



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:54 PM GMT

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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

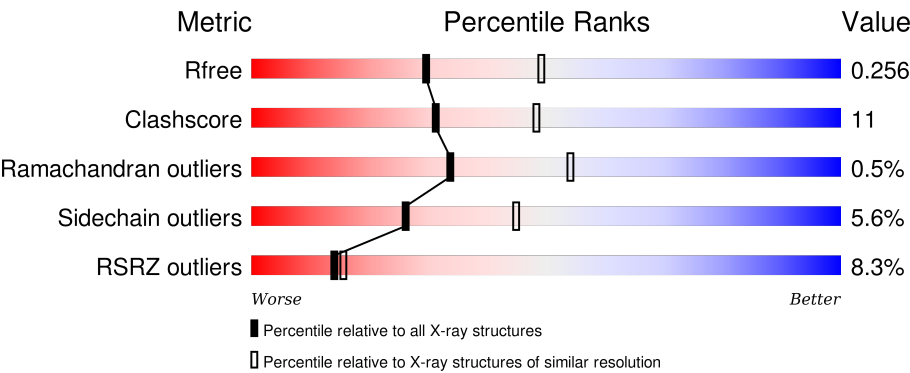
1 Overall quality at a glance i

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}	91344	4549 (2.58-2.50)
Clashscore	102246	5292 (2.58-2.50)
Ramachandran outliers	100387	5194 (2.58-2.50)
Sidechain outliers	100360	5196 (2.58-2.50)
RSRZ outliers	91569	4561 (2.58-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	475	<div><div>5%</div><div><div></div><div>74%</div><div>20%</div><div>• •</div></div></div>
1	C	475	<div><div>3%</div><div><div></div><div>74%</div><div>17%</div><div>• 7%</div></div></div>
1	E	475	<div><div>6%</div><div><div></div><div>72%</div><div>20%</div><div>• 6%</div></div></div>
1	G	475	<div><div>5%</div><div><div></div><div>71%</div><div>20%</div><div>• 5%</div></div></div>
2	B	443	<div><div>2%</div><div><div></div><div>75%</div><div>21%</div><div>• •</div></div></div>

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Mol	Chain	Length	Quality of chain
2	D	443	<div><div></div><div>3%</div><div>74%</div><div>22%</div><div></div><div></div></div>
2	F	443	<div><div></div><div>8%</div><div>75%</div><div>21%</div><div></div><div></div></div>
2	H	443	<div><div></div><div>33%</div><div>73%</div><div>23%</div><div></div><div></div></div>

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

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
2	B	439	Total	C	N	O	S	0	0	0
			3414	2148	591	668	7			
2	D	441	Total	C	N	O	S	0	0	0
			3431	2159	594	671	7			
2	F	440	Total	C	N	O	S	0	0	0
			3422	2154	592	669	7			
2	H	440	Total	C	N	O	S	0	0	0
			3422	2154	592	669	7			

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	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	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	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	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	H	1	Total Zn 1 1	0	0
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

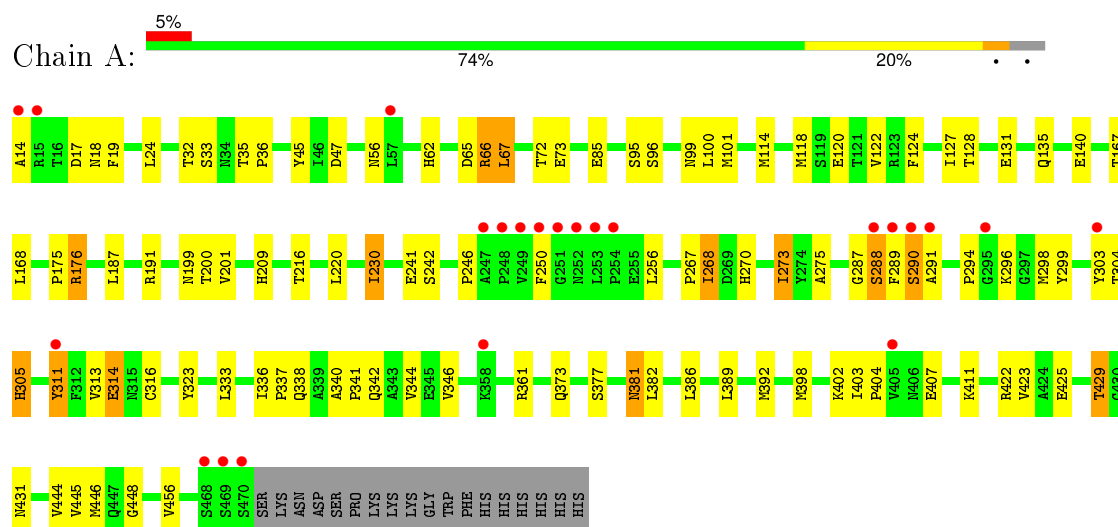
- Molecule 4 is water.

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

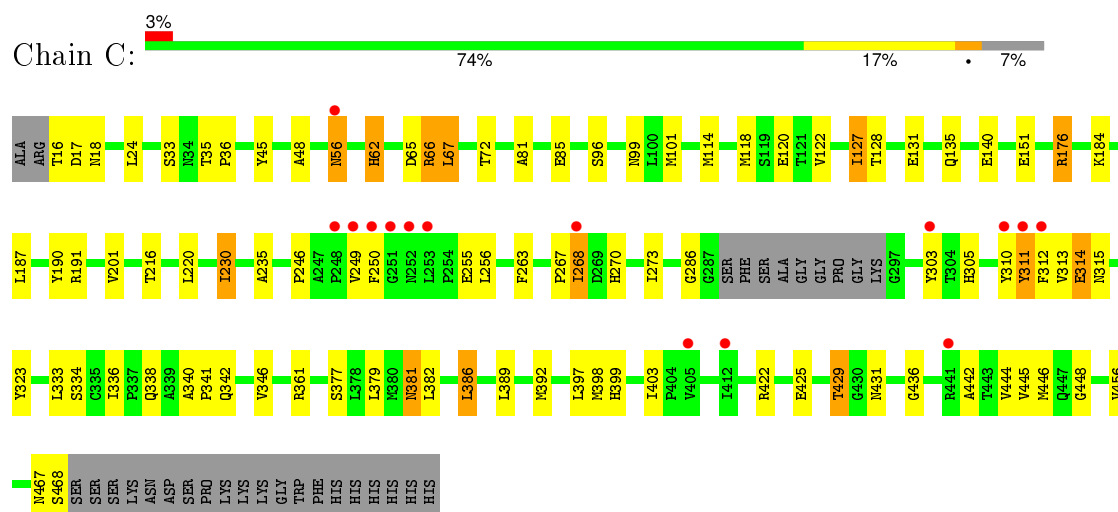
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ($\text{RSRZ} > 2$). 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

