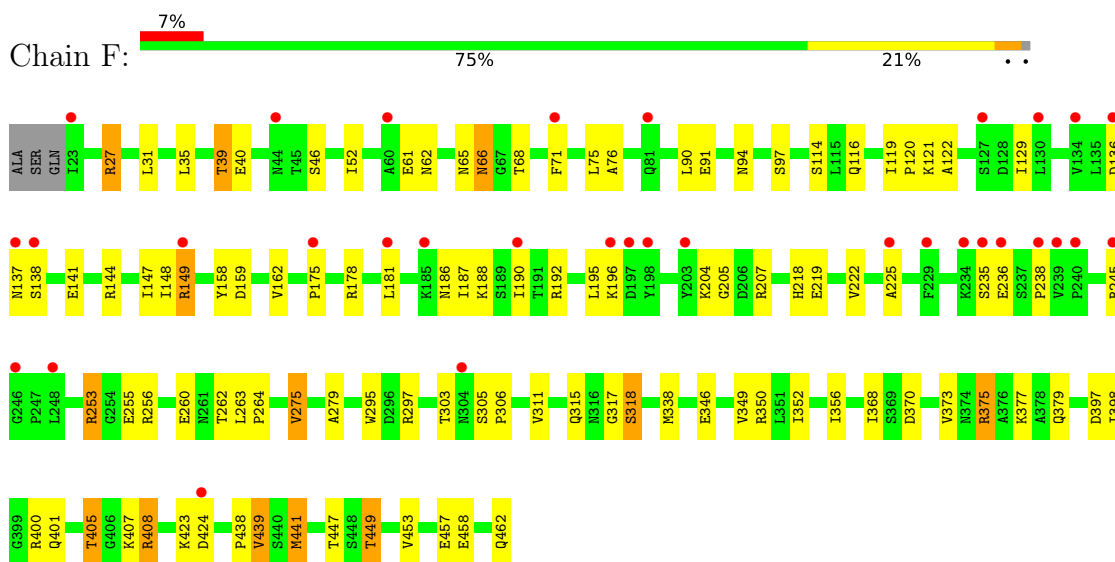


• Molecule 2: MITOCHONDRIAL PROCESSING PEPTIDASE BETA SUBUNIT

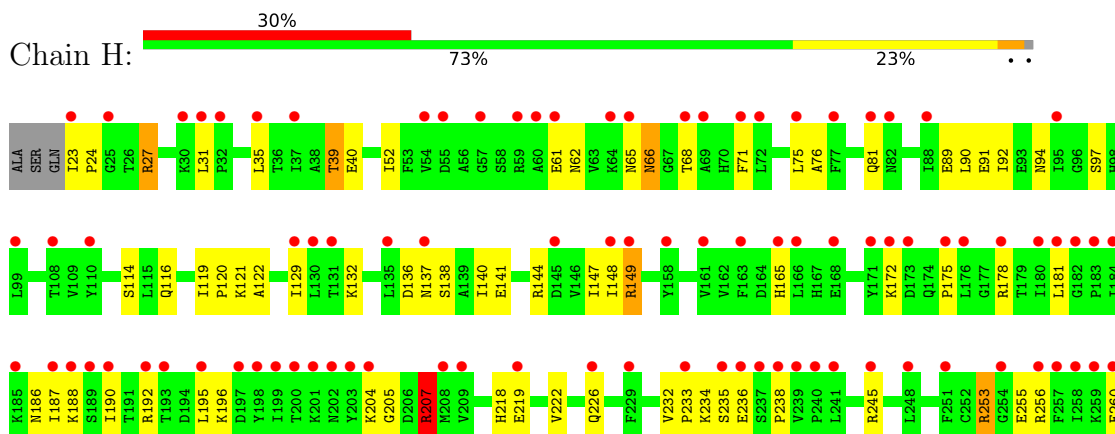


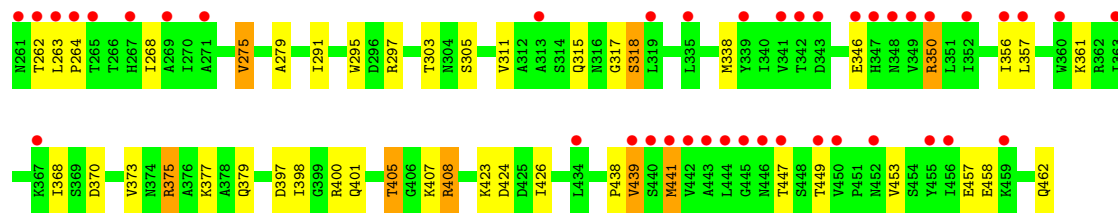


• Molecule 2: MITOCHONDRIAL PROCESSING PEPTIDASE BETA SUBUNIT



• Molecule 2: MITOCHONDRIAL PROCESSING PEPTIDASE BETA SUBUNIT





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	134.20Å 178.62Å 201.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.53 – 2.55 47.53 – 2.54	Depositor EDS
% Data completeness (in resolution range)	98.7 (47.53-2.55) 98.2 (47.53-2.54)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.22 (at 2.54Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.243 , 0.256 0.242 , 0.256	Depositor DCC
$R_{free}$ test set	2025 reflections (1.29%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	53.7	Xtrriage
Anisotropy	0.471	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 44.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	27725	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.08% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

Bond lengths and bond angles in the following residue types are not validated in this section:  
ZN

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	0.64	0/3604	0.76	2/4877 (0.0%)
1	C	0.63	0/3517	0.75	1/4760 (0.0%)
1	E	0.61	0/3548	0.82	4/4800 (0.1%)
1	G	0.59	0/3556	0.75	2/4811 (0.0%)
2	B	0.61	0/3478	0.78	5/4720 (0.1%)
2	D	0.61	1/3495 (0.0%)	0.91	10/4744 (0.2%)
2	F	0.53	0/3486	0.74	5/4732 (0.1%)
2	H	0.53	0/3486	0.87	9/4732 (0.2%)
All	All	0.60	1/28170 (0.0%)	0.80	38/38176 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	236	GLU	CB-CG	-6.03	1.40	1.52

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	149	ARG	NE-CZ-NH2	-17.07	111.76	120.30
2	D	253	ARG	NE-CZ-NH2	16.87	128.73	120.30
2	H	207	ARG	NE-CZ-NH1	-16.50	112.05	120.30
2	H	149	ARG	NE-CZ-NH1	16.43	128.52	120.30
2	D	253	ARG	NE-CZ-NH1	-16.30	112.15	120.30
2	D	350	ARG	NE-CZ-NH2	16.18	128.39	120.30
2	H	207	ARG	NE-CZ-NH2	15.77	128.19	120.30
1	E	422	ARG	NE-CZ-NH1	-15.06	112.77	120.30
2	D	350	ARG	NE-CZ-NH1	-15.04	112.78	120.30
1	E	422	ARG	NE-CZ-NH2	13.97	127.28	120.30
2	D	350	ARG	CG-CD-NE	-10.46	89.83	111.80
2	H	149	ARG	CD-NE-CZ	7.95	134.73	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	253	ARG	CD-NE-CZ	7.81	134.54	123.60
2	B	253	ARG	NE-CZ-NH1	7.77	124.18	120.30
2	F	253	ARG	NE-CZ-NH1	7.68	124.14	120.30
1	E	422	ARG	CD-NE-CZ	7.16	133.62	123.60
2	H	207	ARG	CD-NE-CZ	7.02	133.43	123.60
2	H	253	ARG	NE-CZ-NH1	6.91	123.75	120.30
2	F	253	ARG	NE-CZ-NH2	-6.61	117.00	120.30
1	G	422	ARG	NE-CZ-NH2	-6.43	117.08	120.30
1	E	311	TYR	CB-CG-CD1	-6.34	117.19	121.00
2	D	149	ARG	NE-CZ-NH1	-6.09	117.26	120.30
2	D	350	ARG	CD-NE-CZ	6.05	132.08	123.60
1	G	422	ARG	NE-CZ-NH1	6.05	123.32	120.30
2	D	149	ARG	NE-CZ-NH2	6.00	123.30	120.30
2	H	253	ARG	NE-CZ-NH2	-5.88	117.36	120.30
2	F	149	ARG	NE-CZ-NH1	-5.70	117.45	120.30
1	C	422	ARG	NE-CZ-NH2	-5.69	117.46	120.30
2	B	253	ARG	NE-CZ-NH2	-5.58	117.51	120.30
2	F	207	ARG	NE-CZ-NH2	-5.55	117.52	120.30
1	A	422	ARG	NE-CZ-NH2	-5.51	117.55	120.30
2	B	207	ARG	NE-CZ-NH1	5.43	123.02	120.30
2	F	149	ARG	NE-CZ-NH2	5.39	122.99	120.30
2	H	350	ARG	NE-CZ-NH1	5.36	122.98	120.30
2	D	236	GLU	CB-CA-C	-5.33	99.75	110.40
2	B	149	ARG	NE-CZ-NH2	5.29	122.94	120.30
1	A	422	ARG	NE-CZ-NH1	5.03	122.82	120.30
2	B	207	ARG	NE-CZ-NH2	-5.01	117.79	120.30

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	3531	0	3488	78	0
1	C	3447	0	3406	64	0
1	E	3478	0	3442	77	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	3485	0	3448	82	0
2	B	3414	0	3414	77	0
2	D	3431	0	3432	74	0
2	F	3422	0	3424	75	0
2	H	3422	0	3424	85	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
3	F	1	0	0	0	0
3	H	1	0	0	0	0
4	A	20	0	0	0	0
4	B	27	0	0	0	0
4	C	13	0	0	0	0
4	D	10	0	0	0	0
4	E	9	0	0	0	0
4	F	4	0	0	0	0
4	G	7	0	0	0	0
4	H	1	0	0	0	0
All	All	27725	0	27478	597	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 11.

