



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:22 AM UTC

PDB ID : 1HR6 / pdb_00001hr6
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

<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

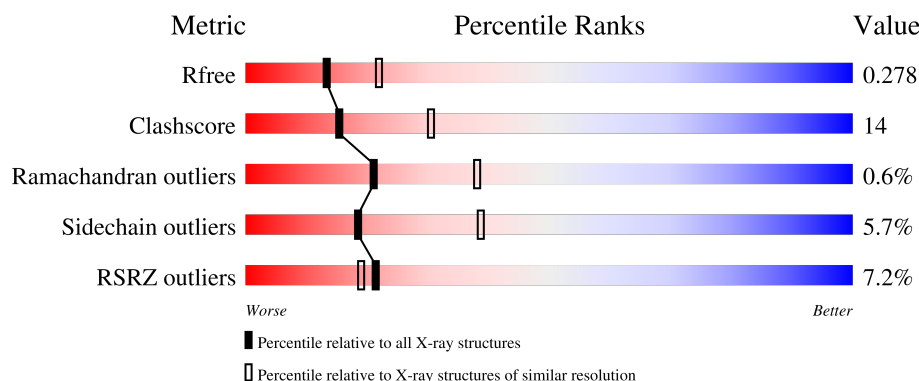
1 Overall quality at a glance

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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 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% 69% 23% . .
1	C	475	 3% 69% 21% 5% .
1	E	475	 6% 71% 21% . .
1	G	475	 5% 67% 26% . .
2	B	443	 3% 70% 25% . .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	D	443	4% 69% 26% 5%
2	F	443	7% 68% 28% 5%
2	H	443	26% 65% 29% 5%

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

Continued on next page...

Continued from previous page...

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

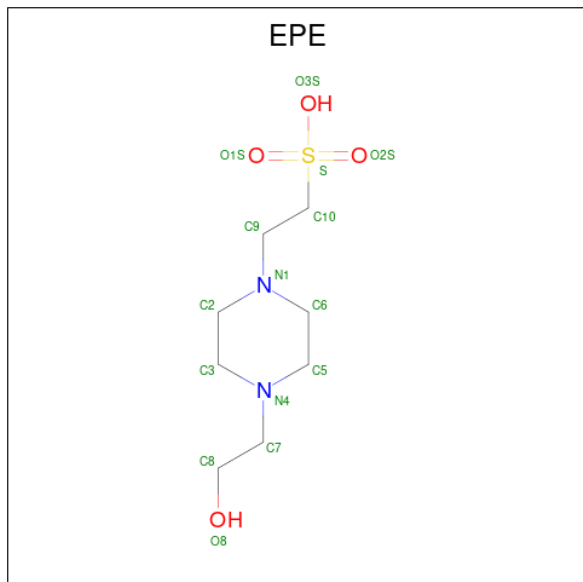
- Molecule 2 is a protein called MITOCHONDRIAL PROCESSING PEPTIDASE BETA SUB-UNIT.

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



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

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

Continued on next page...

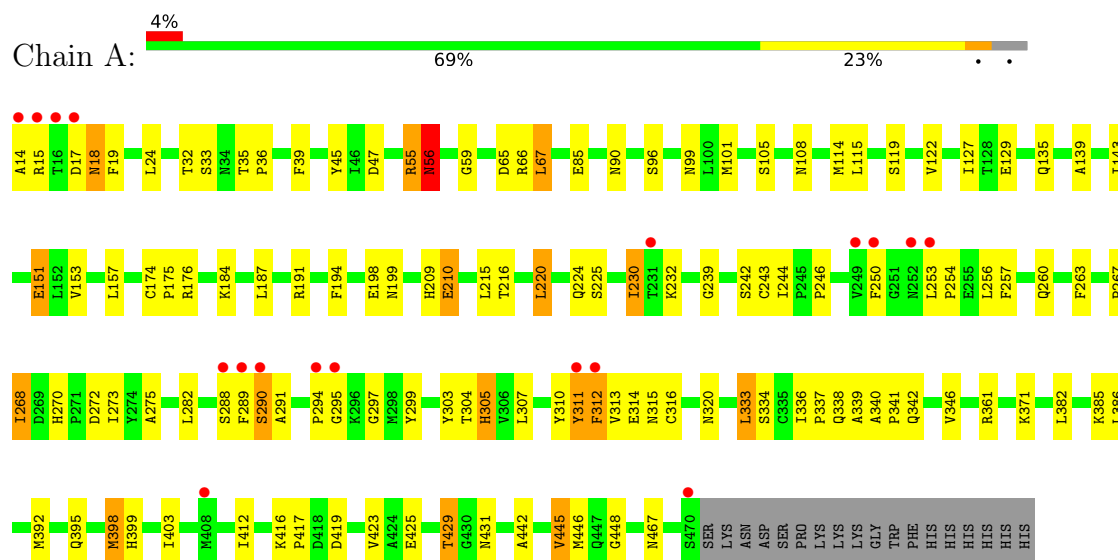
Continued from previous page...