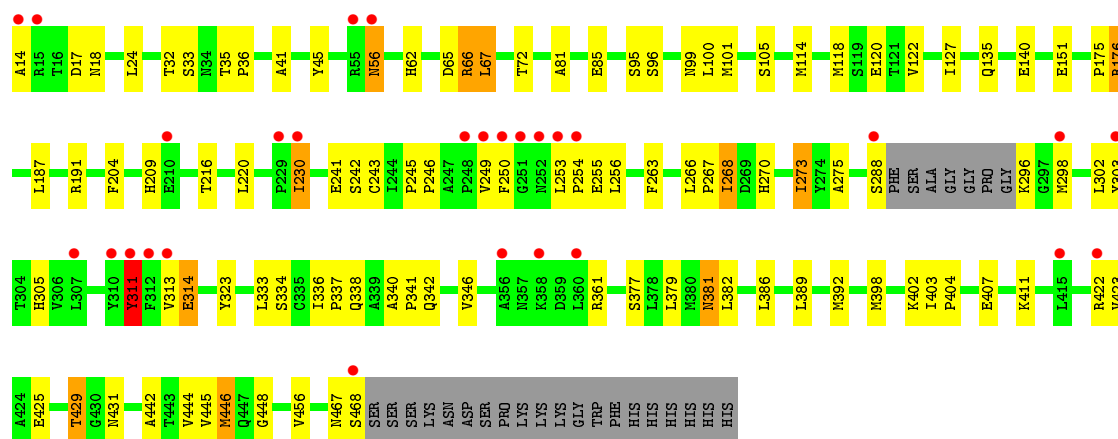


● Molecule 1: MITOCHONDRIAL PROCESSING PEPTIDASE ALPHA SUBUNIT

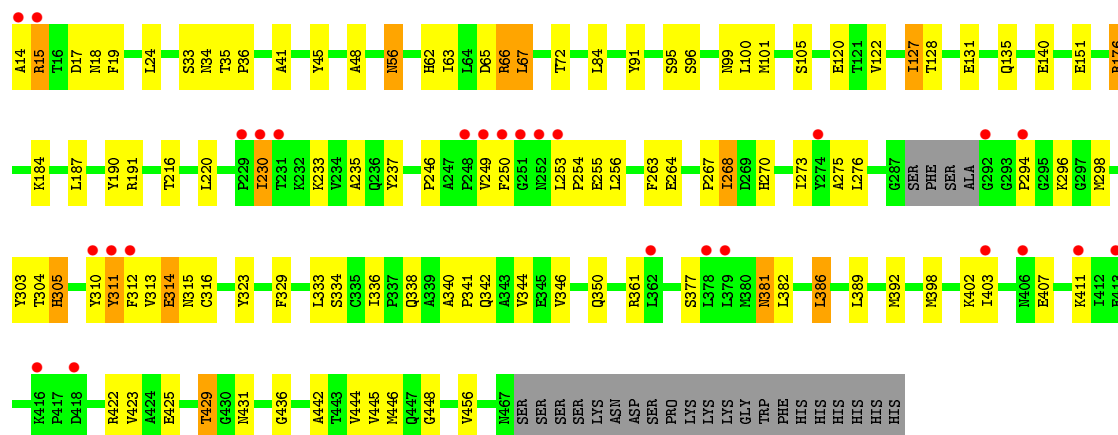


● Molecule 1: MITOCHONDRIAL PROCESSING PEPTIDASE ALPHA SUBUNIT

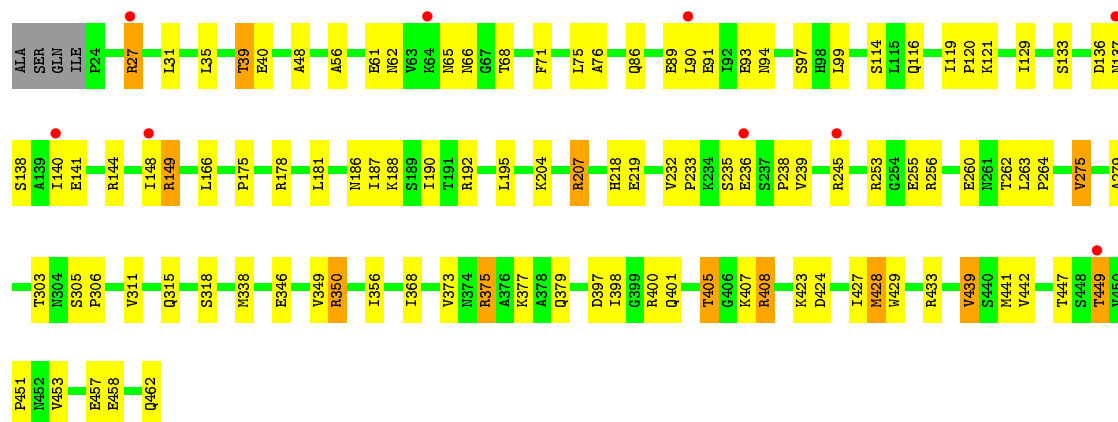
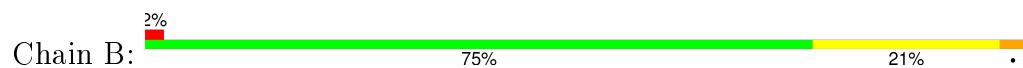




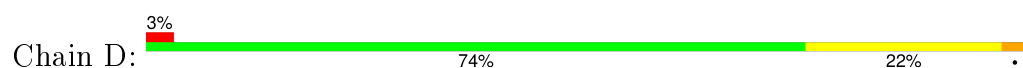
• Molecule 1: MITOCHONDRIAL PROCESSING PEPTIDASE ALPHA SUBUNIT

