Full wwPDB X-ray Structure Validation Report (i)

Jan 30, 2024 – 06:37 PM EST

PDB ID	:	1HR6
Title	:	Yeast Mitochondrial Processing Peptidase
Authors	:	Taylor, A.B.; Smith, B.S.; Kitada, S.; Kojima, K.; Miyaura, H.; Otwinowski, Z.; Ito, A.; Deisenhofer, J.
Deposited on	:	2000-12-21
Resolution	:	2.50 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

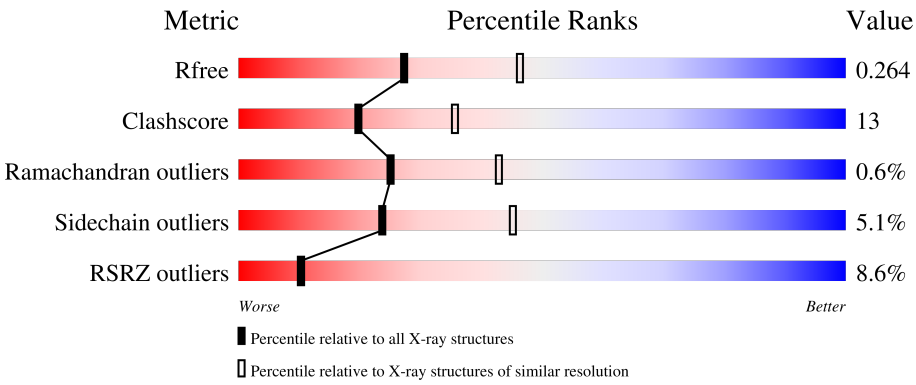
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 <=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	6% 72% 22% • •
1	C	475	4% 72% 21% • 5%
1	E	475	6% 73% 21% • •
1	G	475	6% 70% 23% • •
2	B	443	4% 72% 25% • •

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Mol	Chain	Length	Quality of chain
2	D	443	7% 72% 25%
2	F	443	5% 71% 27%
2	H	443	30% 67% 29%

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	457	3531	2233	599	680	19	0	0	0
1	C	453	3503	2218	592	674	19	0	0	0
1	E	455	3519	2227	597	676	19	0	0	0
1	G	457	3531	2233	599	680	19	0	0	0

There are 32 discrepancies between the modelled and reference sequences:

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

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

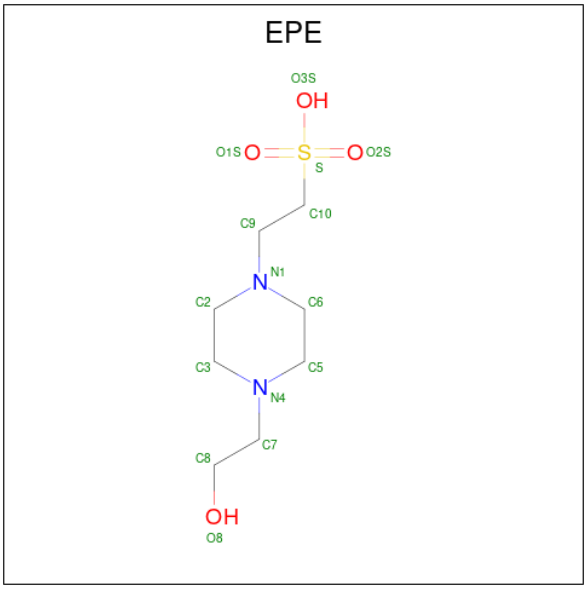
- Molecule 2 is a protein called MITOCHONDRIAL PROCESSING PEPTIDASE BETA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	439	3414	2148	590	669	7	0	0	0
			Total	C	N	O	S			
2	D	443	3442	2165	595	675	7	0	0	0
			Total	C	N	O	S			
2	F	443	3442	2165	595	675	7	0	0	0
			Total	C	N	O	S			
2	H	440	3422	2154	591	670	7	0	0	0

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 (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



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

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 5 is water.

