



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:54 PM GMT

PDB ID : 1HR6
Title : Yeast Mitochondrial Processing Peptidase
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 : 2.50 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

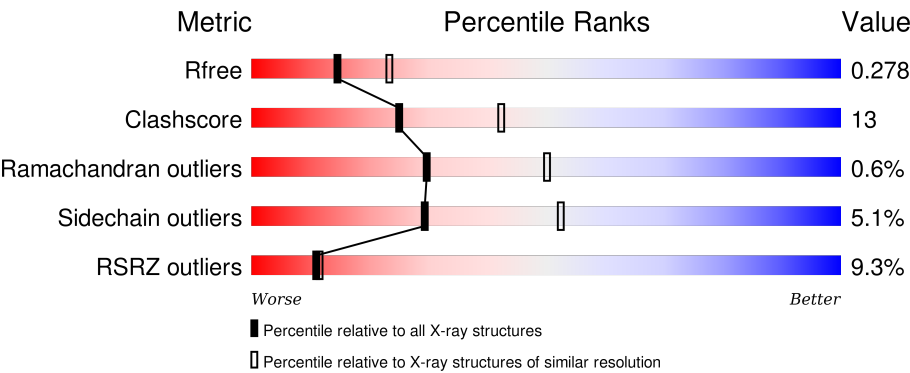
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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>6%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>72%22%••</div></div>
1	C	475	<div><div>4%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>72%21%•5%</div></div>
1	E	475	<div><div>7%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>73%21%••</div></div>
1	G	475	<div><div>8%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>70%23%••</div></div>
2	B	443	<div><div>4%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>72%25%••</div></div>

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

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EPE	G	489	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 28061 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	453	Total	C	N	O	S	0	0	0
			3503	2218	592	674	19			
1	E	455	Total	C	N	O	S	0	0	0
			3519	2227	597	676	19			
1	G	457	Total	C	N	O	S	0	0	0
			3531	2233	599	680	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	590	669	7			
2	D	443	Total	C	N	O	S	0	0	0
			3442	2165	595	675	7			
2	F	443	Total	C	N	O	S	0	0	0
			3442	2165	595	675	7			
2	H	440	Total	C	N	O	S	0	0	0
			3422	2154	591	670	7			

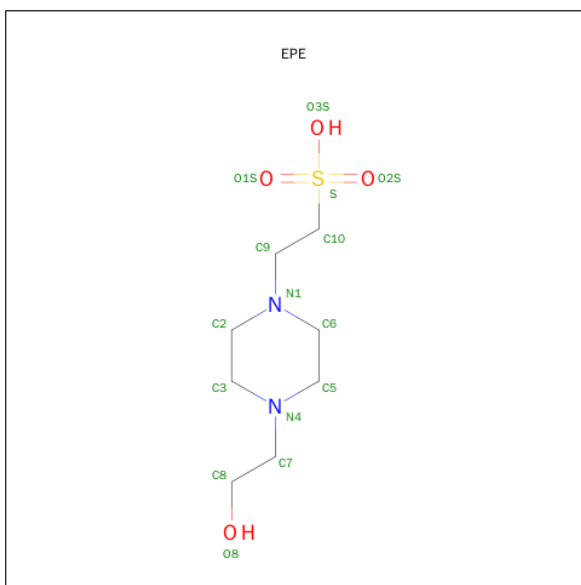
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	20	ALA	-	CLONING ARTIFACT	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	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	84	PRO	SER	SEE REMARK 999	UNP P10507
F	350	ARG	GLN	SEE REMARK 999	UNP P10507
H	20	ALA	-	CLONING ARTIFACT	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	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		
3	F	1	Total	Zn	0	0
			1	1		

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
4	G	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	47	Total	O	0	0
			47	47		
5	B	54	Total	O	0	0
			54	54		

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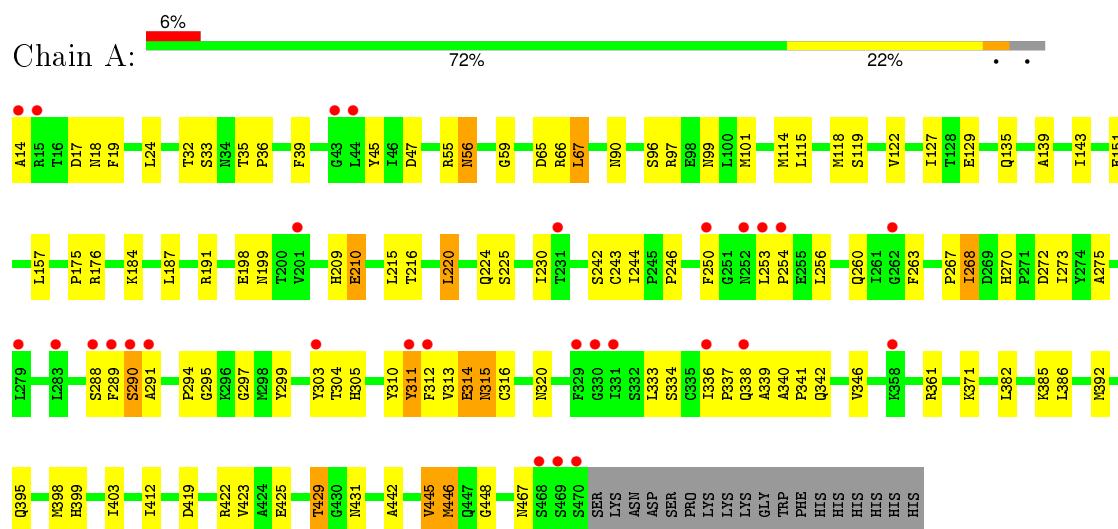
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	28	Total 28	O 28	0	0
5	D	21	Total 21	O 21	0	0
5	E	35	Total 35	O 35	0	0
5	F	10	Total 10	O 10	0	0
5	G	25	Total 25	O 25	0	0
5	H	3	Total 3	O 3	0	0

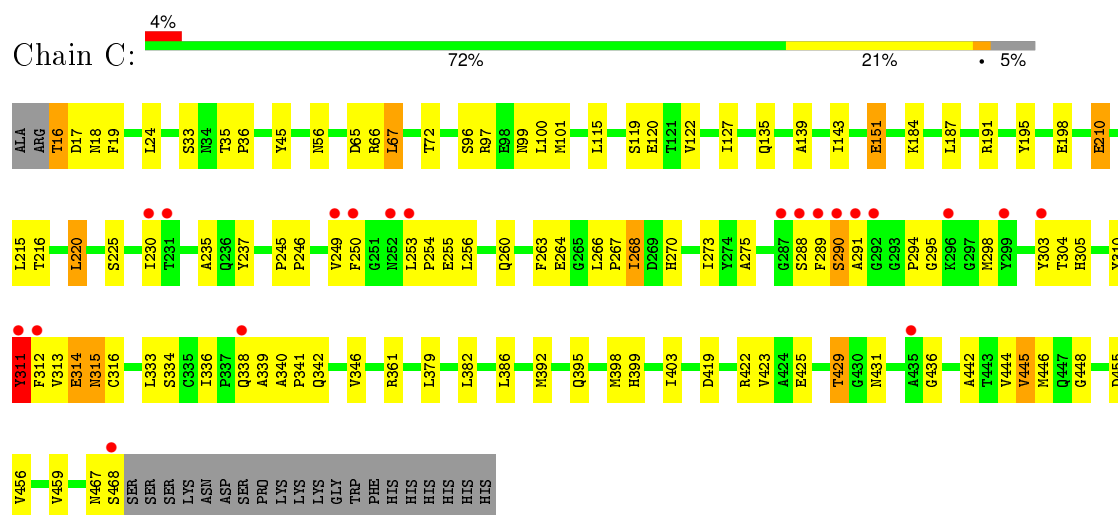
3 Residue-property plots

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 ($RSRZ > 2$). 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