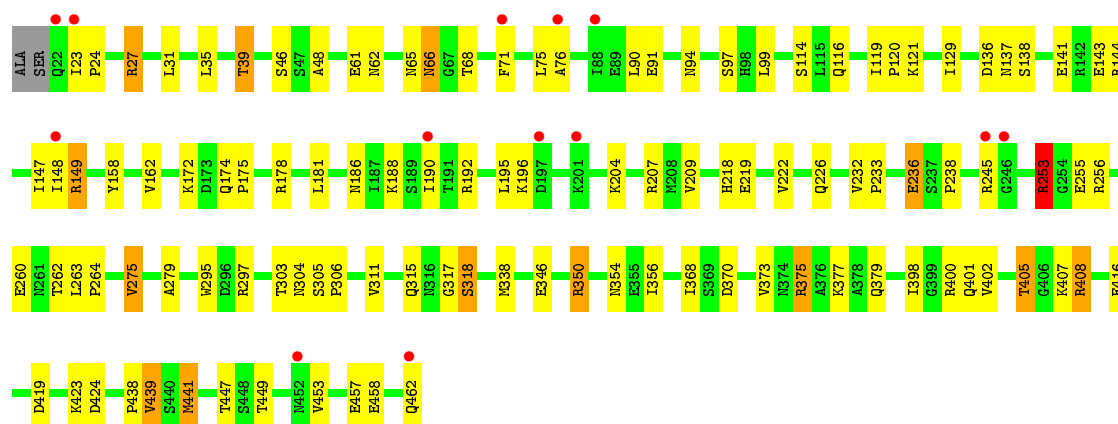


• Molecule 2: MITOCHONDRIAL PROCESSING PEPTIDASE BETA SUBUNIT

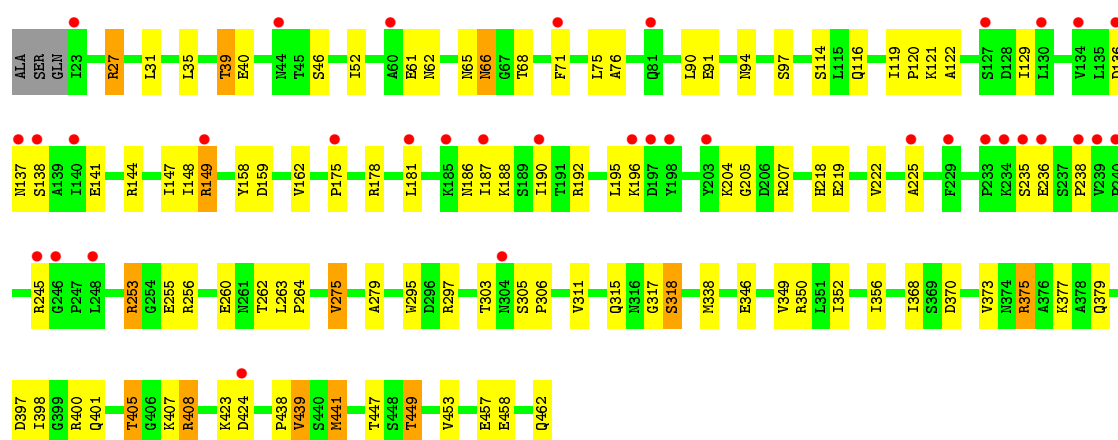
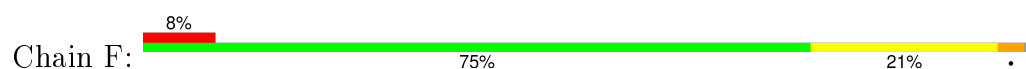


• Molecule 2: MITOCHONDRIAL PROCESSING PEPTIDASE BETA SUBUNIT

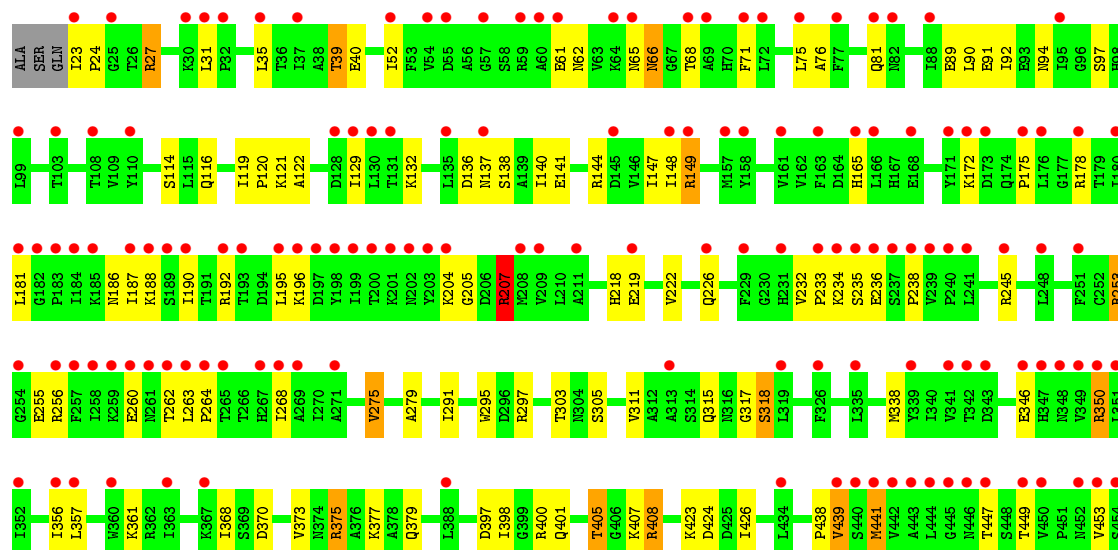
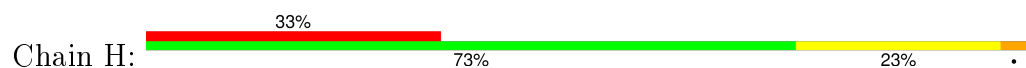