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

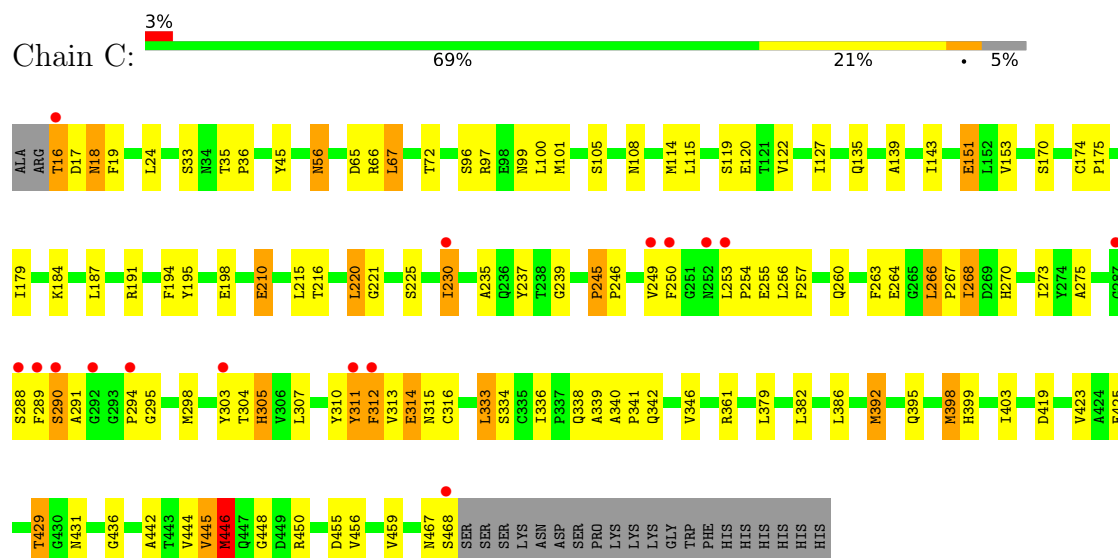
3 Residue-property plots

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

• Molecule 1: MITOCHONDRIAL PROCESSING PEPTIDASE ALPHA SUBUNIT

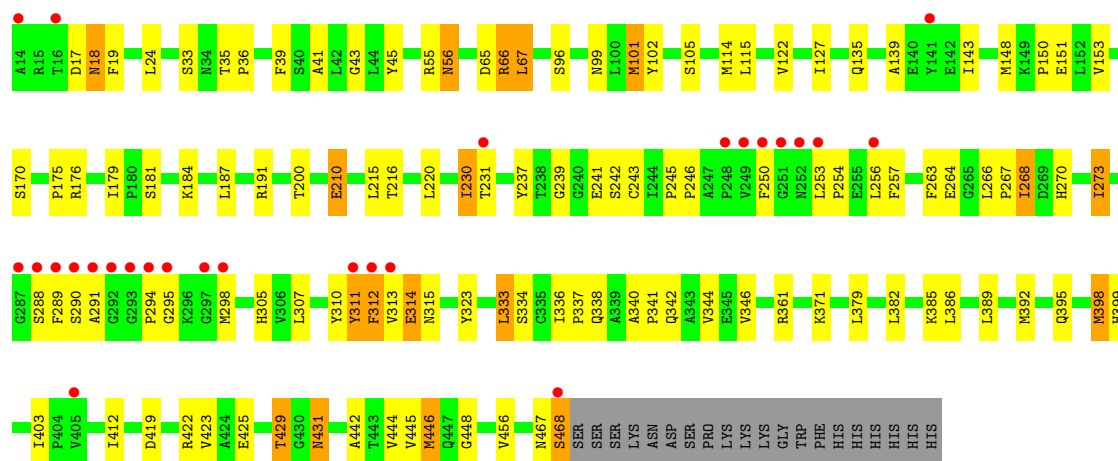


• Molecule 1: MITOCHONDRIAL PROCESSING PEPTIDASE ALPHA SUBUNIT

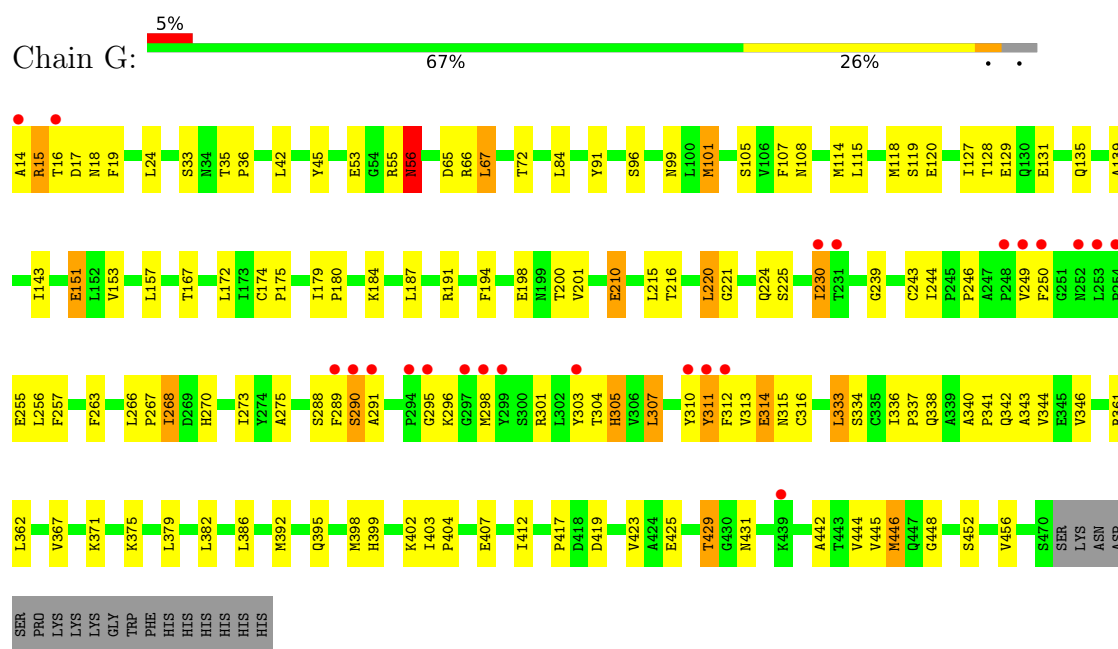


• Molecule 1: MITOCHONDRIAL PROCESSING PEPTIDASE ALPHA SUBUNIT

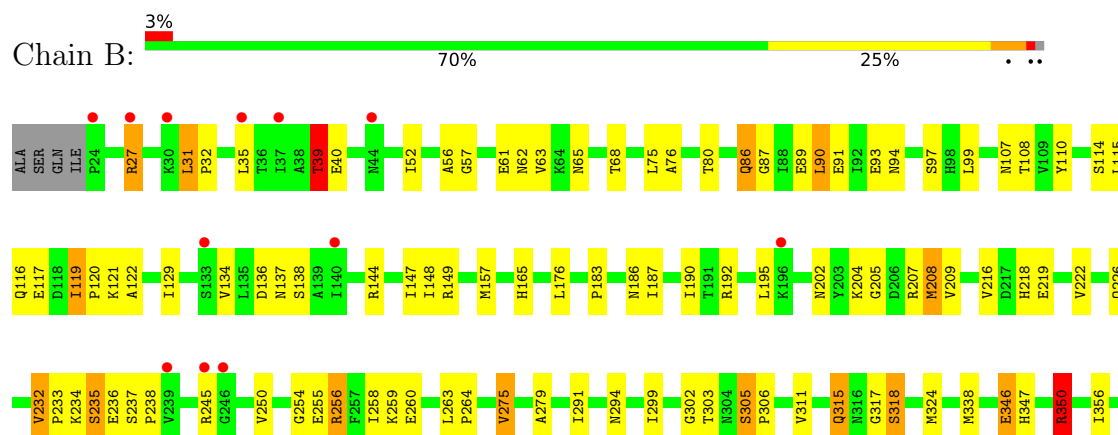




• Molecule 1: MITOCHONDRIAL PROCESSING PEPTIDASE ALPHA SUBUNIT

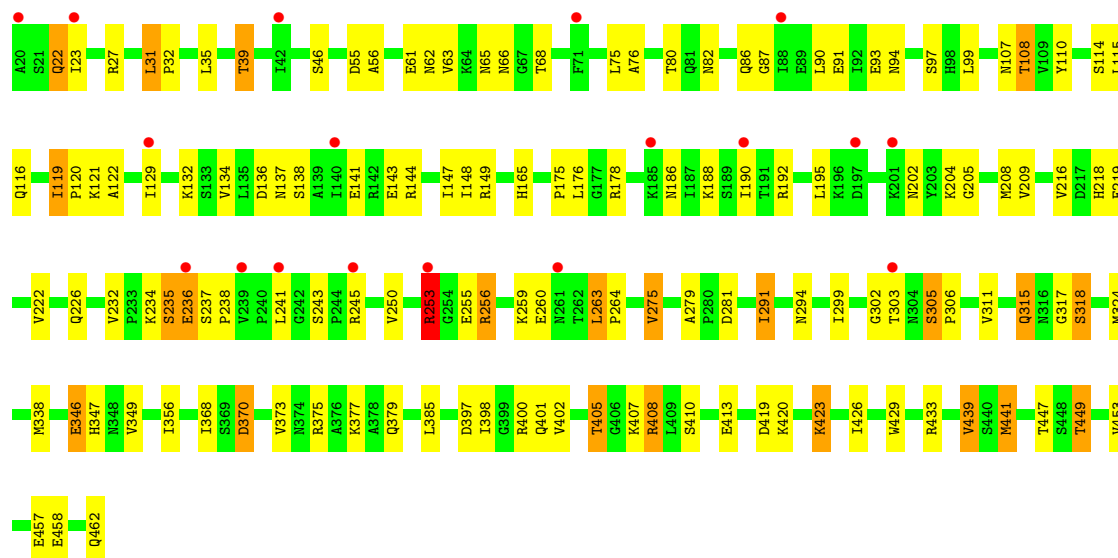


• Molecule 2: MITOCHONDRIAL PROCESSING PEPTIDASE BETA SUBUNIT

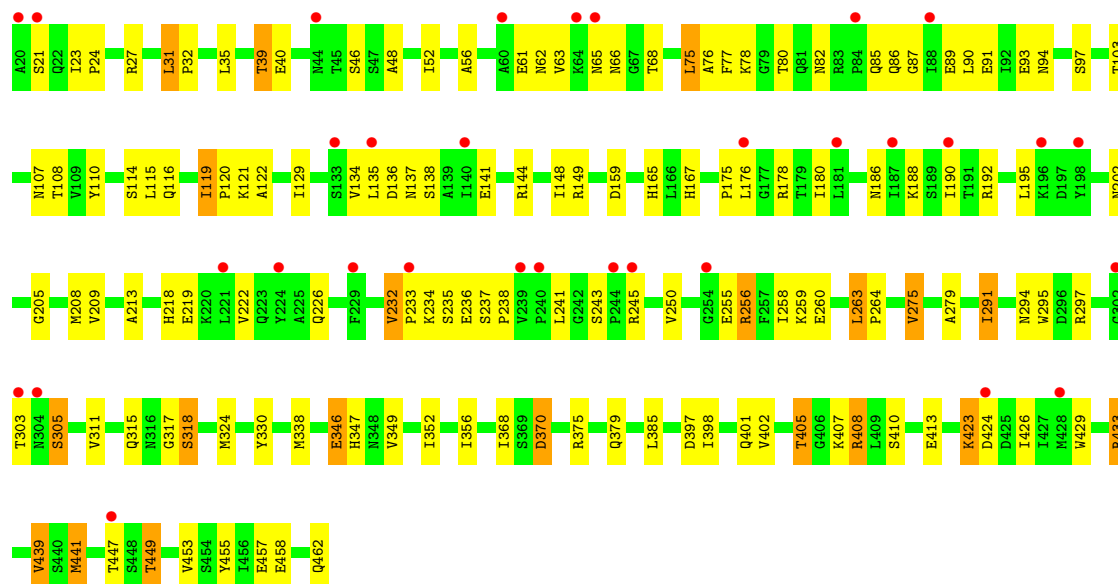




• Molecule 2: MITOCHONDRIAL PROCESSING PEPTIDASE BETA SUBUNIT

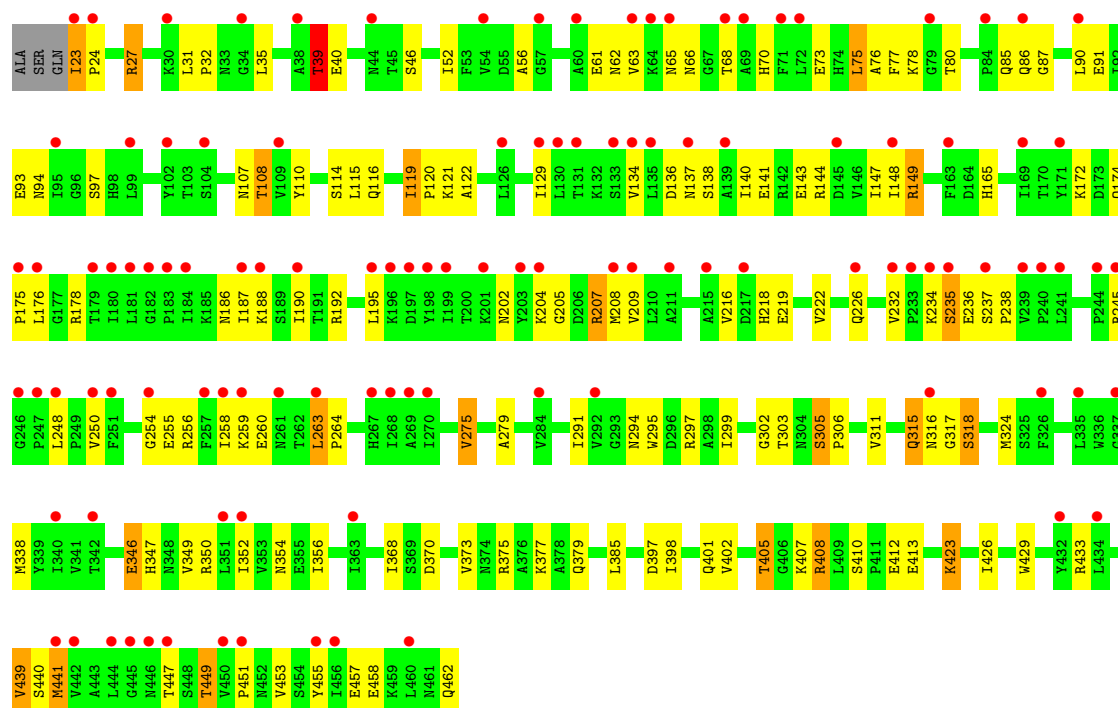


• Molecule 2: MITOCHONDRIAL PROCESSING PEPTIDASE BETA SUBUNIT



• Molecule 2: MITOCHONDRIAL PROCESSING PEPTIDASE BETA SUBUNIT





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, 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) 99.3 (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	Depositor
R, R_{free}	0.245 , 0.279 0.244 , 0.278	Depositor DCC
R_{free} test set	2029 reflections (1.22%)	wwPDB-VP
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 , 40.4	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	0.94	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, 0.333 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: 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	0.85	5/3604 (0.1%)	1.07	14/4877 (0.3%)
1	C	0.78	2/3576 (0.1%)	1.08	18/4840 (0.4%)
1	E	0.76	4/3592 (0.1%)	1.09	18/4861 (0.4%)
1	G	0.73	0/3604	1.06	15/4877 (0.3%)
2	B	0.76	3/3478 (0.1%)	1.12	21/4720 (0.4%)
2	D	0.70	0/3506	1.14	32/4759 (0.7%)
2	F	0.64	1/3506 (0.0%)	1.08	23/4759 (0.5%)
2	H	0.66	3/3486 (0.1%)	1.11	28/4732 (0.6%)
All	All	0.74	18/28352 (0.1%)	1.09	169/38425 (0.4%)

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	114	MET	SD-CE	-8.97	1.57	1.79
1	A	90	ASN	CG-ND2	-8.29	1.15	1.33
1	A	467	ASN	CG-ND2	-8.03	1.16	1.33
1	A	467	ASN	CG-OD1	-7.96	1.08	1.23
1	E	315	ASN	CG-ND2	-7.96	1.16	1.33
1	E	315	ASN	CG-OD1	-7.93	1.08	1.23
1	A	90	ASN	CG-OD1	-7.58	1.09	1.23
2	H	354	ASN	CG-ND2	-7.41	1.17	1.33
2	H	354	ASN	CG-OD1	-7.04	1.10	1.23
1	E	114	MET	SD-CE	-6.86	1.62	1.79
2	F	119	ILE	CA-CB	6.14	1.57	1.54
2	B	52	ILE	CA-CB	5.67	1.60	1.54
1	C	114	MET	SD-CE	-5.57	1.65	1.79
2	B	157	MET	SD-CE	5.56	1.93	1.79
2	H	119	ILE	CA-CB	5.55	1.56	1.54
1	E	298	MET	SD-CE	5.51	1.93	1.79
2	B	441	MET	SD-CE	5.29	1.92	1.79
1	C	392	MET	SD-CE	-5.01	1.67	1.79