All (597) 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:E:33:SER:HB3	1:E:392:MET:HE1	1.30	1.08
1:C:33:SER:HB3	1:C:392:MET:HE1	1.36	1.06
1:G:33:SER:HB3	1:G:392:MET:HE1	1.38	1.04
1:A:33:SER:HB3	1:A:392:MET:HE1	1.40	1.03
1:A:230:ILE:HD12	1:A:230:ILE:H	1.29	0.98
1:G:24:LEU:HD11	1:G:216:THR:HG22	1.43	0.97
1:G:311:TYR:HD2	1:G:311:TYR:N	1.60	0.96
1:C:230:ILE:HD12	1:C:230:ILE:H	1.29	0.95
1:C:24:LEU:HD11	1:C:216:THR:HG22	1.48	0.94
2:D:256:ARG:HG3	2:D:256:ARG:HH11	1.31	0.94
1:G:230:ILE:H	1:G:230:ILE:HD12	1.30	0.93
1:A:24:LEU:HD11	1:A:216:THR:HG22	1.50	0.93
1:E:230:ILE:HD12	1:E:230:ILE:H	1.31	0.92
2:F:256:ARG:HG3	2:F:256:ARG:HH11	1.34	0.91
1:G:311:TYR:N	1:G:311:TYR:CD2	2.35	0.90
2:B:256:ARG:HG3	2:B:256:ARG:HH11	1.32	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:33:SER:HB3	1:G:392:MET:CE	2.03	0.88
1:E:268:ILE:HD11	1:E:398:MET:SD	2.14	0.86
1:E:33:SER:HB3	1:E:392:MET:CE	2.06	0.85
1:C:33:SER:HB3	1:C:392:MET:CE	2.07	0.85
2:H:256:ARG:HH11	2:H:256:ARG:HG3	1.39	0.84
1:E:24:LEU:HD11	1:E:216:THR:HG22	1.59	0.84
1:C:246:PRO:HG3	1:C:448:GLY:HA2	1.59	0.83
2:H:62:ASN:H	2:H:65:ASN:HB3	1.43	0.83
1:G:311:TYR:HD2	1:G:311:TYR:H	0.84	0.83
2:B:62:ASN:H	2:B:65:ASN:HB3	1.43	0.82
2:F:62:ASN:H	2:F:65:ASN:HB3	1.45	0.81
1:A:14:ALA:HB3	1:A:404:PRO:HB3	1.60	0.81
1:A:268:ILE:HD11	1:A:398:MET:SD	2.20	0.81
1:C:429:THR:CG2	1:C:431:ASN:HD22	1.94	0.81
1:C:230:ILE:HD12	1:C:230:ILE:N	1.95	0.80
1:C:268:ILE:HD11	1:C:398:MET:SD	2.22	0.80
1:A:33:SER:HB3	1:A:392:MET:CE	2.12	0.79
1:A:429:THR:CG2	1:A:431:ASN:HD22	1.96	0.79
1:G:268:ILE:HD11	1:G:398:MET:SD	2.23	0.78
2:D:338:MET:HG2	2:D:356:ILE:HD13	1.66	0.77
2:D:62:ASN:H	2:D:65:ASN:HB3	1.49	0.77
1:A:230:ILE:HD12	1:A:230:ILE:N	1.98	0.77
1:G:425:GLU:O	1:G:429:THR:HB	1.85	0.77
1:E:230:ILE:HD12	1:E:230:ILE:N	2.00	0.77
1:A:425:GLU:O	1:A:429:THR:HB	1.85	0.76
1:E:429:THR:CG2	1:E:431:ASN:HD22	1.99	0.76
2:H:275:VAL:HG22	2:H:279:ALA:CB	2.15	0.76
2:H:338:MET:HG2	2:H:356:ILE:HD13	1.68	0.76
1:G:230:ILE:HD12	1:G:230:ILE:N	1.99	0.76
2:H:144:ARG:O	2:H:148:ILE:HG12	1.86	0.75
1:G:429:THR:CG2	1:G:431:ASN:HD22	2.00	0.75
2:B:338:MET:HG2	2:B:356:ILE:HD13	1.69	0.75
1:C:230:ILE:H	1:C:230:ILE:CD1	1.99	0.75
2:F:31:LEU:HD22	2:F:35:LEU:HD23	1.67	0.74
1:G:429:THR:HG21	1:G:431:ASN:HD22	1.52	0.74
1:C:425:GLU:O	1:C:429:THR:HB	1.86	0.74
1:E:246:PRO:HG3	1:E:448:GLY:HA2	1.69	0.74
1:C:429:THR:HG21	1:C:431:ASN:HD22	1.52	0.73
1:C:96:SER:HB3	1:C:99:ASN:OD1	1.89	0.73
2:B:40:GLU:OE1	2:B:408:ARG:NH2	2.20	0.73
1:G:96:SER:HB3	1:G:99:ASN:OD1	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:186:ASN:O	2:H:190:ILE:HG12	1.88	0.73
1:E:425:GLU:O	1:E:429:THR:HB	1.89	0.73
2:B:458:GLU:O	2:B:462:GLN:HB2	1.88	0.73
2:F:245:ARG:HE	2:F:245:ARG:HA	1.54	0.73
2:F:303:THR:HG22	2:F:305:SER:H	1.54	0.73
1:A:230:ILE:H	1:A:230:ILE:CD1	2.00	0.72
2:B:186:ASN:O	2:B:190:ILE:HG12	1.88	0.72
2:F:338:MET:HG2	2:F:356:ILE:HD13	1.72	0.72
2:H:458:GLU:O	2:H:462:GLN:HB2	1.90	0.72
2:F:458:GLU:O	2:F:462:GLN:HB2	1.90	0.72
1:G:230:ILE:H	1:G:230:ILE:CD1	2.02	0.71
1:E:230:ILE:H	1:E:230:ILE:CD1	2.03	0.71
2:D:144:ARG:O	2:D:148:ILE:HG12	1.90	0.71
1:A:429:THR:HG21	1:A:431:ASN:HD22	1.55	0.71
1:G:14:ALA:N	1:G:17:ASP:OD2	2.23	0.71
2:H:31:LEU:HD22	2:H:35:LEU:HD23	1.73	0.71
2:B:144:ARG:O	2:B:148:ILE:HG12	1.91	0.71
1:G:336:ILE:HG22	1:G:338:GLN:OE1	1.91	0.71
2:D:256:ARG:HG3	2:D:256:ARG:NH1	2.03	0.70
2:D:458:GLU:O	2:D:462:GLN:HB2	1.90	0.70
2:B:245:ARG:HE	2:B:245:ARG:HA	1.54	0.70
2:H:303:THR:HG22	2:H:305:SER:H	1.55	0.70
2:D:275:VAL:HG22	2:D:279:ALA:CB	2.22	0.70
1:E:336:ILE:HG22	1:E:338:GLN:OE1	1.92	0.69
2:D:97:SER:OG	2:D:114:SER:HB3	1.92	0.69
2:D:303:THR:HG22	2:D:305:SER:H	1.56	0.69
1:C:62:HIS:CE1	1:C:66:ARG:HD2	2.26	0.69
2:B:350:ARG:NE	2:D:416:GLU:OE2	2.25	0.69
2:D:186:ASN:O	2:D:190:ILE:HG12	1.92	0.69
1:E:429:THR:HG21	1:E:431:ASN:HD22	1.57	0.69
2:F:186:ASN:O	2:F:190:ILE:HG12	1.93	0.69
1:G:246:PRO:HG3	1:G:448:GLY:HA2	1.75	0.69
2:B:97:SER:OG	2:B:114:SER:HB3	1.93	0.68
1:A:14:ALA:CB	1:A:404:PRO:HB3	2.23	0.68
2:D:31:LEU:HD22	2:D:35:LEU:HD23	1.75	0.68
1:A:175:PRO:HB3	1:E:175:PRO:HB3	1.75	0.68
1:A:290:SER:HB3	1:A:303:TYR:OH	1.94	0.68
2:H:23:ILE:HG13	2:H:23:ILE:O	1.94	0.68
2:D:175:PRO:HA	2:D:178:ARG:NH1	2.09	0.68
1:E:96:SER:HB3	1:E:99:ASN:OD1	1.93	0.67
2:F:144:ARG:O	2:F:148:ILE:HG12	1.92	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:256:ARG:HG3	2:B:256:ARG:NH1	2.04	0.67
1:E:311:TYR:C	1:E:313:VAL:H	1.98	0.67
2:B:31:LEU:HD22	2:B:35:LEU:HD23	1.76	0.66
2:B:303:THR:HG22	2:B:305:SER:H	1.61	0.65
2:F:368:ILE:O	2:F:423:LYS:HE3	1.96	0.65
2:H:368:ILE:O	2:H:423:LYS:HE3	1.96	0.65
2:H:76:ALA:HB1	2:H:129:ILE:HG23	1.76	0.65
1:G:15:ARG:HG3	1:G:15:ARG:HH11	1.62	0.64
1:G:311:TYR:C	1:G:313:VAL:H	2.00	0.64
1:A:96:SER:HB3	1:A:99:ASN:OD1	1.96	0.64
2:H:245:ARG:HE	2:H:245:ARG:HA	1.63	0.64
2:H:439:VAL:HG22	2:H:453:VAL:HG13	1.77	0.64
2:B:439:VAL:HG22	2:B:453:VAL:HG13	1.77	0.64
1:A:336:ILE:HG22	1:A:338:GLN:OE1	1.96	0.64
2:H:275:VAL:HG22	2:H:279:ALA:HB3	1.80	0.64
2:H:204:LYS:HA	2:H:233:PRO:O	1.98	0.64
2:H:256:ARG:HG3	2:H:256:ARG:NH1	2.09	0.64
2:B:405:THR:HG22	2:B:407:LYS:H	1.62	0.64
2:B:61:GLU:HA	2:B:65:ASN:HD22	1.64	0.63
1:A:311:TYR:C	1:A:313:VAL:H	2.00	0.63
1:E:311:TYR:C	1:E:313:VAL:N	2.49	0.63
2:F:236:GLU:C	2:F:238:PRO:HD3	2.19	0.63
1:A:311:TYR:C	1:A:313:VAL:N	2.50	0.63
1:C:311:TYR:C	1:C:313:VAL:N	2.50	0.63
2:B:368:ILE:O	2:B:423:LYS:HE3	1.99	0.63
1:C:336:ILE:HG22	1:C:338:GLN:OE1	1.97	0.63
2:D:136:ASP:OD2	2:D:138:SER:HB3	1.99	0.63
1:A:242:SER:OG	1:E:176:ARG:NH2	2.31	0.63
2:F:76:ALA:HB1	2:F:129:ILE:HG23	1.80	0.62
1:G:311:TYR:C	1:G:313:VAL:N	2.48	0.62
2:H:236:GLU:C	2:H:238:PRO:HD3	2.19	0.62
1:C:62:HIS:HE1	1:C:66:ARG:HD2	1.63	0.62
2:F:439:VAL:HG22	2:F:453:VAL:HG13	1.81	0.62
2:H:260:GLU:HG3	2:H:263:LEU:HG	1.81	0.62
1:C:311:TYR:C	1:C:313:VAL:H	2.01	0.62
1:G:268:ILE:HD13	1:G:268:ILE:N	2.14	0.62
1:C:379:LEU:HD13	2:D:46:SER:HB2	1.80	0.62
2:D:245:ARG:HA	2:D:245:ARG:HE	1.65	0.62
2:H:136:ASP:OD2	2:H:138:SER:HB3	2.00	0.62
2:H:90:LEU:HD13	2:H:94:ASN:ND2	2.15	0.62
2:H:39:THR:HG21	2:H:218:HIS:HB2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:PRO:HD2	2:B:99:LEU:HB3	1.81	0.61
2:F:275:VAL:HG22	2:F:279:ALA:CB	2.29	0.61
2:F:260:GLU:HG3	2:F:263:LEU:HG	1.81	0.61
2:F:136:ASP:OD2	2:F:138:SER:HB3	2.00	0.61
2:D:76:ALA:HB1	2:D:129:ILE:HG23	1.81	0.61
2:D:368:ILE:O	2:D:423:LYS:HE3	1.99	0.61
2:D:260:GLU:HG3	2:D:263:LEU:HG	1.81	0.61
2:B:275:VAL:HG22	2:B:279:ALA:CB	2.30	0.61
1:C:342:GLN:O	1:C:346:VAL:HG23	2.00	0.61
1:C:122:VAL:O	1:C:191:ARG:NH2	2.33	0.61
2:H:401:GLN:O	2:H:405:THR:HB	2.01	0.61
1:G:268:ILE:HD13	1:G:268:ILE:H	1.65	0.60
