



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:02 PM UTC

PDB ID : 1HR8 / pdb_00001hr8
Title : Yeast Mitochondrial Processing Peptidase beta-E73Q Mutant Complexed with Cytochrome C Oxidase IV Signal Peptide
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 : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

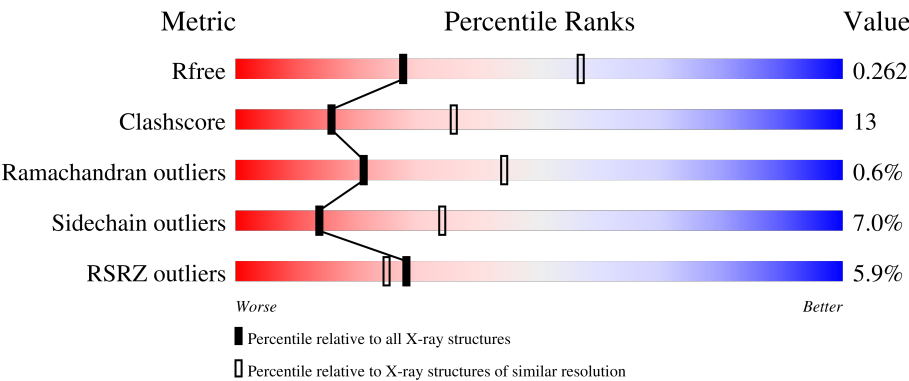
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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

Mol	Chain	Length	Quality of chain
1	A	475	4% 71%20%5%
1	C	475	3% 71%20%6%
1	E	475	4% 69%21%6%
1	G	475	4% 68%22%5%6%
2	B	443	2% 68%26%5%

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Mol	Chain	Length	Quality of chain
2	D	443	4% 69% 26% 5%
2	F	443	4% 70% 26%
2	H	443	16% 69% 26%
3	O	24	42% 12% 25% 12% 46%
3	P	24	25% 8% 21% 8% 63%
3	Q	24	29% 17% 17% 58%
3	R	24	21% 21% 71%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 27990 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	452	Total	C	N	O	S	0	0	0
			3499	2213	594	673	19			
1	C	448	Total	C	N	O	S	0	0	0
			3471	2198	587	667	19			
1	E	445	Total	C	N	O	S	0	0	0
			3459	2190	586	664	19			
1	G	448	Total	C	N	O	S	0	0	0
			3475	2198	589	669	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	443	Total	C	N	O	S	0	0	0
			3442	2165	596	674	7			
2	F	443	Total	C	N	O	S	0	0	0
			3442	2165	596	674	7			
2	H	441	Total	C	N	O	S	0	0	0
			3431	2159	594	671	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 mutation	UNP P10507
B	84	PRO	SER	SEE REMARK 999	UNP P10507
B	350	ARG	GLN	SEE REMARK 999	UNP P10507
D	20	ALA	-	cloning artifact	UNP P10507
D	73	GLN	GLU	engineered mutation	UNP P10507
D	84	PRO	SER	SEE REMARK 999	UNP P10507
D	350	ARG	GLN	SEE REMARK 999	UNP P10507
F	20	ALA	-	cloning artifact	UNP P10507
F	73	GLN	GLU	engineered mutation	UNP P10507
F	84	PRO	SER	SEE REMARK 999	UNP P10507
F	350	ARG	GLN	SEE REMARK 999	UNP P10507
H	20	ALA	-	cloning artifact	UNP P10507

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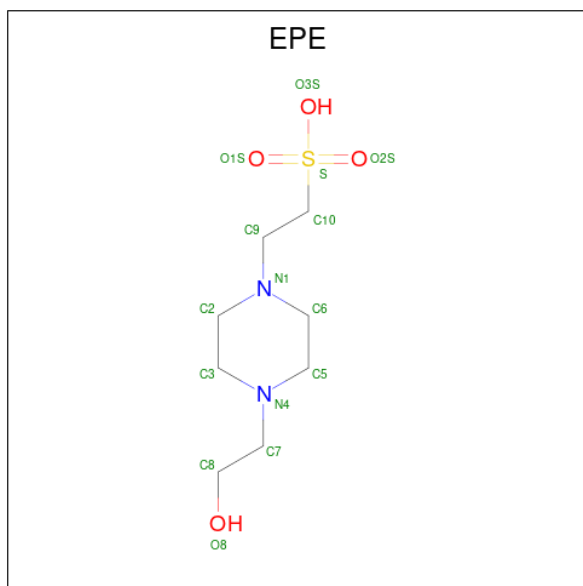
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Chain	Residue	Modelled	Actual	Comment	Reference
H	73	GLN	GLU	engineered mutation	UNP P10507
H	84	PRO	SER	SEE REMARK 999	UNP P10507
H	350	ARG	GLN	SEE REMARK 999	UNP P10507

- Molecule 3 is a protein called CYTOCHROME C OXIDASE POLYPEPTIDE IV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	O	13	Total	C	N	O	S	0	0	0
			107	70	20	16	1			
3	P	9	Total	C	N	O		0	0	0
			76	52	13	11				
3	Q	10	Total	C	N	O	S	0	0	0
			82	55	14	12	1			
3	R	7	Total	C	N	O		0	0	0
			54	34	11	9				

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).



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 ZINC ION (CCD ID: ZN) (formula: Zn).

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

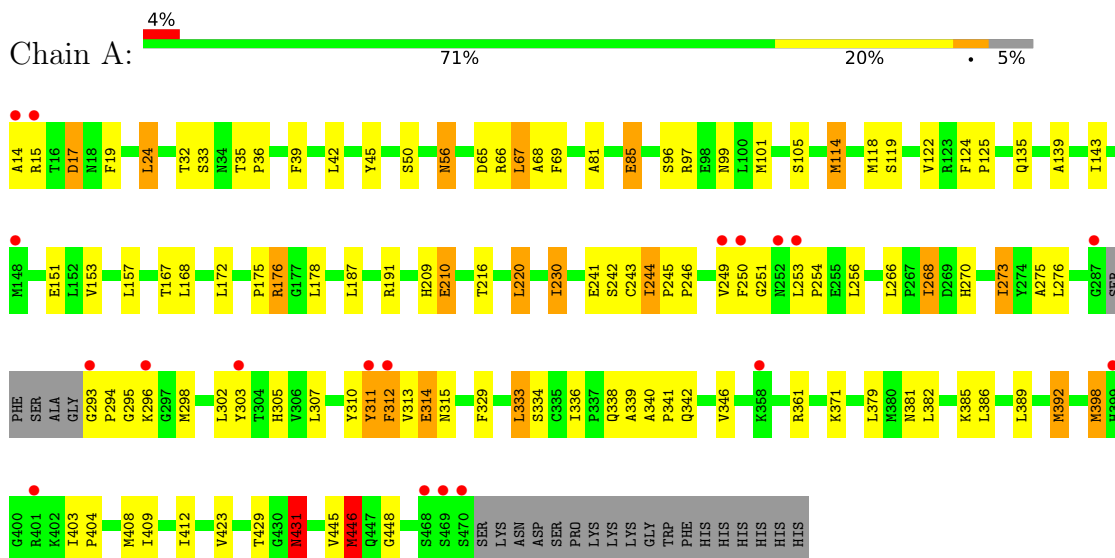
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	1	Total 1	O 1	0	0
6	H	1	Total 1	O 1	0	0
6	O	1	Total 1	O 1	0	0
6	P	1	Total 1	O 1	0	0

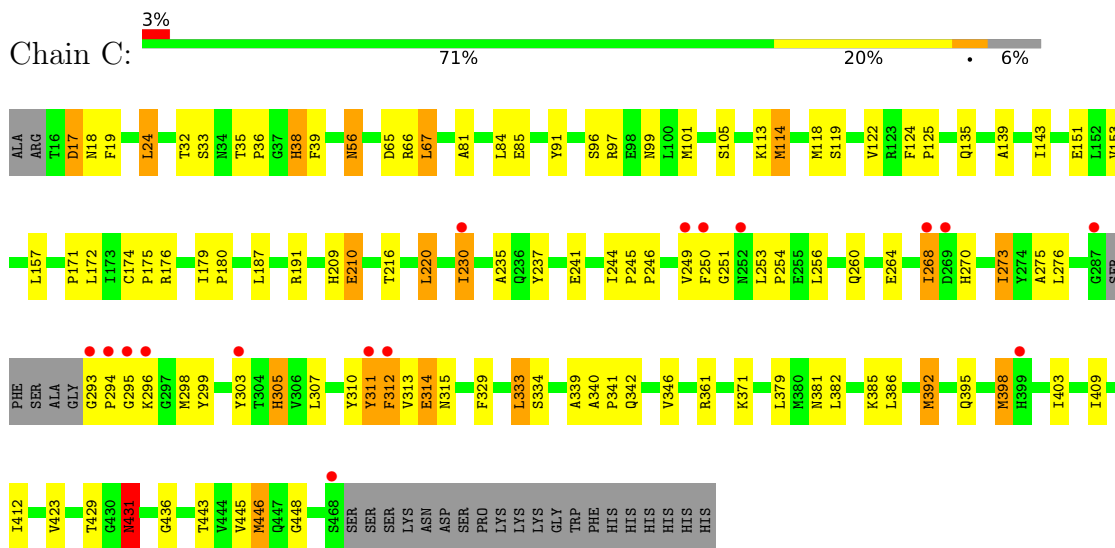
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: MITOCHONDRIAL PROCESSING PEPTIDASE ALPHA SUBUNIT