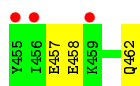


• Molecule 2: MITOCHONDRIAL PROCESSING PEPTIDASE BETA SUBUNIT



• 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	3.22 (at 2.54Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.243 , 0.256 0.242 , 0.256	Depositor DCC
R_{free} test set	2015 reflections (1.29%)	DCC
Wilson B-factor (Å ²)	53.7	Xtriage
Anisotropy	0.471	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 44.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 157262 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	27725	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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:H	1:A:230:ILE:HD12	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:H	1:C:230:ILE:HD12	1.29	0.95
1:C:24:LEU:HD11	1:C:216:THR:HG22	1.48	0.94
2:D:256:ARG:HH11	2:D:256:ARG:HG3	1.31	0.94
1:G:230:ILE:HD12	1:G:230:ILE:H	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:CD2	1:G:311:TYR:N	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:N	1:C:230:ILE:HD12	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:N	1:A:230:ILE:HD12	1.98	0.77
1:G:425:GLU:O	1:G:429:THR:HB	1.85	0.77
1:E:230:ILE:N	1:E:230:ILE:HD12	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
1:C:230:ILE:H	1:C:230:ILE:CD1	1.99	0.75
2:B:338:MET:HG2	2:B:356:ILE:HD13	1.69	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
2:H:186:ASN:O	2:H:190:ILE:HG12	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:96:SER:HB3	1:G:99:ASN:OD1	1.88	0.73
1:E:425:GLU:O	1:E:429:THR:HB	1.89	0.73
2:F:303:THR:HG22	2:F:305:SER:H	1.54	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
1:A:230:ILE:CD1	1:A:230:ILE:H	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:CD1	1:G:230:ILE:H	2.02	0.71
1:E:230:ILE:CD1	1:E:230:ILE:H	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
1:G:336:ILE:HG22	1:G:338:GLN:OE1	1.91	0.71
2:B:144:ARG:O	2:B:148:ILE:HG12	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:HA	2:B:245:ARG:HE	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:303:THR:HG22	2:D:305:SER:H	1.56	0.69
2:D:97:SER:OG	2:D:114:SER:HB3	1.92	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
1:E:429:THR:HG21	1:E:431:ASN:HD22	1.57	0.69
2:D:186:ASN:O	2:D:190:ILE:HG12	1.92	0.69
1:G:246:PRO:HG3	1:G:448:GLY:HA2	1.75	0.69
2:F:186:ASN:O	2:F:190:ILE:HG12	1.93	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:O	2:H:23:ILE:HG13	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:311:TYR:C	1:G:313:VAL:H	2.00	0.64
1:G:15:ARG:HG3	1:G:15:ARG:HH11	1.62	0.64
2:H:439:VAL:HG22	2:H:453:VAL:HG13	1.77	0.64
2:H:245:ARG:HE	2:H:245:ARG:HA	1.63	0.64
1:A:96:SER:HB3	1:A:99:ASN:OD1	1.96	0.64
2:B:439:VAL:HG22	2:B:453:VAL:HG13	1.77	0.64
2:H:275:VAL:HG22	2:H:279:ALA:HB3	1.80	0.64
1:A:336:ILE:HG22	1:A:338:GLN:OE1	1.96	0.64
2:H:204:LYS:HA	2:H:233:PRO:O	1.98	0.64
2:H:256:ARG:NH1	2:H:256:ARG:HG3	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: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:H	2.00	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:D:136:ASP:OD2	2:D:138:SER:HB3	1.99	0.63
1:C:336:ILE:HG22	1:C:338:GLN:OE1	1.97	0.63
2:B:368:ILE:O	2:B:423:LYS:HE3	1.99	0.63
1:A:242:SER:OG	1:E:176:ARG:NH2	2.31	0.63
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
2:F:76:ALA:HB1	2:F:129:ILE:HG23	1.80	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
2:D:245:ARG:HA	2:D:245:ARG:HE	1.65	0.62
1:C:379:LEU:HD13	2:D:46:SER:HB2	1.80	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
1:C:342:GLN:O	1:C:346:VAL:HG23	2.00	0.61
2:B:275:VAL:HG22	2:B:279:ALA:CB	2.30	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:HD13	1:C:268:ILE:N	2.16	0.60
2:F:256:ARG:HG3	2:F:256:ARG:NH1	2.03	0.60
1:G:340:ALA:HB3	1:G:341:PRO:HD3	1.84	0.60
1:G:187:LEU:O	1:G:191:ARG:HG3	2.02	0.60
1:E:14:ALA:HB3	1:E:404:PRO:HB3	1.83	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
1:C:268:ILE:HD13	1:C:268:ILE:H	1.65	0.59
1:C:249:VAL:HG12	1:C:255:GLU:HB2	1.84	0.59
2:F:405:THR:HG22	2:F:407:LYS:H	1.67	0.59
2:B:76:ALA:HB1	2:B:129:ILE:HG23	1.83	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:H	1:A:268:ILE:HD13	1.67	0.59
2:B:39:THR:HG21	2:B:218:HIS:HB2	1.83	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:137:ASN:ND2	2:B:192:ARG:HD2	2.18	0.59
2:B:239:VAL:HG21	2:B:245:ARG:NH2	2.18	0.59
2:H:375:ARG:NH2	2:H:379:GLN:OE1	2.36	0.59
2:D:68:THR:HG23	2:D:195:LEU:HD23	1.83	0.59
2:D:61:GLU:HA	2:D:65:ASN:HD22	1.68	0.58
1:A:187:LEU:O	1:A:191:ARG:HG3	2.03	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:N	1:E:268:ILE:HD13	2.19	0.57
2:H:204:LYS:HG3	2:H:235:SER:OG	2.04	0.57
1:G:294:PRO:HB3	2:H:89:GLU:HA	1.86	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:F:401:GLN:O	2:F:405:THR:HB	2.04	0.56
2:D:236:GLU:C	2:D:238:PRO:HD3	2.25	0.56
1:G:67:LEU:HD13	1:G:135:GLN:HG3	1.86	0.56
2:H:255:GLU:HB3	2:H:453:VAL:HG23	1.87	0.56
1:A:373:GLN:NE2	2:B:93:GLU:OE1	2.37	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
2:H:137:ASN:ND2	2:H:192:ARG:HD2	2.20	0.56
1:E:340:ALA:HB3	1:E:341:PRO:HD3	1.86	0.56
2:F:255:GLU:HB3	2:F:453:VAL:HG23	1.87	0.56
2:D:39:THR:HG21	2:D:218:HIS:HB2	1.87	0.56
2:B:375:ARG:NH2	2:B:379:GLN:OE1	2.38	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
1:E:268:ILE:H	1:E:268:ILE:HD13	1.70	0.55
2:B:245:ARG:NE	2:B:245:ARG:HA	2.19	0.55
2:D:350:ARG:O	2:D:354:ASN:ND2	2.39	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:175:PRO:HA	2:F:178:ARG:NH1	2.21	0.55
2:F:68:THR:HG23	2:F:195:LEU:HD23	1.88	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:C:187:LEU:O	1:C:191:ARG:HG3	2.06	0.55
1:A:67:LEU:HD13	1:A:135:GLN:HG3	1.88	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:F:275:VAL:HG22	2:F:279:ALA:HB3	1.89	0.54
2:D:119:ILE:N	2:D:120:PRO:HD2	2.23	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
1:C:99:ASN:HD22	1:C:101:MET:CE	2.21	0.53
2:B:136:ASP:OD2	2:B:138:SER:HB3	2.08	0.53
1:E:249:VAL:HG12	1:E:255:GLU:HB2	1.91	0.53
2:D:375:ARG:NH2	2:D:379:GLN:OE1	2.41	0.53
2:H:141:GLU:O	2:H:144:ARG:HG3	2.08	0.53
1:A:176:ARG:NH2	1:E:242:SER:OG	2.41	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:397:ASP:OD2	2:B:408:ARG:NH1	2.40	0.52