All (169) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	253	ARG	NE-CZ-NH2	10.28	128.45	119.20
1	A	18	ASN	N-CA-C	-9.71	100.73	112.58
2	D	253	ARG	NE-CZ-NH1	-9.68	111.82	121.50
1	E	422	ARG	NE-CZ-NH2	9.36	127.63	119.20
1	E	422	ARG	NE-CZ-NH1	-9.30	112.20	121.50
2	H	207	ARG	NE-CZ-NH2	9.27	127.55	119.20
2	H	207	ARG	NE-CZ-NH1	-9.04	112.46	121.50
2	D	23	ILE	N-CA-C	-8.51	100.61	108.95
1	C	312	PHE	N-CA-C	-8.38	103.21	113.19
2	H	149	ARG	NE-CZ-NH2	-8.26	111.77	119.20
2	H	232	VAL	CA-C-N	8.22	128.22	119.76
2	H	232	VAL	C-N-CA	8.22	128.22	119.76
2	B	305	SER	CA-C-N	8.15	127.91	119.76
2	B	305	SER	C-N-CA	8.15	127.91	119.76
2	F	305	SER	CA-C-N	8.04	127.97	119.85
2	F	305	SER	C-N-CA	8.04	127.97	119.85
1	E	312	PHE	N-CA-C	-7.98	103.70	113.19
1	A	312	PHE	N-CA-C	-7.88	103.82	113.19
2	D	253	ARG	CD-NE-CZ	7.86	135.41	124.40
2	D	305	SER	CA-C-N	7.71	127.64	119.85
2	D	305	SER	C-N-CA	7.71	127.64	119.85
2	H	235	SER	N-CA-C	-7.51	100.84	110.53
2	D	235	SER	N-CA-C	-7.48	100.88	110.53
2	H	305	SER	CA-C-N	7.37	127.29	119.85
2	H	305	SER	C-N-CA	7.37	127.29	119.85
2	H	149	ARG	CD-NE-CZ	7.35	134.69	124.40
2	F	232	VAL	CA-C-N	7.22	127.26	119.89
2	F	232	VAL	C-N-CA	7.22	127.26	119.89
2	D	23	ILE	CA-C-N	7.16	127.20	119.90
2	D	23	ILE	C-N-CA	7.16	127.20	119.90
1	E	266	LEU	CA-C-N	6.89	126.81	119.85
1	E	266	LEU	C-N-CA	6.89	126.81	119.85
2	F	235	SER	N-CA-C	-6.87	101.66	110.53
2	H	149	ARG	NE-CZ-NH1	6.85	128.35	121.50
2	B	235	SER	N-CA-C	-6.78	102.07	110.41
1	G	55	ARG	N-CA-C	-6.72	105.62	113.88
1	E	422	ARG	CD-NE-CZ	6.69	133.76	124.40
2	B	119	ILE	CB-CA-C	-6.68	107.36	113.70
2	D	347	HIS	N-CA-C	6.55	120.14	109.59
2	D	346	GLU	N-CA-C	6.54	121.33	113.23
2	D	423	LYS	N-CA-C	-6.51	104.18	111.28
2	F	232	VAL	N-CA-C	6.51	114.23	108.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	153	VAL	N-CA-C	6.45	116.59	110.53
2	D	119	ILE	CB-CA-C	-6.43	107.59	113.70
2	D	232	VAL	N-CA-C	6.35	114.09	108.63
1	A	55	ARG	N-CA-C	-6.33	106.10	113.88
1	A	105	SER	N-CA-C	-6.32	99.10	109.40
2	D	385	LEU	N-CA-C	6.31	121.50	113.55
2	H	315	GLN	N-CA-C	6.29	118.83	110.53
2	F	346	GLU	N-CA-C	6.27	121.12	112.90
2	B	107	ASN	N-CA-C	6.27	118.48	109.14
2	D	108	THR	N-CA-C	-6.26	98.70	108.90
2	B	232	VAL	CA-C-N	6.26	126.27	119.89
2	B	232	VAL	C-N-CA	6.26	126.27	119.89
2	H	347	HIS	N-CA-C	6.24	119.63	109.59
2	F	119	ILE	CB-CA-C	-6.22	107.79	113.70
1	G	105	SER	N-CA-C	-6.22	99.26	109.40
2	H	202	ASN	N-CA-C	6.21	121.04	112.90
2	F	202	ASN	N-CA-C	6.21	121.04	112.90
2	F	347	HIS	N-CA-C	6.21	119.95	109.76
2	D	234	LYS	N-CA-C	-6.21	101.33	110.52
2	F	108	THR	N-CA-C	-6.19	98.30	108.76
2	B	350	ARG	NE-CZ-NH2	6.18	124.76	119.20
1	G	257	PHE	N-CA-C	-6.11	100.67	110.14
2	H	207	ARG	CD-NE-CZ	6.09	132.93	124.40
2	H	302	GLY	N-CA-C	-5.99	105.85	115.08
1	E	257	PHE	N-CA-C	-5.98	100.87	110.14
2	H	119	ILE	CB-CA-C	-5.97	108.03	113.70
1	C	245	PRO	CA-C-N	5.96	125.92	119.78
1	C	245	PRO	C-N-CA	5.96	125.92	119.78
2	H	263	LEU	CA-C-N	5.95	125.49	119.19
2	H	263	LEU	C-N-CA	5.95	125.49	119.19
2	H	108	THR	N-CA-C	-5.91	98.77	108.76
2	B	202	ASN	N-CA-C	5.90	120.61	113.41
1	C	257	PHE	N-CA-C	-5.89	101.01	110.14
1	G	153	VAL	N-CA-C	5.88	116.05	110.53
1	A	398	MET	N-CA-C	5.87	118.56	111.40
1	G	194	PHE	N-CA-C	5.83	121.43	113.97
1	E	398	MET	N-CA-C	5.83	118.51	111.40
2	F	263	LEU	CA-C-N	5.83	125.36	119.19
2	F	263	LEU	C-N-CA	5.83	125.36	119.19
2	B	108	THR	N-CA-C	-5.78	99.48	108.90
2	D	232	VAL	CA-C-N	5.77	125.79	119.90
2	D	232	VAL	C-N-CA	5.77	125.79	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	202	ASN	N-CA-C	5.75	120.43	113.41
2	F	234	LYS	N-CA-C	-5.74	101.52	110.42
2	B	346	GLU	N-CA-C	5.74	120.56	113.50
2	B	347	HIS	N-CA-C	5.74	118.83	109.59
2	D	299	ILE	N-CA-C	5.74	119.13	111.44
1	E	239	GLY	N-CA-C	-5.72	103.45	112.61
2	H	346	GLU	N-CA-C	5.70	120.51	113.50
1	C	108	ASN	N-CA-C	5.69	118.22	111.33
1	A	153	VAL	N-CA-C	5.65	115.84	110.53
1	G	56	ASN	N-CA-C	5.64	118.37	111.82
2	D	39	THR	N-CA-C	5.63	117.95	109.23
1	A	56	ASN	N-CA-C	5.63	118.35	111.82
2	B	299	ILE	N-CA-C	5.62	118.97	111.44
2	H	63	VAL	N-CA-C	5.62	117.02	110.62
2	F	63	VAL	N-CA-C	5.60	117.00	110.62
1	G	108	ASN	N-CA-C	5.59	118.09	111.33
1	G	221	GLY	N-CA-C	5.59	119.65	112.83
1	C	398	MET	N-CA-C	5.58	118.21	111.40
1	C	153	VAL	N-CA-C	5.55	115.75	110.53
2	D	241	LEU	N-CA-C	5.55	118.86	111.75
1	C	266	LEU	CA-C-N	5.54	125.44	119.85
1	C	266	LEU	C-N-CA	5.54	125.44	119.85
1	C	194	PHE	N-CA-C	5.53	121.05	113.97
1	C	239	GLY	N-CA-C	-5.52	103.78	112.61
1	A	194	PHE	N-CA-C	5.52	121.03	113.97
1	C	446	MET	N-CA-C	5.52	117.46	109.07
2	H	39	THR	N-CA-C	5.51	117.77	109.23
2	B	39	THR	N-CA-C	5.50	117.63	108.99
1	C	179	ILE	CB-CA-C	-5.46	108.56	114.35
1	G	239	GLY	N-CA-C	-5.46	103.87	112.61
1	C	105	SER	N-CA-C	-5.46	100.50	109.40
1	C	221	GLY	N-CA-C	5.45	119.48	112.83
2	D	263	LEU	CA-C-N	5.44	124.96	119.19
2	D	263	LEU	C-N-CA	5.44	124.96	119.19
1	E	170	SER	N-CA-C	-5.43	101.51	109.50
2	F	107	ASN	N-CA-C	5.43	117.23	109.14
2	H	385	LEU	N-CA-C	5.42	120.39	113.55
2	B	433	ARG	N-CA-C	5.42	119.06	112.23
1	E	56	ASN	N-CA-C	5.41	118.10	111.82
2	H	299	ILE	N-CA-C	5.40	118.68	111.44
2	F	243	SER	CA-C-N	5.40	126.59	119.84
2	F	243	SER	C-N-CA	5.40	126.59	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	207	ARG	CB-CG-CD	-5.40	98.89	111.30
1	C	18	ASN	N-CA-C	-5.39	99.32	110.80
2	F	241	LEU	N-CA-C	5.38	118.63	111.75
1	G	172	LEU	N-CA-C	-5.38	106.56	113.23
2	D	107	ASN	N-CA-C	5.37	117.14	109.14
1	A	15	ARG	N-CA-C	5.36	119.33	111.34
2	D	370	ASP	N-CA-C	-5.36	105.44	111.28
2	H	423	LYS	N-CA-C	-5.36	104.85	111.33
1	E	179	ILE	CB-CA-C	-5.35	108.68	114.35
2	F	39	THR	N-CA-C	5.34	117.51	109.23
2	F	370	ASP	N-CA-C	-5.33	105.47	111.28
1	A	239	GLY	N-CA-C	-5.31	104.12	112.61
2	D	315	GLN	N-CA-C	5.30	117.37	110.53
1	A	232	LYS	N-CA-C	5.30	117.60	107.75
2	H	216	VAL	N-CA-C	5.25	115.67	108.12
1	C	170	SER	N-CA-C	-5.25	101.79	109.50
2	D	216	VAL	N-CA-C	5.24	115.67	108.12
2	B	216	VAL	N-CA-C	5.24	115.66	108.12
1	E	55	ARG	N-CA-C	-5.22	107.04	113.41
2	B	370	ASP	N-CA-C	-5.21	105.60	111.28
1	G	266	LEU	CA-C-N	5.21	125.11	119.85
1	G	266	LEU	C-N-CA	5.21	125.11	119.85
2	F	433	ARG	N-CA-C	5.20	118.78	112.23
1	E	105	SER	N-CA-C	-5.18	100.96	109.40
2	B	208	MET	N-CA-C	5.17	117.05	109.24
1	C	56	ASN	N-CA-C	5.17	117.82	111.82
2	D	243	SER	N-CA-C	5.17	117.21	110.08
2	B	315	GLN	N-CA-C	5.16	117.52	110.55
2	B	302	GLY	N-CA-C	-5.14	107.17	115.08
1	A	85	GLU	N-CA-C	-5.13	105.59	111.14
1	G	101	MET	N-CA-C	5.13	117.18	109.23
1	G	16	THR	N-CA-C	-5.11	107.22	113.50
2	F	385	LEU	N-CA-C	5.10	119.98	113.55
1	E	200	THR	N-CA-C	5.10	117.55	109.50
2	H	107	ASN	N-CA-C	5.08	116.71	109.14
1	A	108	ASN	N-CA-C	5.08	117.48	111.33
1	E	18	ASN	N-CA-C	-5.08	99.98	110.80
1	G	53	GLU	N-CA-C	5.06	119.09	113.01
1	E	101	MET	N-CA-C	5.06	117.07	109.23
2	D	63	VAL	N-CA-C	5.06	116.38	110.62
2	D	302	GLY	N-CA-C	-5.04	107.32	115.08
2	B	63	VAL	N-CA-C	5.04	116.36	110.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	257	PHE	N-CA-C	-5.00	102.67	110.42

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	94	0
1	C	3503	0	3460	89	0
1	E	3519	0	3478	75	0
1	G	3531	0	3488	107	0
2	B	3414	0	3412	101	0
2	D	3442	0	3440	95	0
2	F	3442	0	3440	96	0
2	H	3422	0	3422	118	0
3	A	15	0	17	0	0
3	G	15	0	17	0	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
4	F	1	0	0	0	0
4	H	1	0	0	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	749	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 14.