1:C:268:ILE:N	1:C:268:ILE:HD13	2.16	0.60
1:E:14:ALA:HB3	1:E:404:PRO:HB3	1.83	0.60
2:F:256:ARG:HG3	2:F:256:ARG:NH1	2.03	0.60
1:G:187:LEU:O	1:G:191:ARG:HG3	2.02	0.60
1:G:340:ALA:HB3	1:G:341:PRO:HD3	1.84	0.60
1:A:340:ALA:HB3	1:A:341:PRO:HD3	1.84	0.60
2:B:260:GLU:HG3	2:B:263:LEU:HG	1.83	0.60
2:F:192:ARG:NH1	2:F:196:LYS:HD2	2.17	0.60
1:A:289:PHE:CE2	1:A:291:ALA:HB2	2.37	0.59
2:B:76:ALA:HB1	2:B:129:ILE:HG23	1.83	0.59
1:C:249:VAL:HG12	1:C:255:GLU:HB2	1.84	0.59
1:C:268:ILE:HD13	1:C:268:ILE:H	1.65	0.59
2:F:405:THR:HG22	2:F:407:LYS:H	1.67	0.59
1:A:268:ILE:N	1:A:268:ILE:HD13	2.17	0.59
2:H:175:PRO:HA	2:H:178:ARG:NH1	2.18	0.59
1:A:268:ILE:HD13	1:A:268:ILE:H	1.67	0.59
2:B:39:THR:HG21	2:B:218:HIS:HB2	1.83	0.59
2:B:137:ASN:ND2	2:B:192:ARG:HD2	2.18	0.59
2:H:61:GLU:HA	2:H:65:ASN:HD22	1.66	0.59
2:H:405:THR:HG22	2:H:407:LYS:H	1.67	0.59
2:B:239:VAL:HG21	2:B:245:ARG:NH2	2.18	0.59
2:D:68:THR:HG23	2:D:195:LEU:HD23	1.83	0.59
2:H:375:ARG:NH2	2:H:379:GLN:OE1	2.36	0.59
1:A:187:LEU:O	1:A:191:ARG:HG3	2.03	0.58
2:D:61:GLU:HA	2:D:65:ASN:HD22	1.68	0.58
2:D:439:VAL:HG22	2:D:453:VAL:HG13	1.84	0.58
2:F:137:ASN:ND2	2:F:192:ARG:HD2	2.18	0.58
1:G:267:PRO:HD2	1:G:270:HIS:HB2	1.85	0.58
1:E:187:LEU:O	1:E:191:ARG:HG3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:97:SER:OG	2:F:114:SER:HB3	2.04	0.58
2:F:375:ARG:NH2	2:F:379:GLN:OE1	2.36	0.58
1:E:296:LYS:HE2	1:E:298:MET:CE	2.34	0.58
2:F:91:GLU:OE2	2:F:121:LYS:HD2	2.04	0.58
1:E:268:ILE:HD13	1:E:268:ILE:N	2.19	0.57
1:G:294:PRO:HB3	2:H:89:GLU:HA	1.86	0.57
2:H:204:LYS:HG3	2:H:235:SER:OG	2.04	0.57
1:E:256:LEU:CD1	1:E:314:GLU:HG2	2.34	0.57
2:H:91:GLU:OE2	2:H:121:LYS:HD2	2.05	0.57
2:B:236:GLU:C	2:B:238:PRO:HD3	2.25	0.57
1:C:267:PRO:HD2	1:C:270:HIS:HB2	1.85	0.57
2:D:236:GLU:C	2:D:238:PRO:HD3	2.25	0.56
2:F:401:GLN:O	2:F:405:THR:HB	2.04	0.56
1:G:67:LEU:HD13	1:G:135:GLN:HG3	1.86	0.56
1:A:373:GLN:NE2	2:B:93:GLU:OE1	2.37	0.56
2:H:255:GLU:HB3	2:H:453:VAL:HG23	1.87	0.56
1:E:342:GLN:O	1:E:346:VAL:HG23	2.05	0.56
1:C:256:LEU:CD1	1:C:314:GLU:HG2	2.35	0.56
1:E:340:ALA:HB3	1:E:341:PRO:HD3	1.86	0.56
2:H:137:ASN:ND2	2:H:192:ARG:HD2	2.20	0.56
2:B:375:ARG:NH2	2:B:379:GLN:OE1	2.38	0.56
2:D:39:THR:HG21	2:D:218:HIS:HB2	1.87	0.56
2:F:255:GLU:HB3	2:F:453:VAL:HG23	1.87	0.56
2:H:97:SER:OG	2:H:114:SER:HB3	2.06	0.56
1:A:114:MET:HE2	1:A:118:MET:HG3	1.87	0.56
2:H:311:VAL:O	2:H:315:GLN:HG3	2.05	0.56
2:D:311:VAL:O	2:D:315:GLN:HG3	2.06	0.56
2:B:245:ARG:HA	2:B:245:ARG:NE	2.19	0.55
2:D:350:ARG:O	2:D:354:ASN:ND2	2.39	0.55
1:E:268:ILE:HD13	1:E:268:ILE:H	1.70	0.55
1:C:67:LEU:HD13	1:C:135:GLN:HG3	1.88	0.55
2:F:61:GLU:HA	2:F:65:ASN:HD22	1.72	0.55
2:F:90:LEU:HD13	2:F:94:ASN:ND2	2.21	0.55
2:F:68:THR:HG23	2:F:195:LEU:HD23	1.88	0.55
2:F:175:PRO:HA	2:F:178:ARG:NH1	2.21	0.55
2:D:275:VAL:HG22	2:D:279:ALA:HB3	1.86	0.55
2:B:260:GLU:OE2	2:B:262:THR:HG23	2.07	0.55
2:D:255:GLU:HB3	2:D:453:VAL:HG23	1.88	0.55
1:A:67:LEU:HD13	1:A:135:GLN:HG3	1.88	0.55
1:C:187:LEU:O	1:C:191:ARG:HG3	2.06	0.55
2:B:275:VAL:HG22	2:B:279:ALA:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:249:VAL:HG12	1:G:255:GLU:HB2	1.89	0.55
1:G:256:LEU:CD1	1:G:314:GLU:HG2	2.36	0.55
1:E:122:VAL:O	1:E:191:ARG:NH2	2.40	0.54
1:E:256:LEU:HD11	1:E:314:GLU:HG2	1.89	0.54
1:E:267:PRO:HD2	1:E:270:HIS:HB2	1.88	0.54
2:D:119:ILE:N	2:D:120:PRO:HD2	2.23	0.54
2:F:275:VAL:HG22	2:F:279:ALA:HB3	1.89	0.54
1:C:256:LEU:HD11	1:C:314:GLU:HG2	1.89	0.54
1:G:14:ALA:N	1:G:19:PHE:HB3	2.22	0.54
2:H:192:ARG:NH1	2:H:196:LYS:HD2	2.23	0.54
2:F:116:GLN:O	2:F:119:ILE:HG12	2.08	0.53
2:B:136:ASP:OD2	2:B:138:SER:HB3	2.08	0.53
1:C:99:ASN:HD22	1:C:101:MET:CE	2.21	0.53
2:D:375:ARG:NH2	2:D:379:GLN:OE1	2.41	0.53
1:E:249:VAL:HG12	1:E:255:GLU:HB2	1.91	0.53
1:A:176:ARG:NH2	1:E:242:SER:OG	2.41	0.53
2:H:141:GLU:O	2:H:144:ARG:HG3	2.08	0.53
1:G:296:LYS:HE2	1:G:298:MET:CE	2.38	0.53
2:H:27:ARG:HH11	2:H:27:ARG:HB3	1.73	0.53
2:F:260:GLU:OE2	2:F:262:THR:HG23	2.08	0.53
1:A:99:ASN:HD22	1:A:101:MET:CE	2.22	0.53
1:E:67:LEU:HD13	1:E:135:GLN:HG3	1.91	0.53
1:E:243:CYS:HA	1:E:446:MET:O	2.09	0.53
2:D:192:ARG:NH1	2:D:196:LYS:HD2	2.24	0.52
2:B:311:VAL:O	2:B:315:GLN:HG3	2.10	0.52
2:B:397:ASP:OD2	2:B:408:ARG:NH1	2.40	0.52
2:H:68:THR:HG23	2:H:195:LEU:HD23	1.91	0.52
2:B:401:GLN:O	2:B:405:THR:HB	2.10	0.52
2:D:405:THR:HG22	2:D:407:LYS:H	1.74	0.52
2:F:256:ARG:HH11	2:F:256:ARG:CG	2.15	0.52
1:E:45:TYR:OH	1:E:389:LEU:HG	2.09	0.52
2:F:40:GLU:OE1	2:F:408:ARG:NH2	2.43	0.52
1:A:256:LEU:CD1	1:A:314:GLU:HG2	2.40	0.51
1:A:429:THR:CG2	1:A:431:ASN:ND2	2.71	0.51
2:B:68:THR:HG23	2:B:195:LEU:HD23	1.91	0.51
2:F:119:ILE:N	2:F:120:PRO:HD2	2.26	0.51
2:H:119:ILE:N	2:H:120:PRO:HD2	2.25	0.51
1:A:267:PRO:HD2	1:A:270:HIS:HB2	1.92	0.51
1:A:287:GLY:C	1:A:289:PHE:H	2.13	0.51
2:H:40:GLU:OE1	2:H:408:ARG:NH2	2.43	0.51
1:A:246:PRO:HG3	1:A:448:GLY:HA2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:17:ASP:O	1:C:18:ASN:HB3	2.11	0.51
1:E:241:GLU:HA	1:E:444:VAL:O	2.09	0.51
2:F:39:THR:HG21	2:F:218:HIS:HB2	1.92	0.51
2:H:234:LYS:HG2	2:H:235:SER:O	2.11	0.51
1:A:403:ILE:HG23	1:A:403:ILE:O	2.11	0.51
1:C:429:THR:CG2	1:C:431:ASN:ND2	2.70	0.51
2:F:311:VAL:O	2:F:315:GLN:HG3	2.10	0.51
1:G:140:GLU:HB3	1:G:176:ARG:NH1	2.25	0.51
1:C:45:TYR:OH	1:C:389:LEU:HG	2.11	0.51
2:D:401:GLN:O	2:D:405:THR:HB	2.11	0.51
1:G:19:PHE:HD1	1:G:392:MET:HE1	1.75	0.51
2:H:260:GLU:OE2	2:H:262:THR:HG23	2.11	0.50
2:F:141:GLU:O	2:F:144:ARG:HG3	2.11	0.50
1:C:340:ALA:HB3	1:C:341:PRO:HD3	1.93	0.50
1:G:377:SER:O	1:G:381:ASN:HB2	2.12	0.50
1:C:467:ASN:O	1:C:468:SER:HB2	2.10	0.50
1:A:344:VAL:HG21	1:A:456:VAL:HG22	1.94	0.50
1:E:99:ASN:HD22	1:E:101:MET:CE	2.24	0.50
1:G:48:ALA:HB1	1:G:190:TYR:OH	2.11	0.50
1:G:128:THR:OG1	1:G:131:GLU:HG3	2.12	0.50
1:A:377:SER:O	1:A:381:ASN:HB2	2.12	0.49
2:D:255:GLU:HB3	2:D:453:VAL:CG2	2.42	0.49
2:B:91:GLU:OE2	2:B:121:LYS:HD2	2.12	0.49
1:C:81:ALA:O	1:C:85:GLU:HG3	2.12	0.49
1:C:286:GLY:O	1:C:315:ASN:ND2	2.45	0.49
2:D:48:ALA:HB3	2:D:119:ILE:HD11	1.95	0.49
1:G:256:LEU:HD11	1:G:314:GLU:HG2	1.92	0.49
2:H:207:ARG:HH11	2:H:245:ARG:NH1	2.09	0.49
2:F:255:GLU:HB3	2:F:453:VAL:CG2	2.42	0.49
1:G:99:ASN:HD22	1:G:101:MET:CE	2.24	0.49
2:B:175:PRO:HA	2:B:178:ARG:NH1	2.27	0.49
1:A:35:THR:HB	1:A:36:PRO:CD	2.42	0.49
1:A:342:GLN:O	1:A:346:VAL:HG23	2.13	0.49
1:G:17:ASP:O	1:G:18:ASN:HB3	2.12	0.49
2:B:90:LEU:HD13	2:B:94:ASN:ND2	2.27	0.49
2:F:144:ARG:HH21	2:F:188:LYS:C	2.16	0.49
2:B:62:ASN:OD1	2:B:65:ASN:HB2	2.13	0.49
2:B:373:VAL:O	2:B:377:LYS:HG3	2.13	0.48
1:C:246:PRO:HG3	1:C:448:GLY:CA	2.39	0.48
2:F:137:ASN:HD21	2:F:192:ARG:HD2	1.78	0.48