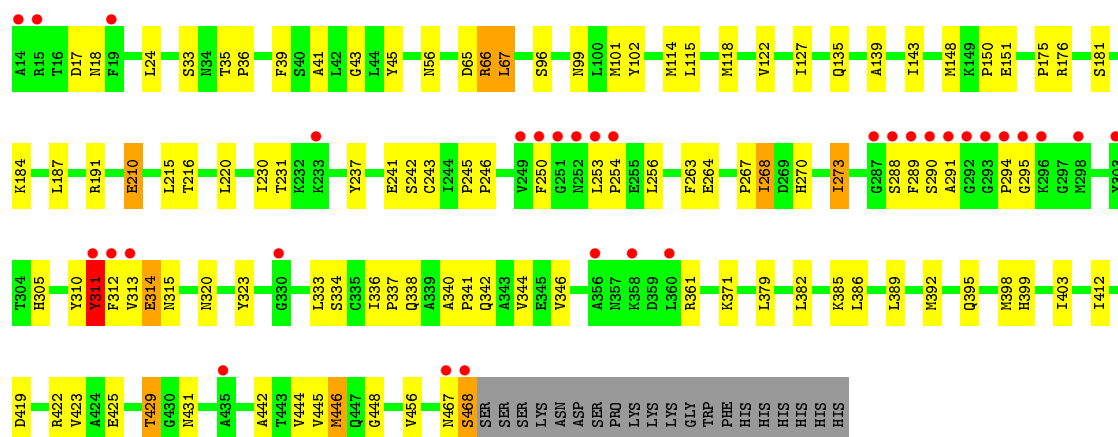


• Molecule 1: MITOCHONDRIAL PROCESSING PEPTIDASE ALPHA SUBUNIT

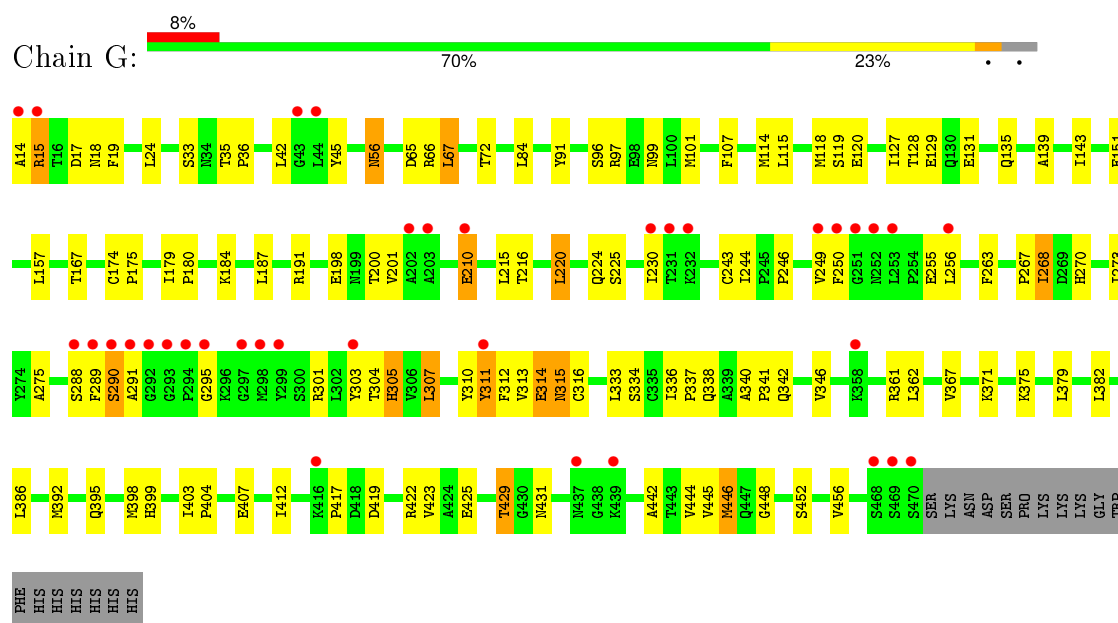


• Molecule 1: MITOCHONDRIAL PROCESSING PEPTIDASE ALPHA SUBUNIT

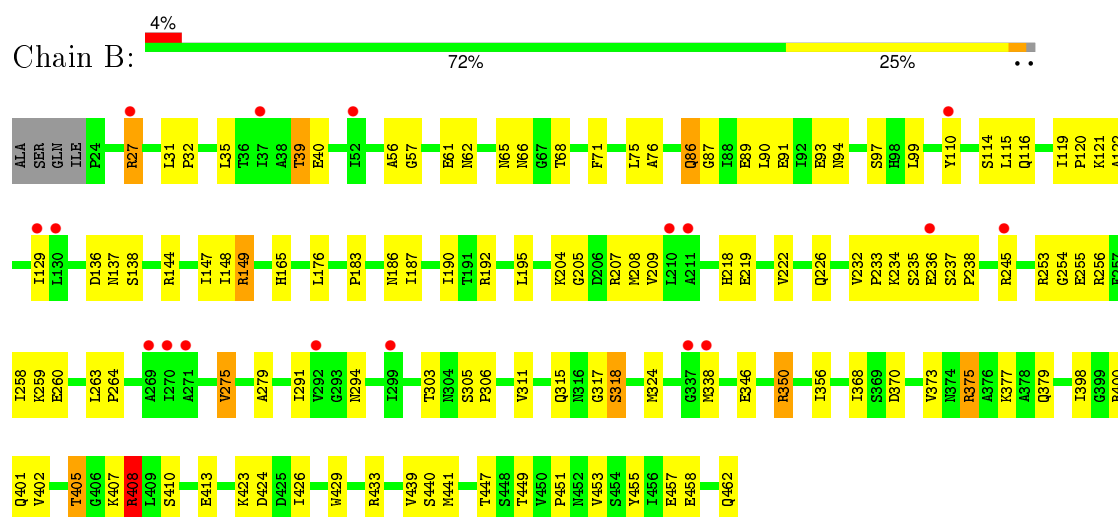




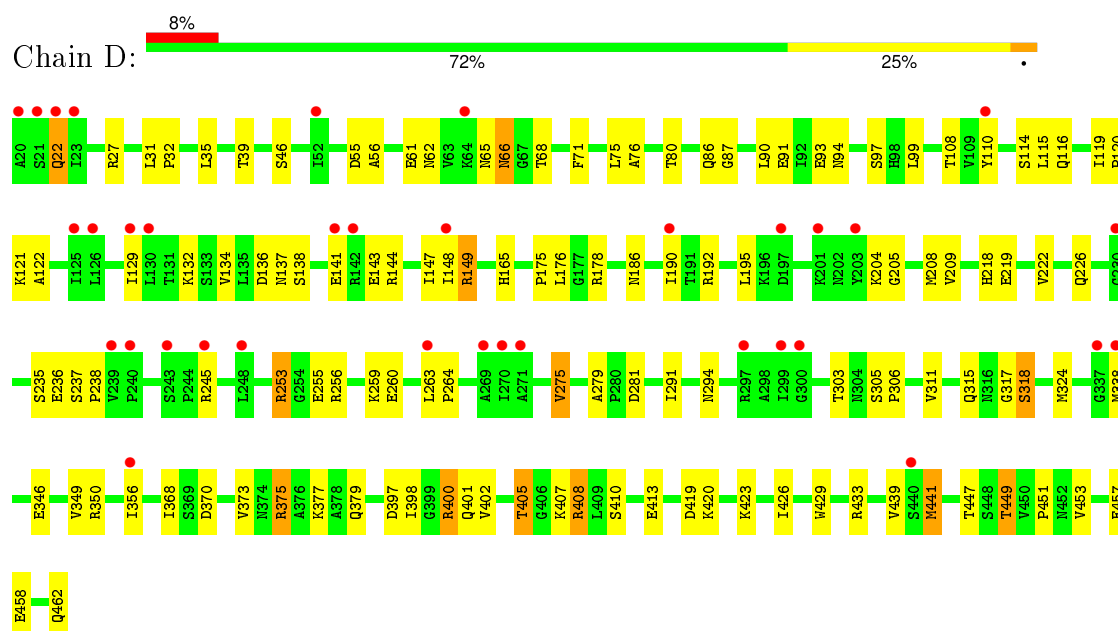
• Molecule 1: MITOCHONDRIAL PROCESSING PEPTIDASE ALPHA SUBUNIT



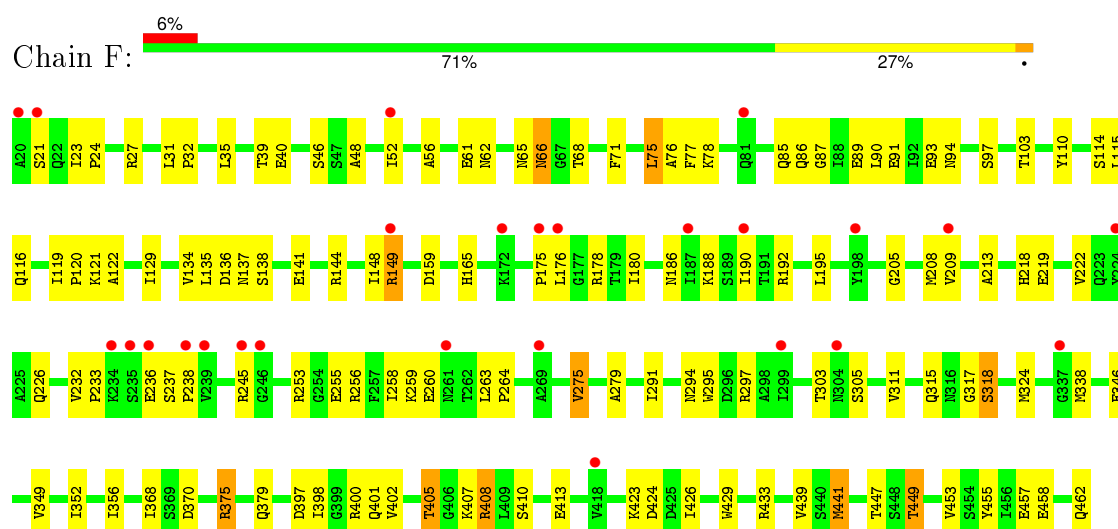
• Molecule 2: MITOCHONDRIAL PROCESSING PEPTIDASE BETA SUBUNIT



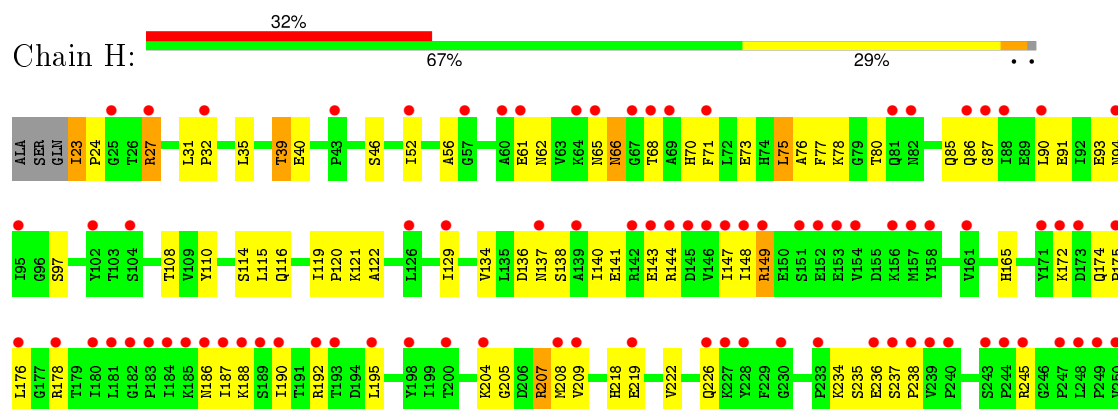
• Molecule 2: MITOCHONDRIAL PROCESSING PEPTIDASE BETA SUBUNIT

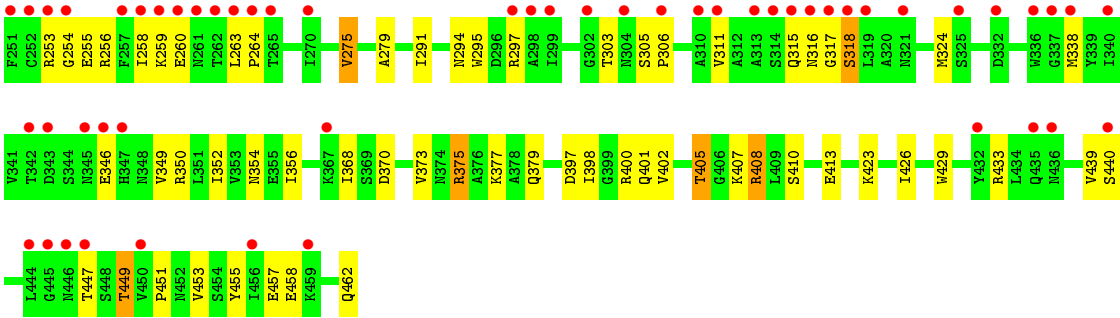


• Molecule 2: MITOCHONDRIAL PROCESSING PEPTIDASE BETA SUBUNIT



• 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	134.18Å 178.50Å 202.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.96 – 2.50 29.96 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.4 (29.96-2.50) 99.1 (29.96-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.68 (at 2.51Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.245 , 0.279 0.244 , 0.278	Depositor DCC
R_{free} test set	2027 reflections (1.22%)	DCC
Wilson B-factor (Å ²)	53.1	Xtriage
Anisotropy	0.297	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 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 166964 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	28061	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 2.32% 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, EPE

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	0.70	4/3604 (0.1%)	0.77	3/4877 (0.1%)
1	C	0.66	1/3576 (0.0%)	0.76	1/4840 (0.0%)
1	E	0.63	2/3592 (0.1%)	0.83	4/4861 (0.1%)
1	G	0.62	0/3604	0.76	3/4877 (0.1%)
2	B	0.62	0/3478	0.80	5/4720 (0.1%)
2	D	0.57	0/3506	0.84	6/4759 (0.1%)
2	F	0.53	0/3506	0.75	4/4759 (0.1%)
2	H	0.56	2/3486 (0.1%)	0.87	7/4732 (0.1%)
All	All	0.61	9/28352 (0.0%)	0.80	33/38425 (0.1%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	467	ASN	CG-OD1	-7.06	1.08	1.24
1	E	315	ASN	CG-OD1	-7.03	1.08	1.24
1	A	90	ASN	CG-ND2	-6.81	1.15	1.32
1	A	90	ASN	CG-OD1	-6.73	1.09	1.24
1	A	467	ASN	CG-ND2	-6.59	1.16	1.32
1	E	315	ASN	CG-ND2	-6.53	1.16	1.32
2	H	354	ASN	CG-OD1	-6.27	1.10	1.24
2	H	354	ASN	CG-ND2	-6.06	1.17	1.32
1	C	311	TYR	CG-CD2	-5.13	1.32	1.39

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	149	ARG	NE-CZ-NH2	-17.06	111.77	120.30
2	D	253	ARG	NE-CZ-NH1	-16.95	111.82	120.30
2	D	253	ARG	NE-CZ-NH2	16.31	128.45	120.30
1	E	422	ARG	NE-CZ-NH1	-16.20	112.20	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	149	ARG	NE-CZ-NH1	16.11	128.35	120.30
2	H	207	ARG	NE-CZ-NH1	-15.68	112.46	120.30
1	E	422	ARG	NE-CZ-NH2	14.66	127.63	120.30
2	H	207	ARG	NE-CZ-NH2	14.49	127.55	120.30
2	B	350	ARG	NE-CZ-NH2	8.93	124.76	120.30
1	E	311	TYR	CB-CG-CD1	-8.77	115.74	121.00
2	D	253	ARG	CD-NE-CZ	8.43	135.41	123.60
2	H	149	ARG	CD-NE-CZ	7.92	134.69	123.60
2	B	350	ARG	NE-CZ-NH1	-7.47	116.56	120.30
1	E	422	ARG	CD-NE-CZ	7.26	133.76	123.60
2	H	207	ARG	CD-NE-CZ	6.66	132.93	123.60
1	G	422	ARG	NE-CZ-NH2	-6.55	117.02	120.30
2	B	253	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	G	97	ARG	NE-CZ-NH1	-6.49	117.06	120.30
1	G	422	ARG	NE-CZ-NH1	6.48	123.54	120.30
2	D	149	ARG	NE-CZ-NH2	6.20	123.40	120.30
2	H	253	ARG	NE-CZ-NH1	6.04	123.32	120.30
2	D	149	ARG	NE-CZ-NH1	-6.03	117.28	120.30
2	F	253	ARG	NE-CZ-NH1	6.01	123.30	120.30
1	C	422	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	A	422	ARG	NE-CZ-NH2	-5.90	117.35	120.30
2	F	149	ARG	NE-CZ-NH2	5.83	123.21	120.30
2	F	149	ARG	NE-CZ-NH1	-5.62	117.49	120.30
1	A	97	ARG	NE-CZ-NH1	-5.61	117.50	120.30
2	B	149	ARG	NE-CZ-NH2	5.52	123.06	120.30
2	F	253	ARG	NE-CZ-NH2	-5.36	117.62	120.30
2	B	408	ARG	NE-CZ-NH1	5.20	122.90	120.30
2	D	350	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	A	422	ARG	NE-CZ-NH1	5.03	122.81	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	85	0
1	C	3503	0	3460	84	0
1	E	3519	0	3478	70	0
1	G	3531	0	3488	97	0
2	B	3414	0	3412	97	0
2	D	3442	0	3440	92	0
2	F	3442	0	3440	90	0
2	H	3422	0	3422	113	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	15	0	17	0	0
4	G	15	0	17	0	0
5	A	47	0	0	3	0
5	B	54	0	0	2	0
5	C	28	0	0	1	0
5	D	21	0	0	0	0
5	E	35	0	0	3	0
5	F	10	0	0	0	0
5	G	25	0	0	1	0
5	H	3	0	0	0	0
All	All	28061	0	27662	703	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 13.