2:B:311:VAL:O	2:B:315:GLN:HG3	2.10	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:CG	2:F:256:ARG:HH11	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: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
1:A:256:LEU:CD1	1:A:314:GLU:HG2	2.40	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
2:H:234:LYS:HG2	2:H:235:SER:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:PRO:HG3	1:A:448:GLY:HA2	1.93	0.51
1:C:17:ASP:O	1:C:18:ASN:HB3	2.11	0.51
2:F:39:THR:HG21	2:F:218:HIS:HB2	1.92	0.51
1:E:241:GLU:HA	1:E:444:VAL:O	2.09	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:A:403:ILE:O	1:A:403:ILE:HG23	2.11	0.51
1:G:140:GLU:HB3	1:G:176:ARG:NH1	2.25	0.51
1:G:19:PHE:HD1	1:G:392:MET:HE1	1.75	0.51
2:D:401:GLN:O	2:D:405:THR:HB	2.11	0.51
1:C:45:TYR:OH	1:C:389:LEU:HG	2.11	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:E:99:ASN:HD22	1:E:101:MET:CE	2.24	0.50
1:A:344:VAL:HG21	1:A:456:VAL:HG22	1.94	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
2:D:255:GLU:HB3	2:D:453:VAL:CG2	2.42	0.49
1:A:377:SER:O	1:A:381:ASN:HB2	2.12	0.49
2:H:207:ARG:HH11	2:H:245:ARG:NH1	2.09	0.49
1:G:256:LEU:HD11	1:G:314:GLU:HG2	1.92	0.49
2:D:48:ALA:HB3	2:D:119:ILE:HD11	1.95	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
1:G:99:ASN:HD22	1:G:101:MET:CE	2.24	0.49
2:F:255:GLU:HB3	2:F:453:VAL:CG2	2.42	0.49
2:B:175:PRO:HA	2:B:178:ARG:NH1	2.27	0.49
1:G:17:ASP:O	1:G:18:ASN:HB3	2.12	0.49
1:A:342:GLN:O	1:A:346:VAL:HG23	2.13	0.49
1:A:35:THR:HB	1:A:36:PRO:CD	2.42	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
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
2:B:373:VAL:O	2:B:377:LYS:HG3	2.13	0.48
2:H:90:LEU:CD1	2:H:94:ASN:HD21	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:CYS:SG	1:A:333:LEU:HD23	2.54	0.48
2:H:144:ARG:HH21	2:H:188:LYS:C	2.15	0.48
1:G:268:ILE:CD1	1:G:268:ILE:H	2.27	0.48
2:D:90:LEU:HD13	2:D:94:ASN:ND2	2.29	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:G:342:GLN:O	1:G:346:VAL:HG23	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
2:D:91:GLU:OE2	2:D:121:LYS:HD2	2.13	0.48
1:C:235:ALA:O	1:C:436:GLY:HA3	2.14	0.48
2:B:428:MET:CE	2:B:428:MET:HA	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
2:D:137:ASN:ND2	2:D:192:ARG:HD2	2.29	0.47
1:C:201:VAL:HG23	1:C:397:LEU:CD1	2.45	0.47
2:D:260:GLU:OE2	2:D:262:THR:HG23	2.13	0.47
2:B:137:ASN:HD21	2:B:192:ARG:HD2	1.77	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:D:141:GLU:O	2:D:144:ARG:HG3	2.14	0.47
2:B:239:VAL:HG21	2:B:245:ARG:HH21	1.79	0.47
1:E:407:GLU:HG2	1:E:411:LYS:HE3	1.97	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
2:H:232:VAL:HG13	2:H:233:PRO:HD2	1.95	0.47
1:G:275:ALA:HB3	1:G:423:VAL:HG21	1.97	0.47
1:E:333:LEU:HD13	1:E:334:SER:N	2.30	0.47
2:F:245:ARG:NE	2:F:245:ARG:HA	2.24	0.47
2:H:370:ASP:OD1	2:H:423:LYS:NZ	2.46	0.47
2:F:295:TRP:CZ2	2:F:297:ARG:HA	2.49	0.47
1:A:392:MET:HE2	1:A:402:LYS:HD2	1.96	0.46
2:H:147:ILE:HG22	2:H:187:ILE:HD13	1.97	0.46
1:C:45:TYR:N	1:C:45:TYR:CD1	2.82	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:H:119:ILE:O	2:H:122:ALA:HB3	2.16	0.46
1:G:72:THR:HG21	1:G:120:GLU:HB3	1.97	0.46
2:F:52:ILE:O	2:F:52:ILE:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:141:GLU:O	2:B:144:ARG:HG3	2.16	0.46
1:A:122:VAL:O	1:A:191:ARG:NH2	2.48	0.46
1:G:62:HIS:CE1	1:G:66:ARG:HD2	2.50	0.46
1:G:429:THR:CG2	1:G:431:ASN:ND2	2.74	0.46
1:G:67:LEU:HD13	1:G:135:GLN:CG	2.46	0.46
2:F:398:ILE:HA	2:F:408:ARG:HG3	1.98	0.46
1:G:407:GLU:HG2	1:G:411:LYS:HE3	1.98	0.46
1:E:429:THR:CG2	1:E:431:ASN:ND2	2.75	0.46
1:E:270:HIS:O	1:E:273:ILE:HB	2.16	0.46
1:E:81:ALA:O	1:E:85:GLU:HG3	2.16	0.46
1:C:35:THR:HB	1:C:36:PRO:CD	2.46	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
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:A:72:THR:HG21	1:A:120:GLU:HB3	1.98	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
2:H:439:VAL:HG13	2:H:457:GLU:HG2	1.98	0.45
1:C:201:VAL:HG23	1:C:397:LEU:HD13	1.98	0.45
2:H:90:LEU:HD13	2:H:94:ASN:HD21	1.77	0.45
1:G:344:VAL:HG21	1:G:456:VAL:HG22	1.98	0.45
1:A:45:TYR:OH	1:A:389:LEU:HG	2.16	0.45
2:F:148:ILE:HD13	2:F:187:ILE:HG21	1.97	0.45
2:B:439:VAL:HG13	2:B:457:GLU:HG2	1.98	0.45
1:E:45:TYR:CD1	1:E:45:TYR:N	2.84	0.45
1:A:403:ILE:O	1:A:403:ILE:CG2	2.65	0.45
1:G:346:VAL:O	1:G:350:GLN:HG2	2.16	0.45
2:H:61:GLU:OE1	2:H:66:ASN:HA	2.17	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:A:256:LEU:HD11	1:A:314:GLU:HG2	1.97	0.45
2:H:116:GLN:O	2:H:119:ILE:HG12	2.16	0.45
1:A:275:ALA:HB3	1:A:423:VAL:HG21	1.97	0.45
2:H:373:VAL:O	2:H:377:LYS:HG3	2.16	0.45
2:H:295:TRP:CZ2	2:H:297:ARG:HA	2.51	0.45
1:G:95:SER:HB3	1:G:100:LEU:HD13	1.98	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:HA	1:G:56:ASN:HD22	1.57	0.45
2:B:61:GLU:OE1	2:B:66:ASN:HA	2.17	0.45
2:H:136:ASP:O	2:H:140:ILE:HG13	2.17	0.45
1:G:304:THR:HG22	1:G:305:HIS:ND1	2.31	0.45
1:G:19:PHE:HD1	1:G:392:MET:CE	2.30	0.44
2:D:27:ARG:HB3	2:D:27:ARG:HH11	1.82	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
2:H:31:LEU:HD21	2:H:226:GLN:HA	1.98	0.44
1:E:336:ILE:HG22	1:E:337:PRO:HD2	1.98	0.44
2:B:255:GLU:HB3	2:B:453:VAL:HG23	1.99	0.44
2:H:218:HIS:O	2:H:222:VAL:HG23	2.17	0.44
1:E:296:LYS:HE2	1:E:298:MET:HE2	1.98	0.44
1:G:127:ILE:HB	1:G:184:LYS:HE3	1.98	0.44
2:F:305:SER:HA	2:F:306:PRO:HD3	1.67	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:F:317:GLY:O	2:F:318:SER:CB	2.64	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:D:245:ARG:HA	2:D:245:ARG:NE	2.30	0.44
2:B:204:LYS:HG3	2:B:235:SER:OG	2.17	0.44
2:D:398:ILE:HA	2:D:408:ARG:HG3	2.00	0.44
1:E:253:LEU:HA	1:E:254:PRO:HD3	1.86	0.44
1:E:17:ASP:O	1:E:18:ASN:HB3	2.17	0.44
2:B:207:ARG:HH11	2:B:245:ARG:NH1	2.15	0.44
1:E:67:LEU:HD13	1:E:135:GLN:CG	2.47	0.44
2:D:317:GLY:O	2:D:318:SER:CB	2.65	0.44
2:B:119:ILE:N	2:B:120:PRO:HD2	2.33	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
2:H:207:ARG:NH1	2:H:245:ARG:NH1	2.65	0.44
1:A:45:TYR:N	1:A:45:TYR:CD1	2.86	0.44
1:E:114:MET:HE2	1:E:118:MET:HG3	1.99	0.44
2:B:255:GLU:HA	2:B:441:MET:O	2.18	0.44
1:A:287:GLY:O	1:A:289:PHE:N	2.51	0.44
2:H:398:ILE:HA	2:H:408:ARG:HG3	1.99	0.44
1:E:32:THR:HG21	1:E:209:HIS:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:444:VAL:HG11	1:E:456:VAL:HG11	1.98	0.44