1:A:316:CYS:SG	1:A:333:LEU:HD23	2.54	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:90:LEU:CD1	2:H:94:ASN:HD21	2.27	0.48
2:H:144:ARG:HH21	2:H:188:LYS:C	2.15	0.48
2:D:90:LEU:HD13	2:D:94:ASN:ND2	2.29	0.48
1:G:268:ILE:H	1:G:268:ILE:CD1	2.27	0.48
2:H:255:GLU:HB3	2:H:453:VAL:CG2	2.43	0.48
1:C:377:SER:O	1:C:381:ASN:HB2	2.14	0.48
1:A:128:THR:OG1	1:A:131:GLU:HG3	2.14	0.48
1:C:114:MET:HE2	1:C:118:MET:HG3	1.96	0.48
1:G:342:GLN:O	1:G:346:VAL:HG23	2.14	0.48
1:C:235:ALA:O	1:C:436:GLY:HA3	2.14	0.48
2:D:91:GLU:OE2	2:D:121:LYS:HD2	2.13	0.48
2:B:428:MET:HA	2:B:428:MET:CE	2.44	0.47
1:C:268:ILE:H	1:C:268:ILE:CD1	2.28	0.47
2:B:441:MET:HE1	2:B:451:PRO:O	2.15	0.47
1:C:201:VAL:HG23	1:C:397:LEU:CD1	2.45	0.47
2:D:137:ASN:ND2	2:D:192:ARG:HD2	2.29	0.47
2:B:137:ASN:HD21	2:B:192:ARG:HD2	1.77	0.47
2:D:260:GLU:OE2	2:D:262:THR:HG23	2.13	0.47
1:E:377:SER:O	1:E:381:ASN:HB2	2.14	0.47
2:F:27:ARG:HB3	2:F:27:ARG:HH11	1.80	0.47
2:B:239:VAL:HG21	2:B:245:ARG:HH21	1.79	0.47
2:D:141:GLU:O	2:D:144:ARG:HG3	2.14	0.47
1:E:407:GLU:HG2	1:E:411:LYS:HE3	1.97	0.47
1:E:333:LEU:HD13	1:E:334:SER:N	2.30	0.47
1:E:392:MET:HE2	1:E:402:LYS:HD2	1.96	0.47
2:F:61:GLU:OE1	2:F:66:ASN:HA	2.14	0.47
1:G:275:ALA:HB3	1:G:423:VAL:HG21	1.97	0.47
2:H:232:VAL:HG13	2:H:233:PRO:HD2	1.95	0.47
2:F:245:ARG:HA	2:F:245:ARG:NE	2.24	0.47
2:F:295:TRP:CZ2	2:F:297:ARG:HA	2.49	0.47
2:H:370:ASP:OD1	2:H:423:LYS:NZ	2.46	0.47
1:A:392:MET:HE2	1:A:402:LYS:HD2	1.96	0.46
1:C:45:TYR:N	1:C:45:TYR:CD1	2.82	0.46
2:H:147:ILE:HG22	2:H:187:ILE:HD13	1.97	0.46
1:E:467:ASN:O	1:E:468:SER:HB2	2.14	0.46
1:A:304:THR:HG22	1:A:305:HIS:ND1	2.29	0.46
1:G:310:TYR:HB3	1:G:312:PHE:CZ	2.51	0.46
2:F:218:HIS:O	2:F:222:VAL:HG23	2.16	0.46
2:F:52:ILE:HG23	2:F:52:ILE:O	2.16	0.46
1:G:72:THR:HG21	1:G:120:GLU:HB3	1.97	0.46
2:H:119:ILE:O	2:H:122:ALA:HB3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:VAL:O	1:A:191:ARG:NH2	2.48	0.46
2:B:141:GLU:O	2:B:144:ARG:HG3	2.16	0.46
1:G:62:HIS:CE1	1:G:66:ARG:HD2	2.50	0.46
2:F:398:ILE:HA	2:F:408:ARG:HG3	1.98	0.46
1:G:67:LEU:HD13	1:G:135:GLN:CG	2.46	0.46
1:G:407:GLU:HG2	1:G:411:LYS:HE3	1.98	0.46
1:G:429:THR:CG2	1:G:431:ASN:ND2	2.74	0.46
1:C:35:THR:HB	1:C:36:PRO:CD	2.46	0.46
1:E:81:ALA:O	1:E:85:GLU:HG3	2.16	0.46
1:E:270:HIS:O	1:E:273:ILE:HB	2.16	0.46
1:E:429:THR:CG2	1:E:431:ASN:ND2	2.75	0.46
2:H:317:GLY:O	2:H:318:SER:CB	2.63	0.46
1:A:19:PHE:HD1	1:A:392:MET:HE1	1.81	0.45
2:D:370:ASP:OD1	2:D:423:LYS:NZ	2.47	0.45
2:F:192:ARG:HH12	2:F:196:LYS:HD2	1.80	0.45
1:A:72:THR:HG21	1:A:120:GLU:HB3	1.98	0.45
2:D:253:ARG:NH2	2:D:457:GLU:OE1	2.49	0.45
2:F:349:VAL:N	2:F:449:THR:OG1	2.49	0.45
1:E:140:GLU:HB3	1:E:176:ARG:NH1	2.31	0.45
1:A:268:ILE:H	1:A:268:ILE:CD1	2.30	0.45
1:C:201:VAL:HG23	1:C:397:LEU:HD13	1.98	0.45
2:H:439:VAL:HG13	2:H:457:GLU:HG2	1.98	0.45
1:G:344:VAL:HG21	1:G:456:VAL:HG22	1.98	0.45
2:H:90:LEU:HD13	2:H:94:ASN:HD21	1.77	0.45
1:A:45:TYR:OH	1:A:389:LEU:HG	2.16	0.45
1:A:403:ILE:O	1:A:403:ILE:CG2	2.65	0.45
2:B:439:VAL:HG13	2:B:457:GLU:HG2	1.98	0.45
1:E:45:TYR:N	1:E:45:TYR:CD1	2.84	0.45
2:F:148:ILE:HD13	2:F:187:ILE:HG21	1.97	0.45
1:G:346:VAL:O	1:G:350:GLN:HG2	2.16	0.45
1:A:256:LEU:HD11	1:A:314:GLU:HG2	1.97	0.45
1:A:275:ALA:HB3	1:A:423:VAL:HG21	1.97	0.45
2:D:439:VAL:HG13	2:D:457:GLU:HG2	1.99	0.45
1:E:296:LYS:HE2	1:E:298:MET:HE1	1.99	0.45
1:G:95:SER:HB3	1:G:100:LEU:HD13	1.98	0.45
2:H:61:GLU:OE1	2:H:66:ASN:HA	2.17	0.45
2:H:116:GLN:O	2:H:119:ILE:HG12	2.16	0.45
2:H:295:TRP:CZ2	2:H:297:ARG:HA	2.51	0.45
2:H:373:VAL:O	2:H:377:LYS:HG3	2.16	0.45
2:B:305:SER:HA	2:B:306:PRO:HD3	1.67	0.45
1:C:267:PRO:HA	1:C:323:TYR:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:41:ALA:HA	1:E:105:SER:HA	1.99	0.45
1:G:45:TYR:CD1	1:G:45:TYR:N	2.85	0.45
1:G:56:ASN:HD22	1:G:56:ASN:HA	1.57	0.45
2:B:61:GLU:OE1	2:B:66:ASN:HA	2.17	0.45
1:G:304:THR:HG22	1:G:305:HIS:ND1	2.31	0.45
2:H:136:ASP:O	2:H:140:ILE:HG13	2.17	0.45
2:D:27:ARG:HB3	2:D:27:ARG:HH11	1.82	0.44
1:G:19:PHE:HD1	1:G:392:MET:CE	2.30	0.44
2:B:255:GLU:HB3	2:B:453:VAL:HG23	1.99	0.44
1:E:33:SER:CB	1:E:392:MET:CE	2.88	0.44
1:E:245:PRO:HA	1:E:246:PRO:HD3	1.80	0.44
1:E:296:LYS:HE2	1:E:298:MET:HE2	1.98	0.44
1:E:336:ILE:HG22	1:E:337:PRO:HD2	1.98	0.44
1:G:127:ILE:HB	1:G:184:LYS:HE3	1.98	0.44
2:H:31:LEU:HD21	2:H:226:GLN:HA	1.98	0.44
2:H:218:HIS:O	2:H:222:VAL:HG23	2.17	0.44
2:F:305:SER:HA	2:F:306:PRO:HD3	1.67	0.44
2:F:317:GLY:O	2:F:318:SER:CB	2.64	0.44
1:G:122:VAL:O	1:G:191:ARG:NH2	2.50	0.44
2:H:397:ASP:OD2	2:H:408:ARG:NH1	2.49	0.44
2:D:303:THR:HG22	2:D:304:ASN:N	2.32	0.44
1:E:379:LEU:HD13	2:F:46:SER:HB2	1.98	0.44
1:G:386:LEU:HD12	1:G:386:LEU:HA	1.80	0.44
2:B:204:LYS:HG3	2:B:235:SER:OG	2.17	0.44
2:D:245:ARG:HA	2:D:245:ARG:NE	2.30	0.44
2:D:398:ILE:HA	2:D:408:ARG:HG3	2.00	0.44
1:E:17:ASP:O	1:E:18:ASN:HB3	2.17	0.44
1:E:253:LEU:HA	1:E:254:PRO:HD3	1.86	0.44
2:B:119:ILE:N	2:B:120:PRO:HD2	2.33	0.44
2:B:207:ARG:HH11	2:B:245:ARG:NH1	2.15	0.44
2:D:317:GLY:O	2:D:318:SER:CB	2.65	0.44
1:E:67:LEU:HD13	1:E:135:GLN:CG	2.47	0.44
1:A:45:TYR:N	1:A:45:TYR:CD1	2.86	0.44
2:B:61:GLU:HA	2:B:65:ASN:ND2	2.31	0.44
2:B:62:ASN:CG	2:B:65:ASN:HB2	2.37	0.44
1:E:114:MET:HE2	1:E:118:MET:HG3	1.99	0.44
2:H:207:ARG:NH1	2:H:245:ARG:NH1	2.65	0.44
1:A:287:GLY:O	1:A:289:PHE:N	2.51	0.44
2:B:255:GLU:HA	2:B:441:MET:O	2.18	0.44
1:E:32:THR:HG21	1:E:209:HIS:HA	2.00	0.44
2:H:398:ILE:HA	2:H:408:ARG:HG3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:LYS:HE2	1:A:298:MET:CE	2.48	0.44
1:C:333:LEU:HD13	1:C:334:SER:N	2.32	0.44
1:E:95:SER:HB3	1:E:100:LEU:HD13	2.00	0.44
1:E:444:VAL:HG11	1:E:456:VAL:HG11	1.98	0.44
1:A:95:SER:HB3	1:A:100:LEU:HD13	2.00	0.43
1:A:294:PRO:HB3	2:B:89:GLU:HA	1.99	0.43
1:A:407:GLU:HG2	1:A:411:LYS:HE3	1.99	0.43
1:C:72:THR:HG21	1:C:120:GLU:HB3	2.00	0.43
1:G:15:ARG:HG3	1:G:15:ARG:NH1	2.31	0.43
2:H:317:GLY:O	2:H:318:SER:OG	2.25	0.43
2:D:158:TYR:O	2:D:162:VAL:HG23	2.19	0.43
1:G:35:THR:HB	1:G:36:PRO:CD	2.48	0.43
2:H:39:THR:HG21	2:H:218:HIS:CB	2.48	0.43
2:H:148:ILE:HD13	2:H:187:ILE:HG21	2.00	0.43
2:H:303:THR:HG22	2:H:305:SER:N	2.29	0.43
2:B:97:SER:OG	2:B:114:SER:CB	2.64	0.43
2:B:144:ARG:HH21	2:B:188:LYS:C	2.21	0.43
1:C:444:VAL:HG11	1:C:456:VAL:HG11	2.00	0.43
2:D:253:ARG:HB3	2:D:438:PRO:HB2	2.00	0.43
1:G:263:PHE:CE2	1:G:442:ALA:HB2	2.53	0.43
2:B:429:TRP:CE2	2:B:433:ARG:HG3	2.54	0.43
2:B:439:VAL:CG2	2:B:453:VAL:HG13	2.47	0.43
1:C:67:LEU:HD13	1:C:135:GLN:CG	2.48	0.43
1:E:35:THR:HB	1:E:36:PRO:CD	2.48	0.43
2:D:97:SER:OG	2:D:114:SER:CB	2.63	0.43
2:D:236:GLU:O	2:D:238:PRO:HD3	2.18	0.43
1:E:99:ASN:HD22	1:E:101:MET:HE3	1.81	0.43
1:E:268:ILE:H	1:E:268:ILE:CD1	2.31	0.43
2:H:137:ASN:HD21	2:H:192:ARG:HD2	1.80	0.43
2:H:268:ILE:HD12	2:H:268:ILE:N	2.33	0.43