All (703) 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	1.28	1.16
2:H:294:ASN:HD22	2:H:324:MET:HA	1.11	1.11
2:B:294:ASN:HD22	2:B:324:MET:HA	1.14	1.07
1:A:33:SER:HB3	1:A:392:MET:HE1	1.42	0.99
1:C:315:ASN:HD22	1:C:316:CYS:N	1.61	0.99
1:G:315:ASN:HD22	1:G:316:CYS:N	1.60	0.98
1:A:315:ASN:HD22	1:A:316:CYS:N	1.63	0.97
1:G:33:SER:HB3	1:G:392:MET:HE1	1.48	0.96
1:E:268:ILE:HD11	1:E:398:MET:SD	2.06	0.95
1:C:24:LEU:HD11	1:C:216:THR:HG22	1.51	0.93
1:G:268:ILE:HD11	1:G:398:MET:SD	2.08	0.92
1:G:24:LEU:HD11	1:G:216:THR:HG22	1.53	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:311:TYR:HD2	1:G:311:TYR:N	1.62	0.90
1:A:268:ILE:HD11	1:A:398:MET:SD	2.12	0.90
1:A:24:LEU:HD11	1:A:216:THR:HG22	1.52	0.89
2:D:256:ARG:HH11	2:D:256:ARG:HG3	1.34	0.89
1:C:33:SER:HB3	1:C:392:MET:HE1	1.54	0.89
1:E:33:SER:HB3	1:E:392:MET:CE	2.03	0.88
1:C:268:ILE:HD11	1:C:398:MET:SD	2.15	0.87
2:B:256:ARG:HG3	2:B:256:ARG:HH11	1.41	0.85
2:F:256:ARG:HG3	2:F:256:ARG:HH11	1.40	0.84
2:H:62:ASN:H	2:H:65:ASN:HB3	1.42	0.84
1:C:33:SER:HB3	1:C:392:MET:CE	2.07	0.84
2:H:294:ASN:ND2	2:H:324:MET:HA	1.93	0.84
2:F:62:ASN:H	2:F:65:ASN:HB3	1.43	0.83
1:G:33:SER:HB3	1:G:392:MET:CE	2.09	0.82
1:C:295:GLY:HA2	2:D:93:GLU:HG2	1.60	0.82
1:A:33:SER:HB3	1:A:392:MET:CE	2.09	0.81
1:A:429:THR:CG2	1:A:431:ASN:HD22	1.93	0.81
1:G:230:ILE:HD12	1:G:230:ILE:H	1.45	0.81
2:B:62:ASN:H	2:B:65:ASN:HB3	1.45	0.81
1:A:425:GLU:O	1:A:429:THR:HB	1.81	0.80
1:G:429:THR:CG2	1:G:431:ASN:HD22	1.94	0.80
1:G:311:TYR:HD2	1:G:311:TYR:H	0.83	0.79
2:H:256:ARG:HH11	2:H:256:ARG:HG3	1.46	0.79
2:B:294:ASN:ND2	2:B:324:MET:HA	1.95	0.79
1:E:24:LEU:HD11	1:E:216:THR:HG22	1.64	0.79
2:D:62:ASN:H	2:D:65:ASN:HB3	1.48	0.79
1:G:14:ALA:N	1:G:19:PHE:HB3	1.97	0.78
1:C:230:ILE:H	1:C:230:ILE:HD12	1.49	0.78
2:H:144:ARG:O	2:H:148:ILE:HG12	1.84	0.78
1:C:246:PRO:HG3	1:C:448:GLY:HA2	1.64	0.78
1:G:311:TYR:CD2	1:G:311:TYR:N	2.35	0.78
2:H:275:VAL:HG22	2:H:279:ALA:CB	2.14	0.77
1:C:429:THR:CG2	1:C:431:ASN:HD22	1.98	0.77
1:E:425:GLU:O	1:E:429:THR:HB	1.84	0.77
2:H:23:ILE:HD13	2:H:23:ILE:N	2.00	0.76
1:C:230:ILE:N	1:C:230:ILE:HD12	2.01	0.76
1:E:429:THR:CG2	1:E:431:ASN:HD22	1.98	0.76
1:G:15:ARG:HG3	1:G:15:ARG:HH11	1.51	0.76
2:B:97:SER:OG	2:B:114:SER:HB3	1.86	0.76
1:A:230:ILE:H	1:A:230:ILE:HD12	1.51	0.76
1:G:425:GLU:O	1:G:429:THR:HB	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:230:ILE:HD12	1:E:230:ILE:H	1.51	0.76
1:C:425:GLU:O	1:C:429:THR:HB	1.87	0.75
1:G:96:SER:HB3	1:G:99:ASN:OD1	1.87	0.75
2:D:338:MET:HG2	2:D:356:ILE:HD13	1.69	0.74
1:E:295:GLY:HA2	2:F:93:GLU:HG2	1.69	0.74
1:G:230:ILE:HD12	1:G:230:ILE:N	2.02	0.74
2:B:294:ASN:HD22	2:B:324:MET:CA	1.99	0.73
2:D:144:ARG:O	2:D:148:ILE:HG12	1.87	0.73
2:F:144:ARG:O	2:F:148:ILE:HG12	1.87	0.73
2:H:76:ALA:HB1	2:H:129:ILE:CG2	2.19	0.73
2:H:294:ASN:HD22	2:H:324:MET:CA	1.96	0.73
2:B:458:GLU:O	2:B:462:GLN:HB2	1.89	0.72
1:G:295:GLY:HA2	2:H:93:GLU:HG2	1.71	0.72
2:B:144:ARG:O	2:B:148:ILE:HG12	1.89	0.72
1:A:230:ILE:N	1:A:230:ILE:HD12	2.04	0.72
2:D:275:VAL:HG22	2:D:279:ALA:CB	2.20	0.71
1:G:246:PRO:HG3	1:G:448:GLY:HA2	1.73	0.71
1:A:175:PRO:HB3	1:E:175:PRO:HB3	1.71	0.71
2:F:275:VAL:HG22	2:F:279:ALA:CB	2.21	0.71
2:H:275:VAL:HG22	2:H:279:ALA:HB3	1.73	0.70
1:G:289:PHE:CE2	1:G:291:ALA:HB2	2.27	0.70
2:F:116:GLN:O	2:F:119:ILE:HG12	1.91	0.70
2:B:76:ALA:HB1	2:B:129:ILE:CG2	2.21	0.70
2:H:338:MET:HG2	2:H:356:ILE:HD13	1.73	0.70
1:E:230:ILE:N	1:E:230:ILE:HD12	2.05	0.70
2:B:294:ASN:ND2	2:B:324:MET:HG3	2.07	0.69
2:F:458:GLU:O	2:F:462:GLN:HB2	1.92	0.69
2:F:76:ALA:HB1	2:F:129:ILE:CG2	2.21	0.69
2:H:294:ASN:ND2	2:H:324:MET:HG3	2.07	0.69
2:H:458:GLU:O	2:H:462:GLN:HB2	1.92	0.68
2:B:256:ARG:HG3	2:B:256:ARG:NH1	2.09	0.68
2:B:275:VAL:HG22	2:B:279:ALA:CB	2.23	0.68
2:D:256:ARG:HG3	2:D:256:ARG:NH1	2.03	0.68
2:D:116:GLN:O	2:D:119:ILE:HG12	1.94	0.68
2:F:256:ARG:HG3	2:F:256:ARG:NH1	2.05	0.67
1:G:14:ALA:N	1:G:17:ASP:OD2	2.27	0.67
2:D:458:GLU:O	2:D:462:GLN:HB2	1.94	0.67
2:H:119:ILE:O	2:H:122:ALA:HB3	1.95	0.67
1:G:429:THR:HG21	1:G:431:ASN:HD22	1.60	0.67
2:B:186:ASN:O	2:B:190:ILE:HG12	1.94	0.66
2:H:116:GLN:O	2:H:119:ILE:HG12	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:96:SER:HB3	1:C:99:ASN:OD1	1.96	0.66
1:C:379:LEU:HD13	2:D:46:SER:HB2	1.77	0.66
2:D:76:ALA:HB1	2:D:129:ILE:CG2	2.25	0.66
2:F:119:ILE:O	2:F:122:ALA:HB3	1.95	0.65
2:F:275:VAL:HG22	2:F:279:ALA:HB3	1.77	0.65
2:B:405:THR:HG22	2:B:407:LYS:H	1.61	0.65
1:C:315:ASN:HD22	1:C:315:ASN:C	2.00	0.65
2:D:97:SER:OG	2:D:114:SER:HB3	1.97	0.65
2:B:275:VAL:HG22	2:B:279:ALA:HB3	1.77	0.65
2:B:338:MET:HG2	2:B:356:ILE:HD13	1.79	0.65
1:E:246:PRO:HG3	1:E:448:GLY:HA2	1.77	0.65
2:H:259:LYS:HG3	2:H:447:THR:HG22	1.78	0.64
2:B:116:GLN:O	2:B:119:ILE:HG12	1.97	0.64
2:D:136:ASP:OD2	2:D:138:SER:HB3	1.98	0.64
1:G:336:ILE:HG22	1:G:338:GLN:OE1	1.98	0.64
2:B:136:ASP:OD2	2:B:138:SER:HB3	1.98	0.64
2:B:245:ARG:HA	2:B:245:ARG:HE	1.61	0.64
2:F:136:ASP:OD2	2:F:138:SER:HB3	1.97	0.64
1:C:295:GLY:CA	2:D:93:GLU:HG2	2.28	0.63
2:F:405:THR:HG22	2:F:407:LYS:H	1.63	0.63
1:G:315:ASN:HD22	1:G:316:CYS:H	1.44	0.63
2:F:186:ASN:O	2:F:190:ILE:HG12	1.99	0.63
1:E:139:ALA:O	1:E:143:ILE:HD13	1.98	0.63
2:H:256:ARG:NH1	2:H:256:ARG:HG3	2.14	0.63
2:H:405:THR:HG22	2:H:407:LYS:H	1.64	0.63
2:H:35:LEU:HD13	2:H:208:MET:HG3	1.81	0.63
2:F:245:ARG:HE	2:F:245:ARG:HA	1.64	0.63
2:D:303:THR:HG22	2:D:305:SER:H	1.64	0.62
1:G:15:ARG:C	1:G:15:ARG:HD3	2.20	0.62
1:E:187:LEU:O	1:E:191:ARG:HG3	1.99	0.62
1:A:96:SER:HB3	1:A:99:ASN:OD1	2.00	0.62
1:C:298:MET:HG2	2:D:93:GLU:OE2	1.99	0.62
1:A:295:GLY:HA2	2:B:93:GLU:HG2	1.79	0.62
2:H:186:ASN:O	2:H:190:ILE:HG12	2.00	0.62
1:A:187:LEU:O	1:A:191:ARG:HG3	2.00	0.62
2:H:236:GLU:C	2:H:238:PRO:HD3	2.21	0.62
2:B:401:GLN:O	2:B:405:THR:HB	1.99	0.62
1:E:336:ILE:HG22	1:E:338:GLN:OE1	1.99	0.62
1:A:315:ASN:HD22	1:A:315:ASN:C	2.00	0.61
1:G:340:ALA:HB3	1:G:341:PRO:HD3	1.82	0.61
1:G:230:ILE:CD1	1:G:230:ILE:H	2.13	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:35:LEU:HD13	2:F:208:MET:HG3	1.82	0.61
2:D:311:VAL:O	2:D:315:GLN:HG3	1.99	0.61
2:H:260:GLU:HG3	2:H:263:LEU:HG	1.83	0.61
1:C:336:ILE:HG22	1:C:338:GLN:OE1	2.01	0.61
1:E:342:GLN:O	1:E:346:VAL:HG23	2.01	0.61
1:E:96:SER:HB3	1:E:99:ASN:OD1	2.01	0.61
1:E:289:PHE:CE2	1:E:291:ALA:HB2	2.35	0.61
2:H:401:GLN:O	2:H:405:THR:HB	2.00	0.61
1:G:187:LEU:O	1:G:191:ARG:HG3	2.01	0.61
1:A:268:ILE:H	1:A:268:ILE:HD13	1.66	0.60
1:C:268:ILE:H	1:C:268:ILE:HD13	1.65	0.60
2:F:338:MET:HG2	2:F:356:ILE:HD13	1.83	0.60
2:H:91:GLU:OE2	2:H:121:LYS:HD2	2.02	0.60
2:B:165:HIS:CD2	2:B:258:ILE:HD11	2.36	0.60
1:G:315:ASN:HD22	1:G:315:ASN:C	2.04	0.60
1:A:139:ALA:O	1:A:143:ILE:HD13	2.01	0.60
1:E:243:CYS:HA	1:E:446:MET:O	2.02	0.60
2:F:97:SER:OG	2:F:114:SER:HB3	2.02	0.60
1:A:224:GLN:CD	1:G:129:GLU:HG3	2.22	0.60
2:F:90:LEU:HD13	2:F:94:ASN:ND2	2.17	0.60
1:A:242:SER:OG	1:E:176:ARG:NH2	2.35	0.60
1:E:340:ALA:HB3	1:E:341:PRO:HD3	1.83	0.60
2:D:186:ASN:O	2:D:190:ILE:HG12	2.00	0.60
1:C:268:ILE:HD13	1:C:268:ILE:N	2.16	0.59
2:D:275:VAL:HG22	2:D:279:ALA:HB3	1.82	0.59
2:H:439:VAL:HG13	2:H:457:GLU:HG2	1.83	0.59
2:H:31:LEU:HG	2:H:32:PRO:HD2	1.82	0.59
2:D:245:ARG:HA	2:D:245:ARG:HE	1.66	0.59
2:H:90:LEU:HD13	2:H:94:ASN:ND2	2.16	0.59
2:H:136:ASP:OD2	2:H:138:SER:HB3	2.01	0.59
2:D:204:LYS:HG3	2:D:235:SER:OG	2.02	0.59
1:G:268:ILE:HD13	1:G:268:ILE:N	2.17	0.59
2:D:260:GLU:HG3	2:D:263:LEU:HG	1.84	0.59
2:D:439:VAL:HG13	2:D:457:GLU:HG2	1.83	0.59
2:B:368:ILE:O	2:B:423:LYS:HE3	2.03	0.59
1:C:419:ASP:O	1:C:423:VAL:HG23	2.03	0.59
2:D:31:LEU:HG	2:D:32:PRO:HD2	1.84	0.59
1:A:342:GLN:O	1:A:346:VAL:HG23	2.03	0.59
2:F:368:ILE:O	2:F:423:LYS:HE3	2.03	0.59
2:F:303:THR:HG22	2:F:305:SER:H	1.66	0.59
1:A:268:ILE:N	1:A:268:ILE:HD13	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:429:THR:HG21	1:C:431:ASN:HD22	1.65	0.59