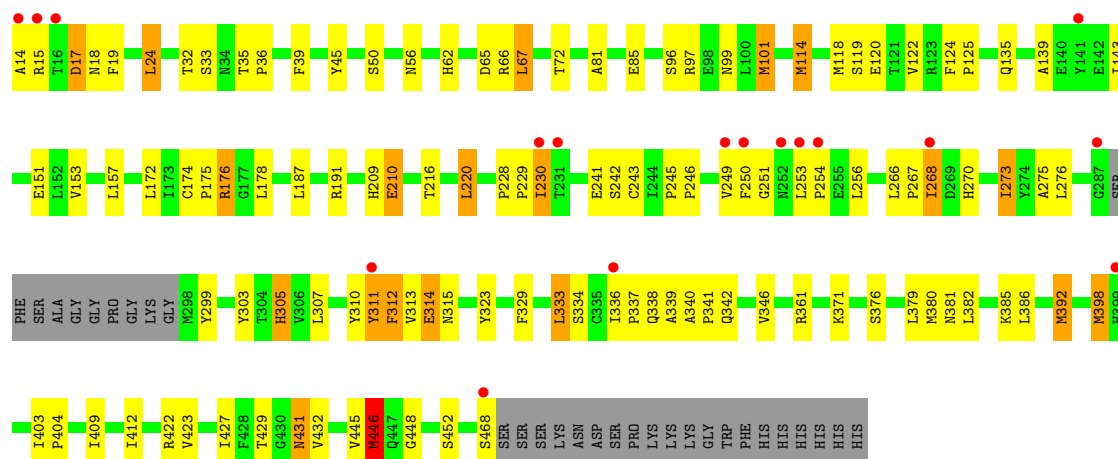


• Molecule 1: MITOCHONDRIAL PROCESSING PEPTIDASE ALPHA SUBUNIT

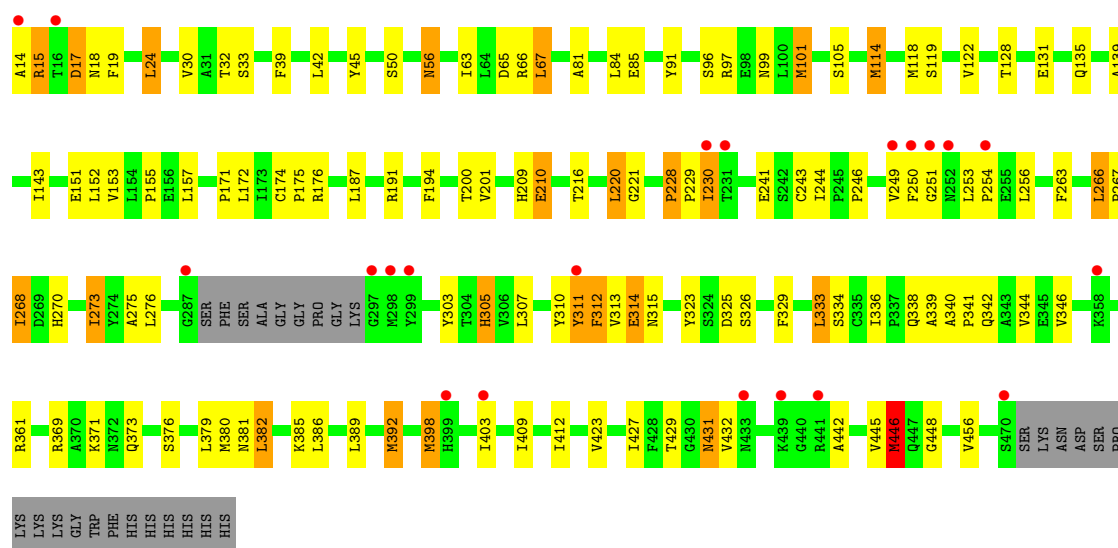


• Molecule 1: MITOCHONDRIAL PROCESSING PEPTIDASE ALPHA SUBUNIT

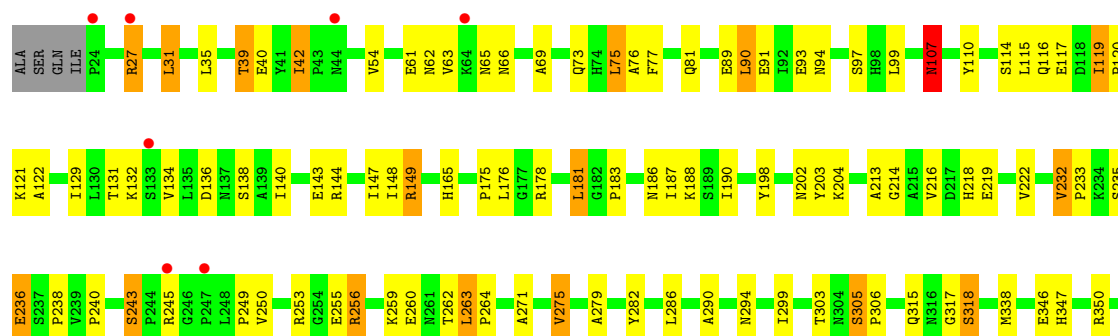




• Molecule 1: MITOCHONDRIAL PROCESSING PEPTIDASE ALPHA SUBUNIT

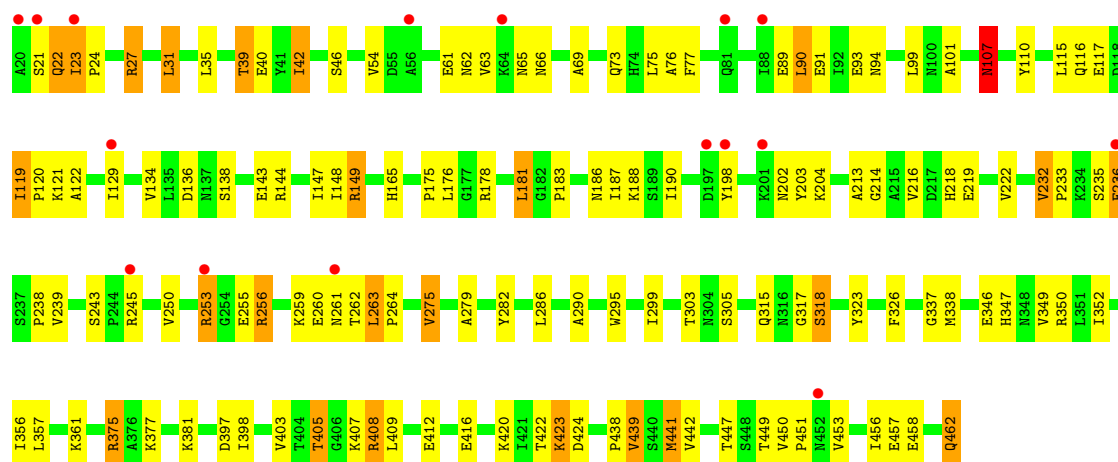


• Molecule 2: MITOCHONDRIAL PROCESSING PEPTIDASE BETA SUBUNIT

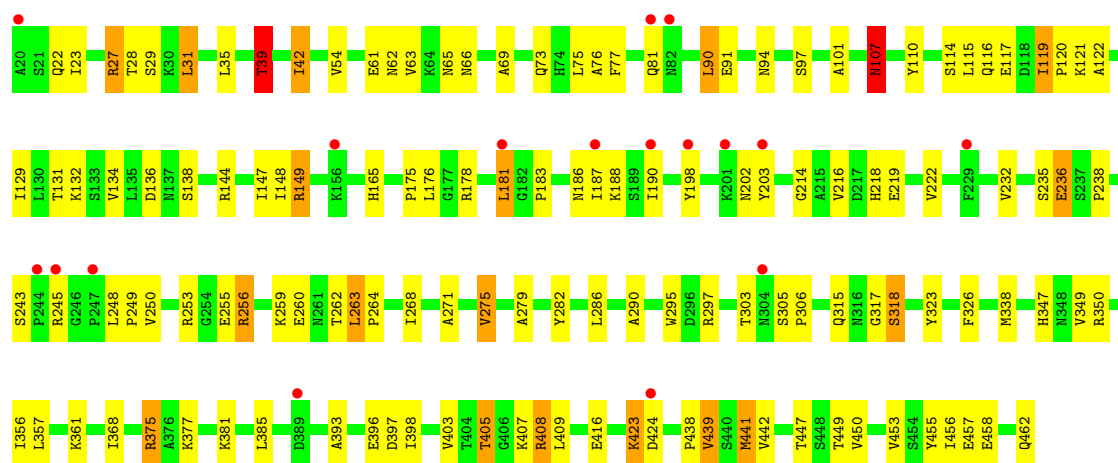




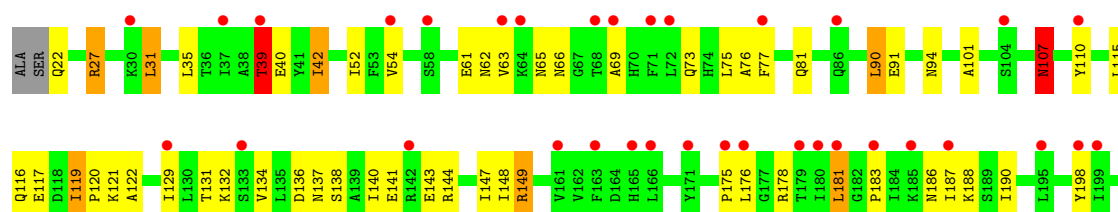
• Molecule 2: MITOCHONDRIAL PROCESSING PEPTIDASE BETA SUBUNIT

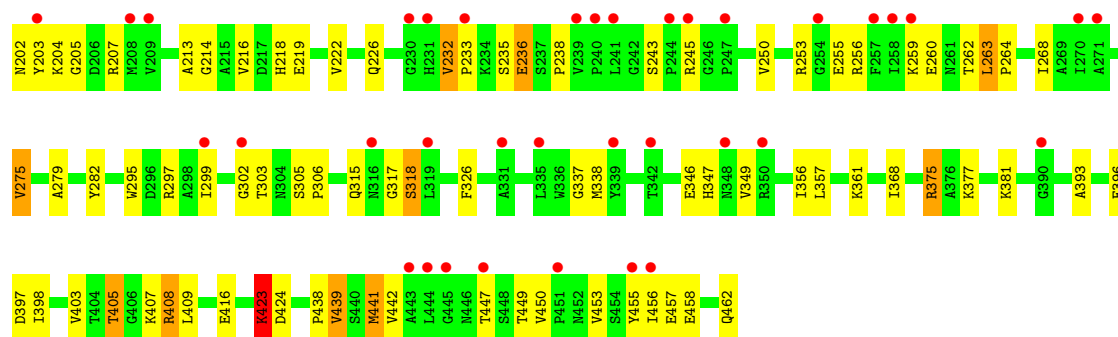


• Molecule 2: MITOCHONDRIAL PROCESSING PEPTIDASE BETA SUBUNIT

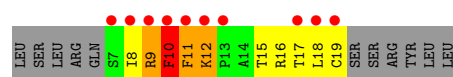
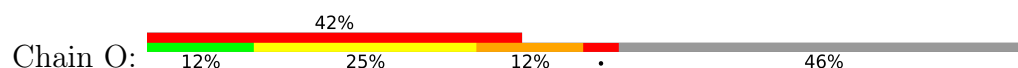


• Molecule 2: MITOCHONDRIAL PROCESSING PEPTIDASE BETA SUBUNIT





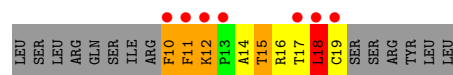
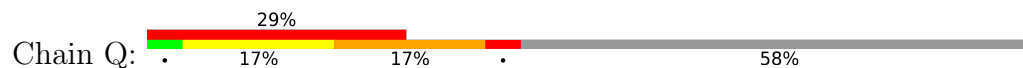
• Molecule 3: CYTOCHROME C OXIDASE POLYPEPTIDE IV



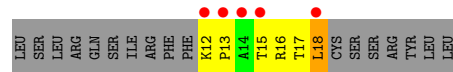
• Molecule 3: CYTOCHROME C OXIDASE POLYPEPTIDE IV



• Molecule 3: CYTOCHROME C OXIDASE POLYPEPTIDE IV



• Molecule 3: CYTOCHROME C OXIDASE POLYPEPTIDE IV



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	134.26Å 178.12Å 202.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.63 – 2.70 48.63 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.63-2.70) 99.9 (48.63-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.61 (at 2.69Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.229 , 0.264 0.228 , 0.262	Depositor DCC
R_{free} test set	2030 reflections (1.51%)	wwPDB-VP
Wilson B-factor (Å ²)	52.9	Xtriage
Anisotropy	0.269	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 47.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	27990	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.35% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: EPE, 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	0.83	6/3570 (0.2%)	1.08	13/4830 (0.3%)
1	C	0.80	7/3542 (0.2%)	1.07	9/4793 (0.2%)
1	E	0.75	6/3529 (0.2%)	1.10	14/4776 (0.3%)
1	G	0.75	4/3545 (0.1%)	1.06	14/4797 (0.3%)
2	B	0.77	0/3478	1.14	27/4720 (0.6%)
2	D	0.81	5/3506 (0.1%)	1.18	25/4759 (0.5%)
2	F	0.61	0/3506	1.14	26/4759 (0.5%)
2	H	0.57	0/3495	1.15	28/4744 (0.6%)
3	O	1.47	0/109	1.92	3/145 (2.1%)
3	P	1.52	0/78	1.48	1/104 (1.0%)
3	Q	1.18	0/84	1.42	2/112 (1.8%)
3	R	1.10	0/54	1.18	0/72
All	All	0.75	28/28496 (0.1%)	1.12	162/38611 (0.4%)

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	462	GLN	CD-NE2	-12.10	1.07	1.33
2	D	261	ASN	CG-ND2	-10.97	1.10	1.33
2	D	261	ASN	CG-OD1	-10.78	1.03	1.23
2	D	462	GLN	CD-OE1	-10.39	1.03	1.23
1	A	392	MET	SD-CE	-10.07	1.54	1.79
1	A	114	MET	SD-CE	-9.15	1.56	1.79
1	A	431	ASN	CG-ND2	-8.04	1.16	1.33
1	C	431	ASN	CG-ND2	-7.76	1.17	1.33
1	G	392	MET	SD-CE	-7.65	1.60	1.79
1	E	431	ASN	CG-ND2	-7.59	1.17	1.33
1	E	114	MET	SD-CE	-7.48	1.60	1.79
1	G	431	ASN	CG-ND2	-7.46	1.17	1.33
1	E	62	HIS	CE1-NE2	-7.32	1.25	1.32
1	G	431	ASN	CG-OD1	-7.28	1.09	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	431	ASN	CG-OD1	-7.26	1.09	1.23
1	C	38	HIS	CE1-NE2	-7.21	1.25	1.32
1	A	431	ASN	CG-OD1	-7.08	1.10	1.23
1	C	431	ASN	CG-OD1	-6.76	1.10	1.23
1	C	392	MET	SD-CE	-6.75	1.62	1.79
1	E	392	MET	SD-CE	-6.74	1.62	1.79
1	C	114	MET	SD-CE	-6.54	1.63	1.79
1	G	114	MET	SD-CE	-6.51	1.63	1.79
1	A	245	PRO	CA-C	5.68	1.55	1.51
1	E	62	HIS	CG-CD2	-5.39	1.29	1.35
1	A	408	MET	SD-CE	5.37	1.93	1.79
1	C	245	PRO	CA-C	5.14	1.56	1.52
2	D	352	ILE	CA-CB	5.12	1.61	1.54
1	C	38	HIS	CG-CD2	-5.01	1.30	1.35