1:E:95:SER:HB3	1:E:100:LEU:HD13	2.00	0.44
1:C:333:LEU:HD13	1:C:334:SER:N	2.32	0.44
1:A:296:LYS:HE2	1:A:298:MET:CE	2.48	0.44
1:G:15:ARG:HG3	1:G:15:ARG:NH1	2.31	0.43
1:A:294:PRO:HB3	2:B:89:GLU:HA	1.99	0.43
2:H:317:GLY:O	2:H:318:SER:OG	2.25	0.43
1:C:72:THR:HG21	1:C:120:GLU:HB3	2.00	0.43
1:A:95:SER:HB3	1:A:100:LEU:HD13	2.00	0.43
1:A:407:GLU:HG2	1:A:411:LYS:HE3	1.99	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:H:39:THR:HG21	2:H:218:HIS:CB	2.48	0.43
1:G:35:THR:HB	1:G:36:PRO:CD	2.48	0.43
2:D:158:TYR:O	2:D:162:VAL:HG23	2.19	0.43
2:B:144:ARG:HH21	2:B:188:LYS:C	2.21	0.43
2:B:97:SER:OG	2:B:114:SER:CB	2.64	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
1:C:444:VAL:HG11	1:C:456:VAL:HG11	2.00	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
2:B:429:TRP:CE2	2:B:433:ARG:HG3	2.54	0.43
1:E:35:THR:HB	1:E:36:PRO:CD	2.48	0.43
1:E:268:ILE:CD1	1:E:268:ILE:H	2.31	0.43
2:D:97:SER:OG	2:D:114:SER:CB	2.63	0.43
1:E:99:ASN:HD22	1:E:101:MET:HE3	1.81	0.43
2:D:236:GLU:O	2:D:238:PRO:HD3	2.18	0.43
2:H:137:ASN:HD21	2:H:192:ARG:HD2	1.80	0.43
2:H:268:ILE:N	2:H:268:ILE:HD12	2.33	0.43
2:D:62:ASN:CG	2:D:65:ASN:HB2	2.39	0.43
2:B:398:ILE:HA	2:B:408:ARG:HG3	2.01	0.43
2:H:291:ILE:HD12	2:H:426:ILE:HD13	2.01	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:D:373:VAL:O	2:D:377:LYS:HG3	2.18	0.43
2:B:350:ARG:NH2	2:D:419:ASP:OD2	2.46	0.43
2:H:263:LEU:HA	2:H:264:PRO:HD3	1.79	0.43
2:B:263:LEU:HA	2:B:264:PRO:HD3	1.82	0.43
1:E:267:PRO:HA	1:E:323:TYR:O	2.19	0.43
2:H:165:HIS:HD2	2:H:256:ARG:HE	1.67	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:F:119:ILE:O	2:F:122:ALA:HB3	2.18	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
2:B:207:ARG:NH1	2:B:245:ARG:NH1	2.66	0.42
1:A:85:GLU:OE2	2:B:303:THR:HG23	2.17	0.42
1:C:311:TYR:O	1:C:313:VAL:N	2.52	0.42
2:B:99:LEU:HD12	2:B:99:LEU:HA	1.91	0.42
1:A:167:THR:OG1	1:A:168:LEU:N	2.51	0.42
2:H:232:VAL:HA	2:H:233:PRO:HD3	1.68	0.42
1:G:403:ILE:HG23	1:G:403:ILE:O	2.17	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
2:H:253:ARG:HB3	2:H:438:PRO:HB2	2.01	0.42
2:F:439:VAL:HG13	2:F:457:GLU:HG2	2.02	0.42
1:A:17:ASP:O	1:A:18:ASN:HB3	2.20	0.42
2:F:204:LYS:HG3	2:F:235:SER:OG	2.19	0.42
1:E:302:LEU:HD23	1:E:302:LEU:HA	1.90	0.42
2:H:81:GLN:HG3	2:H:132:LYS:O	2.20	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:A:267:PRO:HA	1:A:323:TYR:O	2.19	0.42
1:G:315:ASN:OD1	1:G:316:CYS:N	2.52	0.42
1:G:84:LEU:HD13	1:G:91:TYR:CZ	2.55	0.42
1:G:99:ASN:HD22	1:G:101:MET:HE2	1.85	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: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
1:G:392:MET:HE2	1:G:402:LYS:HD2	2.01	0.42
1:C:403:ILE:HG23	1:C:403:ILE:O	2.18	0.42
1:G:276:LEU:HD11	1:G:329:PHE:CD2	2.54	0.42
2:D:305:SER:HA	2:D:306:PRO:HD3	1.68	0.41
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:62:ASN:CG	2:H:65:ASN:HB2	2.40	0.41
2:F:35:LEU:HA	2:F:205:GLY:O	2.20	0.41
2:D:263:LEU:HA	2:D:264:PRO:HD3	1.78	0.41
1:A:35:THR:HB	1:A:36:PRO:HD2	2.02	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:B:166:LEU:HA	2:B:442:VAL:HG21	2.03	0.41
2:H:357:LEU:O	2:H:361:LYS:HG3	2.20	0.41
1:E:263:PHE:CE2	1:E:442:ALA:HB2	2.55	0.41
1:G:444:VAL:HG11	1:G:456:VAL:HG11	2.01	0.41
1:G:235:ALA:O	1:G:436:GLY:HA3	2.20	0.41
2:F:158:TYR:O	2:F:162:VAL:HG23	2.20	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
2:F:90:LEU:CD1	2:F:94:ASN:HD21	2.34	0.41
1:E:403:ILE:O	1:E:403:ILE:HG23	2.20	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: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:G:429:THR:O	1:G:429:THR:CG2	2.69	0.41
2:F:303:THR:HG22	2:F:305:SER:N	2.28	0.41
2:D:31:LEU:HD21	2:D:226:GLN:HA	2.02	0.41
1:C:403:ILE:O	1:C:403:ILE:CG2	2.69	0.41
1:C:127:ILE:HB	1:C:184:LYS:HE3	2.03	0.41
1:E:429:THR:HG22	1:E:431:ASN:HD22	1.83	0.41
1:G:403:ILE:CG2	1:G:403:ILE:O	2.68	0.41
1:C:56:ASN:HA	1:C:56:ASN:HD22	1.55	0.41
1:A:73:GLU:HG2	1:A:124:PHE:HB3	2.02	0.41
1:E:230:ILE:HD13	1:G:233:LYS:CE	2.50	0.41
1:G:268:ILE:N	1:G:268:ILE:CD1	2.82	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
2:F:147:ILE:HG22	2:F:187:ILE:HD13	2.03	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
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
1:A:47:ASP:HB3	1:A:199:ASN:OD1	2.21	0.41
2:H:52:ILE:O	2:H:52:ILE:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:33:SER:CB	1:C:392:MET:CE	2.90	0.41
2:B:136:ASP:O	2:B:140:ILE:HG13	2.21	0.41
2:F:397:ASP:OD2	2:F:408:ARG:NH1	2.50	0.41
2:F:222:VAL:O	2:F:225:ALA:HB3	2.21	0.41
1:G:333:LEU:HD13	1:G:334:SER:N	2.35	0.41
1:C:263:PHE:CE2	1:C:442:ALA:HB2	2.56	0.41
1:E:204:PHE:N	1:E:204:PHE:CD1	2.88	0.41
2:D:61:GLU:OE1	2:D:66:ASN:HA	2.22	0.40
2:B:423:LYS:O	2:B:427:ILE:HG13	2.21	0.40
1:G:63:ILE:HG22	1:G:67:LEU:HD22	2.02	0.40
1:G:45:TYR:OH	1:G:389:LEU:HG	2.21	0.40
2:B:116:GLN:O	2:B:119:ILE:HG12	2.21	0.40
2:F:373:VAL:O	2:F:377:LYS:HG3	2.21	0.40
2:H:172:LYS:HD2	2:H:172:LYS:HA	1.88	0.40
2:F:62:ASN:CG	2:F:65:ASN:HB2	2.42	0.40
2:H:148:ILE:CD1	2:H:187:ILE:HG21	2.52	0.40
2:H:35:LEU:HA	2:H:205:GLY:O	2.22	0.40
1:E:99:ASN:HB2	1:E:101:MET:CE	2.51	0.40
2:B:303:THR:HG22	2:B:305:SER:N	2.32	0.40
2:D:207:ARG:NH1	2:D:245:ARG:NH1	2.69	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
1:G:237:TYR:CG	1:G:264:GLU:HB2	2.56	0.40
1:E:72:THR:HG21	1:E:120:GLU:HB3	2.02	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
1:E:275:ALA:HB3	1:E:423:VAL:HG21	2.03	0.40
2:H:253:ARG:HH21	2:H:457:GLU:CD	2.25	0.40
1:A:99:ASN:HD22	1:A:101:MET:HE3	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
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
1:A:336:ILE:HG22	1:A:337:PRO:HD2	2.04	0.40
2:F:253:ARG:NH2	2:F:457:GLU:OE1	2.55	0.40
1:E:266:LEU:HA	1:E:267:PRO:HD3	1.89	0.40
1:E:35:THR:HB	1:E:36:PRO:HD2	2.03	0.40
2:D:232:VAL:HA	2:D:233:PRO:HD3	1.74	0.40
1:A:241:GLU:HA	1:A:444:VAL:O	2.20	0.40
1:C:140:GLU:HB3	1:C:176:ARG:NH1	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:HIS:CD2	1:A:66:ARG:HD2	2.57	0.40
2:F:159:ASP:OD1	2:F:159:ASP:N	2.54	0.40
2:D:295:TRP:CZ2	2:D:297:ARG:HA	2.57	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
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