2:B:40:GLU:OE1	2:B:408:ARG:NH2	2.35	0.59
1:A:429:THR:HG21	1:A:431:ASN:HD22	1.67	0.58
2:B:260:GLU:HG3	2:B:263:LEU:HG	1.85	0.58
1:C:230:ILE:H	1:C:230:ILE:CD1	2.14	0.58
2:B:259:LYS:HG3	2:B:447:THR:HG22	1.84	0.58
1:C:342:GLN:O	1:C:346:VAL:HG23	2.03	0.58
1:G:311:TYR:C	1:G:313:VAL:H	2.06	0.58
1:G:127:ILE:HB	1:G:184:LYS:HE3	1.86	0.58
1:C:139:ALA:O	1:C:143:ILE:HD13	2.03	0.58
2:D:119:ILE:N	2:D:120:PRO:HD2	2.19	0.58
2:B:439:VAL:HG13	2:B:457:GLU:HG2	1.85	0.58
1:G:268:ILE:HD13	1:G:268:ILE:H	1.68	0.58
2:F:260:GLU:HG3	2:F:263:LEU:HG	1.84	0.58
2:H:207:ARG:NH1	2:H:245:ARG:NH1	2.52	0.58
2:H:207:ARG:HH11	2:H:245:ARG:NH1	2.02	0.58
2:B:76:ALA:O	2:B:129:ILE:HG23	2.04	0.58
2:H:119:ILE:N	2:H:120:PRO:HD2	2.19	0.58
2:H:97:SER:OG	2:H:114:SER:HB3	2.03	0.58
2:D:119:ILE:O	2:D:122:ALA:HB3	2.04	0.58
1:A:340:ALA:HB3	1:A:341:PRO:HD3	1.85	0.58
2:H:311:VAL:O	2:H:315:GLN:HG3	2.03	0.57
1:G:315:ASN:ND2	1:G:316:CYS:N	2.43	0.57
1:E:230:ILE:CD1	1:E:230:ILE:H	2.18	0.57
2:F:303:THR:HG22	2:F:305:SER:N	2.20	0.57
2:H:375:ARG:NH2	2:H:379:GLN:OE1	2.37	0.57
2:D:91:GLU:OE2	2:D:121:LYS:HD2	2.04	0.57
1:G:139:ALA:O	1:G:143:ILE:HD13	2.03	0.57
1:E:429:THR:HG21	1:E:431:ASN:HD22	1.70	0.57
1:A:230:ILE:CD1	1:A:230:ILE:H	2.16	0.57
2:H:31:LEU:HD21	2:H:226:GLN:HA	1.86	0.57
2:D:259:LYS:HG3	2:D:447:THR:HG22	1.86	0.57
2:D:209:VAL:HG21	2:D:402:VAL:HG12	1.86	0.57
2:D:236:GLU:C	2:D:238:PRO:HD3	2.25	0.57
2:H:255:GLU:HB3	2:H:453:VAL:HG23	1.87	0.57
2:B:97:SER:OG	2:B:114:SER:CB	2.53	0.57
2:H:165:HIS:CD2	2:H:258:ILE:HD11	2.39	0.57
1:C:310:TYR:CD1	1:C:312:PHE:CZ	2.92	0.57
1:G:19:PHE:HD1	1:G:392:MET:HE1	1.68	0.56
1:E:268:ILE:N	1:E:268:ILE:HD13	2.20	0.56
2:H:115:LEU:H	2:H:115:LEU:HD12	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:311:TYR:C	1:E:313:VAL:H	2.09	0.56
2:H:303:THR:HG22	2:H:305:SER:H	1.69	0.56
1:C:127:ILE:HB	1:C:184:LYS:HE3	1.87	0.56
1:G:311:TYR:C	1:G:313:VAL:N	2.55	0.56
2:F:291:ILE:HD12	2:F:426:ILE:HD13	1.88	0.56
2:D:405:THR:HG22	2:D:407:LYS:H	1.70	0.56
1:A:99:ASN:HB2	1:A:101:MET:HE3	1.88	0.56
1:A:336:ILE:HG22	1:A:338:GLN:OE1	2.04	0.56
1:E:333:LEU:HD13	1:E:334:SER:N	2.20	0.56
1:E:311:TYR:C	1:E:313:VAL:N	2.58	0.56
2:F:218:HIS:O	2:F:222:VAL:HG23	2.06	0.56
1:A:290:SER:HB3	1:A:303:TYR:OH	2.06	0.56
1:A:289:PHE:CE2	1:A:291:ALA:HB2	2.40	0.56
1:C:340:ALA:HB3	1:C:341:PRO:HD3	1.87	0.55
2:H:234:LYS:HG2	2:H:235:SER:O	2.07	0.55
2:H:137:ASN:ND2	2:H:192:ARG:HD2	2.21	0.55
2:H:398:ILE:HA	2:H:408:ARG:HG3	1.88	0.55
2:F:255:GLU:HB3	2:F:453:VAL:HG23	1.88	0.55
2:F:439:VAL:HG13	2:F:457:GLU:HG2	1.88	0.55
1:C:122:VAL:O	1:C:191:ARG:NH2	2.40	0.55
1:G:342:GLN:O	1:G:346:VAL:HG23	2.07	0.55
2:F:137:ASN:ND2	2:F:192:ARG:HD2	2.22	0.55
2:F:311:VAL:O	2:F:315:GLN:HG3	2.06	0.55
1:A:14:ALA:N	1:A:17:ASP:OD2	2.40	0.54
1:A:299:TYR:OH	2:B:86:GLN:HG2	2.07	0.54
1:C:289:PHE:CE2	1:C:291:ALA:HB2	2.41	0.54
1:A:311:TYR:C	1:A:313:VAL:H	2.08	0.54
2:H:76:ALA:O	2:H:129:ILE:HG23	2.08	0.54
2:B:119:ILE:O	2:B:122:ALA:HB3	2.07	0.54
2:F:91:GLU:OE2	2:F:121:LYS:HD2	2.06	0.54
1:C:19:PHE:HD1	1:C:392:MET:HE1	1.72	0.54
2:F:119:ILE:N	2:F:120:PRO:HD2	2.22	0.54
1:A:127:ILE:HB	1:A:184:LYS:HE3	1.89	0.54
2:H:368:ILE:O	2:H:423:LYS:HE3	2.07	0.54
2:B:137:ASN:ND2	2:B:192:ARG:HD2	2.23	0.54
2:D:255:GLU:HB3	2:D:453:VAL:HG23	1.89	0.54
1:C:187:LEU:O	1:C:191:ARG:HG3	2.07	0.54
1:A:35:THR:HB	1:A:36:PRO:CD	2.37	0.54
1:C:35:THR:HB	1:C:36:PRO:CD	2.38	0.54
1:A:310:TYR:CD1	1:A:312:PHE:CZ	2.96	0.54
1:A:99:ASN:HB2	1:A:101:MET:CE	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:419:ASP:O	1:G:423:VAL:HG23	2.08	0.54
1:C:294:PRO:HD2	2:D:99:LEU:HB3	1.90	0.54
2:F:209:VAL:HG21	2:F:402:VAL:HG12	1.89	0.54
2:F:398:ILE:HA	2:F:408:ARG:HG3	1.91	0.53
1:A:320:ASN:ND2	5:A:492:HOH:O	2.39	0.53
1:A:311:TYR:C	1:A:313:VAL:N	2.60	0.53
2:B:90:LEU:HD13	2:B:94:ASN:ND2	2.22	0.53
2:H:237:SER:N	2:H:238:PRO:HD3	2.23	0.53
2:H:303:THR:HG22	2:H:305:SER:N	2.24	0.53
1:G:403:ILE:HG23	1:G:403:ILE:O	2.07	0.53
2:D:165:HIS:HD2	2:D:256:ARG:CD	2.21	0.53
2:F:401:GLN:O	2:F:405:THR:HB	2.08	0.53
2:H:35:LEU:HD12	2:H:208:MET:O	2.09	0.53
2:F:31:LEU:HG	2:F:32:PRO:HD2	1.90	0.53
2:D:31:LEU:HD21	2:D:226:GLN:HA	1.90	0.53
2:H:245:ARG:HE	2:H:245:ARG:HA	1.73	0.53
1:E:429:THR:HG22	1:E:431:ASN:HD22	1.74	0.53
1:C:311:TYR:C	1:C:313:VAL:H	2.11	0.53
2:B:303:THR:HG22	2:B:305:SER:H	1.73	0.53
1:E:444:VAL:HG11	1:E:456:VAL:HG11	1.91	0.53
2:D:68:THR:HG23	2:D:195:LEU:HD23	1.91	0.53
1:E:268:ILE:H	1:E:268:ILE:HD13	1.74	0.53
1:G:243:CYS:HA	1:G:446:MET:O	2.09	0.53
2:F:375:ARG:NH2	2:F:379:GLN:OE1	2.42	0.53
2:D:76:ALA:CB	2:D:110:TYR:HE2	2.22	0.52
2:D:97:SER:OG	2:D:114:SER:CB	2.57	0.52
1:C:267:PRO:HD2	1:C:270:HIS:HB2	1.90	0.52
1:E:379:LEU:HD13	2:F:46:SER:HB2	1.90	0.52
2:F:259:LYS:HG3	2:F:447:THR:HG22	1.92	0.52
1:E:66:ARG:HD3	5:E:517:HOH:O	2.09	0.52
2:D:303:THR:HG22	2:D:305:SER:N	2.24	0.52
2:H:291:ILE:HD12	2:H:426:ILE:HD13	1.92	0.52
2:B:303:THR:HG22	2:B:305:SER:N	2.25	0.52
2:B:31:LEU:HG	2:B:32:PRO:HD2	1.90	0.52
1:A:19:PHE:HD1	1:A:392:MET:HE1	1.75	0.52
2:B:119:ILE:N	2:B:120:PRO:HD2	2.24	0.52
2:F:90:LEU:CD1	2:F:94:ASN:HD21	2.22	0.52
1:G:256:LEU:CD1	1:G:314:GLU:HG2	2.39	0.52
1:A:246:PRO:HG3	1:A:448:GLY:HA2	1.91	0.52
1:G:67:LEU:HD13	1:G:135:GLN:HG3	1.91	0.52
2:D:375:ARG:NH2	2:D:379:GLN:OE1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:THR:HG22	1:A:431:ASN:HD22	1.73	0.52
2:H:90:LEU:CD1	2:H:94:ASN:HD21	2.23	0.52
2:B:31:LEU:HD21	2:B:226:GLN:HA	1.92	0.52
2:B:91:GLU:OE2	2:B:121:LYS:HD2	2.09	0.52
1:A:230:ILE:CD1	1:A:230:ILE:N	2.73	0.51
1:E:310:TYR:CD1	1:E:312:PHE:CZ	2.99	0.51
2:D:76:ALA:O	2:D:129:ILE:HG23	2.10	0.51
1:C:33:SER:HB3	1:C:392:MET:HE3	1.90	0.51
2:H:61:GLU:HA	2:H:65:ASN:HD22	1.75	0.51
2:D:294:ASN:OD1	2:D:324:MET:HA	2.11	0.51
1:C:235:ALA:O	1:C:436:GLY:HA3	2.10	0.51
1:E:419:ASP:O	1:E:423:VAL:HG23	2.11	0.51
1:E:127:ILE:HB	1:E:184:LYS:HE3	1.91	0.51
2:F:35:LEU:HA	2:F:205:GLY:O	2.11	0.51
2:B:410:SER:OG	2:B:413:GLU:HG3	2.11	0.51
2:D:401:GLN:O	2:D:405:THR:HB	2.10	0.51
2:B:375:ARG:NH2	2:B:379:GLN:OE1	2.43	0.51
2:B:35:LEU:HD13	2:B:208:MET:HG3	1.92	0.51
1:G:429:THR:HG22	1:G:431:ASN:HD22	1.74	0.51
1:C:311:TYR:C	1:C:313:VAL:N	2.60	0.51
2:D:115:LEU:HD12	2:D:115:LEU:H	1.75	0.51
2:D:35:LEU:HD13	2:D:208:MET:HG3	1.93	0.51
1:E:256:LEU:CD1	1:E:314:GLU:HG2	2.41	0.51
2:H:294:ASN:ND2	2:H:324:MET:CG	2.73	0.50
1:E:99:ASN:HB2	1:E:101:MET:CE	2.42	0.50
1:G:375:LYS:HE3	2:H:115:LEU:HD21	1.93	0.50
1:E:256:LEU:HD11	1:E:314:GLU:HG2	1.93	0.50
2:F:294:ASN:OD1	2:F:324:MET:HA	2.10	0.50
2:H:76:ALA:CB	2:H:110:TYR:HE2	2.24	0.50
2:F:76:ALA:O	2:F:129:ILE:HG23	2.11	0.50
2:H:141:GLU:O	2:H:144:ARG:HG3	2.12	0.50
2:D:90:LEU:HD13	2:D:94:ASN:ND2	2.26	0.50
2:F:35:LEU:HD12	2:F:208:MET:O	2.11	0.50
2:B:65:ASN:ND2	5:B:540:HOH:O	2.45	0.50
2:B:27:ARG:NH2	5:B:544:HOH:O	2.45	0.50
1:E:336:ILE:HG22	1:E:337:PRO:HD2	1.93	0.50
2:B:35:LEU:HD12	2:B:208:MET:O	2.11	0.50
1:A:256:LEU:CD1	1:A:314:GLU:HG2	2.42	0.50
2:H:255:GLU:HB3	2:H:453:VAL:CG2	2.42	0.50
2:D:62:ASN:CG	2:D:65:ASN:HB2	2.32	0.49
1:E:241:GLU:HA	1:E:444:VAL:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:373:VAL:O	2:B:377:LYS:HG3	2.12	0.49
2:F:317:GLY:O	2:F:318:SER:CB	2.60	0.49
1:C:315:ASN:HD22	1:C:316:CYS:H	1.50	0.49
2:B:62:ASN:CG	2:B:65:ASN:HB2	2.33	0.49
2:F:237:SER:N	2:F:238:PRO:HD3	2.27	0.49
1:G:15:ARG:HG3	1:G:15:ARG:NH1	2.23	0.49
2:H:175:PRO:HA	2:H:178:ARG:NH1	2.28	0.49
2:B:350:ARG:HD3	2:B:455:TYR:OH	2.12	0.49
2:D:175:PRO:HA	2:D:178:ARG:NH1	2.27	0.49
2:D:368:ILE:O	2:D:423:LYS:HE3	2.12	0.49
1:G:333:LEU:HD13	1:G:334:SER:N	2.27	0.49
1:A:176:ARG:NH2	1:E:242:SER:OG	2.46	0.49
2:B:61:GLU:HA	2:B:65:ASN:HD22	1.76	0.49
2:H:165:HIS:HD2	2:H:256:ARG:CD	2.25	0.49
1:A:395:GLN:OE1	1:A:403:ILE:HG22	2.13	0.49
2:B:39:THR:HG21	2:B:218:HIS:HB2	1.94	0.49