All (162) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	253	ARG	NE-CZ-NH2	12.82	130.74	119.20
2	H	207	ARG	NE-CZ-NH2	12.02	130.02	119.20
2	D	253	ARG	NE-CZ-NH1	-11.87	109.63	121.50
2	F	350	ARG	NE-CZ-NH2	11.86	129.87	119.20
1	E	422	ARG	NE-CZ-NH2	11.48	129.53	119.20
1	E	422	ARG	NE-CZ-NH1	-11.21	110.30	121.50
2	H	207	ARG	NE-CZ-NH1	-11.16	110.34	121.50
1	A	15	ARG	N-CA-C	10.71	122.64	110.97
2	H	149	ARG	NE-CZ-NH2	-10.67	109.60	119.20
2	F	350	ARG	NE-CZ-NH1	-10.21	111.29	121.50
2	H	149	ARG	CD-NE-CZ	10.20	138.69	124.40
1	C	312	PHE	N-CA-C	-9.99	101.11	113.20
2	F	350	ARG	CD-NE-CZ	9.81	138.13	124.40
2	D	253	ARG	CD-NE-CZ	9.72	138.00	124.40
1	G	312	PHE	N-CA-C	-9.65	101.52	113.20
1	E	312	PHE	N-CA-C	-9.62	101.56	113.20
1	A	312	PHE	N-CA-C	-9.48	101.73	113.20
1	E	422	ARG	CD-NE-CZ	9.40	137.56	124.40
3	O	10	PHE	N-CA-C	9.35	125.95	108.65
2	H	149	ARG	NE-CZ-NH1	9.21	130.71	121.50
3	O	9	ARG	N-CA-C	8.97	129.92	110.80
2	B	263	LEU	CA-C-N	8.89	128.61	119.19
2	B	263	LEU	C-N-CA	8.89	128.61	119.19
2	D	232	VAL	CA-C-N	8.33	128.34	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	232	VAL	C-N-CA	8.33	128.34	119.76
2	D	263	LEU	CA-C-N	8.25	127.94	119.19
2	D	263	LEU	C-N-CA	8.25	127.94	119.19
2	H	207	ARG	CD-NE-CZ	8.03	135.64	124.40
2	B	232	VAL	CA-C-N	8.01	128.01	119.76
2	B	232	VAL	C-N-CA	8.01	128.01	119.76
2	H	263	LEU	CA-C-N	7.99	127.65	119.19
2	H	263	LEU	C-N-CA	7.99	127.65	119.19
2	F	263	LEU	CA-C-N	7.98	127.65	119.19
2	F	263	LEU	C-N-CA	7.98	127.65	119.19
2	F	232	VAL	CA-C-N	7.90	127.90	119.76
2	F	232	VAL	C-N-CA	7.90	127.90	119.76
2	H	232	VAL	CA-C-N	7.82	127.82	119.76
2	H	232	VAL	C-N-CA	7.82	127.82	119.76
2	F	63	VAL	N-CA-C	7.80	118.57	110.62
1	E	153	VAL	N-CA-C	7.71	117.82	110.42
2	D	63	VAL	N-CA-C	7.68	118.46	110.62
2	B	63	VAL	N-CA-C	7.65	118.43	110.62
2	H	63	VAL	N-CA-C	7.52	118.29	110.62
3	P	12	LYS	N-CA-C	7.50	121.97	108.55
1	A	153	VAL	N-CA-C	7.42	117.54	110.42
2	B	107	ASN	N-CA-C	7.19	118.66	108.74
1	G	153	VAL	N-CA-C	7.14	117.27	110.42
2	F	23	ILE	CA-C-N	7.11	127.15	119.90
2	F	23	ILE	C-N-CA	7.11	127.15	119.90
2	H	347	HIS	N-CA-C	7.04	120.93	109.59
1	C	153	VAL	N-CA-C	7.00	117.14	110.42
3	O	12	LYS	N-CA-C	6.99	125.25	109.81
2	B	119	ILE	CB-CA-C	-6.93	107.12	113.70
3	Q	12	LYS	N-CA-C	6.90	125.07	109.81
2	F	347	HIS	N-CA-C	6.86	120.64	109.59
2	H	134	VAL	N-CA-C	6.86	117.01	110.42
2	D	462	GLN	OE1-CD-NE2	-6.86	115.74	122.60
2	H	119	ILE	CB-CA-C	-6.79	107.25	113.70
1	C	398	MET	N-CA-C	6.78	119.67	111.40
2	D	347	HIS	N-CA-C	6.76	120.47	109.59
2	F	39	THR	N-CA-C	6.72	120.49	109.06
2	H	423	LYS	N-CA-C	-6.71	103.96	111.28
2	B	134	VAL	N-CA-C	6.70	116.85	110.42
2	H	207	ARG	CB-CG-CD	-6.70	95.90	111.30
2	B	347	HIS	N-CA-C	6.64	120.27	109.59
1	E	398	MET	N-CA-C	6.63	119.49	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	39	THR	N-CA-C	6.63	120.33	109.06
2	H	202	ASN	N-CA-C	6.55	121.56	112.45
1	E	15	ARG	N-CA-C	6.52	121.15	111.96
2	D	202	ASN	N-CA-C	6.51	121.50	112.45
1	C	172	LEU	N-CA-C	-6.51	105.16	113.23
2	B	216	VAL	N-CA-C	6.50	117.47	108.12
2	D	409	LEU	N-CA-C	-6.41	100.79	110.28
2	B	202	ASN	N-CA-C	6.41	121.30	112.90
2	F	119	ILE	CB-CA-C	-6.36	107.65	113.70
2	H	39	THR	N-CA-C	6.35	119.86	109.06
2	H	243	SER	CA-C-N	6.33	126.70	119.93
2	H	243	SER	C-N-CA	6.33	126.70	119.93
2	D	119	ILE	CB-CA-C	-6.32	107.70	113.70
2	D	134	VAL	N-CA-C	6.31	116.48	110.42
2	B	299	ILE	N-CA-C	6.30	117.87	111.00
2	F	134	VAL	N-CA-C	6.30	116.46	110.42
2	F	107	ASN	N-CA-C	6.29	117.41	108.74
2	F	202	ASN	N-CA-C	6.29	121.19	112.45
1	E	266	LEU	CA-C-N	6.28	126.20	119.85
1	E	266	LEU	C-N-CA	6.28	126.20	119.85
1	A	398	MET	N-CA-C	6.22	118.99	111.40
2	D	423	LYS	N-CA-C	-6.22	103.65	111.11
1	C	24	LEU	N-CA-C	-6.21	101.59	110.59
2	D	107	ASN	N-CA-C	6.13	117.20	108.74
1	G	398	MET	N-CA-C	6.12	118.87	111.40
2	D	39	THR	N-CA-C	6.12	119.47	109.06
1	E	24	LEU	N-CA-C	-6.05	101.81	110.59
1	A	244	ILE	CA-C-N	6.03	124.06	119.66
1	A	244	ILE	C-N-CA	6.03	124.06	119.66
2	H	409	LEU	N-CA-C	-6.03	101.36	110.28
2	F	243	SER	CA-C-N	6.03	126.38	119.93
2	F	243	SER	C-N-CA	6.03	126.38	119.93
1	C	38	HIS	ND1-CG-CD2	-6.02	100.08	106.10
1	G	172	LEU	N-CA-C	-6.01	105.03	112.90
2	F	131	THR	N-CA-C	5.96	120.69	113.41
2	H	107	ASN	N-CA-C	5.93	116.93	108.74
2	B	315	GLN	N-CA-C	5.92	118.55	110.55
2	D	216	VAL	N-CA-C	5.89	116.61	108.12
1	C	105	SER	N-CA-C	-5.88	99.81	109.40
2	F	216	VAL	N-CA-C	5.87	116.57	108.12
1	E	101	MET	N-CA-C	5.86	118.31	109.23
1	C	446	MET	N-CA-C	5.84	117.95	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	315	GLN	N-CA-C	5.83	118.42	110.55
1	A	105	SER	N-CA-C	-5.83	99.90	109.40
2	F	315	GLN	N-CA-C	5.82	118.40	110.55
2	B	409	LEU	N-CA-C	-5.81	101.68	110.28
1	A	85	GLU	N-CA-C	-5.79	104.89	111.14
2	H	299	ILE	N-CA-C	5.78	117.30	111.00
2	D	337	GLY	N-CA-C	5.77	118.65	110.74
1	A	266	LEU	CA-C-N	5.71	125.47	119.76
1	A	266	LEU	C-N-CA	5.71	125.47	119.76
1	G	24	LEU	N-CA-C	-5.69	102.33	110.59
1	G	446	MET	N-CA-C	5.66	117.67	109.07
2	D	315	GLN	N-CA-C	5.64	118.16	110.55
1	E	172	LEU	N-CA-C	-5.62	105.15	112.23
1	A	172	LEU	N-CA-C	-5.59	105.19	112.23
2	D	261	ASN	OD1-CG-ND2	-5.59	117.01	122.60
2	D	299	ILE	N-CA-C	5.57	117.07	111.00
2	B	243	SER	CA-C-N	5.55	125.87	119.93
2	B	243	SER	C-N-CA	5.55	125.87	119.93
2	D	243	SER	CA-C-N	5.54	125.86	119.93
2	D	243	SER	C-N-CA	5.54	125.86	119.93
2	B	131	THR	N-CA-C	5.52	120.29	113.50
2	H	216	VAL	N-CA-C	5.51	116.06	108.12
2	D	149	ARG	NE-CZ-NH2	5.46	124.11	119.20
1	G	221	GLY	N-CA-C	5.45	119.27	112.73
1	E	62	HIS	ND1-CG-CD2	-5.43	100.67	106.10
2	F	149	ARG	NE-CZ-NH2	5.39	124.05	119.20
1	A	446	MET	N-CA-C	5.38	117.44	108.99
1	G	105	SER	N-CA-C	-5.38	100.64	109.40
1	G	194	PHE	N-CA-C	5.38	120.49	113.88
2	H	131	THR	N-CA-C	5.38	120.11	113.50
2	H	337	GLY	N-CA-C	5.35	118.08	110.74
2	F	385	LEU	N-CA-C	5.31	119.99	112.93
1	C	443	THR	N-CA-C	-5.31	100.25	108.90
2	F	243	SER	N-CA-C	5.30	115.70	109.60
1	A	24	LEU	N-CA-C	-5.23	103.00	110.59
2	B	149	ARG	NE-CZ-NH2	5.23	123.91	119.20
2	B	271	ALA	N-CA-C	5.21	117.60	109.52
2	B	243	SER	N-CA-C	5.18	115.55	109.60
1	G	228	PRO	CA-C-N	5.17	125.33	119.90
1	G	228	PRO	C-N-CA	5.17	125.33	119.90
1	G	101	MET	N-CA-C	5.17	117.24	109.23
2	F	409	LEU	N-CA-C	-5.14	102.08	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	271	ALA	N-CA-C	5.13	117.47	109.52
2	H	302	GLY	N-CA-C	-5.11	106.07	114.76
2	B	423	LYS	N-CA-C	-5.11	105.15	111.33
1	G	266	LEU	CA-C-N	5.10	125.00	119.85
1	G	266	LEU	C-N-CA	5.10	125.00	119.85
3	Q	18	LEU	N-CA-C	-5.09	99.96	110.80
1	E	446	MET	N-CA-C	5.08	116.80	109.07
2	B	249	PRO	CA-C-N	-5.05	116.52	123.14
2	B	249	PRO	C-N-CA	-5.05	116.52	123.14
2	B	385	LEU	N-CA-C	5.05	119.64	112.93
2	B	305	SER	CA-C-N	5.04	124.94	119.85
2	B	305	SER	C-N-CA	5.04	124.94	119.85