All (749) 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:33:SER:HB3	1:G:392:MET:HE1	1.14	1.11
2:H:294:ASN:HD22	2:H:324:MET:HA	1.11	1.11
1:A:33:SER:HB3	1:A:392:MET:HE1	1.14	1.10
1:C:33:SER:HB3	1:C:392:MET:HE1	1.14	1.08
2:B:294:ASN:HD22	2:B:324:MET:HA	1.14	1.07
1:E:33:SER:HB3	1:E:392:MET:HE1	1.08	1.07
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: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:E:33:SER:CB	1:E:392:MET:HE1	1.99	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
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:HG3	2:D:256:ARG:HH11	1.34	0.89
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
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:C:295:GLY:HA2	2:D:93:GLU:HG2	1.60	0.82
1:A:429:THR:CG2	1:A:431:ASN:HD22	1.93	0.81
1:G:230:ILE:H	1:G:230:ILE:HD12	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:A:33:SER:CB	1:A:392:MET:HE1	2.05	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
1:G:33:SER:CB	1:G:392:MET:HE1	2.06	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
1:A:99:ASN:HB2	1:A:101:MET:HE3	1.63	0.79
2:D:62:ASN:H	2:D:65:ASN:HB3	1.48	0.79
1:C:33:SER:HB3	1:C:392:MET:CE	2.07	0.79
1:E:99:ASN:HB2	1:E:101:MET:HE3	1.64	0.79
1:G:14:ALA:N	1:G:19:PHE:HB3	1.97	0.78
1:C:230:ILE:HD12	1:C:230:ILE:H	1.49	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	1:G:311:TYR:CD2	2.35	0.78
1:E:33:SER:HB3	1:E:392:MET:CE	2.03	0.77
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
1:C:19:PHE:CD1	1:C:392:MET:HE2	2.20	0.77
1:C:99:ASN:HB2	1:C:101:MET:HE3	1.67	0.77
2:H:23:ILE:N	2:H:23:ILE:HD13	2.00	0.76
1:C:230:ILE:HD12	1:C:230:ILE:N	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
1:G:99:ASN:HB2	1:G:101:MET:HE3	1.67	0.76
2:B:97:SER:OG	2:B:114:SER:HB3	1.86	0.76
1:A:230:ILE:HD12	1:A:230:ILE:H	1.51	0.76
1:G:19:PHE:CD1	1:G:392:MET:HE2	2.21	0.76
1:G:425:GLU:O	1:G:429:THR:HB	1.85	0.76
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
2:B:144:ARG:O	2:B:148:ILE:HG12	1.89	0.72
1:G:295:GLY:HA2	2:H:93:GLU:HG2	1.71	0.72
1:A:230:ILE:HD12	1:A:230:ILE:N	2.04	0.72
2:D:275:VAL:HG22	2:D:279:ALA:CB	2.20	0.71
1:A:175:PRO:HB3	1:E:175:PRO:HB3	1.71	0.71
1:G:246:PRO:HG3	1:G:448:GLY:HA2	1.73	0.71
1:A:19:PHE:CD1	1:A:392:MET:HE2	2.26	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:B:76:ALA:HB1	2:B:129:ILE:CG2	2.21	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:116:GLN:O	2:F:119:ILE:HG12	1.91	0.70
2:H:338:MET:HG2	2:H:356:ILE:HD13	1.73	0.70
1:C:315:ASN:HD22	1:C:315:ASN:C	2.00	0.70
1:E:230:ILE:HD12	1:E:230:ILE:N	2.05	0.70
2:B:294:ASN:ND2	2:B:324:MET:HG3	2.07	0.69
2:F:76:ALA:HB1	2:F:129:ILE:CG2	2.21	0.69
2:F:458:GLU:O	2:F:462:GLN:HB2	1.92	0.69
2:H:294:ASN:ND2	2:H:324:MET:HG3	2.07	0.69
1:G:33:SER:HB3	1:G:392:MET:CE	2.09	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:116:GLN:O	2:D:119:ILE:HG12	1.94	0.68
2:D:256:ARG:HG3	2:D:256:ARG:NH1	2.03	0.68
1:C:33:SER:CB	1:C:392:MET:HE1	2.09	0.67
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
1:G:15:ARG:HD3	1:G:15:ARG:C	2.20	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
2:H:441:MET:HE3	2:H:453:VAL:HG23	1.77	0.67
1:G:429:THR:HG21	1:G:431:ASN:HD22	1.60	0.67
2:H:236:GLU:C	2:H:238:PRO:HD3	2.21	0.66
2:B:186:ASN:O	2:B:190:ILE:HG12	1.94	0.66
1:A:315:ASN:HD22	1:A:315:ASN:C	2.00	0.66
2:H:116:GLN:O	2:H:119:ILE:HG12	1.95	0.66
2:D:441:MET:HE3	2:D:453:VAL:HG23	1.77	0.66
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
1:A:99:ASN:HD22	1:A:101:MET:HE3	1.61	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
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
1:G:315:ASN:HD22	1:G:315:ASN:C	2.04	0.65
1:A:224:GLN:CD	1:G:129:GLU:HG3	2.22	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HE	2:B:245:ARG:HA	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:E:139:ALA:O	1:E:143:ILE:HD13	1.98	0.63
2:F:186:ASN:O	2:F:190:ILE:HG12	1.99	0.63
1:G:315:ASN:HD22	1:G:316:CYS:H	1.44	0.63
2:H:256:ARG:HG3	2:H:256:ARG:NH1	2.14	0.63
2:H:405:THR:HG22	2:H:407:LYS:H	1.64	0.63
1:G:311:TYR:C	1:G:313:VAL:H	2.06	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:A:96:SER:HB3	1:A:99:ASN:OD1	2.00	0.62
1:E:187:LEU:O	1:E:191:ARG:HG3	1.99	0.62
1:G:311:TYR:C	1:G:313:VAL:N	2.55	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:F:441:MET:HE3	2:F:453:VAL:HG23	1.79	0.62
2:D:236:GLU:C	2:D:238:PRO:HD3	2.25	0.62
1:A:33:SER:HB3	1:A:392:MET:CE	2.09	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:G:340:ALA:HB3	1:G:341:PRO:HD3	1.82	0.61
2:F:35:LEU:HD13	2:F:208:MET:HG3	1.82	0.61
1:G:230:ILE:H	1:G:230:ILE:CD1	2.13	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:G:99:ASN:HD22	1:G:101:MET:HE3	1.65	0.61
1:E:311:TYR:C	1:E:313:VAL:H	2.09	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
1:G:187:LEU:O	1:G:191:ARG:HG3	2.01	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:401:GLN:O	2:H:405:THR:HB	2.00	0.61
1:A:268:ILE:HD13	1:A:268:ILE:H	1.66	0.60
1:C:268:ILE:HD13	1:C:268:ILE:H	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
1:E:311:TYR:C	1:E:313:VAL:N	2.58	0.60
1:G:19:PHE:HD1	1:G:392:MET:HE2	1.66	0.60
2:B:165:HIS:CD2	2:B:258:ILE:HD11	2.36	0.60
2:B:441:MET:HE3	2:B:453:VAL:HG23	1.82	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
1:C:19:PHE:HD1	1:C:392:MET:HE2	1.65	0.60
2:F:97:SER:OG	2:F:114:SER:HB3	2.02	0.60
1:A:242:SER:OG	1:E:176:ARG:NH2	2.35	0.60
2:F:90:LEU:HD13	2:F:94:ASN:ND2	2.17	0.60
2:D:186:ASN:O	2:D:190:ILE:HG12	2.00	0.60
1:E:340:ALA:HB3	1:E:341:PRO:HD3	1.83	0.60
1:C:268:ILE:HD13	1:C:268:ILE:N	2.16	0.59
2:D:245:ARG:HA	2:D:245:ARG:HE	1.66	0.59
2:D:275:VAL:HG22	2:D:279:ALA:HB3	1.82	0.59
2:H:31:LEU:HG	2:H:32:PRO:HD2	1.82	0.59
2:H:439:VAL:HG13	2:H:457:GLU:HG2	1.83	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
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
1:G:268:ILE:HD13	1:G:268:ILE:N	2.17	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
1:A:99:ASN:ND2	1:A:101:MET:HE3	2.17	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:303:THR:HG22	2:F:305:SER:H	1.66	0.59
2:F:368:ILE:O	2:F:423:LYS:HE3	2.03	0.59
1:A:268:ILE:HD13	1:A:268:ILE:N	2.17	0.59
1:A:311:TYR:C	1:A:313:VAL:H	2.08	0.59
2:B:40:GLU:OE1	2:B:408:ARG:NH2	2.35	0.59
1:C:429:THR:HG21	1:C:431:ASN:HD22	1.65	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:259:LYS:HG3	2:B:447:THR:HG22	1.84	0.58
1:C:230:ILE:H	1:C:230:ILE:CD1	2.14	0.58
1:C:342:GLN:O	1:C:346:VAL:HG23	2.03	0.58
1:C:139:ALA:O	1:C:143:ILE:HD13	2.03	0.58
1:G:127:ILE:HB	1:G:184:LYS:HE3	1.86	0.58
2:B:439:VAL:HG13	2:B:457:GLU:HG2	1.85	0.58
2:D:119:ILE:N	2:D:120:PRO:HD2	2.19	0.58
2:F:260:GLU:HG3	2:F:263:LEU:HG	1.84	0.58
1:G:268:ILE:HD13	1:G:268:ILE:H	1.68	0.58
1:C:99:ASN:HD22	1:C:101:MET:HE3	1.68	0.58
2:H:207:ARG:HH11	2:H:245:ARG:NH1	2.02	0.58
2:H:207:ARG:NH1	2:H:245:ARG:NH1	2.52	0.58
1:A:311:TYR:C	1:A:313:VAL:N	2.60	0.58
2:B:76:ALA:O	2:B:129:ILE:HG23	2.04	0.58
2:H:97:SER:OG	2:H:114:SER:HB3	2.03	0.58
2:H:119:ILE:N	2:H:120:PRO:HD2	2.19	0.58
1:A:340:ALA:HB3	1:A:341:PRO:HD3	1.85	0.58
2:D:119:ILE:O	2:D:122:ALA:HB3	2.04	0.58
2:H:311:VAL:O	2:H:315:GLN:HG3	2.03	0.57
1:C:311:TYR:C	1:C:313:VAL:H	2.11	0.57
1:G:315:ASN:ND2	1:G:316:CYS:N	2.43	0.57
1:E:230:ILE:H	1:E:230:ILE:CD1	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:A:230:ILE:H	1:A:230:ILE:CD1	2.16	0.57
2:D:209:VAL:HG21	2:D:402:VAL:HG12	1.86	0.57
2:D:259:LYS:HG3	2:D:447:THR:HG22	1.86	0.57
1:E:429:THR:HG21	1:E:431:ASN:HD22	1.70	0.57
2:H:31:LEU:HD21	2:H:226:GLN:HA	1.86	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
1:C:310:TYR:CD1	1:C:312:PHE:CZ	2.92	0.57
2:H:165:HIS:CD2	2:H:258:ILE:HD11	2.39	0.57
1:E:268:ILE:HD13	1:E:268:ILE:N	2.20	0.56
2:H:115:LEU:HD12	2:H:115:LEU:H	1.69	0.56
1:C:127:ILE:HB	1:C:184:LYS:HE3	1.87	0.56
2:H:303:THR:HG22	2:H:305:SER:H	1.69	0.56
1:E:99:ASN:HD22	1:E:101:MET:HE3	1.71	0.56
2:F:291:ILE:HD12	2:F:426:ILE:HD13	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:405:THR:HG22	2:D:407:LYS:H	1.70	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
2:F:218:HIS:O	2:F:222:VAL:HG23	2.06	0.56
1:A:289:PHE:CE2	1:A:291:ALA:HB2	2.40	0.56
1:A:290:SER:HB3	1:A:303:TYR:OH	2.06	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
1:C:311:TYR:C	1:C:313:VAL:N	2.60	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
1:C:122:VAL:O	1:C:191:ARG:NH2	2.40	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: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
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
2:H:76:ALA:O	2:H:129:ILE:HG23	2.08	0.54
1:A:127:ILE:HB	1:A:184:LYS:HE3	1.89	0.54
2:B:62:ASN:CG	2:B:65:ASN:HB2	2.33	0.54
2:D:62:ASN:CG	2:D:65:ASN:HB2	2.32	0.54
2:F:119:ILE:N	2:F:120:PRO:HD2	2.22	0.54
1:G:99:ASN:ND2	1:G:101:MET:HE3	2.21	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
1:A:35:THR:HB	1:A:36:PRO:CD	2.37	0.54
1:A:310:TYR:CD1	1:A:312:PHE:CZ	2.96	0.54
1:C:35:THR:HB	1:C:36:PRO:CD	2.38	0.54
1:C:187:LEU:O	1:C:191:ARG:HG3	2.07	0.54
2:D:255:GLU:HB3	2:D:453:VAL:HG23	1.89	0.54
1:E:19:PHE:CD1	1:E:392:MET:HE2	2.43	0.54
1:C:294:PRO:HD2	2:D:99:LEU:HB3	1.90	0.54
1:G:419:ASP:O	1:G:423:VAL:HG23	2.08	0.54
2:F:209:VAL:HG21	2:F:402:VAL:HG12	1.89	0.54
1:A:320:ASN:ND2	5:A:492:HOH:O	2.39	0.53
2:F:398:ILE:HA	2:F:408:ARG:HG3	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:90:LEU:HD13	2:B:94:ASN:ND2	2.22	0.53