2:F:291:ILE:CD1	2:F:426:ILE:HD13	2.42	0.49
1:G:249:VAL:HG12	1:G:255:GLU:HB2	1.95	0.49
1:A:243:CYS:HA	1:A:446:MET:O	2.13	0.49
2:D:22:GLN:HA	2:D:22:GLN:OE1	2.12	0.49
2:F:255:GLU:HB3	2:F:453:VAL:CG2	2.43	0.48
1:E:39:PHE:O	1:E:385:LYS:HE3	2.13	0.48
1:C:16:THR:HG23	1:C:17:ASP:N	2.28	0.48
2:F:52:ILE:O	2:F:52:ILE:HG23	2.12	0.48
2:H:294:ASN:ND2	2:H:324:MET:CA	2.68	0.48
2:H:23:ILE:CD1	2:H:23:ILE:N	2.69	0.48
1:E:403:ILE:O	1:E:403:ILE:HG23	2.13	0.48
1:G:19:PHE:HD1	1:G:392:MET:CE	2.27	0.48
2:H:35:LEU:HA	2:H:205:GLY:O	2.13	0.48
2:F:35:LEU:CD1	2:F:208:MET:HG3	2.43	0.48
2:H:62:ASN:CG	2:H:65:ASN:HB2	2.33	0.48
2:D:255:GLU:HB3	2:D:453:VAL:CG2	2.44	0.48
1:C:249:VAL:HG12	1:C:255:GLU:HB2	1.95	0.48
1:E:210:GLU:HA	1:E:210:GLU:OE1	2.14	0.48
1:C:403:ILE:HG23	1:C:403:ILE:O	2.13	0.48
2:F:62:ASN:CG	2:F:65:ASN:HB2	2.34	0.48
1:A:67:LEU:HD13	1:A:135:GLN:HG3	1.95	0.48
1:A:304:THR:HG22	1:A:305:HIS:ND1	2.29	0.48
1:C:210:GLU:OE1	1:C:210:GLU:HA	2.13	0.48
2:H:35:LEU:CD1	2:H:208:MET:HG3	2.43	0.48
2:H:136:ASP:O	2:H:140:ILE:HG13	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:35:LEU:HA	2:B:205:GLY:O	2.14	0.48
2:F:175:PRO:HA	2:F:178:ARG:NH1	2.29	0.48
2:D:398:ILE:HA	2:D:408:ARG:HG3	1.96	0.48
2:H:370:ASP:OD1	2:H:423:LYS:NZ	2.46	0.48
1:E:115:LEU:HD23	1:E:215:LEU:HB3	1.96	0.48
2:D:317:GLY:O	2:D:318:SER:CB	2.61	0.48
1:E:344:VAL:HG23	5:E:493:HOH:O	2.14	0.48
2:F:61:GLU:OE1	2:F:66:ASN:HA	2.14	0.47
1:C:256:LEU:HD11	1:C:314:GLU:HG2	1.96	0.47
2:F:75:LEU:HA	2:F:78:LYS:HG2	1.96	0.47
1:G:210:GLU:OE1	1:G:210:GLU:HA	2.14	0.47
1:A:336:ILE:HG22	1:A:337:PRO:HD2	1.97	0.47
1:G:157:LEU:HD11	1:G:244:ILE:HD13	1.95	0.47
2:B:90:LEU:CD1	2:B:94:ASN:HD21	2.28	0.47
2:F:76:ALA:CB	2:F:110:TYR:HE2	2.27	0.47
1:A:297:GLY:HA2	2:B:93:GLU:OE1	2.14	0.47
1:G:267:PRO:HD2	1:G:270:HIS:HB2	1.95	0.47
1:C:260:GLN:HB2	1:C:445:VAL:HG12	1.97	0.47
1:G:99:ASN:HB2	1:G:101:MET:CE	2.44	0.47
2:F:97:SER:OG	2:F:114:SER:CB	2.62	0.47
1:C:310:TYR:HD1	1:C:312:PHE:CZ	2.31	0.47
1:C:16:THR:HG23	1:C:18:ASN:H	1.80	0.47
1:A:263:PHE:CE2	1:A:442:ALA:HB2	2.49	0.47
2:D:61:GLU:HA	2:D:65:ASN:HD22	1.78	0.47
2:H:76:ALA:HB1	2:H:129:ILE:HG23	1.93	0.47
2:F:236:GLU:C	2:F:238:PRO:HD3	2.34	0.47
1:G:119:SER:HB2	1:G:220:LEU:CD1	2.45	0.47
1:A:45:TYR:N	1:A:45:TYR:CD1	2.83	0.47
2:F:40:GLU:OE1	2:F:408:ARG:NH2	2.48	0.47
2:H:373:VAL:O	2:H:377:LYS:HG3	2.15	0.47
1:E:45:TYR:CD1	1:E:45:TYR:N	2.82	0.47
1:C:246:PRO:HG3	1:C:448:GLY:CA	2.39	0.47
1:G:15:ARG:CG	1:G:15:ARG:HH11	2.24	0.47
2:B:398:ILE:HA	2:B:408:ARG:HG3	1.97	0.47
1:G:444:VAL:HG11	1:G:456:VAL:HG11	1.97	0.47
2:H:39:THR:HG21	2:H:218:HIS:HB2	1.96	0.47
1:C:429:THR:HG22	1:C:431:ASN:HD22	1.77	0.46
2:B:370:ASP:OD1	2:B:423:LYS:NZ	2.47	0.46
2:H:204:LYS:HG3	2:H:235:SER:OG	2.15	0.46
2:H:397:ASP:OD2	2:H:408:ARG:NH1	2.43	0.46
1:A:115:LEU:HD23	1:A:215:LEU:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:115:LEU:H	2:F:115:LEU:HD12	1.80	0.46
1:C:99:ASN:HB2	1:C:101:MET:CE	2.45	0.46
2:B:305:SER:HA	2:B:306:PRO:HD3	1.68	0.46
2:H:317:GLY:O	2:H:318:SER:CB	2.62	0.46
1:E:467:ASN:O	1:E:468:SER:HB2	2.15	0.46
1:G:114:MET:HE2	1:G:118:MET:HG3	1.96	0.46
2:F:76:ALA:HB1	2:F:129:ILE:HG23	1.96	0.46
2:D:263:LEU:HA	2:D:264:PRO:HD3	1.79	0.46
2:D:253:ARG:HH21	2:D:457:GLU:CD	2.19	0.46
2:B:204:LYS:O	2:B:208:MET:HG2	2.15	0.46
2:B:291:ILE:CD1	2:B:426:ILE:HD13	2.46	0.46
1:A:47:ASP:HB3	1:A:199:ASN:OD1	2.16	0.46
1:C:315:ASN:ND2	1:C:315:ASN:C	2.68	0.46
2:B:245:ARG:NE	2:B:245:ARG:HA	2.30	0.46
2:H:291:ILE:CD1	2:H:426:ILE:HD13	2.46	0.46
1:G:198:GLU:OE1	1:G:225:SER:HB2	2.16	0.46
1:C:19:PHE:HD1	1:C:392:MET:CE	2.28	0.46
2:H:97:SER:OG	2:H:114:SER:CB	2.64	0.46
2:D:429:TRP:CE2	2:D:433:ARG:HG3	2.51	0.46
1:G:310:TYR:CD1	1:G:312:PHE:CZ	3.03	0.46
1:A:403:ILE:O	1:A:403:ILE:HG23	2.16	0.46
1:G:304:THR:HG22	1:G:305:HIS:ND1	2.31	0.46
2:B:165:HIS:HD2	2:B:256:ARG:CD	2.29	0.46
2:H:62:ASN:ND2	2:H:65:ASN:HB2	2.30	0.46
2:B:62:ASN:H	2:B:65:ASN:CB	2.23	0.46
2:B:209:VAL:HG21	2:B:402:VAL:HG12	1.96	0.46
1:C:333:LEU:HD13	1:C:334:SER:N	2.30	0.46
2:F:68:THR:HG23	2:F:195:LEU:HD23	1.97	0.46
2:D:291:ILE:HD12	2:D:426:ILE:HD13	1.97	0.46
2:F:62:ASN:ND2	2:F:65:ASN:HB2	2.30	0.46
2:H:143:GLU:O	2:H:147:ILE:HG12	2.15	0.46
2:B:68:THR:HG23	2:B:195:LEU:HD23	1.98	0.46
1:G:367:VAL:HG21	1:G:417:PRO:HA	1.98	0.46
2:B:294:ASN:ND2	2:B:324:MET:CG	2.77	0.46
1:A:256:LEU:HD11	1:A:314:GLU:HG2	1.98	0.46
2:F:232:VAL:HA	2:F:233:PRO:HD3	1.82	0.46
1:C:444:VAL:HG11	1:C:456:VAL:HG11	1.98	0.46
1:C:268:ILE:H	1:C:268:ILE:CD1	2.29	0.45
1:E:371:LYS:HE3	1:E:412:ILE:O	2.16	0.45
1:C:45:TYR:CD1	1:C:45:TYR:N	2.83	0.45
2:F:90:LEU:HD13	2:F:94:ASN:HD21	1.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:439:VAL:CG1	2:D:457:GLU:HG2	2.46	0.45
1:G:256:LEU:HD11	1:G:314:GLU:HG2	1.97	0.45
2:D:370:ASP:OD1	2:D:423:LYS:NZ	2.48	0.45
1:C:67:LEU:HD13	1:C:135:GLN:HG3	1.98	0.45
1:A:419:ASP:O	1:A:423:VAL:HG23	2.15	0.45
1:A:371:LYS:HE3	1:A:412:ILE:O	2.17	0.45
1:E:267:PRO:HD2	1:E:270:HIS:HB2	1.98	0.45
1:A:315:ASN:C	1:A:315:ASN:ND2	2.69	0.45
2:H:410:SER:OG	2:H:413:GLU:HG3	2.17	0.45
1:A:253:LEU:HA	1:A:254:PRO:HD3	1.80	0.45
2:H:429:TRP:CE2	2:H:433:ARG:HG3	2.50	0.45
1:E:67:LEU:HD13	1:E:135:GLN:HG3	1.97	0.45
1:C:198:GLU:OE1	1:C:225:SER:HB2	2.16	0.45
2:D:143:GLU:O	2:D:147:ILE:HG12	2.16	0.45
1:G:56:ASN:HA	1:G:56:ASN:HD22	1.57	0.45
2:F:429:TRP:CE2	2:F:433:ARG:HG3	2.52	0.45
2:D:62:ASN:ND2	2:D:65:ASN:HB2	2.32	0.45
2:B:263:LEU:HA	2:B:264:PRO:HD3	1.80	0.45
2:B:441:MET:HE1	2:B:451:PRO:O	2.17	0.45
2:F:137:ASN:HD21	2:F:192:ARG:HD2	1.82	0.45
1:C:17:ASP:O	1:C:18:ASN:HB3	2.17	0.45
2:B:232:VAL:HA	2:B:233:PRO:HD3	1.75	0.45
2:B:429:TRP:CE2	2:B:433:ARG:HG3	2.51	0.45
1:A:129:GLU:HG3	1:G:224:GLN:OE1	2.17	0.45
2:H:68:THR:HG23	2:H:195:LEU:HD23	1.97	0.45
1:C:263:PHE:CE2	1:C:442:ALA:HB2	2.52	0.45
1:A:210:GLU:OE1	1:A:210:GLU:HA	2.16	0.45
1:E:295:GLY:CA	2:F:93:GLU:HG2	2.42	0.45
1:C:256:LEU:CD1	1:C:314:GLU:HG2	2.46	0.45
1:G:268:ILE:CD1	1:G:398:MET:SD	2.96	0.45
2:F:370:ASP:OD1	2:F:423:LYS:NZ	2.49	0.45
2:B:204:LYS:HG3	2:B:235:SER:OG	2.16	0.45
1:C:249:VAL:O	1:C:249:VAL:HG23	2.17	0.45
1:G:379:LEU:HD13	2:H:46:SER:HB2	1.99	0.45
2:H:144:ARG:HH21	2:H:188:LYS:C	2.21	0.45
2:F:165:HIS:CD2	2:F:258:ILE:HD11	2.52	0.45
2:F:61:GLU:HA	2:F:65:ASN:HD22	1.81	0.45
1:G:115:LEU:HD23	1:G:215:LEU:HB3	1.98	0.45
1:A:119:SER:HB2	1:A:220:LEU:CD1	2.47	0.45
1:C:315:ASN:ND2	1:C:316:CYS:N	2.46	0.45
1:G:17:ASP:O	1:G:18:ASN:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:137:ASN:HD21	2:H:192:ARG:HD2	1.79	0.45
1:G:395:GLN:OE1	1:G:403:ILE:HG22	2.17	0.45
1:G:310:TYR:HB3	1:G:312:PHE:CZ	2.51	0.45
1:E:35:THR:HB	1:E:36:PRO:CD	2.46	0.45
2:H:80:THR:C	2:H:134:VAL:HG23	2.37	0.45
1:E:294:PRO:HB3	2:F:89:GLU:HA	1.99	0.45
2:D:141:GLU:O	2:D:144:ARG:HG3	2.17	0.44
2:B:218:HIS:O	2:B:222:VAL:HG23	2.18	0.44
1:A:198:GLU:OE1	1:A:225:SER:HB2	2.17	0.44
1:G:99:ASN:HB2	1:G:101:MET:HE2	1.98	0.44
1:C:151:GLU:CD	1:C:151:GLU:H	2.20	0.44
2:B:255:GLU:HB3	2:B:453:VAL:HG23	1.99	0.44
2:D:237:SER:N	2:D:238:PRO:HD3	2.31	0.44
2:B:137:ASN:HD21	2:B:192:ARG:HD2	1.82	0.44
1:A:268:ILE:H	1:A:268:ILE:CD1	2.31	0.44
2:H:352:ILE:O	2:H:356:ILE:HG13	2.18	0.44
1:E:395:GLN:OE1	1:E:403:ILE:HG22	2.17	0.44
1:C:115:LEU:HD23	1:C:215:LEU:HB3	1.98	0.44
2:F:295:TRP:CZ2	2:F:297:ARG:HA	2.52	0.44
1:A:294:PRO:HB3	2:B:89:GLU:HA	1.99	0.44
1:G:268:ILE:CD1	1:G:268:ILE:H	2.31	0.44
2:H:439:VAL:HG22	2:H:453:VAL:HG13	1.99	0.44
2:D:35:LEU:HA	2:D:205:GLY:O	2.17	0.44
1:E:267:PRO:HA	1:E:323:TYR:O	2.17	0.44
2:B:99:LEU:HD12	2:B:99:LEU:HA	1.78	0.44
2:B:311:VAL:O	2:B:315:GLN:HG3	2.17	0.44
2:H:27:ARG:HH11	2:H:27:ARG:HB3	1.82	0.44
2:D:76:ALA:HB1	2:D:129:ILE:HG23	1.99	0.44
1:A:35:THR:HB	1:A:36:PRO:HD2	2.00	0.44
1:C:467:ASN:CG	1:C:468:SER:N	2.71	0.44
2:B:76:ALA:CB	2:B:110:TYR:HE2	2.31	0.44