2:B:398:ILE:HA	2:B:408:ARG:HG3	2.01	0.43
2:D:62:ASN:CG	2:D:65:ASN:HB2	2.39	0.43
2:D:373:VAL:O	2:D:377:LYS:HG3	2.18	0.43
1:E:62:HIS:CE1	1:E:66:ARG:HD2	2.54	0.43
1:G:41:ALA:HA	1:G:105:SER:HA	2.00	0.43
2:H:291:ILE:HD12	2:H:426:ILE:HD13	2.01	0.43
2:B:263:LEU:HA	2:B:264:PRO:HD3	1.82	0.43
2:B:350:ARG:NH2	2:D:419:ASP:OD2	2.46	0.43
1:E:267:PRO:HA	1:E:323:TYR:O	2.19	0.43
2:H:263:LEU:HA	2:H:264:PRO:HD3	1.79	0.43
2:F:119:ILE:O	2:F:122:ALA:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:92:ILE:HG23	2:H:97:SER:HB2	2.01	0.43
2:H:165:HIS:HD2	2:H:256:ARG:HE	1.67	0.43
1:A:311:TYR:O	1:A:313:VAL:N	2.51	0.43
1:A:299:TYR:OH	2:B:86:GLN:HG2	2.19	0.43
2:B:27:ARG:HH11	2:B:27:ARG:HB3	1.82	0.42
1:A:85:GLU:OE2	2:B:303:THR:HG23	2.17	0.42
1:A:167:THR:OG1	1:A:168:LEU:N	2.51	0.42
2:B:99:LEU:HD12	2:B:99:LEU:HA	1.91	0.42
2:B:207:ARG:NH1	2:B:245:ARG:NH1	2.66	0.42
1:C:311:TYR:O	1:C:313:VAL:N	2.52	0.42
1:G:403:ILE:HG23	1:G:403:ILE:O	2.17	0.42
2:H:232:VAL:HA	2:H:233:PRO:HD3	1.68	0.42
2:D:209:VAL:HG21	2:D:402:VAL:HG12	2.02	0.42
2:F:253:ARG:HB3	2:F:438:PRO:HB2	2.01	0.42
2:F:253:ARG:HH21	2:F:457:GLU:CD	2.23	0.42
1:G:267:PRO:HA	1:G:323:TYR:O	2.19	0.42
1:A:17:ASP:O	1:A:18:ASN:HB3	2.20	0.42
1:E:302:LEU:HD23	1:E:302:LEU:HA	1.90	0.42
2:F:204:LYS:HG3	2:F:235:SER:OG	2.19	0.42
2:F:439:VAL:HG13	2:F:457:GLU:HG2	2.02	0.42
2:H:81:GLN:HG3	2:H:132:LYS:O	2.20	0.42
2:H:253:ARG:HB3	2:H:438:PRO:HB2	2.01	0.42
1:A:267:PRO:HA	1:A:323:TYR:O	2.19	0.42
2:B:148:ILE:HD13	2:B:187:ILE:HG21	2.00	0.42
2:D:253:ARG:HH21	2:D:457:GLU:CD	2.23	0.42
2:D:255:GLU:HA	2:D:441:MET:O	2.20	0.42
1:G:84:LEU:HD13	1:G:91:TYR:CZ	2.55	0.42
1:G:315:ASN:OD1	1:G:316:CYS:N	2.52	0.42
1:A:99:ASN:HB2	1:A:101:MET:CE	2.50	0.42
1:A:270:HIS:O	1:A:273:ILE:HB	2.20	0.42
2:B:349:VAL:N	2:B:449:THR:OG1	2.53	0.42
2:D:204:LYS:HA	2:D:233:PRO:O	2.20	0.42
2:F:148:ILE:CD1	2:F:187:ILE:HG21	2.49	0.42
2:F:370:ASP:OD1	2:F:423:LYS:NZ	2.51	0.42
1:G:99:ASN:HD22	1:G:101:MET:HE2	1.85	0.42
1:C:403:ILE:O	1:C:403:ILE:HG23	2.18	0.42
1:G:276:LEU:HD11	1:G:329:PHE:CD2	2.54	0.42
1:G:392:MET:HE2	1:G:402:LYS:HD2	2.01	0.42
1:C:128:THR:OG1	1:C:131:GLU:HG3	2.19	0.41
1:C:310:TYR:CD1	1:C:312:PHE:CZ	3.08	0.41
2:D:305:SER:HA	2:D:306:PRO:HD3	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:THR:HB	1:A:36:PRO:HD2	2.02	0.41
2:B:166:LEU:HA	2:B:442:VAL:HG21	2.03	0.41
2:B:232:VAL:HA	2:B:233:PRO:HD3	1.73	0.41
2:D:23:ILE:HA	2:D:24:PRO:HD3	1.80	0.41
2:D:263:LEU:HA	2:D:264:PRO:HD3	1.78	0.41
1:E:263:PHE:CE2	1:E:442:ALA:HB2	2.55	0.41
2:F:35:LEU:HA	2:F:205:GLY:O	2.20	0.41
2:H:62:ASN:CG	2:H:65:ASN:HB2	2.40	0.41
2:H:357:LEU:O	2:H:361:LYS:HG3	2.20	0.41
2:F:158:TYR:O	2:F:162:VAL:HG23	2.20	0.41
1:G:235:ALA:O	1:G:436:GLY:HA3	2.20	0.41
1:G:444:VAL:HG11	1:G:456:VAL:HG11	2.01	0.41
2:B:48:ALA:HB3	2:B:119:ILE:HD11	2.03	0.41
1:G:253:LEU:HA	1:G:254:PRO:HD3	1.93	0.41
1:E:403:ILE:O	1:E:403:ILE:HG23	2.20	0.41
2:F:90:LEU:CD1	2:F:94:ASN:HD21	2.34	0.41
1:A:32:THR:HG21	1:A:209:HIS:HA	2.02	0.41
1:A:200:THR:HG22	1:A:201:VAL:N	2.35	0.41
1:C:99:ASN:HD22	1:C:101:MET:HE3	1.85	0.41
2:D:116:GLN:O	2:D:119:ILE:HG12	2.20	0.41
1:G:34:ASN:OD1	1:G:35:THR:N	2.43	0.41
1:C:127:ILE:HB	1:C:184:LYS:HE3	2.03	0.41
1:C:403:ILE:O	1:C:403:ILE:CG2	2.69	0.41
2:D:31:LEU:HD21	2:D:226:GLN:HA	2.02	0.41
2:F:303:THR:HG22	2:F:305:SER:N	2.28	0.41
1:G:429:THR:CG2	1:G:429:THR:O	2.69	0.41
1:A:73:GLU:HG2	1:A:124:PHE:HB3	2.02	0.41
1:C:56:ASN:HD22	1:C:56:ASN:HA	1.55	0.41
1:E:429:THR:HG22	1:E:431:ASN:HD22	1.83	0.41
1:G:403:ILE:O	1:G:403:ILE:CG2	2.68	0.41
1:A:47:ASP:HB3	1:A:199:ASN:OD1	2.21	0.41
1:A:287:GLY:C	1:A:289:PHE:N	2.74	0.41
1:C:16:THR:HG23	1:C:18:ASN:H	1.86	0.41
2:D:62:ASN:OD1	2:D:65:ASN:HB2	2.21	0.41
2:D:144:ARG:HH21	2:D:188:LYS:C	2.23	0.41
1:E:230:ILE:HD13	1:G:233:LYS:CE	2.50	0.41
2:F:147:ILE:HG22	2:F:187:ILE:HD13	2.03	0.41
1:G:268:ILE:N	1:G:268:ILE:CD1	2.82	0.41
2:H:52:ILE:HG23	2:H:52:ILE:O	2.21	0.41
2:H:255:GLU:HA	2:H:441:MET:O	2.20	0.41
2:H:439:VAL:CG2	2:H:453:VAL:HG13	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:136:ASP:O	2:B:140:ILE:HG13	2.21	0.41
1:C:33:SER:CB	1:C:392:MET:CE	2.90	0.41
1:C:263:PHE:CE2	1:C:442:ALA:HB2	2.56	0.41
1:E:204:PHE:CD1	1:E:204:PHE:N	2.88	0.41
2:F:222:VAL:O	2:F:225:ALA:HB3	2.21	0.41
2:F:397:ASP:OD2	2:F:408:ARG:NH1	2.50	0.41
1:G:333:LEU:HD13	1:G:334:SER:N	2.35	0.41
2:B:116:GLN:O	2:B:119:ILE:HG12	2.21	0.40
2:B:423:LYS:O	2:B:427:ILE:HG13	2.21	0.40
2:D:61:GLU:OE1	2:D:66:ASN:HA	2.22	0.40
2:F:373:VAL:O	2:F:377:LYS:HG3	2.21	0.40
1:G:45:TYR:OH	1:G:389:LEU:HG	2.21	0.40
1:G:63:ILE:HG22	1:G:67:LEU:HD22	2.02	0.40
2:H:172:LYS:HD2	2:H:172:LYS:HA	1.88	0.40
1:A:67:LEU:HD13	1:A:135:GLN:CG	2.49	0.40
1:A:140:GLU:HB3	1:A:176:ARG:NH1	2.36	0.40
2:B:303:THR:HG22	2:B:305:SER:N	2.32	0.40
2:D:143:GLU:O	2:D:147:ILE:HG12	2.22	0.40
2:D:172:LYS:O	2:D:174:GLN:HG3	2.21	0.40
2:D:207:ARG:NH1	2:D:245:ARG:NH1	2.69	0.40
1:E:72:THR:HG21	1:E:120:GLU:HB3	2.02	0.40
1:E:99:ASN:HB2	1:E:101:MET:CE	2.51	0.40
1:E:275:ALA:HB3	1:E:423:VAL:HG21	2.03	0.40
2:F:62:ASN:CG	2:F:65:ASN:HB2	2.42	0.40
1:G:237:TYR:CG	1:G:264:GLU:HB2	2.56	0.40
2:H:35:LEU:HA	2:H:205:GLY:O	2.22	0.40
2:H:148:ILE:CD1	2:H:187:ILE:HG21	2.52	0.40
1:A:99:ASN:HD22	1:A:101:MET:HE3	1.87	0.40
1:C:48:ALA:HB1	1:C:190:TYR:OH	2.21	0.40
1:C:386:LEU:HD12	1:C:386:LEU:HA	1.91	0.40
2:D:99:LEU:HD12	2:D:99:LEU:HA	1.87	0.40
2:F:255:GLU:HA	2:F:441:MET:O	2.21	0.40
2:F:349:VAL:O	2:F:352:ILE:HG22	2.22	0.40
2:H:253:ARG:HH21	2:H:457:GLU:CD	2.25	0.40
1:A:62:HIS:CD2	1:A:66:ARG:HD2	2.57	0.40
1:A:241:GLU:HA	1:A:444:VAL:O	2.20	0.40
1:A:336:ILE:HG22	1:A:337:PRO:HD2	2.04	0.40
1:C:140:GLU:HB3	1:C:176:ARG:NH1	2.37	0.40
2:D:232:VAL:HA	2:D:233:PRO:HD3	1.74	0.40
2:D:295:TRP:CZ2	2:D:297:ARG:HA	2.57	0.40
1:E:35:THR:HB	1:E:36:PRO:HD2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:266:LEU:HA	1:E:267:PRO:HD3	1.89	0.40
2:F:159:ASP:OD1	2:F:159:ASP:N	2.54	0.40
2:F:253:ARG:NH2	2:F:457:GLU:OE1	2.55	0.40
2:D:218:HIS:O	2:D:222:VAL:HG23	2.21	0.40
1:E:56:ASN:HD22	1:E:56:ASN:HA	1.58	0.40
1:E:230:ILE:HD13	1:G:233:LYS:HE3	2.02	0.40
2:F:263:LEU:HA	2:F:264:PRO:HD3	1.79	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	455/475 (96%)	435 (96%)	16 (4%)	4 (1%)	17 24
1	C	440/475 (93%)	421 (96%)	17 (4%)	2 (0%)	29 40
1	E	444/475 (94%)	422 (95%)	20 (4%)	2 (0%)	29 40
1	G	446/475 (94%)	425 (95%)	19 (4%)	2 (0%)	34 46
2	B	437/443 (99%)	423 (97%)	12 (3%)	2 (0%)	29 40
2	D	439/443 (99%)	423 (96%)	15 (3%)	1 (0%)	47 60
2	F	438/443 (99%)	421 (96%)	16 (4%)	1 (0%)	47 60
2	H	438/443 (99%)	420 (96%)	16 (4%)	2 (0%)	29 40
All	All	3537/3672 (96%)	3390 (96%)	131 (4%)	16 (0%)	29 40