1:G:403:ILE:HG23	1:G:403:ILE:O	2.07	0.53
2:H:303:THR:HG22	2:H:305:SER:N	2.24	0.53
2:D:165:HIS:HD2	2:D:256:ARG:CD	2.21	0.53
2:F:31:LEU:HG	2:F:32:PRO:HD2	1.90	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: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
2:B:303:THR:HG22	2:B:305:SER:H	1.73	0.53
1:E:429:THR:HG22	1:E:431:ASN:HD22	1.74	0.53
2:H:62:ASN:CG	2:H:65:ASN:HB2	2.33	0.53
2:D:68:THR:HG23	2:D:195:LEU:HD23	1.91	0.53
1:E:444:VAL:HG11	1:E:456:VAL:HG11	1.91	0.53
2:F:62:ASN:CG	2:F:65:ASN:HB2	2.34	0.53
1:E:268:ILE:HD13	1:E:268:ILE:H	1.74	0.53
2:F:375:ARG:NH2	2:F:379:GLN:OE1	2.42	0.53
1:G:243:CYS:HA	1:G:446:MET:O	2.09	0.53
2:H:237:SER:N	2:H:238:PRO:HD3	2.23	0.53
1:C:267:PRO:HD2	1:C:270:HIS:HB2	1.90	0.52
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:E:379:LEU:HD13	2:F:46:SER:HB2	1.90	0.52
1:E:66:ARG:HD3	5:E:517:HOH:O	2.09	0.52
2:F:259:LYS:HG3	2:F:447:THR:HG22	1.92	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:31:LEU:HG	2:B:32:PRO:HD2	1.90	0.52
2:B:303:THR:HG22	2:B:305:SER:N	2.25	0.52
1:A:246:PRO:HG3	1:A:448:GLY:HA2	1.91	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:67:LEU:HD13	1:G:135:GLN:HG3	1.91	0.52
1:G:256:LEU:CD1	1:G:314:GLU:HG2	2.39	0.52
2:D:375:ARG:NH2	2:D:379:GLN:OE1	2.43	0.52
1:A:429:THR:HG22	1:A:431:ASN:HD22	1.73	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
2:H:90:LEU:CD1	2:H:94:ASN:HD21	2.23	0.52
1:A:230:ILE:N	1:A:230:ILE:CD1	2.73	0.51
1:E:310:TYR:CD1	1:E:312:PHE:CZ	2.99	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:76:ALA:O	2:D:129:ILE:HG23	2.10	0.51
2:F:236:GLU:C	2:F:238:PRO:HD3	2.34	0.51
2:D:294:ASN:OD1	2:D:324:MET:HA	2.11	0.51
2:H:61:GLU:HA	2:H:65:ASN:HD22	1.75	0.51
1:C:235:ALA:O	1:C:436:GLY:HA3	2.10	0.51
1:E:127:ILE:HB	1:E:184:LYS:HE3	1.91	0.51
1:E:419:ASP:O	1:E:423:VAL:HG23	2.11	0.51
2:B:410:SER:OG	2:B:413:GLU:HG3	2.11	0.51
2:F:35:LEU:HA	2:F:205:GLY:O	2.11	0.51
2:B:375:ARG:NH2	2:B:379:GLN:OE1	2.43	0.51
2:D:401:GLN:O	2:D:405:THR:HB	2.10	0.51
2:B:35:LEU:HD13	2:B:208:MET:HG3	1.92	0.51
2:D:253:ARG:HH21	2:D:457:GLU:CD	2.19	0.51
2:D:115:LEU:HD12	2:D:115:LEU:H	1.75	0.51
1:G:429:THR:HG22	1:G:431:ASN:HD22	1.74	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
1:E:256:LEU:HD11	1:E:314:GLU:HG2	1.93	0.50
1:G:375:LYS:HE3	2:H:115:LEU:HD21	1.93	0.50
2:H:294:ASN:ND2	2:H:324:MET:CG	2.73	0.50
2:F:294:ASN:OD1	2:F:324:MET:HA	2.10	0.50
2:F:76:ALA:O	2:F:129:ILE:HG23	2.11	0.50
2:H:76:ALA:CB	2:H:110:TYR:HE2	2.24	0.50
2:D:90:LEU:HD13	2:D:94:ASN:ND2	2.26	0.50
2:H:141:GLU:O	2:H:144:ARG:HG3	2.12	0.50
1:A:99:ASN:CB	1:A:101:MET:HE3	2.37	0.50
1:A:315:ASN:C	1:A:315:ASN:ND2	2.69	0.50
2:F:35:LEU:HD12	2:F:208:MET:O	2.11	0.50
2:B:27:ARG:NH2	5:B:544:HOH:O	2.45	0.50
2:B:65:ASN:ND2	5:B:540:HOH:O	2.45	0.50
1:A:256:LEU:CD1	1:A:314:GLU:HG2	2.42	0.50
2:B:35:LEU:HD12	2:B:208:MET:O	2.11	0.50
1:E:336:ILE:HG22	1:E:337:PRO:HD2	1.93	0.50
1:G:315:ASN:C	1:G:315:ASN:ND2	2.69	0.50
1:A:99:ASN:HB2	1:A:101:MET:CE	2.38	0.50
2:H:255:GLU:HB3	2:H:453:VAL:CG2	2.42	0.50
2:B:373:VAL:O	2:B:377:LYS:HG3	2.12	0.49
1:E:241:GLU:HA	1:E:444:VAL:O	2.11	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:F:237:SER:N	2:F:238:PRO:HD3	2.27	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:350:ARG:HD3	2:B:455:TYR:OH	2.12	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: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
2:H:80:THR:C	2:H:134:VAL:HG23	2.37	0.49
1:A:19:PHE:HD1	1:A:392:MET:HE2	1.77	0.49
1:A:176:ARG:NH2	1:E:242:SER:OG	2.46	0.49
1:C:151:GLU:CD	1:C:151:GLU:H	2.20	0.49
1:G:333:LEU:HD13	1:G:334:SER:N	2.27	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: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
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:OE1	2:D:22:GLN:HA	2.12	0.49
1:C:16:THR:HG23	1:C:17:ASP:N	2.28	0.48
1:C:467:ASN:CG	1:C:468:SER:N	2.71	0.48
1:E:39:PHE:O	1:E:385:LYS:HE3	2.13	0.48
2:F:52:ILE:HG23	2:F:52:ILE:O	2.12	0.48
2:F:255:GLU:HB3	2:F:453:VAL:CG2	2.43	0.48
2:H:144:ARG:HH21	2:H:188:LYS:C	2.21	0.48
1:E:403:ILE:HG23	1:E:403:ILE:O	2.13	0.48
2:H:23:ILE:N	2:H:23:ILE:CD1	2.69	0.48
2:H:294:ASN:ND2	2:H:324:MET:CA	2.68	0.48
2:B:236:GLU:C	2:B:238:PRO:HD3	2.38	0.48
2:F:35:LEU:CD1	2:F:208:MET:HG3	2.43	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
1:C:249:VAL:HG12	1:C:255:GLU:HB2	1.95	0.48
2:D:255:GLU:HB3	2:D:453:VAL:CG2	2.44	0.48
1:E:210:GLU:HA	1:E:210:GLU:OE1	2.14	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:HA	1:C:210:GLU:OE1	2.13	0.48
2:B:35:LEU:HA	2:B:205:GLY:O	2.14	0.48
2:D:398:ILE:HA	2:D:408:ARG:HG3	1.96	0.48
2:F:175:PRO:HA	2:F:178:ARG:NH1	2.29	0.48
2:H:35:LEU:CD1	2:H:208:MET:HG3	2.43	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:136:ASP:O	2:H:140:ILE:HG13	2.14	0.48
2:H:370:ASP:OD1	2:H:423:LYS:NZ	2.46	0.48
2:D:317:GLY:O	2:D:318:SER:CB	2.61	0.48
1:E:115:LEU:HD23	1:E:215:LEU:HB3	1.96	0.48
1:E:344:VAL:HG23	5:E:493:HOH:O	2.14	0.48
1:C:99:ASN:ND2	1:C:101:MET:HE3	2.29	0.47
1:C:256:LEU:HD11	1:C:314:GLU:HG2	1.96	0.47
2:F:61:GLU:OE1	2:F:66:ASN:HA	2.14	0.47
1:C:403:ILE:O	1:C:403:ILE:HG23	2.13	0.47
2:F:75:LEU:HA	2:F:78:LYS:HG2	1.96	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:F:455:TYR:CD1	2:F:455:TYR:C	2.92	0.47
1:G:210:GLU:OE1	1:G:210:GLU:HA	2.14	0.47
2:B:90:LEU:CD1	2:B:94:ASN:HD21	2.28	0.47
1:A:297:GLY:HA2	2:B:93:GLU:OE1	2.14	0.47
1:C:260:GLN:HB2	1:C:445:VAL:HG12	1.97	0.47
2:F:76:ALA:CB	2:F:110:TYR:HE2	2.27	0.47
1:G:267:PRO:HD2	1:G:270:HIS:HB2	1.95	0.47
1:A:263:PHE:CE2	1:A:442:ALA:HB2	2.49	0.47
1:C:16:THR:HG23	1:C:18:ASN:H	1.80	0.47
1:C:19:PHE:CE1	1:C:392:MET:HE2	2.48	0.47
1:C:310:TYR:HD1	1:C:312:PHE:CZ	2.31	0.47
2:F:97:SER:OG	2:F:114:SER:CB	2.62	0.47
2:H:455:TYR:CD1	2:H:455:TYR:C	2.92	0.47
1:A:45:TYR:N	1:A:45:TYR:CD1	2.83	0.47
2:D:61:GLU:HA	2:D:65:ASN:HD22	1.78	0.47
1:G:119:SER:HB2	1:G:220:LEU:CD1	2.45	0.47
2:H:76:ALA:HB1	2:H:129:ILE:HG23	1.93	0.47
1:E:45:TYR:N	1:E:45:TYR:CD1	2.82	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
2:B:398:ILE:HA	2:B:408:ARG:HG3	1.97	0.47
1:C:246:PRO:HG3	1:C:448:GLY:CA	2.39	0.47
1:G:15:ARG:HH11	1:G:15:ARG:CG	2.24	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:A:115:LEU:HD23	1:A:215:LEU:HB3	1.97	0.46
2:B:370:ASP:OD1	2:B:423:LYS:NZ	2.47	0.46
1:C:429:THR:HG22	1:C:431:ASN:HD22	1.77	0.46
2:F:115:LEU:HD12	2:F:115:LEU:H	1.80	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:47:ASP:HB3	1:A:199:ASN:OD1	2.16	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
2:D:263:LEU:HA	2:D:264:PRO:HD3	1.79	0.46
1:E:99:ASN:ND2	1:E:101:MET:HE3	2.31	0.46
2:F:76:ALA:HB1	2:F:129:ILE:HG23	1.96	0.46
2:B:245:ARG:HA	2:B:245:ARG:NE	2.30	0.46
1:G:198:GLU:OE1	1:G:225:SER:HB2	2.16	0.46
2:H:291:ILE:CD1	2:H:426:ILE:HD13	2.46	0.46
1:C:19:PHE:HD1	1:C:392:MET:CE	2.28	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
2:H:97:SER:OG	2:H:114:SER:CB	2.64	0.46
1:A:403:ILE:HG23	1:A:403:ILE:O	2.16	0.46
1:G:304:THR:HG22	1:G:305:HIS:ND1	2.31	0.46
2:B:62:ASN:H	2:B:65:ASN:CB	2.23	0.46
2:B:165:HIS:HD2	2:B:256:ARG:CD	2.29	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:D:291:ILE:HD12	2:D:426:ILE:HD13	1.97	0.46
2:F:68:THR:HG23	2:F:195:LEU:HD23	1.97	0.46
2:H:62:ASN:ND2	2:H:65:ASN:HB2	2.30	0.46
2:B:68:THR:HG23	2:B:195:LEU:HD23	1.98	0.46
2:F:62:ASN:ND2	2:F:65:ASN:HB2	2.30	0.46
1:G:367:VAL:HG21	1:G:417:PRO:HA	1.98	0.46
2:H:143:GLU:O	2:H:147:ILE:HG12	2.15	0.46
1:A:256:LEU:HD11	1:A:314:GLU:HG2	1.98	0.46
2:B:294:ASN:ND2	2:B:324:MET:CG	2.77	0.46
1:C:444:VAL:HG11	1:C:456:VAL:HG11	1.98	0.46
2:F:232:VAL:HA	2:F:233:PRO:HD3	1.82	0.46
1:C:45:TYR:N	1:C:45:TYR:CD1	2.83	0.45
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
2:F:144:ARG:HH21	2:F:188:LYS:C	2.24	0.45
2:H:441:MET:HE3	2:H:453:VAL:CG2	2.46	0.45
1:A:371:LYS:HE3	1:A:412:ILE:O	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:ASP:O	1:A:423:VAL:HG23	2.15	0.45
1:C:67:LEU:HD13	1:C:135:GLN:HG3	1.98	0.45
2:D:80:THR:C	2:D:134:VAL:HG23	2.41	0.45
2:D:370:ASP:OD1	2:D:423:LYS:NZ	2.48	0.45
2:D:439:VAL:CG1	2:D:457:GLU:HG2	2.46	0.45
1:E:267:PRO:HD2	1:E:270:HIS:HB2	1.98	0.45
2:F:90:LEU:HD13	2:F:94:ASN:HD21	1.79	0.45
1:G:256:LEU:HD11	1:G:314:GLU:HG2	1.97	0.45
1:A:253:LEU:HA	1:A:254:PRO:HD3	1.80	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:E:67:LEU:HD13	1:E:135:GLN:HG3	1.97	0.45
2:F:429:TRP:CE2	2:F:433:ARG:HG3	2.52	0.45
1:G:56:ASN:HD22	1:G:56:ASN:HA	1.57	0.45
2:H:410:SER:OG	2:H:413:GLU:HG3	2.17	0.45
2:H:429:TRP:CE2	2:H:433:ARG:HG3	2.50	0.45
1:A:129:GLU:HG3	1:G:224:GLN:OE1	2.17	0.45
1:A:210:GLU:OE1	1:A:210:GLU:HA	2.16	0.45
2:B:232:VAL:HA	2:B:233:PRO:HD3	1.75	0.45
2:B:263:LEU:HA	2:B:264:PRO:HD3	1.80	0.45
2:B:429:TRP:CE2	2:B:433:ARG:HG3	2.51	0.45
1:C:17:ASP:O	1:C:18:ASN:HB3	2.17	0.45
1:C:263:PHE:CE2	1:C:442:ALA:HB2	2.52	0.45
2:D:62:ASN:ND2	2:D:65:ASN:HB2	2.32	0.45
2:F:137:ASN:HD21	2:F:192:ARG:HD2	1.82	0.45
1:G:174:CYS:O	1:G:175:PRO:C	2.60	0.45
2:H:68:THR:HG23	2:H:195:LEU:HD23	1.97	0.45
1:C:256:LEU:CD1	1:C:314:GLU:HG2	2.46	0.45
1:E:295:GLY:CA	2:F:93:GLU:HG2	2.42	0.45
2:B:204:LYS:HG3	2:B:235:SER:OG	2.16	0.45
1:C:249:VAL:HG23	1:C:249:VAL:O	2.17	0.45
2:D:55:ASP:OD1	2:D:55:ASP:C	2.59	0.45
2:F:370:ASP:OD1	2:F:423:LYS:NZ	2.49	0.45
1:G:268:ILE:CD1	1:G:398:MET:SD	2.96	0.45