1:E:122:VAL:O	1:E:191:ARG:NH2	2.51	0.44
1:C:35:THR:HB	1:C:36:PRO:HD2	2.00	0.44
2:F:103:THR:O	2:F:180:ILE:HD13	2.18	0.44
1:G:371:LYS:HE3	1:G:412:ILE:O	2.18	0.44
1:A:315:ASN:HD22	1:A:316:CYS:H	1.57	0.44
2:B:236:GLU:C	2:B:238:PRO:HD3	2.38	0.44
1:G:315:ASN:HB3	1:G:334:SER:HB2	2.00	0.43
1:G:263:PHE:CE2	1:G:442:ALA:HB2	2.53	0.43
2:F:87:GLY:O	2:F:91:GLU:HB2	2.18	0.43
1:A:294:PRO:HD2	2:B:99:LEU:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:263:PHE:CE2	1:E:442:ALA:HB2	2.53	0.43
1:E:99:ASN:HB2	1:E:101:MET:HE3	2.00	0.43
2:B:90:LEU:HD13	2:B:94:ASN:HD21	1.83	0.43
2:F:31:LEU:HD21	2:F:226:GLN:HA	1.99	0.43
2:B:87:GLY:O	2:B:91:GLU:HB2	2.19	0.43
2:B:317:GLY:O	2:B:318:SER:CB	2.65	0.43
1:G:35:THR:HB	1:G:36:PRO:CD	2.48	0.43
2:D:137:ASN:ND2	2:D:192:ARG:HD2	2.33	0.43
2:D:349:VAL:N	2:D:449:THR:OG1	2.51	0.43
2:D:87:GLY:O	2:D:91:GLU:HB2	2.18	0.43
2:H:147:ILE:HG22	2:H:187:ILE:HD13	2.01	0.43
1:G:290:SER:HB3	1:G:303:TYR:OH	2.19	0.43
1:C:312:PHE:CD1	1:C:339:ALA:CB	3.01	0.43
2:F:397:ASP:OD2	2:F:408:ARG:NH1	2.44	0.43
2:F:23:ILE:HA	2:F:24:PRO:HD3	1.89	0.43
1:E:43:GLY:HA2	1:E:102:TYR:O	2.19	0.43
1:E:17:ASP:O	1:E:18:ASN:HB3	2.19	0.43
2:B:350:ARG:HH12	2:D:419:ASP:HB3	1.84	0.43
1:C:395:GLN:OE1	1:C:403:ILE:HG22	2.18	0.43
2:D:291:ILE:CD1	2:D:426:ILE:HD13	2.48	0.43
1:C:304:THR:HG22	1:C:305:HIS:ND1	2.33	0.43
2:B:294:ASN:ND2	2:B:324:MET:CA	2.71	0.43
2:D:108:THR:CG2	2:D:110:TYR:HE1	2.31	0.43
2:B:255:GLU:HA	2:B:441:MET:O	2.18	0.43
2:B:115:LEU:HD12	2:B:115:LEU:H	1.83	0.43
1:G:315:ASN:C	1:G:315:ASN:ND2	2.69	0.43
1:G:19:PHE:CD1	1:G:392:MET:CE	3.01	0.43
2:H:61:GLU:OE1	2:H:66:ASN:HA	2.19	0.43
1:G:15:ARG:CG	1:G:15:ARG:NH1	2.82	0.43
2:B:183:PRO:HD2	2:B:186:ASN:HB2	2.01	0.43
2:D:305:SER:HA	2:D:306:PRO:HD3	1.66	0.43
1:A:310:TYR:HD1	1:A:312:PHE:CZ	2.37	0.43
2:F:410:SER:OG	2:F:413:GLU:HG3	2.19	0.43
1:G:200:THR:HG22	1:G:201:VAL:N	2.34	0.43
2:B:207:ARG:NH1	2:B:245:ARG:NH1	2.67	0.43
2:H:115:LEU:N	2:H:115:LEU:HD12	2.34	0.43
1:A:267:PRO:HD2	1:A:270:HIS:HB2	2.01	0.43
1:C:245:PRO:HA	1:C:246:PRO:HD3	1.90	0.42
1:E:245:PRO:HA	1:E:246:PRO:HD3	1.78	0.42
1:C:275:ALA:CB	1:C:423:VAL:HG21	2.49	0.42
1:G:275:ALA:HB3	1:G:423:VAL:HG21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:349:VAL:N	2:F:449:THR:OG1	2.52	0.42
2:F:455:TYR:C	2:F:455:TYR:CD1	2.92	0.42
1:G:45:TYR:N	1:G:45:TYR:CD1	2.87	0.42
2:F:141:GLU:O	2:F:144:ARG:HG3	2.20	0.42
1:E:270:HIS:O	1:E:273:ILE:HB	2.19	0.42
2:B:237:SER:N	2:B:238:PRO:HD3	2.34	0.42
1:G:84:LEU:HD13	1:G:91:TYR:CZ	2.55	0.42
1:C:19:PHE:CD1	1:C:392:MET:CE	3.02	0.42
2:B:291:ILE:HD12	2:B:426:ILE:HD13	1.99	0.42
1:E:41:ALA:HB1	1:E:389:LEU:HD22	2.01	0.42
1:A:260:GLN:HB2	1:A:445:VAL:HG12	2.01	0.42
2:H:349:VAL:N	2:H:449:THR:OG1	2.53	0.42
1:E:148:MET:O	1:E:150:PRO:HD3	2.18	0.42
2:H:263:LEU:HA	2:H:264:PRO:HD3	1.77	0.42
2:D:439:VAL:HG22	2:D:453:VAL:HG13	2.01	0.42
2:F:263:LEU:HA	2:F:264:PRO:HD3	1.76	0.42
1:G:303:TYR:HA	1:G:307:LEU:HB2	2.02	0.42
2:D:410:SER:OG	2:D:413:GLU:HG3	2.19	0.42
2:H:455:TYR:C	2:H:455:TYR:CD1	2.92	0.42
1:A:333:LEU:HD13	1:A:334:SER:N	2.34	0.42
2:B:147:ILE:HG22	2:B:187:ILE:HD13	2.00	0.42
1:G:72:THR:HG21	1:G:120:GLU:HB3	2.00	0.42
2:H:209:VAL:HG21	2:H:402:VAL:HG12	2.00	0.42
2:H:305:SER:HA	2:H:306:PRO:HD3	1.73	0.42
1:C:237:TYR:CG	1:C:264:GLU:HB2	2.55	0.42
2:H:70:HIS:O	2:H:73:GLU:HB3	2.19	0.42
1:E:237:TYR:CG	1:E:264:GLU:HB2	2.55	0.42
2:H:165:HIS:HD2	2:H:256:ARG:HD2	1.84	0.42
2:H:259:LYS:HG3	2:H:447:THR:CG2	2.48	0.42
2:B:439:VAL:HG22	2:B:453:VAL:HG13	2.01	0.42
1:C:266:LEU:HA	1:C:267:PRO:HD3	1.90	0.42
2:D:397:ASP:OD2	2:D:408:ARG:NH1	2.43	0.42
1:C:290:SER:HB3	1:C:303:TYR:OH	2.20	0.42
2:F:77:PHE:O	2:F:85:GLN:HG3	2.20	0.42
2:D:165:HIS:HD2	2:D:256:ARG:NE	2.18	0.42
1:G:246:PRO:HG3	1:G:448:GLY:CA	2.47	0.42
2:F:439:VAL:HG22	2:F:453:VAL:HG13	2.01	0.42
1:G:128:THR:OG1	1:G:131:GLU:HG3	2.20	0.42
1:C:100:LEU:HD21	1:C:195:TYR:OH	2.20	0.42
2:H:87:GLY:O	2:H:91:GLU:HB2	2.20	0.42
2:D:255:GLU:HA	2:D:441:MET:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:336:ILE:HG22	1:G:337:PRO:HD2	2.01	0.41
2:H:375:ARG:HB3	2:H:375:ARG:HH11	1.85	0.41
1:A:272:ASP:HA	5:A:493:HOH:O	2.20	0.41
2:D:80:THR:HB	2:D:132:LYS:O	2.19	0.41
2:B:76:ALA:HB1	2:B:129:ILE:HG23	2.00	0.41
1:G:275:ALA:CB	1:G:423:VAL:HG21	2.49	0.41
2:F:48:ALA:HB1	2:F:213:ALA:O	2.20	0.41
2:D:373:VAL:O	2:D:377:LYS:HG3	2.20	0.41
2:D:204:LYS:O	2:D:208:MET:HG2	2.20	0.41
2:B:350:ARG:HH11	2:D:420:LYS:HB3	1.83	0.41
2:F:349:VAL:O	2:F:352:ILE:HG22	2.20	0.41
2:D:218:HIS:O	2:D:222:VAL:HG23	2.20	0.41
2:H:40:GLU:OE1	2:H:408:ARG:NH2	2.54	0.41
1:C:455:ASP:O	1:C:459:VAL:HG23	2.20	0.41
1:A:114:MET:HE2	1:A:118:MET:HG3	2.01	0.41
1:C:253:LEU:HA	1:C:254:PRO:HD3	1.87	0.41
2:H:295:TRP:CZ2	2:H:297:ARG:HA	2.56	0.41
2:H:75:LEU:HA	2:H:78:LYS:HG2	2.03	0.41
2:F:144:ARG:HH21	2:F:188:LYS:C	2.24	0.41
1:G:289:PHE:HE2	1:G:291:ALA:HB2	1.79	0.41
2:H:172:LYS:O	2:H:174:GLN:HG3	2.20	0.41
1:A:122:VAL:O	1:A:191:ARG:NH2	2.54	0.41
1:C:72:THR:HG21	1:C:120:GLU:HB3	2.03	0.41
2:B:294:ASN:HD21	2:B:324:MET:HG3	1.83	0.41
1:A:315:ASN:HB3	1:A:334:SER:HB2	2.03	0.41
2:H:108:THR:HG22	2:H:110:TYR:HE1	1.85	0.41
2:D:108:THR:HG22	2:D:110:TYR:HE1	1.86	0.41
2:F:259:LYS:HB2	2:F:259:LYS:HE3	1.87	0.41
2:D:90:LEU:CD1	2:D:94:ASN:HD21	2.34	0.41
2:H:218:HIS:O	2:H:222:VAL:HG23	2.20	0.41
1:A:275:ALA:CB	1:A:423:VAL:HG21	2.51	0.41
1:G:107:PHE:HA	5:G:494:HOH:O	2.21	0.41
1:E:253:LEU:HA	1:E:254:PRO:HD3	1.85	0.41
1:A:157:LEU:HD11	1:A:244:ILE:HD13	2.03	0.41
1:C:119:SER:HB2	1:C:220:LEU:CD1	2.50	0.41
1:A:32:THR:HG21	1:A:209:HIS:HA	2.03	0.41
1:A:39:PHE:O	1:A:385:LYS:HE3	2.21	0.41
1:G:404:PRO:HG2	1:G:407:GLU:HB2	2.03	0.41
1:C:19:PHE:CD1	1:C:392:MET:HE2	2.56	0.41
2:D:400:ARG:NH2	2:D:401:GLN:HG2	2.35	0.41
2:F:255:GLU:HA	2:F:441:MET:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:172:LYS:HD2	2:H:172:LYS:HA	1.93	0.41
1:C:97:ARG:NH1	5:C:513:HOH:O	2.54	0.41
2:H:254:GLY:O	2:H:440:SER:HA	2.21	0.41
1:E:114:MET:HE2	1:E:118:MET:HG3	2.02	0.41
2:B:97:SER:CB	2:B:114:SER:HB3	2.50	0.40
1:A:312:PHE:CD1	1:A:339:ALA:CB	3.04	0.40
1:G:119:SER:HB2	1:G:220:LEU:HD13	2.02	0.40
1:G:174:CYS:O	1:G:175:PRO:C	2.60	0.40
2:H:350:ARG:HG3	2:H:451:PRO:HB3	2.02	0.40
1:A:55:ARG:NH1	1:E:181:SER:OG	2.52	0.40
1:A:429:THR:O	1:A:429:THR:CG2	2.70	0.40
1:C:96:SER:CB	1:C:99:ASN:OD1	2.67	0.40
1:A:59:GLY:HA2	5:A:497:HOH:O	2.21	0.40
1:A:56:ASN:HD22	1:A:56:ASN:HA	1.63	0.40
2:H:77:PHE:O	2:H:85:GLN:HG3	2.21	0.40
2:D:61:GLU:OE1	2:D:66:ASN:HA	2.21	0.40
2:H:349:VAL:HG23	2:H:449:THR:HG23	2.02	0.40
2:F:159:ASP:OD1	2:F:159:ASP:N	2.52	0.40
2:D:55:ASP:C	2:D:55:ASP:OD1	2.59	0.40
1:G:301:ARG:NH2	1:G:362:LEU:HD23	2.37	0.40
2:D:349:VAL:HG23	2:D:449:THR:HG23	2.03	0.40
2:D:80:THR:C	2:D:134:VAL:HG23	2.41	0.40
1:G:179:ILE:N	1:G:180:PRO:CD	2.84	0.40
2:B:254:GLY:O	2:B:440:SER:HA	2.21	0.40
1:G:42:LEU:HD23	1:G:42:LEU:N	2.36	0.40
2:H:52:ILE:HG23	2:H:52:ILE:O	2.20	0.40
1:E:429:THR:O	1:E:429:THR:CG2	2.68	0.40
2:D:279:ALA:HB1	2:D:281:ASP:OD1	2.21	0.40
2:H:90:LEU:HD13	2:H:94:ASN:HD21	1.80	0.40
2:D:441:MET:HE1	2:D:451:PRO:O	2.21	0.40
2:H:375:ARG:NH1	2:H:375:ARG:HB3	2.37	0.40
1:A:17:ASP:O	1:A:18:ASN:HB3	2.22	0.40
1:E:231:THR:O	5:E:505:HOH:O	2.22	0.40
2:F:134:VAL:O	2:F:135:LEU:HB2	2.21	0.40
2:B:234:LYS:HB2	2:B:234:LYS:HE3	1.82	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	455/475 (96%)	436 (96%)	17 (4%)	2 (0%)	39	61
1	C	451/475 (95%)	433 (96%)	16 (4%)	2 (0%)	39	61
1	E	453/475 (95%)	435 (96%)	16 (4%)	2 (0%)	39	61
1	G	455/475 (96%)	434 (95%)	17 (4%)	4 (1%)	21	37
2	B	437/443 (99%)	423 (97%)	11 (2%)	3 (1%)	26	46
2	D	441/443 (100%)	426 (97%)	12 (3%)	3 (1%)	26	46
2	F	441/443 (100%)	425 (96%)	13 (3%)	3 (1%)	26	46
2	H	438/443 (99%)	423 (97%)	11 (2%)	4 (1%)	21	37
All	All	3571/3672 (97%)	3435 (96%)	113 (3%)	23 (1%)	30	50