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	250	PHE
1	G	250	PHE
2	H	24	PRO

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Mol	Chain	Res	Type
1	A	250	PHE
1	A	288	SER
2	B	318	SER
2	D	318	SER
1	E	250	PHE
2	F	318	SER
2	H	318	SER
1	A	290	SER
2	B	56	ALA
1	A	127	ILE
1	C	127	ILE
1	E	127	ILE
1	G	127	ILE

### 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	384/401 (96%)	364 (95%)	20 (5%)	23	30
1	C	376/401 (94%)	353 (94%)	23 (6%)	18	24
1	E	379/401 (94%)	357 (94%)	22 (6%)	20	26
1	G	378/401 (94%)	356 (94%)	22 (6%)	20	26
2	B	376/379 (99%)	356 (95%)	20 (5%)	22	30
2	D	378/379 (100%)	358 (95%)	20 (5%)	22	30
2	F	377/379 (100%)	357 (95%)	20 (5%)	22	30
2	H	377/379 (100%)	356 (94%)	21 (6%)	21	28
All	All	3025/3120 (97%)	2857 (94%)	168 (6%)	21	28

All (168) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	ASN
1	A	65	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	66	ARG
1	A	67	LEU
1	A	176	ARG
1	A	220	LEU
1	A	230	ILE
1	A	268	ILE
1	A	273	ILE
1	A	288	SER
1	A	305	HIS
1	A	311	TYR
1	A	314	GLU
1	A	361	ARG
1	A	381	ASN
1	A	382	LEU
1	A	386	LEU
1	A	429	THR
1	A	445	VAL
1	A	446	MET
2	B	27	ARG
2	B	39	THR
2	B	71	PHE
2	B	75	LEU
2	B	133	SER
2	B	149	ARG
2	B	181	LEU
2	B	219	GLU
2	B	275	VAL
2	B	346	GLU
2	B	350	ARG
2	B	375	ARG
2	B	400	ARG
2	B	405	THR
2	B	408	ARG
2	B	424	ASP
2	B	428	MET
2	B	439	VAL
2	B	447	THR
2	B	449	THR
1	C	56	ASN
1	C	62	HIS
1	C	65	ASP
1	C	66	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	67	LEU
1	C	151	GLU
1	C	176	ARG
1	C	220	LEU
1	C	230	ILE
1	C	268	ILE
1	C	273	ILE
1	C	303	TYR
1	C	305	HIS
1	C	311	TYR
1	C	314	GLU
1	C	361	ARG
1	C	381	ASN
1	C	382	LEU
1	C	386	LEU
1	C	399	HIS
1	C	429	THR
1	C	445	VAL
1	C	446	MET
2	D	27	ARG
2	D	39	THR
2	D	66	ASN
2	D	71	PHE
2	D	75	LEU
2	D	149	ARG
2	D	181	LEU
2	D	219	GLU
2	D	253	ARG
2	D	275	VAL
2	D	346	GLU
2	D	375	ARG
2	D	400	ARG
2	D	405	THR
2	D	408	ARG
2	D	424	ASP
2	D	439	VAL
2	D	441	MET
2	D	447	THR
2	D	449	THR
1	E	56	ASN
1	E	65	ASP
1	E	66	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	E	67	LEU
1	E	151	GLU
1	E	176	ARG
1	E	220	LEU
1	E	230	ILE
1	E	268	ILE
1	E	273	ILE
1	E	288	SER
1	E	303	TYR
1	E	305	HIS
1	E	311	TYR
1	E	314	GLU
1	E	361	ARG
1	E	381	ASN
1	E	382	LEU
1	E	386	LEU
1	E	429	THR
1	E	445	VAL
1	E	446	MET
2	F	27	ARG
2	F	39	THR
2	F	66	ASN
2	F	71	PHE
2	F	75	LEU
2	F	149	ARG
2	F	181	LEU
2	F	219	GLU
2	F	275	VAL
2	F	346	GLU
2	F	350	ARG
2	F	375	ARG
2	F	400	ARG
2	F	405	THR
2	F	408	ARG
2	F	424	ASP
2	F	439	VAL
2	F	441	MET
2	F	447	THR
2	F	449	THR
1	G	15	ARG
1	G	56	ASN
1	G	65	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	G	66	ARG
1	G	67	LEU
1	G	151	GLU
1	G	176	ARG
1	G	220	LEU
1	G	230	ILE
1	G	268	ILE
1	G	273	ILE
1	G	303	TYR
1	G	305	HIS
1	G	311	TYR
1	G	314	GLU
1	G	361	ARG
1	G	381	ASN
1	G	382	LEU
1	G	386	LEU
1	G	429	THR
1	G	445	VAL
1	G	446	MET
2	H	27	ARG
2	H	39	THR
2	H	66	ASN
2	H	71	PHE
2	H	75	LEU
2	H	149	ARG
2	H	181	LEU
2	H	207	ARG
2	H	219	GLU
2	H	275	VAL
2	H	346	GLU
2	H	350	ARG
2	H	375	ARG
2	H	400	ARG
2	H	405	THR
2	H	408	ARG
2	H	424	ASP
2	H	439	VAL
2	H	441	MET
2	H	447	THR
2	H	449	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	ASN
1	A	62	HIS
1	A	99	ASN
1	A	320	ASN
1	A	349	GLN
1	A	406	ASN
1	A	431	ASN
2	B	44	ASN
2	B	65	ASN
2	B	137	ASN
2	B	165	HIS
2	B	223	GLN
2	B	304	ASN
2	B	374	ASN
1	C	56	ASN
1	C	99	ASN
1	C	315	ASN
1	C	320	ASN
1	C	406	ASN
1	C	431	ASN
2	D	44	ASN
2	D	65	ASN
2	D	66	ASN
2	D	107	ASN
2	D	137	ASN
2	D	186	ASN
2	D	223	GLN
2	D	354	ASN
2	D	374	ASN
1	E	56	ASN
1	E	99	ASN
1	E	236	GLN
1	E	320	ASN
1	E	406	ASN
1	E	431	ASN
2	F	44	ASN
2	F	65	ASN
2	F	107	ASN
2	F	137	ASN
2	F	165	HIS
2	F	186	ASN
2	F	223	GLN
2	F	374	ASN