1:G:379:LEU:HD13	2:H:46:SER:HB2	1.99	0.45
2:B:441:MET:HE3	2:B:441:MET:HB3	1.84	0.45
2:F:165:HIS:CD2	2:F:258:ILE:HD11	2.52	0.45
1:A:119:SER:HB2	1:A:220:LEU:CD1	2.47	0.45
2:F:61:GLU:HA	2:F:65:ASN:HD22	1.81	0.45
2:F:167:HIS:NE2	2:F:330:TYR:OH	2.44	0.45
1:G:115:LEU:HD23	1:G:215:LEU:HB3	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:315:ASN:ND2	1:C:316:CYS:N	2.46	0.45
1:E:35:THR:HB	1:E:36:PRO:CD	2.46	0.45
1:E:294:PRO:HB3	2:F:89:GLU:HA	1.99	0.45
1:G:17:ASP:O	1:G:18:ASN:HB3	2.16	0.45
1:G:310:TYR:HB3	1:G:312:PHE:CZ	2.51	0.45
1:G:395:GLN:OE1	1:G:403:ILE:HG22	2.17	0.45
2:H:137:ASN:HD21	2:H:192:ARG:HD2	1.79	0.45
1:A:198:GLU:OE1	1:A:225:SER:HB2	2.17	0.44
2:B:218:HIS:O	2:B:222:VAL:HG23	2.18	0.44
2:D:141:GLU:O	2:D:144:ARG:HG3	2.17	0.44
1:A:129:GLU:HG3	1:G:224:GLN:CD	2.41	0.44
2:B:137:ASN:HD21	2:B:192:ARG:HD2	1.82	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
1:A:268:ILE:H	1:A:268:ILE:CD1	2.31	0.44
1:C:115:LEU:HD23	1:C:215:LEU:HB3	1.98	0.44
1:E:99:ASN:HB2	1:E:101:MET:CE	2.42	0.44
1:E:395:GLN:OE1	1:E:403:ILE:HG22	2.17	0.44
2:F:295:TRP:CZ2	2:F:297:ARG:HA	2.52	0.44
2:H:352:ILE:O	2:H:356:ILE:HG13	2.18	0.44
1:A:294:PRO:HB3	2:B:89:GLU:HA	1.99	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:D:35:LEU:HA	2:D:205:GLY:O	2.17	0.44
2:D:144:ARG:HH21	2:D:188:LYS:C	2.25	0.44
1:E:267:PRO:HA	1:E:323:TYR:O	2.17	0.44
2:F:80:THR:C	2:F:134:VAL:HG23	2.43	0.44
1:G:268:ILE:H	1:G:268:ILE:CD1	2.31	0.44
2:H:27:ARG:HH11	2:H:27:ARG:HB3	1.82	0.44
2:H:439:VAL:HG22	2:H:453:VAL:HG13	1.99	0.44
1:A:35:THR:HB	1:A:36:PRO:HD2	2.00	0.44
2:D:76:ALA:HB1	2:D:129:ILE:HG23	1.99	0.44
2:B:76:ALA:CB	2:B:110:TYR:HE2	2.31	0.44
1:C:35:THR:HB	1:C:36:PRO:HD2	2.00	0.44
1:E:122:VAL:O	1:E:191:ARG:NH2	2.51	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
1:G:263:PHE:CE2	1:G:442:ALA:HB2	2.53	0.43
1:G:315:ASN:HB3	1:G:334:SER:HB2	2.00	0.43
1:A:294:PRO:HD2	2:B:99:LEU:HB3	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:263:PHE:CE2	1:E:442:ALA:HB2	2.53	0.43
2:F:87:GLY:O	2:F:91:GLU:HB2	2.18	0.43
2:H:317:GLY:O	2:H:318:SER:OG	2.35	0.43
2:B:87:GLY:O	2:B:91:GLU:HB2	2.19	0.43
2:B:90:LEU:HD13	2:B:94:ASN:HD21	1.83	0.43
2:B:317:GLY:O	2:B:318:SER:CB	2.65	0.43
2:F:31:LEU:HD21	2:F:226:GLN:HA	1.99	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:441:MET:HE3	2:D:441:MET:HB3	1.85	0.43
2:D:87:GLY:O	2:D:91:GLU:HB2	2.18	0.43
2:F:80:THR:C	2:F:82:ASN:H	2.27	0.43
1:G:114:MET:HE2	1:G:118:MET:HG3	2.00	0.43
1:G:290:SER:HB3	1:G:303:TYR:OH	2.19	0.43
2:H:147:ILE:HG22	2:H:187:ILE:HD13	2.01	0.43
1:C:312:PHE:CD1	1:C:339:ALA:CB	3.01	0.43
1:E:17:ASP:O	1:E:18:ASN:HB3	2.19	0.43
1:E:43:GLY:HA2	1:E:102:TYR:O	2.19	0.43
2:F:23:ILE:HA	2:F:24:PRO:HD3	1.89	0.43
2:F:397:ASP:OD2	2:F:408:ARG:NH1	2.44	0.43
2:B:350:ARG:HH12	2:D:419:ASP:HB3	1.84	0.43
2:B:455:TYR:CD1	2:B:455:TYR:C	2.96	0.43
1:C:304:THR:HG22	1:C:305:HIS:ND1	2.33	0.43
1:C:315:ASN:C	1:C:315:ASN:ND2	2.68	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:G:19:PHE:CE1	1:G:392:MET:HE2	2.54	0.43
1:G:151:GLU:CD	1:G:151:GLU:H	2.25	0.43
2:B:80:THR:C	2:B:134:VAL:HG23	2.43	0.43
2:B:115:LEU:HD12	2:B:115:LEU:H	1.83	0.43
2:B:255:GLU:HA	2:B:441:MET:O	2.18	0.43
2:B:294:ASN:ND2	2:B:324:MET:CA	2.71	0.43
1:C:101:MET:HE2	1:C:101:MET:HB3	1.93	0.43
2:D:108:THR:CG2	2:D:110:TYR:HE1	2.31	0.43
1:A:310:TYR:HD1	1:A:312:PHE:CZ	2.37	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
2:F:410:SER:OG	2:F:413:GLU:HG3	2.19	0.43
1:G:15:ARG:NH1	1:G:15:ARG:CG	2.82	0.43
1:G:200:THR:HG22	1:G:201:VAL:N	2.34	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:61:GLU:OE1	2:H:66:ASN:HA	2.19	0.43
1:A:267:PRO:HD2	1:A:270:HIS:HB2	2.01	0.43
2:B:207:ARG:NH1	2:B:245:ARG:NH1	2.67	0.43
2:H:115:LEU:HD12	2:H:115:LEU:N	2.34	0.43
1:C:245:PRO:HA	1:C:246:PRO:HD3	1.90	0.42
1:C:275:ALA:CB	1:C:423:VAL:HG21	2.49	0.42
1:E:245:PRO:HA	1:E:246:PRO:HD3	1.78	0.42
2:F:349:VAL:N	2:F:449:THR:OG1	2.52	0.42
1:G:45:TYR:CD1	1:G:45:TYR:N	2.87	0.42
1:G:275:ALA:HB3	1:G:423:VAL:HG21	2.02	0.42
2:B:237:SER:N	2:B:238:PRO:HD3	2.34	0.42
1:E:270:HIS:O	1:E:273:ILE:HB	2.19	0.42
1:E:333:LEU:HD13	1:E:333:LEU:C	2.44	0.42
2:F:141:GLU:O	2:F:144:ARG:HG3	2.20	0.42
1:G:84:LEU:HD13	1:G:91:TYR:CZ	2.55	0.42
2:B:291:ILE:HD12	2:B:426:ILE:HD13	1.99	0.42
1:A:260:GLN:HB2	1:A:445:VAL:HG12	2.01	0.42
1:E:41:ALA:HB1	1:E:389:LEU:HD22	2.01	0.42
1:E:148:MET:O	1:E:150:PRO:HD3	2.18	0.42
2:H:349:VAL:N	2:H:449:THR:OG1	2.53	0.42
2:D:410:SER:OG	2:D:413:GLU:HG3	2.19	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:H:263:LEU:HA	2:H:264:PRO:HD3	1.77	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
2:F:441:MET:HE3	2:F:441:MET:HB3	1.87	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:441:MET:HE3	2:H:441:MET:HB3	1.85	0.42
1:C:237:TYR:CG	1:C:264:GLU:HB2	2.55	0.42
1:E:237:TYR:CG	1:E:264:GLU:HB2	2.55	0.42
2:F:317:GLY:O	2:F:318:SER:OG	2.37	0.42
2:H:70:HIS:O	2:H:73:GLU:HB3	2.19	0.42
2:H:305:SER:HA	2:H:306:PRO:HD3	1.73	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
1:C:290:SER:HB3	1:C:303:TYR:OH	2.20	0.42
2:D:397:ASP:OD2	2:D:408:ARG:NH1	2.43	0.42
2:F:77:PHE:O	2:F:85:GLN:HG3	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:416:LYS:O	1:A:417:PRO:C	2.62	0.42
1:C:100:LEU:HD21	1:C:195:TYR:OH	2.20	0.42
2:D:165:HIS:HD2	2:D:256:ARG:NE	2.18	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:G:246:PRO:HG3	1:G:448:GLY:CA	2.47	0.42
2:D:255:GLU:HA	2:D:441:MET:O	2.20	0.42
2:H:87:GLY:O	2:H:91:GLU:HB2	2.20	0.42
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
1:G:99:ASN:CB	1:G:101:MET:HE3	2.42	0.41
1:G:336:ILE:HG22	1:G:337:PRO:HD2	2.01	0.41
2:H:375:ARG:HH11	2:H:375:ARG:HB3	1.85	0.41
2:B:76:ALA:HB1	2:B:129:ILE:HG23	2.00	0.41
2:D:373:VAL:O	2:D:377:LYS:HG3	2.20	0.41
2:F:48:ALA:HB1	2:F:213:ALA:O	2.20	0.41
1:G:275:ALA:CB	1:G:423:VAL:HG21	2.49	0.41
2:B:350:ARG:HH11	2:D:420:LYS:HB3	1.83	0.41
2:D:204:LYS:O	2:D:208:MET:HG2	2.20	0.41
2:D:218:HIS:O	2:D:222:VAL:HG23	2.20	0.41
2:F:349:VAL:O	2:F:352:ILE:HG22	2.20	0.41
2:H:412:GLU:CD	2:H:412:GLU:H	2.28	0.41
1:C:455:ASP:O	1:C:459:VAL:HG23	2.20	0.41
2:H:40:GLU:OE1	2:H:408:ARG:NH2	2.54	0.41
1:A:174:CYS:O	1:A:175:PRO:C	2.63	0.41
1:C:253:LEU:HA	1:C:254:PRO:HD3	1.87	0.41
2:H:75:LEU:HA	2:H:78:LYS:HG2	2.03	0.41
2:H:295:TRP:CZ2	2:H:297:ARG:HA	2.56	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
1:C:174:CYS:O	1:C:175:PRO:C	2.63	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:A:157:LEU:HD11	1:A:244:ILE:HD13	2.03	0.41
1:A:275:ALA:CB	1:A:423:VAL:HG21	2.51	0.41
1:A:315:ASN:HB3	1:A:334:SER:HB2	2.03	0.41
2:B:294:ASN:HD21	2:B:324:MET:HG3	1.83	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119:SER:HB2	1:C:220:LEU:CD1	2.50	0.41
2:D:90:LEU:CD1	2:D:94:ASN:HD21	2.34	0.41
2:D:108:THR:HG22	2:D:110:TYR:HE1	1.86	0.41
1:E:253:LEU:HA	1:E:254:PRO:HD3	1.85	0.41
2:F:259:LYS:HB2	2:F:259:LYS:HE3	1.87	0.41
1:G:99:ASN:HB2	1:G:101:MET:CE	2.44	0.41
1:G:107:PHE:HA	5:G:494:HOH:O	2.21	0.41
1:G:404:PRO:HG2	1:G:407:GLU:HB2	2.03	0.41
2:H:108:THR:HG22	2:H:110:TYR:HE1	1.85	0.41
2:H:218:HIS:O	2:H:222:VAL:HG23	2.20	0.41
1:C:97:ARG:NH1	5:C:513:HOH:O	2.54	0.41
2:D:400:ARG:NH2	2:D:401:GLN:HG2	2.35	0.41
1:E:19:PHE:HD1	1:E:392:MET:HE2	1.82	0.41
2:F:255:GLU:HA	2:F:441:MET:O	2.21	0.41
2:H:172:LYS:HA	2:H:172:LYS:HD2	1.93	0.41
2:H:254:GLY:O	2:H:440:SER:HA	2.21	0.41
1:A:55:ARG:NH1	1:E:181:SER:OG	2.52	0.40
1:A:312:PHE:CD1	1:A:339:ALA:CB	3.04	0.40
1:A:339:ALA:O	1:A:340:ALA:C	2.65	0.40
2:B:97:SER:CB	2:B:114:SER:HB3	2.50	0.40
2:D:80:THR:C	2:D:82:ASN:H	2.28	0.40
1:G:119:SER:HB2	1:G:220:LEU:HD13	2.02	0.40
1:G:343:ALA:O	1:G:344:VAL:C	2.65	0.40
2:H:350:ARG:HG3	2:H:451:PRO:HB3	2.02	0.40
1:A:56:ASN:HD22	1:A:56:ASN:HA	1.63	0.40
1:A:59:GLY:HA2	5:A:497:HOH:O	2.21	0.40
1:A:151:GLU:CD	1:A:151:GLU:H	2.30	0.40
1:C:96:SER:CB	1:C:99:ASN:OD1	2.67	0.40
2:H:77:PHE:O	2:H:85:GLN:HG3	2.21	0.40
1:A:282:LEU:HD23	1:A:282:LEU:C	2.47	0.40
2:D:61:GLU:OE1	2:D:66:ASN:HA	2.21	0.40
2:F:159:ASP:OD1	2:F:159:ASP:N	2.52	0.40
1:G:296:LYS:HG2	1:G:298:MET:HE2	2.04	0.40
1:G:301:ARG:NH2	1:G:362:LEU:HD23	2.37	0.40
2:H:349:VAL:HG23	2:H:449:THR:HG23	2.02	0.40
2:B:254:GLY:O	2:B:440:SER:HA	2.21	0.40
2:D:349:VAL:HG23	2:D:449:THR:HG23	2.03	0.40
1:G:42:LEU:N	1:G:42:LEU:HD23	2.36	0.40
1:G:179:ILE:N	1:G:180:PRO:CD	2.84	0.40
2:H:52:ILE:O	2:H:52:ILE:HG23	2.20	0.40
1:A:17:ASP:O	1:A:18:ASN:HB3	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:234:LYS:HB2	2:B:234:LYS:HE3	1.82	0.40
2:B:317:GLY:O	2:B:318:SER:OG	2.38	0.40
1:C:446:MET:HE3	1:C:450:ARG:CD	2.52	0.40
2:D:279:ALA:HB1	2:D:281:ASP:OD1	2.21	0.40
1:E:231:THR:O	5:E:505:HOH:O	2.22	0.40
1:E:429:THR:CG2	1:E:429:THR:O	2.68	0.40
2:F:134:VAL:O	2:F:135:LEU:HB2	2.21	0.40
1:G:392:MET:HE3	1:G:402:LYS:HD2	2.03	0.40
2:H:90:LEU:HD13	2:H:94:ASN:HD21	1.80	0.40
2:H:375:ARG:HB3	2:H:375:ARG:NH1	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	455/475 (96%)	436 (96%)	17 (4%)	2 (0%)	30	49
1	C	451/475 (95%)	433 (96%)	16 (4%)	2 (0%)	30	49
1	E	453/475 (95%)	435 (96%)	16 (4%)	2 (0%)	30	49
1	G	455/475 (96%)	434 (95%)	17 (4%)	4 (1%)	14	27
2	B	437/443 (99%)	423 (97%)	11 (2%)	3 (1%)	18	34
2	D	441/443 (100%)	426 (97%)	12 (3%)	3 (1%)	18	34
2	F	441/443 (100%)	425 (96%)	13 (3%)	3 (1%)	18	34
2	H	438/443 (99%)	423 (97%)	11 (2%)	4 (1%)	14	27
All	All	3571/3672 (97%)	3435 (96%)	113 (3%)	23 (1%)	21	38