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	250	PHE
2	B	57	GLY
1	C	250	PHE
1	C	290	SER
2	D	318	SER
1	E	250	PHE
2	F	318	SER
1	G	250	PHE
1	A	290	SER
2	B	56	ALA
2	B	318	SER
2	D	56	ALA
1	G	290	SER
2	H	56	ALA
2	H	318	SER
1	E	290	SER
2	F	21	SER

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Mol	Chain	Res	Type
2	F	56	ALA
1	G	452	SER
2	D	22	GLN
1	G	167	THR
2	H	24	PRO
2	H	316	ASN

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	51
1	C	381/401 (95%)	360 (94%)	21 (6%)	27	48
1	E	382/401 (95%)	360 (94%)	22 (6%)	25	45
1	G	384/401 (96%)	361 (94%)	23 (6%)	24	43
2	B	376/379 (99%)	359 (96%)	17 (4%)	34	59
2	D	379/379 (100%)	362 (96%)	17 (4%)	34	59
2	F	379/379 (100%)	361 (95%)	18 (5%)	32	56
2	H	377/379 (100%)	360 (96%)	17 (4%)	34	59
All	All	3042/3120 (98%)	2887 (95%)	155 (5%)	29	52

All (155) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	ASN
1	A	65	ASP
1	A	66	ARG
1	A	67	LEU
1	A	151	GLU
1	A	210	GLU
1	A	220	LEU
1	A	268	ILE
1	A	273	ILE

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Mol	Chain	Res	Type
1	A	288	SER
1	A	311	TYR
1	A	314	GLU
1	A	315	ASN
1	A	361	ARG
1	A	382	LEU
1	A	386	LEU
1	A	399	HIS
1	A	429	THR
1	A	445	VAL
1	A	446	MET
2	B	27	ARG
2	B	39	THR
2	B	66	ASN
2	B	71	PHE
2	B	75	LEU
2	B	86	GLN
2	B	149	ARG
2	B	176	LEU
2	B	219	GLU
2	B	275	VAL
2	B	346	GLU
2	B	375	ARG
2	B	400	ARG
2	B	405	THR
2	B	408	ARG
2	B	424	ASP
2	B	449	THR
1	C	16	THR
1	C	56	ASN
1	C	65	ASP
1	C	66	ARG
1	C	67	LEU
1	C	151	GLU
1	C	210	GLU
1	C	220	LEU
1	C	268	ILE
1	C	273	ILE
1	C	288	SER
1	C	311	TYR
1	C	314	GLU
1	C	315	ASN

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Mol	Chain	Res	Type
1	C	361	ARG
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	86	GLN
2	D	149	ARG
2	D	176	LEU
2	D	219	GLU
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	441	MET
2	D	449	THR
1	E	56	ASN
1	E	65	ASP
1	E	66	ARG
1	E	67	LEU
1	E	151	GLU
1	E	210	GLU
1	E	220	LEU
1	E	268	ILE
1	E	273	ILE
1	E	288	SER
1	E	305	HIS
1	E	311	TYR
1	E	314	GLU
1	E	320	ASN
1	E	361	ARG
1	E	382	LEU
1	E	386	LEU
1	E	399	HIS

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Mol	Chain	Res	Type
1	E	429	THR
1	E	445	VAL
1	E	446	MET
1	E	468	SER
2	F	27	ARG
2	F	39	THR
2	F	66	ASN
2	F	71	PHE
2	F	75	LEU
2	F	86	GLN
2	F	149	ARG
2	F	176	LEU
2	F	219	GLU
2	F	275	VAL
2	F	346	GLU
2	F	375	ARG
2	F	400	ARG
2	F	405	THR
2	F	408	ARG
2	F	424	ASP
2	F	441	MET
2	F	449	THR
1	G	15	ARG
1	G	56	ASN
1	G	65	ASP
1	G	66	ARG
1	G	67	LEU
1	G	151	GLU
1	G	210	GLU
1	G	220	LEU
1	G	268	ILE
1	G	273	ILE
1	G	288	SER
1	G	305	HIS
1	G	307	LEU
1	G	311	TYR
1	G	314	GLU
1	G	315	ASN
1	G	361	ARG
1	G	382	LEU
1	G	386	LEU
1	G	399	HIS

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Mol	Chain	Res	Type
1	G	429	THR
1	G	445	VAL
1	G	446	MET
2	H	23	ILE
2	H	27	ARG
2	H	39	THR
2	H	66	ASN
2	H	71	PHE
2	H	75	LEU
2	H	86	GLN
2	H	149	ARG
2	H	176	LEU
2	H	219	GLU
2	H	275	VAL
2	H	346	GLU
2	H	375	ARG
2	H	400	ARG
2	H	405	THR
2	H	408	ARG
2	H	449	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	ASN
1	A	99	ASN
1	A	315	ASN
1	A	320	ASN
1	A	349	GLN
1	A	381	ASN
1	A	406	ASN
1	A	431	ASN
1	A	467	ASN
2	B	44	ASN
2	B	137	ASN
2	B	165	HIS
2	B	186	ASN
2	B	223	GLN
2	B	294	ASN
2	B	354	ASN
2	B	374	ASN
1	C	56	ASN

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Mol	Chain	Res	Type
1	C	315	ASN
1	C	320	ASN
1	C	349	GLN
1	C	381	ASN
1	C	406	ASN
1	C	431	ASN
2	D	44	ASN
2	D	66	ASN
2	D	137	ASN
2	D	165	HIS
2	D	223	GLN
2	D	354	ASN
2	D	374	ASN
1	E	56	ASN
1	E	320	ASN
1	E	349	GLN
1	E	381	ASN
1	E	406	ASN
1	E	431	ASN
2	F	44	ASN
2	F	137	ASN
2	F	165	HIS
2	F	223	GLN
2	F	354	ASN
2	F	374	ASN
1	G	56	ASN
1	G	315	ASN
1	G	320	ASN
1	G	349	GLN
1	G	381	ASN
1	G	406	ASN
1	G	431	ASN
2	H	44	ASN
2	H	65	ASN
2	H	66	ASN
2	H	137	ASN
2	H	165	HIS
2	H	186	ASN
2	H	223	GLN
2	H	294	ASN
2	H	354	ASN
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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	EPE	A	489	-	14,15,15	1.10	1 (7%)	18,20,20	1.09	1 (5%)
4	EPE	G	489	-	14,15,15	1.17	1 (7%)	18,20,20	1.13	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EPE	A	489	-	-	0/9/19/19	0/1/1/1
4	EPE	G	489	-	-	0/9/19/19	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	489	EPE	C6-N1	2.02	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	489	EPE	C6-N1	2.37	1.53	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	489	EPE	O1S-S-C10	-2.39	104.87	106.91
4	A	489	EPE	C7-N4-C5	-2.09	105.91	111.27