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%)	21	36
1	C	440/475 (93%)	421 (96%)	17 (4%)	2 (0%)	34	54
1	E	444/475 (94%)	422 (95%)	20 (4%)	2 (0%)	34	54
1	G	446/475 (94%)	425 (95%)	19 (4%)	2 (0%)	39	60
2	B	437/443 (99%)	423 (97%)	12 (3%)	2 (0%)	34	54
2	D	439/443 (99%)	423 (96%)	15 (3%)	1 (0%)	52	73
2	F	438/443 (99%)	421 (96%)	16 (4%)	1 (0%)	52	73
2	H	438/443 (99%)	420 (96%)	16 (4%)	2 (0%)	34	54
All	All	3537/3672 (96%)	3390 (96%)	131 (4%)	16 (0%)	34	54

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 ⓘ

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%)	29	49
1	C	376/401 (94%)	353 (94%)	23 (6%)	23	40
1	E	379/401 (94%)	357 (94%)	22 (6%)	25	43
1	G	378/401 (94%)	356 (94%)	22 (6%)	25	43
2	B	376/379 (99%)	356 (95%)	20 (5%)	28	48
2	D	378/379 (100%)	358 (95%)	20 (5%)	28	48
2	F	377/379 (100%)	357 (95%)	20 (5%)	28	48
2	H	377/379 (100%)	356 (94%)	21 (6%)	26	45
All	All	3025/3120 (97%)	2857 (94%)	168 (6%)	26	45

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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Mol	Chain	Res	Type
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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Mol	Chain	Res	Type
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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Mol	Chain	Res	Type
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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Mol	Chain	Res	Type
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

Some 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 ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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

There are no such residues in this entry.

5.8 Polymer linkage issues

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	457/475 (96%)	0.66	23 (5%) 32 38	31, 49, 83, 101	0
1	C	444/475 (93%)	0.43	15 (3%) 49 55	30, 50, 75, 101	0
1	E	448/475 (94%)	0.62	28 (6%) 23 27	34, 53, 80, 101	0
1	G	450/475 (94%)	0.61	26 (5%) 26 31	35, 54, 82, 101	0
2	B	439/443 (99%)	0.52	9 (2%) 67 72	30, 51, 76, 95	0
2	D	441/443 (99%)	0.46	13 (2%) 55 61	33, 58, 79, 97	0
2	F	440/443 (99%)	0.68	36 (8%) 14 16	44, 67, 86, 97	0
2	H	440/443 (99%)	1.51	147 (33%) 0 0	52, 75, 91, 99	0
All	All	3559/3672 (96%)	0.68	297 (8%) 14 15	30, 58, 85, 101	0

All (297) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	250	PHE	9.5
1	E	250	PHE	8.7
1	C	252	ASN	7.9
2	H	456	ILE	7.8
2	H	198	TYR	7.8
2	H	71	PHE	7.4
1	C	249	VAL	6.9
1	G	249	VAL	6.6
2	H	190	ILE	6.6
2	H	444	LEU	6.6
1	E	253	LEU	6.5
1	A	250	PHE	6.4
1	E	249	VAL	6.4
1	A	311	TYR	6.3
1	A	252	ASN	6.2
1	G	252	ASN	6.1