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
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%)	363 (94%)	21 (6%)	19	40
1	C	381/401 (95%)	357 (94%)	24 (6%)	16	34
1	E	382/401 (95%)	357 (94%)	25 (6%)	15	32
1	G	384/401 (96%)	360 (94%)	24 (6%)	16	34
2	B	376/379 (99%)	355 (94%)	21 (6%)	19	39
2	D	379/379 (100%)	359 (95%)	20 (5%)	20	42
2	F	379/379 (100%)	359 (95%)	20 (5%)	20	42

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	377/379 (100%)	360 (96%)	17 (4%)	24	49
All	All	3042/3120 (98%)	2870 (94%)	172 (6%)	18	39

All (172) 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	230	ILE
1	A	268	ILE
1	A	273	ILE
1	A	288	SER
1	A	305	HIS
1	A	307	LEU
1	A	311	TYR
1	A	333	LEU
1	A	361	ARG
1	A	382	LEU
1	A	386	LEU
1	A	399	HIS
1	A	429	THR
1	A	445	VAL
2	B	27	ARG
2	B	31	LEU
2	B	39	THR
2	B	75	LEU
2	B	86	GLN
2	B	90	LEU
2	B	117	GLU
2	B	149	ARG
2	B	176	LEU
2	B	219	GLU
2	B	250	VAL
2	B	256	ARG
2	B	275	VAL
2	B	346	GLU
2	B	350	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	405	THR
2	B	408	ARG
2	B	424	ASP
2	B	439	VAL
2	B	441	MET
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	230	ILE
1	C	268	ILE
1	C	273	ILE
1	C	288	SER
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	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	31	LEU
2	D	39	THR
2	D	75	LEU
2	D	86	GLN
2	D	149	ARG
2	D	176	LEU
2	D	219	GLU
2	D	236	GLU
2	D	250	VAL
2	D	253	ARG
2	D	256	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	275	VAL
2	D	291	ILE
2	D	346	GLU
2	D	405	THR
2	D	408	ARG
2	D	439	VAL
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	230	ILE
1	E	268	ILE
1	E	273	ILE
1	E	288	SER
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	382	LEU
1	E	386	LEU
1	E	399	HIS
1	E	429	THR
1	E	431	ASN
1	E	445	VAL
1	E	446	MET
1	E	468	SER
2	F	27	ARG
2	F	31	LEU
2	F	39	THR
2	F	75	LEU
2	F	86	GLN
2	F	149	ARG
2	F	176	LEU
2	F	219	GLU
2	F	250	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	256	ARG
2	F	275	VAL
2	F	291	ILE
2	F	346	GLU
2	F	405	THR
2	F	408	ARG
2	F	423	LYS
2	F	424	ASP
2	F	439	VAL
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	230	ILE
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	333	LEU
1	G	361	ARG
1	G	382	LEU
1	G	386	LEU
1	G	399	HIS
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	75	LEU
2	H	86	GLN
2	H	149	ARG
2	H	176	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	219	GLU
2	H	248	LEU
2	H	250	VAL
2	H	275	VAL
2	H	346	GLU
2	H	405	THR
2	H	408	ARG
2	H	439	VAL
2	H	441	MET
2	H	449	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	ASN
1	A	227	HIS
1	A	315	ASN
1	A	320	ASN
1	A	349	GLN
1	A	381	ASN
1	A	406	ASN
1	A	431	ASN
2	B	44	ASN
2	B	65	ASN
2	B	85	GLN
2	B	137	ASN
2	B	165	HIS
2	B	223	GLN
2	B	294	ASN
2	B	354	ASN
2	B	374	ASN
2	B	436	ASN
1	C	56	ASN
1	C	315	ASN
1	C	320	ASN
1	C	381	ASN
1	C	406	ASN
1	C	431	ASN
1	C	447	GLN
2	D	44	ASN
2	D	65	ASN
2	D	66	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	85	GLN
2	D	137	ASN
2	D	165	HIS
2	D	223	GLN
2	D	354	ASN
2	D	374	ASN
2	D	462	GLN
1	E	56	ASN
1	E	252	ASN
1	E	320	ASN
1	E	349	GLN
1	E	381	ASN
1	E	406	ASN
1	E	431	ASN
1	E	447	GLN
2	F	44	ASN
2	F	66	ASN
2	F	85	GLN
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	227	HIS
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	85	GLN
2	H	137	ASN
2	H	165	HIS
2	H	223	GLN
2	H	294	ASN
2	H	304	ASN
2	H	315	GLN
2	H	354	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	374	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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$
3	EPE	A	489	-	15,15,15	1.29	2 (13%)	19,20,20	0.99	1 (5%)
3	EPE	G	489	-	15,15,15	1.43	3 (20%)	19,20,20	0.94	0