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Mol	Chain	Res	Type
1	G	56	ASN
1	G	99	ASN
1	G	320	ASN
1	G	349	GLN
1	G	406	ASN
1	G	431	ASN
2	H	44	ASN
2	H	65	ASN
2	H	66	ASN
2	H	107	ASN
2	H	137	ASN
2	H	165	HIS
2	H	186	ASN
2	H	223	GLN
2	H	374	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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	457/475 (96%)	0.59	22 (4%) 30 37	31, 49, 83, 101	0
1	C	444/475 (93%)	0.36	14 (3%) 47 55	30, 50, 75, 101	0
1	E	448/475 (94%)	0.55	24 (5%) 25 30	34, 53, 80, 101	0
1	G	450/475 (94%)	0.53	20 (4%) 34 41	35, 54, 82, 101	0
2	B	439/443 (99%)	0.45	8 (1%) 68 74	30, 51, 76, 95	0
2	D	441/443 (99%)	0.39	12 (2%) 54 61	33, 58, 79, 97	0
2	F	440/443 (99%)	0.60	33 (7%) 14 17	44, 67, 86, 97	0
2	H	440/443 (99%)	1.41	133 (30%) 0 0	52, 75, 91, 99	0
All	All	3559/3672 (96%)	0.61	266 (7%) 14 17	30, 58, 85, 101	0