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, 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%)	0.27	29 (6%)	23	26	30, 46, 85, 101	0
1	C	453/475 (95%)	0.21	20 (4%)	38	43	31, 49, 82, 101	0
1	E	455/475 (95%)	0.40	32 (7%)	19	22	33, 53, 85, 101	0
1	G	457/475 (96%)	0.39	36 (7%)	15	17	35, 54, 89, 101	0
2	B	439/443 (99%)	0.19	17 (3%)	43	48	28, 49, 75, 96	0
2	D	443/443 (100%)	0.44	35 (7%)	15	17	34, 58, 84, 101	0
2	F	443/443 (100%)	0.54	26 (5%)	26	29	45, 68, 88, 100	0
2	H	440/443 (99%)	1.58	140 (31%)	1	0	54, 78, 93, 100	0
All	All	3587/3672 (97%)	0.50	335 (9%)	11	11	28, 58, 88, 101	0

All (335) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	187	ILE	9.2
2	H	184	ILE	8.9
1	C	289	PHE	8.2
2	F	21	SER	8.1
1	C	290	SER	7.8
1	E	289	PHE	7.8
2	H	71	PHE	7.7
2	H	181	LEU	7.7
1	E	292	GLY	7.5
2	H	188	LYS	7.3
1	E	293	GLY	7.1
2	D	20	ALA	7.1
2	H	171	TYR	6.7
1	G	470	SER	6.5
1	C	291	ALA	6.5
1	G	311	TYR	6.4

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Mol	Chain	Res	Type	RSRZ
1	E	288	SER	6.3
2	D	21	SER	6.3
1	G	291	ALA	6.3
2	F	245	ARG	6.2
2	H	149	ARG	6.1
1	G	250	PHE	6.1
1	E	291	ALA	6.1
1	A	469	SER	6.0
1	G	252	ASN	6.0
2	H	445	GLY	5.9
2	H	90	LEU	5.9
1	A	470	SER	5.8
2	H	245	ARG	5.8
1	C	288	SER	5.7
2	H	190	ILE	5.7
1	G	290	SER	5.6
1	E	311	TYR	5.5
1	E	312	PHE	5.5
2	H	251	PHE	5.5
1	A	252	ASN	5.5
2	F	20	ALA	5.5
2	H	86	GLN	5.4
2	H	226	GLN	5.4
1	E	14	ALA	5.4
1	A	289	PHE	5.4
2	H	185	LYS	5.4
1	G	289	PHE	5.4
1	C	311	TYR	5.3
2	H	238	PRO	5.2
1	E	252	ASN	5.2
1	G	295	GLY	5.2
1	A	14	ALA	5.2
2	H	148	ILE	5.2
1	G	230	ILE	5.1
1	G	469	SER	5.1
1	A	311	TYR	5.0
1	C	252	ASN	5.0
2	H	298	ALA	5.0
2	H	367	LYS	5.0
1	C	312	PHE	4.9
2	H	262	THR	4.8
2	H	157	MET	4.8

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Mol	Chain	Res	Type	RSRZ
2	H	248	LEU	4.7
2	H	145	ASP	4.7
2	H	189	SER	4.7
2	H	236	GLU	4.6
2	H	432	TYR	4.6
2	D	270	ILE	4.6
2	H	65	ASN	4.5
2	H	239	VAL	4.5
1	G	299	TYR	4.5
2	H	297	ARG	4.5
1	E	290	SER	4.5
2	H	198	TYR	4.4
2	H	237	SER	4.4
2	D	337	GLY	4.4
1	C	292	GLY	4.4
2	H	146	VAL	4.4
2	H	180	ILE	4.3
1	E	250	PHE	4.3
1	G	294	PRO	4.2
1	E	468	SER	4.2
2	H	258	ILE	4.2
2	H	249	PRO	4.2
2	B	299	ILE	4.2
1	A	250	PHE	4.1
2	H	299	ILE	4.1
1	A	312	PHE	4.1
1	E	287	GLY	4.0
1	A	253	LEU	4.0
2	H	317	GLY	4.0
1	E	296	LYS	4.0
2	H	147	ILE	4.0
2	D	126	LEU	4.0
2	H	263	LEU	4.0
1	E	295	GLY	4.0
1	A	290	SER	4.0
2	H	195	LEU	3.9
2	H	144	ARG	3.9
2	H	64	LYS	3.9
2	H	126	LEU	3.9
2	F	190	ILE	3.9
1	G	14	ALA	3.9
2	H	233	PRO	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	291	ALA	3.8
2	H	153	GLU	3.8
1	G	298	MET	3.8
2	H	68	THR	3.8
2	H	347	HIS	3.8
1	E	251	GLY	3.8
2	H	32	PRO	3.8
1	E	249	VAL	3.7
1	A	15	ARG	3.7
1	A	358	LYS	3.7
2	H	60	ALA	3.7
2	H	137	ASN	3.7
1	G	249	VAL	3.7
2	H	154	VAL	3.7
2	H	173	ASP	3.7
2	H	182	GLY	3.7
2	F	187	ILE	3.7
2	F	239	VAL	3.7
2	H	315	GLN	3.7
2	H	314	SER	3.7
1	G	292	GLY	3.6
1	G	253	LEU	3.6
2	H	337	GLY	3.6
2	H	152	GLU	3.6
1	G	297	GLY	3.6
1	C	250	PHE	3.6
1	G	231	THR	3.6
2	H	250	VAL	3.6
2	D	245	ARG	3.5
2	D	338	MET	3.5
1	C	468	SER	3.5
2	H	25	GLY	3.5
2	H	436	ASN	3.5
2	H	193	THR	3.4
2	H	82	ASN	3.4
2	H	161	VAL	3.4
2	H	447	THR	3.4
2	H	311	VAL	3.4
2	H	259	LYS	3.4
2	D	129	ILE	3.4
2	D	23	ILE	3.3
1	G	203	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
2	H	321	ASN	3.3
2	H	265	THR	3.3
2	H	176	LEU	3.3
2	H	346	GLU	3.3
2	F	81	GLN	3.3
1	A	468	SER	3.2
2	H	446	ASN	3.2
2	D	248	LEU	3.2
2	F	235	SER	3.2
2	H	342	THR	3.2
2	D	52	ILE	3.2
2	H	304	ASN	3.2
2	D	130	LEU	3.2
2	H	260	GLU	3.2
2	D	197	ASP	3.2
2	H	338	MET	3.2
2	H	252	CYS	3.1
1	G	468	SER	3.1
2	H	318	SER	3.1
1	E	358	LYS	3.1
2	H	192	ARG	3.1
1	A	331	ILE	3.1
2	D	190	ILE	3.1
2	F	236	GLU	3.1
2	H	319	LEU	3.1
2	H	456	ILE	3.1
2	F	149	ARG	3.1
2	H	219	GLU	3.1
1	C	338	GLN	3.0
2	H	88	ILE	3.0
2	H	158	TYR	3.0
2	H	444	LEU	3.0
2	B	236	GLU	3.0
1	C	299	TYR	3.0
2	H	208	MET	3.0
2	D	271	ALA	3.0
1	C	249	VAL	2.9
1	E	253	LEU	2.9
2	D	240	PRO	2.9
2	H	264	PRO	2.9
2	D	110	TYR	2.9
2	B	27	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
2	H	257	PHE	2.9
2	D	125	ILE	2.9
1	E	15	ARG	2.8
2	F	304	ASN	2.8
2	B	130	LEU	2.8
2	H	332	ASP	2.8
2	B	338	MET	2.8
2	H	200	THR	2.8
1	G	288	SER	2.8
2	H	156	LYS	2.8
2	H	240	PRO	2.8
2	H	310	ALA	2.8
2	B	52	ILE	2.7
2	H	253	ARG	2.7
2	F	299	ILE	2.7
1	A	44	LEU	2.7
1	A	283	LEU	2.7
1	G	439	LYS	2.7
1	C	296	LYS	2.7
1	A	330	GLY	2.7
2	H	69	ALA	2.7
2	D	356	ILE	2.7
2	H	261	ASN	2.7
2	F	238	PRO	2.7
2	H	244	PRO	2.7
1	A	329	PHE	2.7
1	G	210	GLU	2.7
2	H	94	ASN	2.7
2	F	52	ILE	2.7
2	H	52	ILE	2.6
1	A	254	PRO	2.6
2	H	175	PRO	2.6
2	H	435	GLN	2.6
1	E	303	TYR	2.6
1	A	288	SER	2.6
2	H	95	ILE	2.6
2	D	201	LYS	2.6
2	F	234	LYS	2.6
2	D	269	ALA	2.6
2	D	239	VAL	2.6
2	B	245	ARG	2.6
2	H	270	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	271	ALA	2.6
2	D	203	TYR	2.5
2	F	172	LYS	2.5
2	H	227	LYS	2.5
1	A	201	VAL	2.5
1	A	303	TYR	2.5
1	A	231	THR	2.5
2	D	142	ARG	2.5
1	G	202	ALA	2.5
1	A	262	GLY	2.5
2	B	292	VAL	2.5
2	H	243	SER	2.5
2	H	302	GLY	2.5
2	H	27	ARG	2.5
1	C	303	TYR	2.5
2	H	450	VAL	2.5
2	D	243	SER	2.5
2	F	418	VAL	2.5
2	H	143	GLU	2.5
2	H	102	TYR	2.5
1	A	338	GLN	2.5
1	G	15	ARG	2.5
2	H	209	VAL	2.5
2	D	297	ARG	2.5
2	H	142	ARG	2.5
2	H	316	ASN	2.4
2	H	343	ASP	2.4
1	G	416	LYS	2.4
2	B	270	ILE	2.4
2	D	141	GLU	2.4
2	H	345	ASN	2.4
1	E	298	MET	2.4
2	H	139	ALA	2.4
2	B	337	GLY	2.4
2	D	299	ILE	2.4
1	E	467	ASN	2.4
1	G	303	TYR	2.4
2	H	87	GLY	2.4
2	H	81	GLN	2.4
2	H	340	ILE	2.4
2	B	269	ALA	2.4
2	F	337	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	263	LEU	2.3
1	C	230	ILE	2.3
2	F	261	ASN	2.3
2	H	254	GLY	2.3
2	F	209	VAL	2.3
2	H	247	PRO	2.3
2	H	183	PRO	2.3
2	H	104	SER	2.3
2	H	186	ASN	2.3
2	D	230	GLY	2.3
2	D	22	GLN	2.3
2	F	176	LEU	2.3
1	E	356	ALA	2.2
1	E	435	ALA	2.2
2	F	224	TYR	2.2
2	H	61	GLU	2.2
1	E	294	PRO	2.2
2	B	211	ALA	2.2
1	E	233	LYS	2.2
1	A	336	ILE	2.2
2	B	37	ILE	2.2
2	B	129	ILE	2.2
2	H	67	GLY	2.2
2	H	129	ILE	2.2
1	C	253	LEU	2.2
1	E	254	PRO	2.2
2	H	172	LYS	2.2
2	H	459	LYS	2.2
2	H	57	GLY	2.2
1	C	435	ALA	2.2
1	A	43	GLY	2.2
2	F	246	GLY	2.2
2	H	151	SER	2.2
1	E	19	PHE	2.2
1	E	330	GLY	2.1
2	H	440	SER	2.1
2	H	178	ARG	2.1
2	H	336	TRP	2.1
2	D	300	GLY	2.1
2	H	230	GLY	2.1
1	G	358	LYS	2.1
1	G	43	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	232	LYS	2.1
2	H	204	LYS	2.1
1	E	313	VAL	2.1
1	G	44	LEU	2.1
2	B	110	TYR	2.1
2	F	198	TYR	2.1
2	B	210	LEU	2.1
2	F	269	ALA	2.1
1	E	360	LEU	2.1
1	C	231	THR	2.1
1	G	251	GLY	2.1
1	G	256	LEU	2.1
2	H	43	PRO	2.1
2	H	325	SER	2.1
2	H	313	ALA	2.0
2	H	306	PRO	2.0
2	D	64	LYS	2.0
1	C	287	GLY	2.0
1	G	293	GLY	2.0
2	D	148	ILE	2.0
2	F	175	PRO	2.0
1	A	279	LEU	2.0
2	D	440	SER	2.0
2	H	228	TYR	2.0
1	G	437	ASN	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 ⓘ

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(\AA^2)	Q<0.9
4	EPE	G	489	15/15	0.91	0.26	2.24	70,78,84,85	0
4	EPE	A	489	15/15	0.96	0.23	1.48	68,73,80,81	0
3	ZN	H	504	1/1	0.94	0.13	-1.32	101,101,101,101	0
3	ZN	F	503	1/1	0.83	0.06	-	84,84,84,84	0
3	ZN	D	502	1/1	0.95	0.06	-	79,79,79,79	0
3	ZN	B	501	1/1	0.98	0.04	-	62,62,62,62	0

6.5 Other polymers [i](#)

There are no such residues in this entry.