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3499	0	3460	84	0
1	C	3471	0	3432	87	0
1	E	3459	0	3421	85	0
1	G	3475	0	3434	96	0
2	B	3414	0	3414	104	0
2	D	3442	0	3442	106	0
2	F	3442	0	3442	97	0
2	H	3431	0	3432	94	0
3	O	107	0	114	15	0
3	P	76	0	80	10	0
3	Q	82	0	85	14	0
3	R	54	0	62	7	0
4	A	15	0	17	0	0
4	G	15	0	17	0	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
5	F	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	H	1	0	0	0	0
6	F	1	0	0	0	0
6	H	1	0	0	0	0
6	O	1	0	0	0	0
6	P	1	0	0	0	0
All	All	27990	0	27852	745	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 (745) 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:G:14:ALA:N	1:G:19:PHE:HB3	1.64	1.11
2:D:256:ARG:HG3	2:D:256:ARG:HH11	1.33	0.93
2:F:256:ARG:HG3	2:F:256:ARG:HH11	1.34	0.91
2:B:256:ARG:HG3	2:B:256:ARG:HH11	1.34	0.91
1:C:295:GLY:HA2	2:D:93:GLU:HG2	1.52	0.90
1:G:33:SER:HB3	1:G:392:MET:HE1	1.57	0.85
2:H:256:ARG:HH11	2:H:256:ARG:HG3	1.37	0.84
1:E:268:ILE:HD11	1:E:398:MET:SD	2.19	0.82
1:A:268:ILE:HD11	1:A:398:MET:SD	2.19	0.82
1:A:295:GLY:HA2	2:B:93:GLU:HG2	1.61	0.81
1:C:230:ILE:HD12	1:C:230:ILE:H	1.46	0.80
1:E:33:SER:HB3	1:E:392:MET:HE1	1.62	0.80
1:C:268:ILE:HD11	1:C:398:MET:SD	2.21	0.80
1:G:230:ILE:H	1:G:230:ILE:HD12	1.48	0.79
1:E:33:SER:HB3	1:E:392:MET:CE	2.13	0.79
2:H:186:ASN:O	2:H:190:ILE:HG12	1.83	0.78
1:G:268:ILE:HD11	1:G:398:MET:SD	2.24	0.78
1:G:33:SER:HB3	1:G:392:MET:CE	2.12	0.78
1:G:157:LEU:HB3	1:G:445:VAL:HG21	1.65	0.78
2:B:115:LEU:HD12	2:B:115:LEU:H	1.49	0.77
2:B:144:ARG:O	2:B:148:ILE:HG12	1.86	0.76
2:B:62:ASN:H	2:B:65:ASN:HB3	1.51	0.76
2:H:144:ARG:O	2:H:148:ILE:HG12	1.85	0.76
2:F:186:ASN:O	2:F:190:ILE:HG12	1.85	0.76
2:F:375:ARG:HB3	2:F:375:ARG:NH1	2.01	0.75
1:A:230:ILE:HD12	1:A:230:ILE:H	1.49	0.75
2:D:338:MET:HG2	2:D:356:ILE:HD13	1.67	0.75
2:H:115:LEU:HD12	2:H:115:LEU:H	1.51	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:62:ASN:H	2:H:65:ASN:HB3	1.52	0.75
2:B:186:ASN:O	2:B:190:ILE:HG12	1.87	0.74
2:F:144:ARG:O	2:F:148:ILE:HG12	1.87	0.74
2:H:338:MET:HG2	2:H:356:ILE:HD13	1.68	0.74
1:A:33:SER:HB3	1:A:392:MET:HE1	1.67	0.74
1:A:19:PHE:CD1	1:A:392:MET:HE2	2.23	0.74
2:D:186:ASN:O	2:D:190:ILE:HG12	1.88	0.74
2:B:405:THR:HG22	2:B:407:LYS:H	1.52	0.74
2:H:181:LEU:HD13	3:R:16:ARG:HG3	1.70	0.73
1:E:230:ILE:HD12	1:E:230:ILE:H	1.51	0.73
1:C:33:SER:HB3	1:C:392:MET:HE1	1.70	0.73
2:F:62:ASN:H	2:F:65:ASN:HB3	1.54	0.73
2:D:375:ARG:HB3	2:D:375:ARG:NH1	2.04	0.73
2:B:338:MET:HG2	2:B:356:ILE:HD13	1.69	0.72
1:E:99:ASN:HD22	1:E:101:MET:HE3	1.53	0.72
2:F:405:THR:HG22	2:F:407:LYS:H	1.54	0.72
2:D:62:ASN:H	2:D:65:ASN:HB3	1.53	0.72
2:H:375:ARG:NH1	2:H:375:ARG:HB3	2.04	0.72
1:A:33:SER:HB3	1:A:392:MET:CE	2.20	0.72
1:C:230:ILE:HD12	1:C:230:ILE:N	2.05	0.72
2:D:144:ARG:O	2:D:148:ILE:HG12	1.89	0.72
2:F:256:ARG:HG3	2:F:256:ARG:NH1	2.05	0.71
1:A:99:ASN:HD22	1:A:101:MET:HE3	1.56	0.71
2:H:136:ASP:OD2	2:H:138:SER:HB3	1.90	0.71
2:F:338:MET:HG2	2:F:356:ILE:HD13	1.71	0.70
2:H:76:ALA:HB1	2:H:129:ILE:CG2	2.22	0.70
2:B:375:ARG:HB3	2:B:375:ARG:NH1	2.06	0.70
2:D:77:PHE:CD1	3:P:18:LEU:HD22	2.27	0.70
1:C:33:SER:HB3	1:C:392:MET:CE	2.22	0.70
2:F:136:ASP:OD2	2:F:138:SER:HB3	1.91	0.70
2:H:303:THR:HG22	2:H:305:SER:H	1.57	0.70
2:B:303:THR:HG22	2:B:305:SER:H	1.57	0.69
2:H:405:THR:HG22	2:H:407:LYS:H	1.57	0.69
2:B:441:MET:HE3	2:B:453:VAL:HG23	1.75	0.69
2:D:441:MET:HE3	2:D:453:VAL:HG23	1.73	0.69
1:G:99:ASN:HB2	1:G:101:MET:HE3	1.75	0.69
2:D:136:ASP:OD2	2:D:138:SER:HB3	1.92	0.68
1:A:99:ASN:HB2	1:A:101:MET:HE3	1.74	0.68
1:E:246:PRO:HG3	1:E:448:GLY:HA2	1.74	0.68
2:D:303:THR:HG22	2:D:305:SER:H	1.57	0.68
2:H:90:LEU:HD13	2:H:94:ASN:ND2	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:LYS:HG2	1:A:298:MET:HE2	1.74	0.68
1:G:230:ILE:HD12	1:G:230:ILE:N	2.08	0.68
2:F:115:LEU:HD12	2:F:115:LEU:H	1.59	0.68
1:G:19:PHE:CD1	1:G:392:MET:HE2	2.29	0.68
2:F:76:ALA:HB1	2:F:129:ILE:CG2	2.22	0.68
1:E:99:ASN:HB2	1:E:101:MET:HE3	1.75	0.68
1:A:175:PRO:HB3	1:E:175:PRO:HB3	1.75	0.67
2:D:115:LEU:HD12	2:D:115:LEU:H	1.57	0.67
1:A:230:ILE:HD12	1:A:230:ILE:N	2.09	0.67
2:B:350:ARG:HH11	2:D:420:LYS:HB3	1.58	0.67
1:E:99:ASN:ND2	1:E:101:MET:HE3	2.10	0.67
1:E:157:LEU:HB3	1:E:445:VAL:HG21	1.75	0.67
1:E:230:ILE:HD12	1:E:230:ILE:N	2.09	0.67
2:F:441:MET:HE3	2:F:453:VAL:HG23	1.76	0.67
1:C:38:HIS:HD2	2:D:412:GLU:OE2	1.78	0.67
2:F:303:THR:HG22	2:F:305:SER:H	1.60	0.66
2:B:136:ASP:OD2	2:B:138:SER:HB3	1.95	0.66
2:D:175:PRO:HA	2:D:178:ARG:NH1	2.11	0.66
2:D:405:THR:HG22	2:D:407:LYS:H	1.59	0.66
2:H:275:VAL:HG22	2:H:279:ALA:CB	2.25	0.66
1:C:295:GLY:CA	2:D:93:GLU:HG2	2.26	0.66
2:B:76:ALA:HB1	2:B:129:ILE:CG2	2.26	0.66
2:H:441:MET:HE3	2:H:453:VAL:HG23	1.78	0.65
2:D:76:ALA:HB1	2:D:129:ILE:CG2	2.27	0.65
2:B:77:PHE:CD1	3:O:18:LEU:HD22	2.30	0.65
2:B:256:ARG:HG3	2:B:256:ARG:NH1	2.07	0.65
1:G:24:LEU:HD11	1:G:216:THR:HG22	1.78	0.65
2:H:275:VAL:HG11	2:H:282:TYR:HA	1.78	0.65
2:H:256:ARG:HG3	2:H:256:ARG:NH1	2.10	0.65
1:C:99:ASN:HB2	1:C:101:MET:HE3	1.78	0.65
2:D:165:HIS:HD2	2:D:256:ARG:HE	1.44	0.65
1:G:99:ASN:HD22	1:G:101:MET:HE3	1.62	0.65
2:H:458:GLU:O	2:H:462:GLN:HB2	1.96	0.65
1:C:122:VAL:O	1:C:191:ARG:NH2	2.30	0.65
2:H:39:THR:HB	2:H:218:HIS:HD2	1.62	0.64
1:A:99:ASN:ND2	1:A:101:MET:HE3	2.12	0.64
1:C:99:ASN:HD22	1:C:101:MET:HE3	1.61	0.64
1:G:14:ALA:N	1:G:17:ASP:OD2	2.30	0.64
1:C:157:LEU:HB3	1:C:445:VAL:HG21	1.79	0.64
1:A:19:PHE:HD1	1:A:392:MET:CE	2.11	0.64
2:B:458:GLU:O	2:B:462:GLN:HB2	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:246:PRO:HG3	1:G:448:GLY:HA2	1.80	0.64
2:H:77:PHE:CE1	3:R:18:LEU:HD22	2.31	0.64
2:D:181:LEU:HD13	3:P:16:ARG:HG3	1.79	0.63
2:H:175:PRO:HA	2:H:178:ARG:NH1	2.13	0.63
2:H:236:GLU:C	2:H:238:PRO:HD3	2.23	0.63
2:H:181:LEU:CD1	3:R:16:ARG:HG3	2.28	0.63
1:E:243:CYS:HA	1:E:446:MET:O	1.97	0.63
1:E:210:GLU:HA	1:E:210:GLU:OE1	1.98	0.63
1:A:157:LEU:HB3	1:A:445:VAL:HG21	1.80	0.63
1:G:19:PHE:HD1	1:G:392:MET:CE	2.12	0.63
3:Q:17:THR:C	3:Q:19:CYS:H	2.07	0.62
1:A:210:GLU:OE1	1:A:210:GLU:HA	1.99	0.62
2:B:290:ALA:HB2	3:O:10:PHE:CZ	2.34	0.62
2:D:458:GLU:O	2:D:462:GLN:HB2	1.99	0.62
1:C:210:GLU:HA	1:C:210:GLU:OE1	1.99	0.62
2:F:458:GLU:O	2:F:462:GLN:HB2	1.99	0.62
2:B:245:ARG:HE	2:B:245:ARG:HA	1.65	0.62
1:C:19:PHE:CD1	1:C:392:MET:HE2	2.35	0.62
2:F:275:VAL:HG11	2:F:282:TYR:HA	1.82	0.62
2:H:76:ALA:O	2:H:129:ILE:HG23	2.00	0.62
1:A:19:PHE:CE1	1:A:392:MET:HE2	2.34	0.62
2:B:90:LEU:HD13	2:B:94:ASN:ND2	2.15	0.62
2:H:27:ARG:HH11	2:H:27:ARG:HB3	1.64	0.62
1:A:242:SER:OG	1:E:176:ARG:NH2	2.33	0.62
2:F:90:LEU:HD13	2:F:94:ASN:ND2	2.14	0.62
1:G:210:GLU:OE1	1:G:210:GLU:HA	2.00	0.61
3:O:17:THR:HG22	3:O:19:CYS:N	2.15	0.61
2:B:54:VAL:O	2:B:107:ASN:HB3	2.00	0.61
2:D:90:LEU:HD13	2:D:94:ASN:ND2	2.16	0.61
2:D:441:MET:HE2	2:D:456:ILE:HD12	1.83	0.61
2:F:375:ARG:HB3	2:F:375:ARG:CZ	2.31	0.61
1:C:24:LEU:HD11	1:C:216:THR:HG22	1.82	0.61
1:C:246:PRO:HG3	1:C:448:GLY:HA2	1.81	0.61
2:F:175:PRO:HA	2:F:178:ARG:NH1	2.16	0.61
1:C:19:PHE:HD1	1:C:392:MET:CE	2.13	0.60
2:D:275:VAL:HG11	2:D:282:TYR:HA	1.83	0.60
2:D:116:GLN:O	2:D:119:ILE:HG12	2.01	0.60
1:C:298:MET:HG2	2:D:93:GLU:OE2	2.01	0.60
2:D:236:GLU:C	2:D:238:PRO:HD3	2.27	0.60
2:F:76:ALA:O	2:F:129:ILE:HG23	2.02	0.60
2:F:101:ALA:O	3:Q:17:THR:HG23	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:99:ASN:ND2	1:G:101:MET:HE3	2.17	0.60
1:A:19:PHE:CD1	1:A:392:MET:CE	2.86	0.59
2:B:175:PRO:HA	2:B:178:ARG:NH1	2.17	0.59
2:B:441:MET:HE3	2:B:453:VAL:CG2	2.33	0.59
2:D:375:ARG:HB3	2:D:375:ARG:CZ	2.32	0.59
2:F:236:GLU:C	2:F:238:PRO:HD3	2.26	0.59
1:G:15:ARG:HG3	1:G:15:ARG:HH11	1.66	0.59
2:B:275:VAL:HG11	2:B:282:TYR:HA	1.83	0.59
2:H:375:ARG:HB3	2:H:375:ARG:CZ	2.33	0.59
1:A:114:MET:HE2	1:A:118:MET:HE3	1.84	0.59
2:H:90:LEU:CD1	2:H:94:ASN:HD21	2.15	0.59
3:P:10:PHE:O	3:P:12:LYS:HE2	2.03	0.59
2:F:27:ARG:HB3	2:F:27:ARG:HH11	1.66	0.59
2:D:256:ARG:HG3	2:D:256:ARG:NH1	2.06	0.58
2:F:275:VAL:HG22	2:F:279:ALA:CB	2.32	0.58
1:E:187:LEU:O	1:E:191:ARG:HG3	2.03	0.58
2:B:236:GLU:C	2:B:238:PRO:HD3	2.28	0.58
2:F:116:GLN:O	2:F:119:ILE:HG12	2.03	0.58
1:G:275:ALA:HB3	1:G:423:VAL:HG21	1.85	0.58
2:B:181:LEU:HD13	3:O:16:ARG:HG3	1.86	0.58
2:D:290:ALA:HB2	3:P:10:PHE:CZ	2.39	0.58
1:G:157:LEU:CB	1:G:445:VAL:HG21	2.33	0.58
2:H:54:VAL:O	2:H:107:ASN:HB3	2.04	0.58
2:H:116:GLN:O	2:H:119:ILE:HG12	2.02	0.58
1:A:294:PRO:HB3	2:B:89:GLU:HA	1.86	0.58
2:F:181:LEU:HD13	3:Q:16:ARG:HG3	1.85	0.58
2:F:441:MET:HE3	2:F:453:VAL:CG2	2.33	0.58
1:G:114:MET:HE2	1:G:118:MET:HE3	1.86	0.58
1:C:38:HIS:CD2	2:D:412:GLU:OE2	2.56	0.58
1:C:230:ILE:H	1:C:230:ILE:CD1	2.16	0.58
2:H:76:ALA:HB1	2:H:129:ILE:HG22	1.86	0.58
1:E:19:PHE:CD1	1:E:392:MET:HE2	2.39	0.57
2:H:101:ALA:O	3:R:17:THR:HG23	2.02	0.57
1:G:122:VAL:O	1:G:191:ARG:NH2	2.36	0.57
1:G:187:LEU:O	1:G:191:ARG:HG3	2.04	0.57
1:C:429:THR:CG2	1:C:431:ASN:HD22	2.16	0.57
2:D:181:LEU:CD1	3:P:16:ARG:HG3	2.34	0.57
2:F:39:THR:HB	2:F:218:HIS:HD2	1.70	0.57
1:C:114:MET:HE2	1:C:118:MET:HE3	1.85	0.57
1:G:119:SER:HB3	1:G:220:LEU:HD11	1.86	0.57
2:H:39:THR:HB	2:H:218:HIS:CD2	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:439:VAL:HG13	2:B:457:GLU:HG2	1.86	0.57
2:D:165:HIS:HD2	2:D:256:ARG:NE	2.02	0.57
2:F:76:ALA:HB1	2:F:129:ILE:HG22	1.86	0.57
2:H:218:HIS:O	2:H:222:VAL:HG23	2.05	0.57
2:D:441:MET:HE3	2:D:453:VAL:CG2	2.35	0.57
2:F:218:HIS:O	2:F:222:VAL:HG23	2.05	0.56
2:B:375:ARG:HB3	2:B:375:ARG:CZ	2.35	0.56
2:B:115:LEU:HD12	2:B:115:LEU:N	2.20	0.56
2:B:275:VAL:HG22	2:B:279:ALA:CB	2.36	0.56
1:C:119:SER:HB3	1:C:220:LEU:HD11	1.88	0.56
2:D:286:LEU:HD21	3:P:11:PHE:CE1	2.40	0.56
1:G:15:ARG:HG3	1:G:15:ARG:NH1	2.20	0.56
1:G:19:PHE:CD1	1:G:392:MET:CE	2.88	0.56
2:H:441:MET:HE3	2:H:453:VAL:CG2	2.34	0.56
2:D:275:VAL:HG22	2:D:279:ALA:CB	2.35	0.56
2:F:377:LYS:O	2:F:381:LYS:HG3	2.05	0.56
2:F:290:ALA:HB2	3:Q:10:PHE:CE1	2.39	0.56
2:D:27:ARG:HB3	2:D:27:ARG:HH11	1.71	0.56
2:B:62:ASN:OD1	2:B:65:ASN:HB2	2.04	0.56
1:C:19:PHE:CD1	1:C:392:MET:CE	2.89	0.56
1:C:99:ASN:ND2	1:C:101:MET:HE3	2.19	0.56
2:D:439:VAL:HG13	2:D:457:GLU:HG2	1.87	0.56
2:F:290:ALA:HB2	3:Q:10:PHE:CZ	2.41	0.56
1:A:187:LEU:O	1:A:191:ARG:HG3	2.06	0.56
1:G:268:ILE:HD13	1:G:268:ILE:N	2.20	0.56
2:D:62:ASN:OD1	2:D:65:ASN:HB2	2.05	0.56
2:F:245:ARG:HE	2:F:245:ARG:HA	1.70	0.56
2:D:218:HIS:O	2:D:222:VAL:HG23	2.06	0.55
2:D:290:ALA:HB2	3:P:10:PHE:CE1	2.41	0.55
1:E:139:ALA:O	1:E:143:ILE:HD13	2.07	0.55
1:C:187:LEU:O	1:C:191:ARG:HG3	2.05	0.55
1:E:122:VAL:O	1:E:191:ARG:NH2	2.40	0.55
2:H:115:LEU:HD12	2:H:115:LEU:N	2.22	0.55
1:C:429:THR:HG22	1:C:431:ASN:HD22	1.70	0.55
2:D:441:MET:HG2	2:D:442:VAL:N	2.22	0.55
1:E:14:ALA:HB3	1:E:404:PRO:HB3	1.87	0.55
1:E:114:MET:HE2	1:E:118:MET:HE3	1.88	0.55
3:O:17:THR:C	3:O:19:CYS:H	2.15	0.55
1:C:157:LEU:CB	1:C:445:VAL:HG21	2.36	0.55
2:D:204:LYS:HG3	2:D:235:SER:OG	2.07	0.55
2:B:116:GLN:O	2:B:119:ILE:HG12	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:19:PHE:CE1	1:G:392:MET:HE2	2.42	0.55
2:B:76:ALA:O	2:B:129:ILE:HG23	2.08	0.54
2:B:90:LEU:CD1	2:B:94:ASN:HD21	2.20	0.54
2:B:27:ARG:HH11	2:B:27:ARG:HB3	1.71	0.54
1:C:299:TYR:CZ	2:D:90:LEU:HD23	2.43	0.54
2:H:439:VAL:HG13	2:H:457:GLU:HG2	1.89	0.54
2:B:181:LEU:CD1	3:O:16:ARG:HG3	2.37	0.54
1:C:379:LEU:HD13	2:D:46:SER:HB2	1.90	0.54
2:D:245:ARG:HA	2:D:245:ARG:HE	1.73	0.54
1:G:96:SER:HB3	1:G:99:ASN:OD1	2.07	0.54
2:B:218:HIS:O	2:B:222:VAL:HG23	2.08	0.54
2:D:76:ALA:O	2:D:129:ILE:HG23	2.07	0.54
2:D:441:MET:HE2	2:D:456:ILE:CD1	2.38	0.54
2:H:62:ASN:OD1	2:H:65:ASN:HB2	2.08	0.54
2:F:90:LEU:CD1	2:F:94:ASN:HD21	2.21	0.54
2:F:181:LEU:CD1	3:Q:16:ARG:HG3	2.37	0.54
2:B:77:PHE:CE1	3:O:18:LEU:HD22	2.42	0.54
1:C:96:SER:HB3	1:C:99:ASN:OD1	2.08	0.54
1:E:157:LEU:CB	1:E:445:VAL:HG21	2.38	0.53
1:E:270:HIS:O	1:E:273:ILE:HB	2.08	0.53
2:H:397:ASP:OD2	2:H:408:ARG:NH1	2.41	0.53
2:B:40:GLU:OE1	2:B:408:ARG:NH2	2.41	0.53
1:C:268:ILE:N	1:C:268:ILE:HD13	2.23	0.53
1:C:19:PHE:CE1	1:C:392:MET:HE2	2.43	0.53
2:F:119:ILE:O	2:F:122:ALA:HB3	2.08	0.53
2:H:441:MET:HE2	2:H:456:ILE:HD12	1.90	0.53
2:F:54:VAL:O	2:F:107:ASN:HB3	2.09	0.53
1:A:230:ILE:H	1:A:230:ILE:CD1	2.18	0.53
1:A:24:LEU:HD11	1:A:216:THR:HG22	1.91	0.53
2:B:290:ALA:HB2	3:O:10:PHE:HZ	1.73	0.53
1:A:268:ILE:N	1:A:268:ILE:HD13	2.24	0.53
1:A:333:LEU:HD13	1:A:334:SER:N	2.24	0.53
2:B:31:LEU:HD22	2:B:35:LEU:HD23	1.91	0.53
2:B:441:MET:HG2	2:B:442:VAL:N	2.24	0.52
1:E:39:PHE:CE1	1:E:385:LYS:HD2	2.44	0.52
1:E:119:SER:HB3	1:E:220:LEU:HD11	1.90	0.52
2:F:31:LEU:HD22	2:F:35:LEU:HD23	1.92	0.52
1:A:429:THR:O	1:A:429:THR:HG22	2.09	0.52
1:E:24:LEU:HD11	1:E:216:THR:HG22	1.90	0.52
1:A:122:VAL:O	1:A:191:ARG:NH2	2.42	0.52
2:B:377:LYS:O	2:B:381:LYS:HG3	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:253:ARG:HB3	2:D:438:PRO:HB2	1.92	0.52
1:A:429:THR:CG2	1:A:431:ASN:HD22	2.22	0.52
2:D:62:ASN:CG	2:D:65:ASN:HB2	2.35	0.52
2:F:439:VAL:HG13	2:F:457:GLU:HG2	1.90	0.52
1:A:403:ILE:HG23	1:A:403:ILE:O	2.10	0.52
2:H:90:LEU:CD1	2:H:94:ASN:ND2	2.71	0.52
1:A:139:ALA:O	1:A:143:ILE:HD13	2.09	0.52
1:C:32:THR:C	1:C:392:MET:HE1	2.35	0.52
1:G:379:LEU:HD11	1:G:409:ILE:HD11	1.91	0.52
1:A:176:ARG:NH2	1:E:242:SER:OG	2.43	0.52
1:C:403:ILE:O	1:C:403:ILE:HG23	2.10	0.52
1:E:32:THR:HG21	1:E:209:HIS:HA	1.92	0.52
1:E:268:ILE:HD13	1:E:268:ILE:N	2.25	0.52
1:C:249:VAL:HG23	1:C:249:VAL:O	2.10	0.51
1:C:429:THR:HG22	1:C:429:THR:O	2.09	0.51
1:E:19:PHE:HD1	1:E:392:MET:CE	2.23	0.51
1:G:157:LEU:HB3	1:G:445:VAL:CG2	2.38	0.51
1:G:230:ILE:H	1:G:230:ILE:CD1	2.18	0.51
1:E:33:SER:HB3	1:E:392:MET:HE3	1.90	0.51
1:E:299:TYR:CZ	2:F:90:LEU:HD23	2.44	0.51
2:H:441:MET:HG2	2:H:442:VAL:N	2.25	0.51
1:A:371:LYS:HE3	1:A:412:ILE:O	2.11	0.51
2:F:62:ASN:OD1	2:F:65:ASN:HB2	2.10	0.51
2:F:441:MET:HG2	2:F:442:VAL:N	2.25	0.51
2:H:69:ALA:HB2	2:H:198:TYR:CZ	2.45	0.51
1:A:119:SER:HB3	1:A:220:LEU:HD11	1.91	0.51
2:B:76:ALA:HB1	2:B:129:ILE:HG22	1.93	0.51
1:E:33:SER:CB	1:E:392:MET:HE1	2.39	0.51
2:B:62:ASN:CG	2:B:65:ASN:HB2	2.36	0.51
1:E:96:SER:HB3	1:E:99:ASN:OD1	2.11	0.51
1:G:333:LEU:HD13	1:G:334:SER:N	2.26	0.51
2:B:286:LEU:HD21	3:O:11:PHE:CE1	2.46	0.51
2:B:350:ARG:NH1	2:D:420:LYS:HB3	2.25	0.51
1:C:81:ALA:O	1:C:85:GLU:HG3	2.10	0.51
2:D:76:ALA:HB1	2:D:129:ILE:HG22	1.93	0.51
2:H:62:ASN:CG	2:H:65:ASN:HB2	2.35	0.51
1:E:81:ALA:O	1:E:85:GLU:HG3	2.11	0.50
2:D:42:ILE:HG13	2:D:214:GLY:HA2	1.92	0.50
3:R:12:LYS:N	3:R:13:PRO:HD3	2.27	0.50
1:A:157:LEU:CB	1:A:445:VAL:HG21	2.42	0.50
1:A:379:LEU:HD11	1:A:409:ILE:HD11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:39:THR:HB	2:F:218:HIS:CD2	2.45	0.50
2:F:397:ASP:OD2	2:F:408:ARG:NH1	2.43	0.50
1:A:342:GLN:O	1:A:346:VAL:HG23	2.11	0.50
2:B:245:ARG:HA	2:B:245:ARG:NE	2.26	0.50
2:F:255:GLU:HB3	2:F:453:VAL:HG23	1.94	0.50
1:E:230:ILE:H	1:E:230:ILE:CD1	2.21	0.50
2:H:453:VAL:O	2:H:457:GLU:HG3	2.11	0.50
2:B:119:ILE:O	2:B:122:ALA:HB3	2.12	0.50
2:B:416:GLU:HA	2:B:416:GLU:OE1	2.11	0.50
1:C:314:GLU:OE2	1:C:315:ASN:HB2	2.12	0.50
1:G:276:LEU:HD11	1:G:329:PHE:CD2	2.47	0.50
1:G:310:TYR:HB3	1:G:312:PHE:CZ	2.46	0.50
2:H:119:ILE:O	2:H:122:ALA:HB3	2.12	0.50
2:F:61:GLU:OE1	2:F:66:ASN:HA	2.12	0.50
1:G:139:ALA:O	1:G:143:ILE:HD13	2.11	0.50
1:G:243:CYS:HA	1:G:446:MET:O	2.11	0.50
1:G:371:LYS:HE3	1:G:412:ILE:O	2.12	0.50
3:Q:10:PHE:O	3:Q:11:PHE:O	2.30	0.50
2:B:42:ILE:HG13	2:B:214:GLY:HA2	1.93	0.49
1:A:314:GLU:OE2	1:A:315:ASN:HB2	2.12	0.49
1:E:340:ALA:HB3	1:E:341:PRO:HD3	1.94	0.49
1:G:270:HIS:O	1:G:273:ILE:HB	2.13	0.49
1:A:270:HIS:O	1:A:273:ILE:HB	2.12	0.49
2:D:115:LEU:HD12	2:D:115:LEU:N	2.26	0.49
2:F:441:MET:HE2	2:F:456:ILE:HD12	1.94	0.49
2:H:255:GLU:HB3	2:H:453:VAL:HG23	1.94	0.49
3:O:11:PHE:O	3:O:12:LYS:HG2	2.11	0.49
1:E:67:LEU:HD13	1:E:135:GLN:HG3	1.95	0.49
2:F:253:ARG:HB3	2:F:438:PRO:HB2	1.95	0.49
2:H:144:ARG:HH21	2:H:188:LYS:C	2.21	0.49
2:H:317:GLY:O	2:H:318:SER:CB	2.60	0.49
2:F:69:ALA:HB2	2:F:198:TYR:CZ	2.48	0.49
3:Q:11:PHE:O	3:Q:12:LYS:HG2	2.13	0.49
2:D:77:PHE:CE1	3:P:18:LEU:HD22	2.47	0.49
2:F:62:ASN:CG	2:F:65:ASN:HB2	2.38	0.49
1:G:81:ALA:O	1:G:85:GLU:HG3	2.13	0.49
1:A:32:THR:HG21	1:A:209:HIS:HA	1.94	0.48
1:A:429:THR:HG22	1:A:431:ASN:HD22	1.78	0.48
2:B:69:ALA:HB2	2:B:198:TYR:CZ	2.48	0.48
1:G:249:VAL:O	1:G:249:VAL:HG23	2.13	0.48
2:H:31:LEU:HD22	2:H:35:LEU:HD23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:119:ILE:O	2:D:122:ALA:HB3	2.13	0.48
1:G:67:LEU:HD13	1:G:135:GLN:HG3	1.94	0.48
1:E:249:VAL:HG23	1:E:249:VAL:O	2.13	0.48
1:A:81:ALA:O	1:A:85:GLU:HG3	2.14	0.48
1:A:96:SER:HB3	1:A:99:ASN:OD1	2.13	0.48
2:F:90:LEU:CD1	2:F:94:ASN:ND2	2.76	0.48
1:G:32:THR:HG21	1:G:209:HIS:HA	1.94	0.48
2:H:253:ARG:HB3	2:H:438:PRO:HB2	1.95	0.48
1:C:371:LYS:HE3	1:C:412:ILE:O	2.13	0.48
1:A:340:ALA:HB3	1:A:341:PRO:HD3	1.95	0.48
2:B:76:ALA:HB1	2:B:129:ILE:HG23	1.95	0.48
2:B:90:LEU:CD1	2:B:94:ASN:ND2	2.77	0.48
2:D:377:LYS:O	2:D:381:LYS:HG3	2.14	0.48
2:F:144:ARG:HH21	2:F:188:LYS:C	2.21	0.48
2:B:368:ILE:O	2:B:423:LYS:HE3	2.13	0.48
1:C:340:ALA:HB3	1:C:341:PRO:HD3	1.95	0.48