All (266) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	250	PHE	9.2
1	E	250	PHE	8.5
1	C	252	ASN	7.7
2	H	456	ILE	7.5
2	H	198	TYR	7.5
2	H	71	PHE	7.1
1	C	249	VAL	6.6
2	H	190	ILE	6.4
2	H	444	LEU	6.3
1	E	253	LEU	6.3
1	G	249	VAL	6.3
1	A	250	PHE	6.2
1	A	311	TYR	6.1
1	E	249	VAL	6.1
1	A	252	ASN	6.0
1	G	252	ASN	5.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	H	171	TYR	5.8
2	H	263	LEU	5.8
1	C	250	PHE	5.7
2	H	184	ILE	5.7
2	F	198	TYR	5.6
2	H	257	PHE	5.6
2	H	239	VAL	5.5
1	A	253	LEU	5.5
2	H	195	LEU	5.5
2	H	233	PRO	5.4
1	A	14	ALA	5.4
2	H	258	ILE	5.2
1	A	249	VAL	5.1
1	G	311	TYR	5.1
1	A	288	SER	4.9
2	H	339	TYR	4.9
1	E	311	TYR	4.8
1	E	14	ALA	4.7
2	H	187	ILE	4.7
1	E	251	GLY	4.6
1	C	312	PHE	4.5
1	A	15	ARG	4.5
2	H	182	GLY	4.5
2	D	245	ARG	4.4
2	H	251	PHE	4.4
1	C	253	LEU	4.4
2	H	440	SER	4.4
2	D	88	ILE	4.3
2	H	64	LYS	4.2
1	E	252	ASN	4.2
1	G	294	PRO	4.2
2	H	342	THR	4.2
2	H	181	LEU	4.2
1	G	253	LEU	4.1
1	A	289	PHE	4.1
2	H	163	PHE	4.1
2	D	197	ASP	4.1
2	F	190	ILE	4.1
2	F	229	PHE	4.0
1	A	248	PRO	4.0
2	H	193	THR	4.0
2	H	161	VAL	3.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	358	LYS	3.9
2	H	269	ALA	3.9
2	H	238	PRO	3.9
2	H	237	SER	3.9
2	H	166	LEU	3.9
1	G	14	ALA	3.9
1	A	469	SER	3.9
2	H	450	VAL	3.8
1	A	254	PRO	3.8
1	A	290	SER	3.8
1	C	311	TYR	3.8
2	H	208	MET	3.7
2	H	54	VAL	3.7
2	H	357	LEU	3.7
2	H	262	THR	3.7
2	H	203	TYR	3.7
2	H	200	THR	3.6
2	H	447	THR	3.6
1	G	251	GLY	3.6
2	F	136	ASP	3.5
2	H	189	SER	3.5
2	H	165	HIS	3.5
1	E	312	PHE	3.4
2	H	176	LEU	3.4
1	A	470	SER	3.4
2	H	65	ASN	3.4
2	H	72	LEU	3.4
2	H	226	GLN	3.4
2	H	236	GLU	3.4
2	H	99	LEU	3.4
2	H	267	HIS	3.4
2	D	71	PHE	3.4
2	H	55	ASP	3.4
2	F	246	GLY	3.3
2	H	434	LEU	3.3
2	F	60	ALA	3.3
1	E	288	SER	3.3
2	F	245	ARG	3.3
2	D	190	ILE	3.3
2	H	60	ALA	3.3
2	H	350	ARG	3.3
2	H	204	LYS	3.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	H	443	ALA	3.2
2	H	449	THR	3.2
1	E	468	SER	3.2
2	H	260	GLU	3.2
2	H	77	PHE	3.2
2	F	138	SER	3.2
2	H	173	ASP	3.2
2	H	445	GLY	3.2
2	H	256	ARG	3.2
2	H	37	ILE	3.2
2	H	254	GLY	3.1
2	H	68	THR	3.1
2	D	148	ILE	3.1
2	H	180	ILE	3.0
2	H	229	PHE	3.0
1	C	303	TYR	3.0
2	H	459	LYS	3.0
2	H	145	ASP	3.0
2	H	31	LEU	3.0
2	H	69	ALA	3.0
2	F	130	LEU	3.0
2	H	95	ILE	2.9
2	H	335	LEU	2.9
2	H	446	ASN	2.9
2	H	35	LEU	2.9
2	H	248	LEU	2.9
2	B	27	ARG	2.9
1	E	15	ARG	2.8
1	A	291	ALA	2.8
2	H	197	ASP	2.8
2	H	199	ILE	2.8
1	G	231	THR	2.8
2	H	23	ILE	2.8
1	A	251	GLY	2.8
1	E	356	ALA	2.8
2	H	352	ILE	2.8
2	F	239	VAL	2.8
2	H	202	ASN	2.8
2	H	346	GLU	2.8
2	H	110	TYR	2.7
2	H	148	ILE	2.7
2	H	149	ARG	2.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	310	TYR	2.7
2	F	181	LEU	2.7
2	D	201	LYS	2.7
2	H	137	ASN	2.7
2	H	452	ASN	2.7
2	F	203	TYR	2.7
2	H	188	LYS	2.7
1	A	303	TYR	2.7
1	E	254	PRO	2.7
2	H	245	ARG	2.7
2	H	264	PRO	2.7
2	H	185	LYS	2.7
2	H	61	GLU	2.7
2	H	265	THR	2.7
2	H	363	ILE	2.7
1	C	405	VAL	2.6
2	F	127	SER	2.6
1	G	416	LYS	2.6
2	H	240	PRO	2.6
2	D	462	GLN	2.6
2	H	158	TYR	2.6
1	G	15	ARG	2.6
2	H	261	ASN	2.6
2	F	23	ILE	2.6
2	H	135	LEU	2.6
2	B	140	ILE	2.6
2	H	235	SER	2.6
2	D	246	GLY	2.6
2	H	59	ARG	2.6
2	H	219	GLU	2.6
1	C	268	ILE	2.5
2	F	235	SER	2.5
2	H	441	MET	2.5
2	H	192	ARG	2.5
1	E	313	VAL	2.5
2	F	225	ALA	2.5
1	C	412	ILE	2.5
2	F	196	LYS	2.5
2	H	341	VAL	2.5
1	G	312	PHE	2.5
2	F	240	PRO	2.5
2	H	439	VAL	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	B	236	GLU	2.4
2	F	185	LYS	2.4
2	H	241	LEU	2.4
2	H	259	LYS	2.4
1	G	292	GLY	2.4
1	G	229	PRO	2.4
2	H	271	ALA	2.4
1	C	248	PRO	2.4
2	D	76	ALA	2.4
2	H	343	ASP	2.4
2	H	178	ARG	2.4
2	H	360	TRP	2.4
2	H	75	LEU	2.4
2	H	348	ASN	2.4
2	H	201	LYS	2.3
1	G	403	ILE	2.3
2	H	175	PRO	2.3
1	G	274	TYR	2.3
2	H	313	ALA	2.3
2	H	347	HIS	2.3
2	H	108	THR	2.3
2	F	236	GLU	2.3
2	B	64	LYS	2.3
2	H	30	LYS	2.3
1	E	248	PRO	2.3
2	H	319	LEU	2.3
2	B	137	ASN	2.3
2	F	137	ASN	2.3
2	H	82	ASN	2.3
2	H	172	LYS	2.2
2	H	349	VAL	2.2
2	H	442	VAL	2.2
2	H	81	GLN	2.2
1	E	415	LEU	2.2
1	A	468	SER	2.2
1	A	57	LEU	2.2
2	F	238	PRO	2.2
2	F	71	PHE	2.2
2	F	248	LEU	2.2
2	F	44	ASN	2.2
2	H	455	TYR	2.2
1	G	230	ILE	2.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	D	23	ILE	2.2
2	H	356	ILE	2.2
2	H	25	GLY	2.2
1	E	358	LYS	2.2
2	H	32	PRO	2.2
2	F	149	ARG	2.2
2	H	131	THR	2.2
2	F	424	ASP	2.1
2	B	245	ARG	2.1
1	G	411	LYS	2.1
2	F	81	GLN	2.1
1	A	247	ALA	2.1
2	H	209	VAL	2.1
1	G	248	PRO	2.1
2	F	134	VAL	2.1
2	H	129	ILE	2.1
1	C	441	ARG	2.1
2	H	367	LYS	2.1
2	F	304	ASN	2.1
1	C	251	GLY	2.1
2	B	148	ILE	2.1
1	E	56	ASN	2.1
2	H	168	GLU	2.1
2	F	175	PRO	2.1
2	F	234	LYS	2.1
1	E	303	TYR	2.1
2	B	90	LEU	2.1
2	D	22	GLN	2.1
1	E	298	MET	2.0
1	E	360	LEU	2.0
1	G	413	GLU	2.0
1	A	295	GLY	2.0
1	E	55	ARG	2.0
2	F	197	ASP	2.0
2	H	57	GLY	2.0
2	H	88	ILE	2.0
2	H	130	LEU	2.0
1	E	422	ARG	2.0
1	E	210	GLU	2.0
2	H	183	PRO	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	ZN	H	504	1/1	0.84	0.10	100,100,100,100	0
3	ZN	D	502	1/1	0.94	0.14	64,64,64,64	0
3	ZN	F	503	1/1	0.96	0.14	73,73,73,73	0
3	ZN	B	501	1/1	0.98	0.17	46,46,46,46	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.