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Mol	Chain	Res	Type	RSRZ
2	H	171	TYR	6.0
2	H	263	LEU	6.0
2	H	184	ILE	5.9
1	C	250	PHE	5.9
2	F	198	TYR	5.8
2	H	239	VAL	5.8
2	H	257	PHE	5.8
2	H	233	PRO	5.7
1	A	253	LEU	5.7
2	H	195	LEU	5.7
1	A	14	ALA	5.6
1	A	249	VAL	5.4
2	H	258	ILE	5.4
1	G	311	TYR	5.2
1	A	288	SER	5.1
2	H	339	TYR	5.0
1	E	311	TYR	5.0
1	E	14	ALA	4.9
1	E	251	GLY	4.9
2	H	187	ILE	4.9
2	H	182	GLY	4.7
1	A	15	ARG	4.7
1	C	312	PHE	4.7
2	D	245	ARG	4.6
2	H	440	SER	4.6
1	C	253	LEU	4.6
2	H	251	PHE	4.6
2	D	88	ILE	4.5
1	G	294	PRO	4.4
2	H	342	THR	4.4
2	H	64	LYS	4.4
2	H	181	LEU	4.4
1	E	252	ASN	4.4
1	G	253	LEU	4.3
2	D	197	ASP	4.3
1	A	248	PRO	4.3
1	A	289	PHE	4.2
2	H	163	PHE	4.2
2	F	190	ILE	4.2
2	F	229	PHE	4.2
2	H	193	THR	4.2
2	H	161	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
2	H	269	ALA	4.1
2	H	238	PRO	4.1
1	G	14	ALA	4.1
1	A	358	LYS	4.0
2	H	237	SER	4.0
2	H	166	LEU	4.0
1	A	469	SER	4.0
2	H	450	VAL	4.0
1	A	254	PRO	4.0
2	H	208	MET	4.0
1	A	290	SER	3.9
2	H	54	VAL	3.9
2	H	357	LEU	3.9
1	C	311	TYR	3.9
2	H	262	THR	3.9
2	H	203	TYR	3.8
2	H	447	THR	3.8
2	H	200	THR	3.8
1	G	251	GLY	3.7
2	F	136	ASP	3.7
2	H	189	SER	3.6
2	H	165	HIS	3.6
2	H	72	LEU	3.6
2	H	176	LEU	3.6
2	H	65	ASN	3.6
1	A	470	SER	3.6
1	E	312	PHE	3.6
2	H	55	ASP	3.6
2	H	99	LEU	3.6
2	H	226	GLN	3.6
2	F	246	GLY	3.6
2	H	236	GLU	3.5
2	D	71	PHE	3.5
2	F	60	ALA	3.5
2	H	60	ALA	3.5
2	H	267	HIS	3.5
2	H	434	LEU	3.5
2	H	443	ALA	3.4
2	D	190	ILE	3.4
1	E	288	SER	3.4
2	H	350	ARG	3.4
2	F	245	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
2	H	445	GLY	3.4
2	H	173	ASP	3.4
2	H	204	LYS	3.4
2	H	449	THR	3.4
2	H	260	GLU	3.3
1	E	468	SER	3.3
2	H	77	PHE	3.3
2	H	254	GLY	3.3
2	H	37	ILE	3.3
2	H	256	ARG	3.3
2	F	138	SER	3.3
2	D	148	ILE	3.3
2	H	68	THR	3.3
2	H	180	ILE	3.2
2	H	229	PHE	3.2
2	H	69	ALA	3.2
2	H	145	ASP	3.1
1	C	303	TYR	3.1
2	F	130	LEU	3.1
2	H	31	LEU	3.1
2	H	459	LYS	3.1
2	H	95	ILE	3.1
2	H	35	LEU	3.0
2	H	335	LEU	3.0
2	H	446	ASN	3.0
1	G	231	THR	3.0
2	H	197	ASP	3.0
2	H	248	LEU	3.0
1	A	291	ALA	3.0
2	B	27	ARG	3.0
1	A	251	GLY	3.0
1	E	356	ALA	3.0
1	E	15	ARG	3.0
2	H	199	ILE	3.0
2	H	23	ILE	3.0
2	F	239	VAL	2.9
2	H	346	GLU	2.9
2	H	202	ASN	2.9
2	H	352	ILE	2.9
2	H	148	ILE	2.9
2	F	181	LEU	2.9
2	H	110	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
2	H	149	ARG	2.9
1	E	254	PRO	2.9
2	H	264	PRO	2.9
1	C	310	TYR	2.8
2	H	137	ASN	2.8
2	H	452	ASN	2.8
2	F	203	TYR	2.8
2	D	201	LYS	2.8
2	H	188	LYS	2.8
2	H	265	THR	2.8
2	H	240	PRO	2.8
1	A	303	TYR	2.8
2	H	245	ARG	2.8
1	C	405	VAL	2.8
2	H	61	GLU	2.8
1	G	416	LYS	2.8
2	F	127	SER	2.8
2	H	363	ILE	2.8
2	D	462	GLN	2.8
2	H	158	TYR	2.8
2	H	261	ASN	2.8
1	G	15	ARG	2.8
2	H	185	LYS	2.8
2	F	23	ILE	2.7
2	H	135	LEU	2.7
2	B	140	ILE	2.7
2	D	246	GLY	2.7
2	H	59	ARG	2.7
2	H	235	SER	2.7
2	H	219	GLU	2.7
2	H	441	MET	2.7
2	F	235	SER	2.7
1	C	268	ILE	2.7
1	E	313	VAL	2.7
2	F	225	ALA	2.7
2	H	341	VAL	2.6
2	H	192	ARG	2.6
1	C	412	ILE	2.6
2	F	240	PRO	2.6
2	H	439	VAL	2.6
2	F	196	LYS	2.6
1	G	312	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	248	PRO	2.6
1	G	229	PRO	2.6
2	H	241	LEU	2.6
2	H	343	ASP	2.5
2	F	185	LYS	2.5
2	H	271	ALA	2.5
2	B	236	GLU	2.5
2	D	76	ALA	2.5
1	G	292	GLY	2.5
2	H	259	LYS	2.5
2	H	178	ARG	2.5
2	H	75	LEU	2.5
2	H	348	ASN	2.5
2	H	360	TRP	2.5
1	G	403	ILE	2.5
2	H	313	ALA	2.5
2	H	175	PRO	2.5
2	H	347	HIS	2.5
1	G	274	TYR	2.4
2	H	319	LEU	2.4
2	H	108	THR	2.4
2	H	201	LYS	2.4
2	F	236	GLU	2.4
1	E	248	PRO	2.4
2	H	82	ASN	2.4
2	H	349	VAL	2.4
2	H	442	VAL	2.4
2	B	64	LYS	2.4
2	H	30	LYS	2.4
2	B	137	ASN	2.4
1	A	468	SER	2.4
2	F	238	PRO	2.4
2	F	137	ASN	2.4
2	H	172	LYS	2.4
1	A	57	LEU	2.4
1	E	415	LEU	2.4
2	H	25	GLY	2.3
1	G	230	ILE	2.3
2	F	71	PHE	2.3
2	H	81	GLN	2.3
2	F	248	LEU	2.3
2	F	44	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	23	ILE	2.3
2	H	356	ILE	2.3
2	H	32	PRO	2.3
2	H	455	TYR	2.3
2	H	131	THR	2.3
2	F	424	ASP	2.3
1	E	358	LYS	2.3
2	F	134	VAL	2.3
1	G	248	PRO	2.3
2	B	245	ARG	2.3
2	F	149	ARG	2.3
1	A	247	ALA	2.2
1	G	411	LYS	2.2
2	H	209	VAL	2.2
2	F	81	GLN	2.2
1	E	298	MET	2.2
2	B	148	ILE	2.2
2	H	129	ILE	2.2
1	C	251	GLY	2.2
2	F	304	ASN	2.2
1	C	441	ARG	2.2
2	F	175	PRO	2.2
1	E	56	ASN	2.2
2	H	367	LYS	2.2
1	A	295	GLY	2.2
2	D	22	GLN	2.2
1	E	360	LEU	2.2
2	B	90	LEU	2.2
2	H	168	GLU	2.2
2	F	197	ASP	2.2
1	E	303	TYR	2.2
2	H	88	ILE	2.2
2	F	234	LYS	2.2
2	H	57	GLY	2.1
1	G	413	GLU	2.1
2	F	187	ILE	2.1
1	E	55	ARG	2.1
2	H	52	ILE	2.1
2	H	130	LEU	2.1
2	H	183	PRO	2.1
2	H	453	VAL	2.1
1	E	210	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
2	H	128	ASP	2.1
1	G	406	ASN	2.1
1	E	422	ARG	2.1
1	E	307	LEU	2.1
1	G	378	LEU	2.1
1	G	379	LEU	2.1
2	F	233	PRO	2.1
1	A	405	VAL	2.1
1	G	418	ASP	2.1
2	H	157	MET	2.1
1	C	56	ASN	2.1
1	E	310	TYR	2.1
2	F	140	ILE	2.1
2	H	454	SER	2.1
1	E	230	ILE	2.1
2	H	268	ILE	2.1
2	H	231	HIS	2.1
2	H	211	ALA	2.0
2	B	449	THR	2.0
2	H	103	THR	2.0
2	H	326	PHE	2.0
2	D	452	ASN	2.0
1	E	229	PRO	2.0
2	H	234	LYS	2.0
1	G	362	LEU	2.0
2	H	351	LEU	2.0
2	H	388	LEU	2.0
1	G	310	TYR	2.0
2	H	196	LYS	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 [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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	LLDF	B-factors(Å ²)	Q<0.9
3	ZN	H	504	1/1	0.84	0.10	-1.29	100,100,100,100	0
3	ZN	B	501	1/1	0.98	0.17	-	46,46,46,46	0
3	ZN	F	503	1/1	0.96	0.14	-	73,73,73,73	0
3	ZN	D	502	1/1	0.94	0.14	-	64,64,64,64	0

6.5 Other polymers [i](#)

There are no such residues in this entry.