2:D:235:SER:O	2:D:238:PRO:HG3	2.13	0.48
2:H:42:ILE:HG13	2:H:214:GLY:HA2	1.95	0.48
1:C:294:PRO:HB3	2:D:89:GLU:HA	1.96	0.48
2:D:90:LEU:CD1	2:D:94:ASN:HD21	2.27	0.48
1:E:314:GLU:OE2	1:E:315:ASN:HB2	2.14	0.48
1:E:371:LYS:HE3	1:E:412:ILE:O	2.14	0.48
2:H:119:ILE:N	2:H:120:PRO:HD2	2.29	0.48
2:H:398:ILE:HA	2:H:408:ARG:HG3	1.96	0.48
2:B:183:PRO:HD2	2:B:186:ASN:HB2	1.96	0.47
2:B:458:GLU:CD	2:D:422:THR:HB	2.39	0.47
2:D:54:VAL:O	2:D:107:ASN:HB3	2.14	0.47
2:F:375:ARG:HB3	2:F:375:ARG:HH11	1.78	0.47
2:H:91:GLU:OE2	2:H:121:LYS:HD2	2.14	0.47
1:A:293:GLY:HA3	2:B:99:LEU:O	2.14	0.47
1:C:275:ALA:HB3	1:C:423:VAL:HG21	1.96	0.47
2:D:143:GLU:O	2:D:147:ILE:HG12	2.13	0.47
1:E:333:LEU:HD13	1:E:334:SER:N	2.28	0.47
2:H:245:ARG:HE	2:H:245:ARG:HA	1.79	0.47
1:C:276:LEU:HD11	1:C:329:PHE:CD2	2.49	0.47
2:D:232:VAL:HA	2:D:233:PRO:HD3	1.67	0.47
3:R:16:ARG:HA	3:R:16:ARG:HD3	1.67	0.47
1:A:45:TYR:N	1:A:45:TYR:CD1	2.83	0.47
2:F:115:LEU:HD12	2:F:115:LEU:N	2.28	0.47
1:G:275:ALA:CB	1:G:423:VAL:HG21	2.44	0.47
2:D:91:GLU:OE2	2:D:121:LYS:HD2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:73:GLN:HA	2:F:110:TYR:OH	2.15	0.47
1:G:429:THR:HG22	1:G:429:THR:O	2.15	0.47
2:H:77:PHE:CD1	3:R:18:LEU:HD22	2.50	0.47
2:B:61:GLU:OE1	2:B:66:ASN:HA	2.14	0.47
1:C:235:ALA:O	1:C:436:GLY:HA3	2.14	0.47
2:D:101:ALA:O	3:P:17:THR:HG23	2.15	0.47
1:E:99:ASN:HB2	1:E:101:MET:CE	2.44	0.47
2:F:22:GLN:OE1	2:F:22:GLN:HA	2.14	0.47
2:F:255:GLU:HB3	2:F:453:VAL:CG2	2.45	0.47
2:H:368:ILE:O	2:H:423:LYS:HE3	2.15	0.47
2:H:377:LYS:O	2:H:381:LYS:HG3	2.14	0.47
1:A:249:VAL:HG23	1:A:249:VAL:O	2.15	0.47
1:C:342:GLN:O	1:C:346:VAL:HG23	2.15	0.47
2:F:183:PRO:HD2	2:F:186:ASN:HB2	1.97	0.47
1:A:67:LEU:HD13	1:A:135:GLN:HG3	1.97	0.47
1:C:32:THR:HG21	1:C:209:HIS:HA	1.96	0.47
1:A:32:THR:C	1:A:392:MET:HE1	2.40	0.47
2:D:439:VAL:CG1	2:D:457:GLU:HG2	2.45	0.47
2:F:263:LEU:HA	2:F:264:PRO:HD3	1.69	0.47
3:Q:17:THR:C	3:Q:19:CYS:N	2.68	0.47
1:G:403:ILE:HG23	1:G:403:ILE:O	2.13	0.46
1:A:35:THR:HB	1:A:36:PRO:CD	2.44	0.46
1:A:42:LEU:HD23	1:A:42:LEU:N	2.30	0.46
2:B:439:VAL:HG22	2:B:453:VAL:HG13	1.96	0.46
2:B:441:MET:HE2	2:B:456:ILE:HD12	1.96	0.46
2:F:42:ILE:HG13	2:F:214:GLY:HA2	1.97	0.46
1:C:270:HIS:O	1:C:273:ILE:HB	2.14	0.46
2:D:317:GLY:O	2:D:318:SER:CB	2.64	0.46
1:E:19:PHE:HD1	1:E:392:MET:HE2	1.79	0.46
2:F:245:ARG:HA	2:F:245:ARG:NE	2.31	0.46
1:G:39:PHE:CE1	1:G:385:LYS:HD2	2.51	0.46
2:H:439:VAL:CG1	2:H:457:GLU:HG2	2.46	0.46
2:D:349:VAL:HG11	2:D:450:VAL:HG22	1.97	0.46
2:H:357:LEU:O	2:H:361:LYS:HG3	2.16	0.46
1:C:429:THR:CG2	1:C:429:THR:O	2.63	0.46
2:H:76:ALA:HB1	2:H:129:ILE:HG23	1.97	0.46
2:H:255:GLU:HB3	2:H:453:VAL:CG2	2.46	0.46
2:H:441:MET:HE2	2:H:456:ILE:CD1	2.45	0.46
1:A:275:ALA:HB3	1:A:423:VAL:HG21	1.97	0.46
2:B:253:ARG:HB3	2:B:438:PRO:HB2	1.98	0.46
2:B:439:VAL:CG1	2:B:457:GLU:HG2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:398:ILE:HA	2:D:408:ARG:HG3	1.97	0.46
2:F:349:VAL:HG11	2:F:450:VAL:HG22	1.98	0.46
2:H:349:VAL:HG11	2:H:450:VAL:HG22	1.97	0.46
1:A:33:SER:HB3	1:A:392:MET:HE3	1.98	0.46
2:B:453:VAL:O	2:B:457:GLU:HG3	2.16	0.46
1:C:333:LEU:HD13	1:C:334:SER:N	2.31	0.46
1:G:268:ILE:N	1:G:268:ILE:CD1	2.79	0.46
2:H:61:GLU:OE1	2:H:66:ASN:HA	2.16	0.46
1:A:178:LEU:HD11	1:E:178:LEU:HD11	1.97	0.46
2:H:81:GLN:HG3	2:H:132:LYS:O	2.16	0.46
2:D:40:GLU:O	2:D:213:ALA:HA	2.16	0.46
1:E:311:TYR:C	1:E:311:TYR:CD2	2.94	0.46
2:F:76:ALA:HB1	2:F:129:ILE:HG23	1.97	0.46
1:A:114:MET:CE	1:A:118:MET:HG3	2.46	0.45
1:A:253:LEU:HA	1:A:254:PRO:HD3	1.80	0.45
2:D:31:LEU:HD22	2:D:35:LEU:HD23	1.98	0.45
2:D:263:LEU:HA	2:D:264:PRO:HD3	1.67	0.45
2:F:91:GLU:OE2	2:F:121:LYS:HD2	2.16	0.45
1:G:256:LEU:CD1	1:G:314:GLU:HG2	2.46	0.45
1:G:340:ALA:HB3	1:G:341:PRO:HD3	1.97	0.45
2:B:397:ASP:OD2	2:B:408:ARG:NH1	2.47	0.45
2:D:73:GLN:HA	2:D:110:TYR:OH	2.17	0.45
1:E:311:TYR:C	1:E:313:VAL:H	2.24	0.45
1:E:429:THR:HG22	1:E:429:THR:O	2.16	0.45
2:F:119:ILE:N	2:F:120:PRO:HD2	2.32	0.45
2:F:235:SER:O	2:F:238:PRO:HG3	2.16	0.45
2:B:263:LEU:HA	2:B:264:PRO:HD3	1.67	0.45
2:B:357:LEU:O	2:B:361:LYS:HG3	2.16	0.45
2:B:97:SER:OG	2:B:114:SER:HB3	2.17	0.45
1:C:139:ALA:O	1:C:143:ILE:HD13	2.17	0.45
2:D:119:ILE:N	2:D:120:PRO:HD2	2.32	0.45
1:E:342:GLN:O	1:E:346:VAL:HG23	2.17	0.45
1:E:403:ILE:HG23	1:E:403:ILE:O	2.16	0.45
2:F:286:LEU:HD21	3:Q:11:PHE:CE1	2.51	0.45
2:H:143:GLU:O	2:H:147:ILE:HG12	2.17	0.45
2:B:260:GLU:HG3	2:B:263:LEU:HG	1.98	0.45
2:F:165:HIS:HD2	2:F:256:ARG:HE	1.65	0.45
2:F:295:TRP:CZ2	2:F:297:ARG:HA	2.52	0.45
2:F:368:ILE:O	2:F:423:LYS:HE3	2.15	0.45
2:D:260:GLU:HG3	2:D:263:LEU:HG	1.98	0.45
2:B:203:TYR:N	2:B:203:TYR:CD1	2.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:441:MET:HE3	2:B:441:MET:HB3	1.83	0.45
2:D:255:GLU:HB3	2:D:453:VAL:HG23	1.98	0.45
2:B:73:GLN:HA	2:B:110:TYR:OH	2.16	0.45
1:C:17:ASP:O	1:C:18:ASN:HB3	2.17	0.45
2:H:40:GLU:O	2:H:213:ALA:HA	2.17	0.45
2:B:290:ALA:HB2	3:O:10:PHE:CE1	2.52	0.45
2:D:76:ALA:HB1	2:D:129:ILE:HG23	1.99	0.45
2:D:397:ASP:OD2	2:D:408:ARG:NH1	2.49	0.45
1:E:379:LEU:HD11	1:E:409:ILE:HD11	1.99	0.45
2:F:357:LEU:O	2:F:361:LYS:HG3	2.17	0.45
1:G:33:SER:HB3	1:G:392:MET:HE3	1.96	0.45
1:C:157:LEU:HD11	1:C:244:ILE:HD13	1.98	0.44
2:D:260:GLU:CG	2:D:263:LEU:HG	2.47	0.44
1:E:67:LEU:HD13	1:E:135:GLN:CG	2.47	0.44
2:F:398:ILE:HA	2:F:408:ARG:HG3	1.99	0.44
2:B:147:ILE:HG22	2:B:187:ILE:HD13	2.00	0.44
1:A:243:CYS:HA	1:A:446:MET:O	2.17	0.44
2:B:260:GLU:CG	2:B:263:LEU:HG	2.48	0.44
1:C:311:TYR:C	1:C:311:TYR:CD2	2.96	0.44
2:D:144:ARG:HH21	2:D:188:LYS:C	2.24	0.44
1:E:256:LEU:CD1	1:E:314:GLU:HG2	2.47	0.44
1:G:314:GLU:OE2	1:G:315:ASN:HB2	2.16	0.44
1:A:35:THR:HB	1:A:36:PRO:HD2	1.98	0.44
2:B:240:PRO:O	2:B:243:SER:OG	2.35	0.44
1:E:157:LEU:HB3	1:E:445:VAL:CG2	2.44	0.44
1:E:310:TYR:HB3	1:E:312:PHE:CZ	2.53	0.44
2:F:326:PHE:CD1	2:F:326:PHE:C	2.95	0.44
1:A:429:THR:O	1:A:429:THR:CG2	2.66	0.44
1:C:310:TYR:CD1	1:C:312:PHE:CZ	3.06	0.44
2:D:61:GLU:OE1	2:D:66:ASN:HA	2.17	0.44
1:G:311:TYR:C	1:G:311:TYR:CD2	2.95	0.44
2:D:90:LEU:CD1	2:D:94:ASN:ND2	2.80	0.44
2:F:77:PHE:CE1	3:Q:18:LEU:HD22	2.53	0.44
1:G:96:SER:OG	1:G:97:ARG:N	2.50	0.44
2:B:317:GLY:O	2:B:318:SER:CB	2.65	0.44
1:E:124:PHE:N	1:E:125:PRO:CD	2.80	0.44
1:G:50:SER:OG	1:G:97:ARG:HA	2.17	0.44
1:G:344:VAL:HG21	1:G:456:VAL:HG22	2.00	0.44
2:H:73:GLN:HA	2:H:110:TYR:OH	2.17	0.44
3:Q:14:ALA:C	3:Q:15:THR:HG22	2.42	0.44
2:D:23:ILE:HA	2:D:24:PRO:HD3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:32:THR:C	1:E:392:MET:HE1	2.43	0.44
1:G:63:ILE:HG22	1:G:67:LEU:HD22	2.00	0.44
2:H:90:LEU:HD13	2:H:94:ASN:HD21	1.77	0.44
2:D:349:VAL:HG23	2:D:449:THR:HG23	2.00	0.44
1:E:427:ILE:HD13	1:E:432:VAL:CG2	2.47	0.44
2:H:295:TRP:CZ2	2:H:297:ARG:HA	2.53	0.44
1:A:56:ASN:HD22	1:A:56:ASN:HA	1.62	0.43
1:A:295:GLY:CA	2:B:93:GLU:HG2	2.41	0.43
1:A:311:TYR:C	1:A:311:TYR:CD2	2.95	0.43
1:C:296:LYS:HE2	1:C:298:MET:HE2	2.00	0.43
1:E:336:ILE:HG22	1:E:338:GLN:OE1	2.18	0.43
2:H:259:LYS:HG3	2:H:447:THR:HG22	2.00	0.43
1:E:256:LEU:HD23	1:E:336:ILE:HD13	2.01	0.43
2:F:97:SER:OG	2:F:114:SER:HB3	2.18	0.43
1:G:32:THR:C	1:G:392:MET:HE1	2.43	0.43
3:O:8:ILE:O	3:O:9:ARG:HG3	2.18	0.43
1:A:157:LEU:HD11	1:A:244:ILE:HD13	2.00	0.43
2:D:203:TYR:N	2:D:203:TYR:CD1	2.85	0.43
1:E:275:ALA:HB3	1:E:423:VAL:HG21	2.00	0.43
1:G:266:LEU:HA	1:G:267:PRO:HD3	1.85	0.43
1:G:310:TYR:CD1	1:G:312:PHE:CZ	3.06	0.43
2:H:260:GLU:CG	2:H:263:LEU:HG	2.49	0.43
1:A:311:TYR:C	1:A:313:VAL:H	2.26	0.43
2:B:350:ARG:HD2	2:D:420:LYS:HB2	1.99	0.43
2:D:21:SER:OG	2:D:22:GLN:N	2.51	0.43
2:D:453:VAL:O	2:D:457:GLU:HG3	2.18	0.43
1:C:119:SER:HB3	1:C:220:LEU:CD1	2.49	0.43
1:C:256:LEU:CD1	1:C:314:GLU:HG2	2.49	0.43
1:C:294:PRO:HD2	2:D:99:LEU:HB3	1.99	0.43
1:E:311:TYR:C	1:E:313:VAL:N	2.75	0.43
2:F:77:PHE:CD1	3:Q:18:LEU:HD22	2.54	0.43
2:F:393:ALA:O	2:F:396:GLU:HB3	2.19	0.43
2:F:416:GLU:OE1	2:F:416:GLU:HA	2.19	0.43
1:G:17:ASP:O	1:G:18:ASN:HB3	2.18	0.43
3:O:17:THR:C	3:O:19:CYS:N	2.75	0.43
3:Q:16:ARG:HA	3:Q:16:ARG:HD3	1.74	0.43
1:C:311:TYR:CD2	1:C:311:TYR:N	2.84	0.43
2:F:305:SER:HA	2:F:306:PRO:HD3	1.81	0.43
1:G:339:ALA:O	1:G:340:ALA:C	2.61	0.43
2:H:183:PRO:HD2	2:H:186:ASN:HB2	2.01	0.43
2:H:204:LYS:HG3	2:H:235:SER:OG	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:326:PHE:CD1	2:H:326:PHE:C	2.96	0.43
2:H:416:GLU:OE1	2:H:416:GLU:HA	2.19	0.43
1:A:276:LEU:HD11	1:A:329:PHE:CD2	2.53	0.43
2:B:305:SER:HA	2:B:306:PRO:HD3	1.83	0.43
2:B:350:ARG:NH1	2:D:416:GLU:OE2	2.52	0.43
1:C:311:TYR:C	1:C:313:VAL:H	2.26	0.43
1:E:305:HIS:ND1	1:E:305:HIS:N	2.67	0.43
3:O:10:PHE:O	3:O:11:PHE:O	2.37	0.43
1:C:84:LEU:HD13	1:C:91:TYR:CZ	2.54	0.43
1:C:253:LEU:HA	1:C:254:PRO:HD3	1.80	0.43
1:E:35:THR:HB	1:E:36:PRO:CD	2.49	0.43
2:F:259:LYS:HG3	2:F:447:THR:HG22	2.01	0.43
2:F:439:VAL:CG1	2:F:457:GLU:HG2	2.49	0.43
2:F:441:MET:HE2	2:F:456:ILE:CD1	2.49	0.43
1:G:152:LEU:O	1:G:155:PRO:HD2	2.18	0.43
1:G:305:HIS:ND1	1:G:305:HIS:N	2.67	0.43
2:D:69:ALA:HB2	2:D:198:TYR:CZ	2.53	0.43
1:E:19:PHE:CD1	1:E:392:MET:CE	3.01	0.43
1:E:228:PRO:HA	1:E:229:PRO:HD3	1.86	0.43
1:E:276:LEU:HD11	1:E:329:PHE:CD2	2.52	0.43
1:G:67:LEU:HD13	1:G:135:GLN:CG	2.49	0.43
1:G:84:LEU:HD13	1:G:91:TYR:CZ	2.54	0.43
1:G:310:TYR:HB3	1:G:312:PHE:CE2	2.54	0.43
1:A:339:ALA:O	1:A:340:ALA:C	2.62	0.43
2:B:31:LEU:HA	2:B:31:LEU:HD12	1.80	0.43
2:D:326:PHE:CD1	2:D:326:PHE:C	2.96	0.43
1:E:376:SER:O	1:E:380:MET:HG3	2.19	0.43
3:P:16:ARG:HA	3:P:16:ARG:HD3	1.92	0.43
1:A:50:SER:OG	1:A:97:ARG:HA	2.18	0.42
1:A:256:LEU:CD1	1:A:314:GLU:HG2	2.49	0.42
1:A:311:TYR:CD2	1:A:311:TYR:N	2.83	0.42
2:B:232:VAL:HA	2:B:233:PRO:HD3	1.73	0.42
2:B:393:ALA:O	2:B:396:GLU:HB3	2.19	0.42
2:F:317:GLY:O	2:F:318:SER:CB	2.66	0.42
1:G:174:CYS:HA	1:G:175:PRO:HD3	1.94	0.42
1:G:325:ASP:O	1:G:326:SER:HB2	2.18	0.42
2:H:260:GLU:HG3	2:H:263:LEU:HG	2.00	0.42
1:A:124:PHE:N	1:A:125:PRO:CD	2.82	0.42
1:A:311:TYR:C	1:A:313:VAL:N	2.77	0.42
2:D:183:PRO:HD2	2:D:186:ASN:HB2	2.01	0.42
2:D:255:GLU:HB3	2:D:453:VAL:CG2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:50:SER:OG	1:E:97:ARG:HA	2.19	0.42
1:E:311:TYR:C	1:E:311:TYR:HD2	2.26	0.42
2:F:260:GLU:HG3	2:F:263:LEU:HG	2.01	0.42
2:B:144:ARG:HH21	2:B:188:LYS:C	2.26	0.42
1:E:45:TYR:N	1:E:45:TYR:CD1	2.87	0.42
2:F:147:ILE:HG22	2:F:187:ILE:HD13	2.01	0.42
2:F:165:HIS:HD2	2:F:256:ARG:NE	2.16	0.42
2:F:260:GLU:CG	2:F:263:LEU:HG	2.50	0.42
2:H:137:ASN:O	2:H:141:GLU:HG2	2.19	0.42
2:B:91:GLU:OE2	2:B:121:LYS:HD2	2.19	0.42
1:C:67:LEU:HD13	1:C:135:GLN:HG3	2.01	0.42
1:G:157:LEU:HD11	1:G:244:ILE:HD13	2.01	0.42
2:H:136:ASP:O	2:H:140:ILE:HG13	2.19	0.42
2:B:398:ILE:HA	2:B:408:ARG:HG3	2.02	0.42
1:G:311:TYR:C	1:G:313:VAL:H	2.26	0.42
2:H:147:ILE:HG22	2:H:187:ILE:HD13	2.02	0.42
2:H:268:ILE:HD12	2:H:268:ILE:N	2.35	0.42
2:B:259:LYS:HG3	2:B:447:THR:HG22	2.00	0.42
2:D:147:ILE:HG22	2:D:187:ILE:HD13	2.02	0.42
2:B:255:GLU:HB3	2:B:453:VAL:HG23	2.00	0.42
2:D:350:ARG:HG3	2:D:451:PRO:HB3	2.02	0.42
1:G:45:TYR:OH	1:G:389:LEU:HG	2.20	0.42
1:G:311:TYR:C	1:G:313:VAL:N	2.76	0.42
2:B:165:HIS:HD2	2:B:256:ARG:NE	2.18	0.42
2:B:401:GLN:O	2:B:405:THR:HB	2.20	0.42
1:C:395:GLN:OE1	1:C:403:ILE:HG22	2.20	0.42
2:D:165:HIS:CD2	2:D:256:ARG:HE	2.31	0.42
1:E:19:PHE:CE1	1:E:392:MET:HE2	2.54	0.42
2:F:81:GLN:HG3	2:F:132:LYS:O	2.19	0.42
2:F:453:VAL:O	2:F:457:GLU:HG3	2.20	0.42
1:A:14:ALA:N	1:A:17:ASP:OD2	2.52	0.42
1:A:39:PHE:O	1:A:385:LYS:HE3	2.19	0.42
1:A:99:ASN:CB	1:A:101:MET:HE3	2.47	0.42
1:C:56:ASN:HD22	1:C:56:ASN:HA	1.56	0.42
1:C:96:SER:OG	1:C:97:ARG:N	2.53	0.42
1:C:124:PHE:N	1:C:125:PRO:CD	2.83	0.42
1:C:237:TYR:CG	1:C:264:GLU:HB2	2.54	0.42
1:C:310:TYR:HB3	1:C:312:PHE:CZ	2.54	0.42
2:F:203:TYR:N	2:F:203:TYR:CD1	2.88	0.42
1:G:119:SER:HB3	1:G:220:LEU:CD1	2.48	0.42
1:A:311:TYR:C	1:A:311:TYR:HD2	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:245:ARG:HA	2:D:245:ARG:NE	2.33	0.42
1:E:311:TYR:CD2	1:E:311:TYR:N	2.81	0.42
1:G:311:TYR:C	1:G:311:TYR:HD2	2.28	0.42
2:B:40:GLU:O	2:B:213:ALA:HA	2.20	0.41
1:C:157:LEU:HB3	1:C:445:VAL:CG2	2.48	0.41
1:E:267:PRO:HA	1:E:323:TYR:O	2.20	0.41
2:H:305:SER:HA	2:H:306:PRO:HD3	1.83	0.41
2:H:439:VAL:HG22	2:H:453:VAL:HG13	2.02	0.41
1:E:96:SER:OG	1:E:97:ARG:N	2.51	0.41
1:E:245:PRO:HA	1:E:246:PRO:HD3	1.87	0.41
1:G:33:SER:CB	1:G:392:MET:HE1	2.39	0.41
2:H:349:VAL:HG23	2:H:449:THR:HG23	2.03	0.41
1:A:68:ALA:O	1:A:69:PHE:HB2	2.20	0.41
1:A:167:THR:OG1	1:A:168:LEU:N	2.52	0.41
1:C:339:ALA:O	1:C:340:ALA:C	2.63	0.41
1:E:174:CYS:HA	1:E:175:PRO:HD3	1.97	0.41
1:G:200:THR:HG22	1:G:201:VAL:N	2.34	0.41
1:G:267:PRO:HA	1:G:323:TYR:O	2.20	0.41
2:H:232:VAL:HA	2:H:233:PRO:HD3	1.70	0.41
1:C:260:GLN:HB2	1:C:445:VAL:HG12	2.03	0.41
1:C:311:TYR:C	1:C:311:TYR:HD2	2.28	0.41
1:C:379:LEU:HD11	1:C:409:ILE:HD11	2.03	0.41
2:D:31:LEU:HD12	2:D:31:LEU:HA	1.90	0.41
1:E:310:TYR:CD1	1:E:312:PHE:CZ	3.08	0.41
1:G:30:VAL:HG22	1:G:216:THR:HG21	2.03	0.41
1:G:268:ILE:CD1	1:G:268:ILE:H	2.33	0.41
1:G:427:ILE:HD13	1:G:432:VAL:CG2	2.50	0.41
2:B:203:TYR:N	2:B:203:TYR:HD1	2.19	0.41
2:B:204:LYS:HG3	2:B:235:SER:OG	2.21	0.41
1:G:128:THR:OG1	1:G:131:GLU:HG3	2.21	0.41
1:G:228:PRO:HA	1:G:229:PRO:HD3	1.83	0.41
2:H:455:TYR:CD1	2:H:455:TYR:C	2.98	0.41
1:A:14:ALA:N	1:A:404:PRO:HB3	2.36	0.41
1:C:268:ILE:N	1:C:268:ILE:CD1	2.83	0.41
2:D:295:TRP:HB3	2:D:323:TYR:CE2	2.54	0.41
1:E:72:THR:HG21	1:E:120:GLU:HB3	2.02	0.41
1:E:101:MET:HE2	1:E:101:MET:HB3	1.95	0.41
1:G:42:LEU:N	1:G:42:LEU:HD23	2.34	0.41
1:G:263:PHE:CE2	1:G:442:ALA:HB2	2.55	0.41
1:G:369:ARG:O	1:G:373:GLN:HG3	2.20	0.41
1:A:99:ASN:HB2	1:A:101:MET:CE	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:375:ARG:HB3	2:B:375:ARG:HH11	1.82	0.41
1:C:33:SER:HB3	1:C:392:MET:HE3	2.00	0.41
1:C:273:ILE:HD13	1:C:273:ILE:HA	1.88	0.41
1:C:293:GLY:HA3	2:D:99:LEU:O	2.20	0.41
1:C:305:HIS:ND1	1:C:305:HIS:N	2.68	0.41
2:D:286:LEU:HD23	2:D:286:LEU:HA	1.88	0.41
1:G:45:TYR:CD1	1:G:45:TYR:N	2.88	0.41
1:G:99:ASN:HB2	1:G:101:MET:CE	2.49	0.41
1:G:376:SER:O	1:G:380:MET:HG3	2.21	0.41
2:B:75:LEU:HD21	2:B:140:ILE:HG12	2.02	0.41
1:G:119:SER:CB	1:G:220:LEU:HD11	2.50	0.41
2:H:203:TYR:N	2:H:203:TYR:CD1	2.89	0.41
1:A:268:ILE:N	1:A:268:ILE:CD1	2.83	0.41
2:B:143:GLU:O	2:B:147:ILE:HG12	2.20	0.41
2:B:441:MET:HE2	2:B:456:ILE:CD1	2.50	0.41
1:E:17:ASP:O	1:E:18:ASN:HB3	2.21	0.41
2:F:28:THR:HG22	2:F:29:SER:N	2.35	0.41
2:F:248:LEU:HA	2:F:249:PRO:HD3	1.92	0.41
2:F:295:TRP:HB3	2:F:323:TYR:CE2	2.56	0.41
2:H:35:LEU:HA	2:H:205:GLY:O	2.20	0.41
2:B:423:LYS:O	2:B:427:ILE:HG13	2.20	0.41
2:D:203:TYR:N	2:D:203:TYR:HD1	2.19	0.41
1:E:253:LEU:HA	1:E:254:PRO:HD3	1.81	0.41
1:G:382:LEU:HD12	1:G:382:LEU:HA	1.91	0.41
1:G:429:THR:O	1:G:429:THR:CG2	2.69	0.41
2:H:263:LEU:HA	2:H:264:PRO:HD3	1.67	0.41
1:C:113:LYS:HA	1:C:113:LYS:HD2	1.92	0.40
1:C:311:TYR:C	1:C:313:VAL:N	2.76	0.40
1:E:114:MET:CE	1:E:118:MET:HG3	2.51	0.40
2:F:455:TYR:CD1	2:F:455:TYR:C	3.00	0.40
1:G:56:ASN:HD22	1:G:56:ASN:HA	1.58	0.40
1:G:253:LEU:HA	1:G:254:PRO:HD3	1.82	0.40
2:B:119:ILE:N	2:B:120:PRO:HD2	2.36	0.40
2:D:357:LEU:O	2:D:361:LYS:HG3	2.21	0.40
1:E:268:ILE:N	1:E:268:ILE:CD1	2.84	0.40
1:A:310:TYR:HB3	1:A:312:PHE:CZ	2.56	0.40
2:B:294:ASN:ND2	3:O:9:ARG:HA	2.36	0.40
1:C:35:THR:HB	1:C:36:PRO:CD	2.51	0.40
1:C:179:ILE:N	1:C:180:PRO:CD	2.84	0.40
2:D:259:LYS:HG3	2:D:447:THR:HG22	2.03	0.40
2:F:268:ILE:N	2:F:268:ILE:HD12	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:114:MET:CE	1:G:118:MET:HG3	2.52	0.40
1:G:342:GLN:O	1:G:346:VAL:HG23	2.22	0.40
2:H:31:LEU:HD21	2:H:226:GLN:HA	2.03	0.40
2:H:52:ILE:HG23	2:H:52:ILE:O	2.21	0.40
2:H:317:GLY:O	2:H:318:SER:OG	2.39	0.40
1:A:302:LEU:HA	1:A:302:LEU:HD23	1.85	0.40
2:B:373:VAL:O	2:B:377:LYS:HG3	2.22	0.40
1:C:101:MET:HE2	1:C:101:MET:HB3	1.86	0.40
1:C:174:CYS:HA	1:C:175:PRO:HD3	1.90	0.40
1:E:339:ALA:O	1:E:340:ALA:C	2.64	0.40
1:A:45:TYR:OH	1:A:389:LEU:HG	2.21	0.40
1:A:246:PRO:HG3	1:A:448:GLY:HA2	2.02	0.40
1:A:336:ILE:HG22	1:A:338:GLN:OE1	2.21	0.40
2:B:81:GLN:HG3	2:B:132:LYS:O	2.21	0.40
1:C:39:PHE:CE1	1:C:385:LYS:HD2	2.57	0.40
1:E:336:ILE:HG23	1:E:337:PRO:HD2	2.04	0.40
2:F:256:ARG:NH1	2:F:256:ARG:CG	2.78	0.40
2:F:349:VAL:HG23	2:F:449:THR:HG23	2.03	0.40
1:G:336:ILE:HG22	1:G:338:GLN:OE1	2.22	0.40
2:H:393:ALA:O	2:H:396:GLU:HB3	2.21	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	448/475 (94%)	427 (95%)	19 (4%)	2 (0%)	30 54
1	C	444/475 (94%)	426 (96%)	15 (3%)	3 (1%)	18 41
1	E	441/475 (93%)	423 (96%)	15 (3%)	3 (1%)	18 41
1	G	444/475 (94%)	424 (96%)	16 (4%)	4 (1%)	14 35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	437/443 (99%)	420 (96%)	16 (4%)	1 (0%)	43	68
2	D	441/443 (100%)	420 (95%)	19 (4%)	2 (0%)	24	48
2	F	441/443 (100%)	425 (96%)	15 (3%)	1 (0%)	43	68
2	H	439/443 (99%)	422 (96%)	16 (4%)	1 (0%)	43	68
3	O	11/24 (46%)	6 (54%)	4 (36%)	1 (9%)	0	0
3	P	7/24 (29%)	5 (71%)	1 (14%)	1 (14%)	0	0
3	Q	8/24 (33%)	3 (38%)	4 (50%)	1 (12%)	0	0
3	R	5/24 (21%)	4 (80%)	1 (20%)	0	100	100
All	All	3566/3768 (95%)	3405 (96%)	141 (4%)	20 (1%)	21	44