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
3	EPE	A	489	-	-	2/9/19/19	0/1/1/1
3	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)
3	G	489	EPE	C10-S	2.95	1.81	1.77
3	A	489	EPE	C10-S	2.47	1.81	1.77
3	G	489	EPE	C6-N1	2.42	1.53	1.46
3	A	489	EPE	C6-N1	2.06	1.52	1.46
3	G	489	EPE	C7-N4	2.02	1.52	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	489	EPE	C7-N4-C5	-2.00	105.91	111.24

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	489	EPE	C10-C9-N1-C2
3	G	489	EPE	C10-C9-N1-C6
3	A	489	EPE	C10-C9-N1-C2
3	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	457/475 (96%)	0.08	18 (3%)	43	38	30, 46, 85, 101	0
1	C	453/475 (95%)	0.20	16 (3%)	47	42	31, 49, 82, 101	0
1	E	455/475 (95%)	0.30	27 (5%)	28	24	33, 53, 85, 101	0
1	G	457/475 (96%)	0.37	23 (5%)	34	30	35, 54, 89, 101	0
2	B	439/443 (99%)	0.21	13 (2%)	52	48	28, 49, 75, 96	0
2	D	443/443 (100%)	0.45	18 (4%)	41	37	34, 58, 84, 101	0
2	F	443/443 (100%)	0.79	32 (7%)	21	19	45, 68, 88, 100	0
2	H	440/443 (99%)	1.49	113 (25%)	1	1	54, 78, 93, 100	0
All	All	3587/3672 (97%)	0.48	260 (7%)	21	19	28, 58, 88, 101	0

All (260) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	23	ILE	6.2
1	E	311	TYR	5.3
1	E	289	PHE	5.3
2	H	71	PHE	5.2
1	G	14	ALA	5.0
1	E	293	GLY	5.0
1	E	312	PHE	4.9
2	H	187	ILE	4.6
2	D	20	ALA	4.5
2	H	181	LEU	4.5
2	B	24	PRO	4.4
1	G	250	PHE	4.4
1	G	294	PRO	4.3
2	D	197	ASP	4.3
1	C	250	PHE	4.3
1	E	14	ALA	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	H	239	VAL	4.2
1	C	249	VAL	4.2
1	C	311	TYR	4.2
1	G	311	TYR	4.2
1	C	289	PHE	4.2
1	E	291	ALA	4.2
1	A	311	TYR	4.1
1	G	299	TYR	4.0
2	H	180	ILE	3.8
1	A	14	ALA	3.8
1	E	250	PHE	3.8
2	H	24	PRO	3.7
2	D	190	ILE	3.7
2	H	198	TYR	3.7
1	E	292	GLY	3.7
1	G	295	GLY	3.7
1	G	231	THR	3.6
1	C	288	SER	3.6
1	C	312	PHE	3.6
1	G	249	VAL	3.6
2	F	187	ILE	3.6
2	H	190	ILE	3.6
1	E	249	VAL	3.6
1	C	290	SER	3.6
1	C	230	ILE	3.6
2	F	190	ILE	3.6
2	H	171	TYR	3.5
2	H	195	LEU	3.5
2	D	245	ARG	3.4
2	F	20	ALA	3.4
1	G	289	PHE	3.4
2	H	68	THR	3.4
1	A	253	LEU	3.4
1	E	295	GLY	3.4
1	A	250	PHE	3.4
1	G	230	ILE	3.4
2	F	245	ARG	3.3
2	H	247	PRO	3.3
2	H	248	LEU	3.3
2	H	184	ILE	3.3
1	A	312	PHE	3.2
1	C	468	SER	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	236	GLU	3.2
1	G	291	ALA	3.1
2	B	245	ARG	3.1
2	H	72	LEU	3.1
2	H	455	TYR	3.1
1	E	288	SER	3.1
1	C	292	GLY	3.1
2	H	240	PRO	3.1
2	H	63	VAL	3.1
2	F	198	TYR	3.0
2	H	456	ILE	3.0
2	H	211	ALA	3.0
2	H	84	PRO	3.0
1	E	253	LEU	3.0
1	G	298	MET	3.0
2	H	60	ALA	3.0
2	H	451	PRO	2.9
2	H	226	GLN	2.9
2	H	209	VAL	2.9
2	H	30	LYS	2.9
2	H	445	GLY	2.9
2	F	424	ASP	2.9
2	H	208	MET	2.9
2	H	251	PHE	2.9
2	H	69	ALA	2.8
1	A	295	GLY	2.8
1	G	439	LYS	2.8
2	H	246	GLY	2.8
1	G	252	ASN	2.8
2	H	139	ALA	2.8
2	F	133	SER	2.8
2	H	335	LEU	2.8
1	A	289	PHE	2.8
2	H	342	THR	2.7
2	H	79	GLY	2.7
2	F	88	ILE	2.7
2	H	258	ILE	2.7
2	H	233	PRO	2.7
2	H	133	SER	2.7
2	H	434	LEU	2.7
2	H	86	GLN	2.7
1	E	256	LEU	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	H	245	ARG	2.7
2	H	34	GLY	2.6
2	H	244	PRO	2.6
1	A	249	VAL	2.6
2	H	109	VAL	2.6
2	H	232	VAL	2.6
2	H	131	THR	2.6
2	H	203	TYR	2.6
2	D	140	ILE	2.6
2	F	244	PRO	2.6
1	A	288	SER	2.6
2	H	269	ALA	2.6
2	H	57	GLY	2.6
2	H	254	GLY	2.6
1	E	294	PRO	2.6
2	H	129	ILE	2.6
2	H	351	LEU	2.6
2	B	239	VAL	2.6
2	F	302	GLY	2.6
1	G	253	LEU	2.6
1	C	303	TYR	2.6
2	B	27	ARG	2.5
1	A	408	MET	2.5
2	D	23	ILE	2.5
2	H	340	ILE	2.5
1	A	470	SER	2.5
1	E	252	ASN	2.5
1	E	313	VAL	2.5
2	B	452	ASN	2.5
1	A	231	THR	2.5
1	E	290	SER	2.5
2	H	447	THR	2.5
2	H	199	ILE	2.5
2	F	181	LEU	2.5
2	H	126	LEU	2.5
2	B	44	ASN	2.5
1	E	16	THR	2.5
2	F	140	ILE	2.4
2	H	95	ILE	2.4
2	H	148	ILE	2.4
2	H	104	SER	2.4
2	H	183	PRO	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	H	64	LYS	2.4
2	H	169	ILE	2.4
1	E	141	TYR	2.4
1	G	312	PHE	2.4
2	D	239	VAL	2.4
2	F	304	ASN	2.4
2	H	134	VAL	2.4
1	E	298	MET	2.4
2	F	428	MET	2.4
2	F	60	ALA	2.4
1	C	253	LEU	2.4
2	H	444	LEU	2.4
2	D	71	PHE	2.4
2	H	441	MET	2.4
1	G	290	SER	2.3
2	H	135	LEU	2.3
2	H	145	ASP	2.3
2	F	224	TYR	2.3
2	H	204	LYS	2.3
2	H	292	VAL	2.3
2	H	261	ASN	2.3
2	F	240	PRO	2.3
1	E	287	GLY	2.3
2	H	337	GLY	2.3
2	H	137	ASN	2.3
2	D	303	THR	2.3
2	H	176	LEU	2.3
1	E	297	GLY	2.2
2	D	201	LYS	2.2
2	F	21	SER	2.2
2	H	235	SER	2.2
2	H	270	ILE	2.2
1	A	15	ARG	2.2
2	D	261	ASN	2.2
2	H	182	GLY	2.2
2	H	188	LYS	2.2
2	F	221	LEU	2.2
2	B	37	ILE	2.2
2	F	229	PHE	2.2
1	G	248	PRO	2.2
2	F	239	VAL	2.2
2	F	65	ASN	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	F	176	LEU	2.2
2	H	263	LEU	2.2
1	C	16	THR	2.2
2	F	254	GLY	2.2
2	F	196	LYS	2.2
2	H	259	LYS	2.2
1	E	405	VAL	2.1
2	H	250	VAL	2.1
2	H	38	ALA	2.1
2	H	316	ASN	2.1
2	H	130	LEU	2.1
1	A	294	PRO	2.1
1	E	248	PRO	2.1
2	H	284	VAL	2.1
2	H	442	VAL	2.1
1	G	16	THR	2.1
1	G	297	GLY	2.1
2	F	303	THR	2.1
2	H	90	LEU	2.1
2	H	460	LEU	2.1
2	D	88	ILE	2.1
2	D	185	LYS	2.1
2	F	64	LYS	2.1
2	H	201	LYS	2.1
1	G	254	PRO	2.1
2	H	54	VAL	2.1
2	B	35	LEU	2.1
2	D	253	ARG	2.1
2	D	129	ILE	2.1
2	H	352	ILE	2.1
2	H	363	ILE	2.1
2	H	102	TYR	2.1
2	B	30	LYS	2.1
2	H	175	PRO	2.1
2	H	450	VAL	2.1
1	A	252	ASN	2.1
2	D	241	LEU	2.1
2	F	135	LEU	2.1
2	H	44	ASN	2.1
2	H	99	LEU	2.1
2	H	446	ASN	2.1
1	E	251	GLY	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	H	179	THR	2.1
2	D	42	ILE	2.1
2	H	234	LYS	2.1
2	H	197	ASP	2.1
1	E	468	SER	2.1
2	H	237	SER	2.1
2	F	84	PRO	2.1
2	H	326	PHE	2.0
1	C	252	ASN	2.0
2	F	44	ASN	2.0
2	H	65	ASN	2.0
2	H	241	LEU	2.0
1	C	287	GLY	2.0
2	B	246	GLY	2.0
1	A	16	THR	2.0
1	E	231	THR	2.0
2	B	140	ILE	2.0
2	F	447	THR	2.0
2	H	196	LYS	2.0
1	A	17	ASP	2.0
1	A	290	SER	2.0
1	C	294	PRO	2.0
1	G	303	TYR	2.0
2	H	217	ASP	2.0
2	H	163	PHE	2.0
2	H	257	PHE	2.0
2	H	215	ALA	2.0
2	B	196	LYS	2.0
2	H	268	ILE	2.0
2	F	233	PRO	2.0
1	G	310	TYR	2.0
2	B	133	SER	2.0
2	H	267	HIS	2.0
2	H	432	TYR	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 [i](#)

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($\text{\AA}^2$)	Q<0.9
3	EPE	G	489	15/15	0.91	0.15	70,78,84,85	0
3	EPE	A	489	15/15	0.92	0.14	68,73,80,81	0
4	ZN	F	503	1/1	0.95	0.06	84,84,84,84	0
4	ZN	D	502	1/1	0.97	0.05	79,79,79,79	0
4	ZN	B	501	1/1	0.98	0.04	62,62,62,62	0
4	ZN	H	504	1/1	0.98	0.12	101,101,101,101	0

6.5 Other polymers [i](#)

There are no such residues in this entry.