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	O	11	PHE
3	P	11	PHE
3	Q	11	PHE
1	C	250	PHE
1	G	15	ARG
1	G	250	PHE
1	A	250	PHE
2	B	318	SER
2	D	318	SER
1	E	250	PHE
1	E	251	GLY
2	F	318	SER
2	H	318	SER
1	A	251	GLY
2	D	22	GLN
1	E	452	SER
1	G	251	GLY
1	C	251	GLY
1	C	171	PRO
1	G	171	PRO

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	381/401 (95%)	356 (93%)	25 (7%)	15	36
1	C	378/401 (94%)	353 (93%)	25 (7%)	15	36
1	E	377/401 (94%)	351 (93%)	26 (7%)	14	34
1	G	379/401 (94%)	354 (93%)	25 (7%)	15	36
2	B	376/379 (99%)	349 (93%)	27 (7%)	13	32
2	D	379/379 (100%)	351 (93%)	28 (7%)	13	32
2	F	379/379 (100%)	354 (93%)	25 (7%)	15	36
2	H	378/379 (100%)	352 (93%)	26 (7%)	14	34
3	O	12/23 (52%)	10 (83%)	2 (17%)	2	6
3	P	8/23 (35%)	7 (88%)	1 (12%)	4	11
3	Q	9/23 (39%)	6 (67%)	3 (33%)	0	1
3	R	6/23 (26%)	4 (67%)	2 (33%)	0	1
All	All	3062/3212 (95%)	2847 (93%)	215 (7%)	14	34

All (215) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ASP
1	A	56	ASN
1	A	65	ASP
1	A	66	ARG
1	A	67	LEU
1	A	151	GLU
1	A	176	ARG
1	A	210	GLU
1	A	220	LEU
1	A	230	ILE
1	A	241	GLU
1	A	268	ILE
1	A	273	ILE
1	A	303	TYR
1	A	305	HIS
1	A	307	LEU
1	A	311	TYR
1	A	314	GLU
1	A	333	LEU

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Mol	Chain	Res	Type
1	A	361	ARG
1	A	381	ASN
1	A	382	LEU
1	A	386	LEU
1	A	431	ASN
1	A	446	MET
2	B	27	ARG
2	B	31	LEU
2	B	39	THR
2	B	42	ILE
2	B	75	LEU
2	B	90	LEU
2	B	107	ASN
2	B	117	GLU
2	B	149	ARG
2	B	176	LEU
2	B	181	LEU
2	B	219	GLU
2	B	236	GLU
2	B	250	VAL
2	B	256	ARG
2	B	262	THR
2	B	275	VAL
2	B	346	GLU
2	B	375	ARG
2	B	403	VAL
2	B	405	THR
2	B	408	ARG
2	B	423	LYS
2	B	424	ASP
2	B	439	VAL
2	B	441	MET
2	B	449	THR
1	C	17	ASP
1	C	56	ASN
1	C	65	ASP
1	C	66	ARG
1	C	67	LEU
1	C	151	GLU
1	C	176	ARG
1	C	210	GLU
1	C	220	LEU

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Mol	Chain	Res	Type
1	C	230	ILE
1	C	241	GLU
1	C	268	ILE
1	C	273	ILE
1	C	303	TYR
1	C	305	HIS
1	C	307	LEU
1	C	311	TYR
1	C	314	GLU
1	C	333	LEU
1	C	361	ARG
1	C	381	ASN
1	C	382	LEU
1	C	386	LEU
1	C	431	ASN
1	C	446	MET
2	D	23	ILE
2	D	27	ARG
2	D	31	LEU
2	D	39	THR
2	D	42	ILE
2	D	75	LEU
2	D	90	LEU
2	D	107	ASN
2	D	117	GLU
2	D	149	ARG
2	D	176	LEU
2	D	181	LEU
2	D	219	GLU
2	D	236	GLU
2	D	239	VAL
2	D	250	VAL
2	D	256	ARG
2	D	262	THR
2	D	275	VAL
2	D	346	GLU
2	D	375	ARG
2	D	403	VAL
2	D	405	THR
2	D	408	ARG
2	D	423	LYS
2	D	424	ASP

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Mol	Chain	Res	Type
2	D	439	VAL
2	D	441	MET
1	E	17	ASP
1	E	56	ASN
1	E	65	ASP
1	E	66	ARG
1	E	67	LEU
1	E	151	GLU
1	E	176	ARG
1	E	210	GLU
1	E	220	LEU
1	E	230	ILE
1	E	241	GLU
1	E	268	ILE
1	E	273	ILE
1	E	303	TYR
1	E	305	HIS
1	E	307	LEU
1	E	311	TYR
1	E	314	GLU
1	E	333	LEU
1	E	361	ARG
1	E	381	ASN
1	E	382	LEU
1	E	386	LEU
1	E	431	ASN
1	E	446	MET
1	E	468	SER
2	F	27	ARG
2	F	31	LEU
2	F	39	THR
2	F	42	ILE
2	F	75	LEU
2	F	90	LEU
2	F	107	ASN
2	F	117	GLU
2	F	149	ARG
2	F	176	LEU
2	F	181	LEU
2	F	219	GLU
2	F	236	GLU
2	F	250	VAL

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Mol	Chain	Res	Type
2	F	256	ARG
2	F	262	THR
2	F	275	VAL
2	F	375	ARG
2	F	403	VAL
2	F	405	THR
2	F	408	ARG
2	F	423	LYS
2	F	424	ASP
2	F	439	VAL
2	F	441	MET
1	G	17	ASP
1	G	56	ASN
1	G	65	ASP
1	G	66	ARG
1	G	67	LEU
1	G	151	GLU
1	G	176	ARG
1	G	210	GLU
1	G	220	LEU
1	G	230	ILE
1	G	241	GLU
1	G	268	ILE
1	G	273	ILE
1	G	303	TYR
1	G	305	HIS
1	G	307	LEU
1	G	311	TYR
1	G	314	GLU
1	G	333	LEU
1	G	361	ARG
1	G	381	ASN
1	G	382	LEU
1	G	386	LEU
1	G	431	ASN
1	G	446	MET
2	H	22	GLN
2	H	27	ARG
2	H	31	LEU
2	H	39	THR
2	H	42	ILE
2	H	75	LEU

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Mol	Chain	Res	Type
2	H	90	LEU
2	H	107	ASN
2	H	117	GLU
2	H	149	ARG
2	H	176	LEU
2	H	181	LEU
2	H	219	GLU
2	H	236	GLU
2	H	250	VAL
2	H	262	THR
2	H	275	VAL
2	H	346	GLU
2	H	375	ARG
2	H	403	VAL
2	H	405	THR
2	H	408	ARG
2	H	423	LYS
2	H	424	ASP
2	H	439	VAL
2	H	441	MET
3	O	10	PHE
3	O	15	THR
3	P	15	THR
3	Q	10	PHE
3	Q	15	THR
3	Q	18	LEU
3	R	15	THR
3	R	18	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	ASN
1	A	99	ASN
1	A	320	ASN
1	A	349	GLN
1	A	350	GLN
1	A	381	ASN
1	A	406	ASN
1	A	431	ASN
2	B	44	ASN
2	B	66	ASN

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Mol	Chain	Res	Type
2	B	85	GLN
2	B	137	ASN
2	B	165	HIS
2	B	223	GLN
2	B	354	ASN
2	B	374	ASN
1	C	38	HIS
1	C	56	ASN
1	C	135	GLN
1	C	320	ASN
1	C	349	GLN
1	C	350	GLN
1	C	381	ASN
1	C	406	ASN
1	C	431	ASN
2	D	44	ASN
2	D	66	ASN
2	D	85	GLN
2	D	165	HIS
2	D	223	GLN
2	D	261	ASN
2	D	304	ASN
2	D	316	ASN
2	D	354	ASN
2	D	374	ASN
1	E	56	ASN
1	E	236	GLN
1	E	315	ASN
1	E	320	ASN
1	E	349	GLN
1	E	350	GLN
1	E	381	ASN
1	E	406	ASN
1	E	447	GLN
1	E	467	ASN
2	F	44	ASN
2	F	66	ASN
2	F	85	GLN
2	F	137	ASN
2	F	165	HIS
2	F	218	HIS
2	F	223	GLN

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Mol	Chain	Res	Type
2	F	374	ASN
2	F	462	GLN
1	G	56	ASN
1	G	315	ASN
1	G	320	ASN
1	G	349	GLN
1	G	350	GLN
1	G	381	ASN
1	G	406	ASN
2	H	66	ASN
2	H	85	GLN
2	H	137	ASN
2	H	165	HIS
2	H	218	HIS
2	H	223	GLN
2	H	316	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 oligosaccharides 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	-	15,15,15	1.64	3 (20%)	19,20,20	0.89	1 (5%)
4	EPE	G	489	-	15,15,15	1.25	2 (13%)	19,20,20	0.94	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	-	-	2/9/19/19	0/1/1/1
4	EPE	G	489	-	-	2/9/19/19	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	489	EPE	C10-S	3.97	1.83	1.77
4	A	489	EPE	C6-N1	2.55	1.53	1.46
4	A	489	EPE	C2-N1	2.09	1.52	1.46
4	G	489	EPE	C10-S	2.05	1.80	1.77
4	G	489	EPE	C6-N1	2.03	1.52	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	489	EPE	C7-N4-C5	-2.07	105.73	111.24
4	G	489	EPE	C7-N4-C5	-2.02	105.85	111.24

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	489	EPE	C10-C9-N1-C2
4	G	489	EPE	C10-C9-N1-C2
4	G	489	EPE	C10-C9-N1-C6
4	A	489	EPE	C10-C9-N1-C6

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	452/475 (95%)	0.02	19 (4%) 40 37	22, 43, 88, 101	0
1	C	448/475 (94%)	-0.04	16 (3%) 46 42	25, 43, 80, 101	0
1	E	445/475 (93%)	0.15	17 (3%) 44 40	27, 51, 88, 101	0
1	G	448/475 (94%)	0.10	21 (4%) 36 33	29, 49, 86, 101	0
2	B	439/443 (99%)	0.01	8 (1%) 67 65	22, 43, 76, 101	0
2	D	443/443 (100%)	0.21	16 (3%) 46 42	27, 52, 84, 101	0
2	F	443/443 (100%)	0.58	17 (3%) 44 40	33, 68, 98, 101	0
2	H	441/443 (99%)	1.10	70 (15%) 5 4	43, 91, 101, 101	0
3	O	13/24 (54%)	3.44	10 (76%) 0 0	52, 95, 101, 101	0
3	P	9/24 (37%)	2.98	6 (66%) 0 0	61, 77, 99, 101	0
3	Q	10/24 (41%)	2.95	7 (70%) 0 0	64, 101, 101, 101	0
3	R	7/24 (29%)	2.49	5 (71%) 0 0	89, 96, 101, 101	0
All	All	3598/3768 (95%)	0.30	212 (5%) 28 25	22, 53, 100, 101	0

All (212) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	O	11	PHE	6.5
3	P	11	PHE	6.2
1	A	14	ALA	5.9
3	O	8	ILE	5.7
3	Q	11	PHE	5.7
1	E	14	ALA	5.7
3	Q	10	PHE	5.5
1	G	311	TYR	5.2
3	O	13	PRO	5.0
1	E	250	PHE	5.0
1	E	311	TYR	4.9

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Mol	Chain	Res	Type	RSRZ
3	P	13	PRO	4.8
3	Q	13	PRO	4.7
3	O	12	LYS	4.7
2	B	24	PRO	4.7
1	A	287	GLY	4.7
1	G	250	PHE	4.6
1	A	250	PHE	4.6
1	G	287	GLY	4.5
1	G	230	ILE	4.4
1	C	468	SER	4.4
1	E	230	ILE	4.4
1	A	311	TYR	4.3
1	C	250	PHE	4.3
1	G	249	VAL	4.2
1	C	249	VAL	4.2
1	C	312	PHE	4.1
2	D	197	ASP	4.1
3	O	10	PHE	4.0
1	C	311	TYR	3.9
1	E	249	VAL	3.8
1	E	287	GLY	3.8
2	F	424	ASP	3.8
1	G	14	ALA	3.8
1	E	253	LEU	3.7
2	H	171	TYR	3.7
1	A	312	PHE	3.7
2	H	198	TYR	3.7
1	A	249	VAL	3.7
3	O	17	THR	3.6
3	P	10	PHE	3.6
3	O	18	LEU	3.6
2	H	451	PRO	3.5
1	E	468	SER	3.5
2	B	245	ARG	3.5
2	H	444	LEU	3.5
3	O	7	SER	3.5
3	R	13	PRO	3.4
2	B	452	ASN	3.3
1	G	231	THR	3.3
1	C	252	ASN	3.3
1	A	253	LEU	3.2
2	D	88	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
2	H	69	ALA	3.2
2	D	261	ASN	3.2
3	P	12	LYS	3.1
3	R	12	LYS	3.1
2	D	129	ILE	3.1
2	F	245	ARG	3.1
3	P	18	LEU	3.0
2	H	254	GLY	3.0
2	H	71	PHE	3.0
2	H	180	ILE	2.9
2	H	233	PRO	2.9
1	G	297	GLY	2.9
3	Q	12	LYS	2.9
1	G	399	HIS	2.9
1	A	470	SER	2.9
1	C	287	GLY	2.9
1	G	16	THR	2.9
3	R	18	LEU	2.9
2	D	245	ARG	2.8
2	H	176	LEU	2.8
2	D	236	GLU	2.8
1	C	296	LYS	2.8
2	F	198	TYR	2.8
2	H	443	ALA	2.8
1	C	230	ILE	2.8
2	H	299	ILE	2.8
2	H	72	LEU	2.8
1	E	399	HIS	2.8
2	H	30	LYS	2.7
2	H	270	ILE	2.7
2	H	331	ALA	2.7
1	A	15	ARG	2.7
2	H	247	PRO	2.7
2	H	258	ILE	2.7
2	H	195	LEU	2.7
1	E	231	THR	2.7
2	D	64	LYS	2.7
2	H	244	PRO	2.7
1	C	268	ILE	2.7
2	H	133	SER	2.7
2	H	316	ASN	2.7
1	A	296	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
2	D	20	ALA	2.6
2	B	44	ASN	2.6
2	H	161	VAL	2.6
2	B	27	ARG	2.6
2	H	199	ILE	2.6
1	A	293	GLY	2.6
2	F	20	ALA	2.6
3	R	14	ALA	2.6
1	E	268	ILE	2.5
2	H	335	LEU	2.5
2	D	201	LYS	2.5
1	A	303	TYR	2.5
1	G	299	TYR	2.5
1	C	293	GLY	2.5
1	E	254	PRO	2.5
2	H	203	TYR	2.5
1	C	295	GLY	2.5
3	O	19	CYS	2.5
2	H	37	ILE	2.5
2	H	245	ARG	2.5
2	H	239	VAL	2.5
2	F	229	PHE	2.5
3	R	15	THR	2.5
2	H	259	LYS	2.5
2	H	129	ILE	2.5
2	H	64	LYS	2.4
2	H	165	HIS	2.4
2	H	455	TYR	2.4
1	A	468	SER	2.4
1	A	469	SER	2.4
1	C	269	ASP	2.4
1	G	298	MET	2.4
1	C	294	PRO	2.4
1	G	254	PRO	2.4
1	G	439	LYS	2.4
2	F	247	PRO	2.4
2	H	86	GLN	2.4
1	E	15	ARG	2.4
1	E	141	TYR	2.4
1	G	441	ARG	2.4
2	H	110	TYR	2.4
2	F	304	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
2	H	175	PRO	2.4
2	H	183	PRO	2.4
2	H	445	GLY	2.4
2	F	81	GLN	2.4
2	H	241	LEU	2.3
2	H	348	ASN	2.3
1	A	358	LYS	2.3
2	H	104	SER	2.3
2	H	319	LEU	2.3
2	F	201	LYS	2.3
2	B	133	SER	2.3
2	H	350	ARG	2.3
3	O	9	ARG	2.3
1	E	16	THR	2.3
2	H	339	TYR	2.3
1	E	252	ASN	2.3
1	A	401	ARG	2.3
2	H	209	VAL	2.3
3	Q	19	CYS	2.3
2	F	190	ILE	2.3
1	A	399	HIS	2.3
1	G	358	LYS	2.3
1	A	252	ASN	2.3
1	G	252	ASN	2.3
2	H	240	PRO	2.3
2	F	181	LEU	2.3
2	H	63	VAL	2.3
3	Q	18	LEU	2.3
2	B	64	LYS	2.2
2	F	156	LYS	2.2
1	G	470	SER	2.2
2	H	231	HIS	2.2
2	B	247	PRO	2.2
2	D	81	GLN	2.2
2	H	58	SER	2.2
2	H	181	LEU	2.2
2	H	208	MET	2.2
2	H	447	THR	2.2
3	P	15	THR	2.2
2	H	185	LYS	2.2
1	G	403	ILE	2.2
2	H	39	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	303	TYR	2.2
2	D	198	TYR	2.2
2	D	452	ASN	2.2
2	D	21	SER	2.2
2	F	203	TYR	2.1
2	H	271	ALA	2.1
2	H	68	THR	2.1
2	F	244	PRO	2.1
2	F	82	ASN	2.1
2	H	456	ILE	2.1
2	D	56	ALA	2.1
2	H	142	ARG	2.1
1	A	148	MET	2.1
1	G	251	GLY	2.1
2	H	187	ILE	2.1
2	F	389	ASP	2.1
2	H	77	PHE	2.1
2	D	253	ARG	2.1
3	Q	17	THR	2.1
2	H	166	LEU	2.1
1	G	433	ASN	2.1
2	H	390	GLY	2.1
2	D	23	ILE	2.1
2	H	163	PHE	2.1
2	H	257	PHE	2.1
1	E	336	ILE	2.0
2	F	187	ILE	2.0
2	H	302	GLY	2.0
2	H	179	THR	2.0
2	H	342	THR	2.0
1	C	399	HIS	2.0
2	H	230	GLY	2.0
2	H	54	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors(Å ²)	Q<0.9
4	EPE	G	489	15/15	0.86	0.22	87,87,87,87	0
4	EPE	A	489	15/15	0.88	0.17	81,81,81,81	0
5	ZN	F	503	1/1	0.95	0.07	101,101,101,101	0
5	ZN	D	502	1/1	0.98	0.05	91,91,91,91	0
5	ZN	B	501	1/1	0.99	0.06	72,72,72,72	0
5	ZN	H	504	1/1	0.99	0.11	101,101,101,101	0

6.5 Other polymers [i](#)

There are no such residues in this entry.