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

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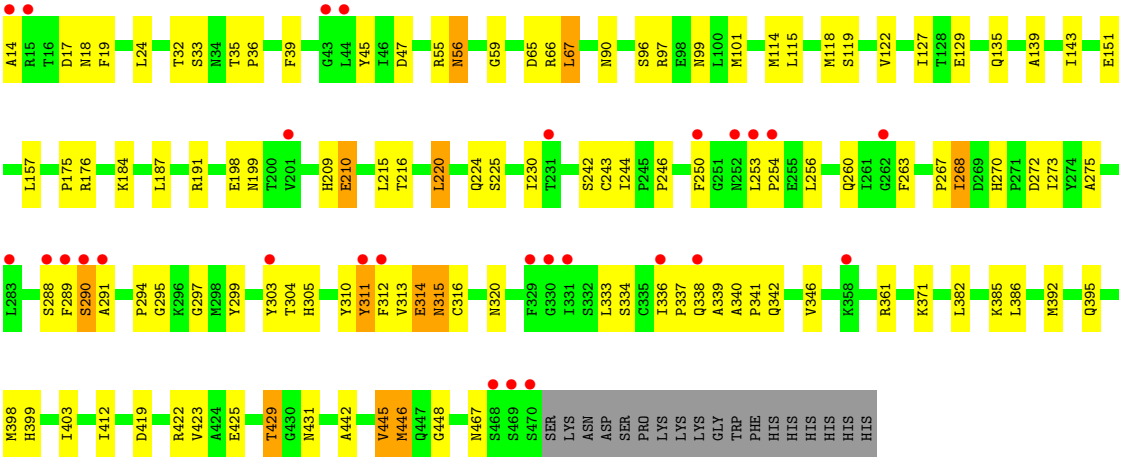
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	C	28	28	28	0	0
			Total	O		
5	D	21	21	21	0	0
			Total	O		
5	E	35	35	35	0	0
			Total	O		
5	F	10	10	10	0	0
			Total	O		
5	G	25	25	25	0	0
			Total	O		
5	H	3	3	3	0	0

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.

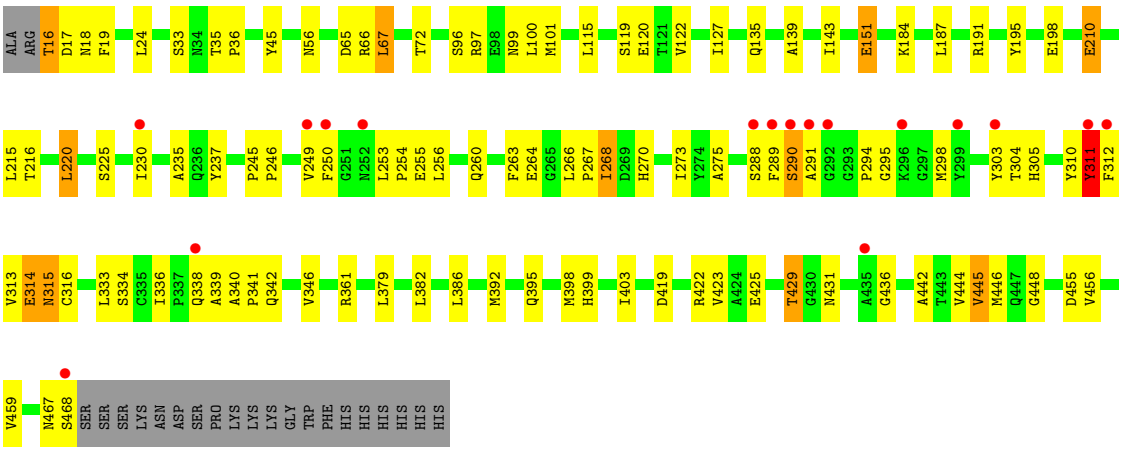
• Molecule 1: MITOCHONDRIAL PROCESSING PEPTIDASE ALPHA SUBUNIT

Chain A:



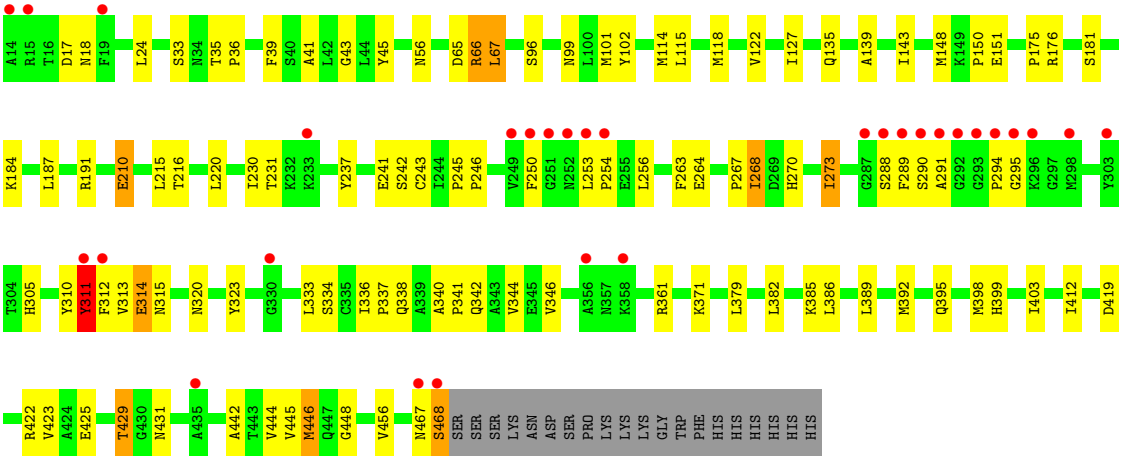
• Molecule 1: MITOCHONDRIAL PROCESSING PEPTIDASE ALPHA SUBUNIT

Chain C:



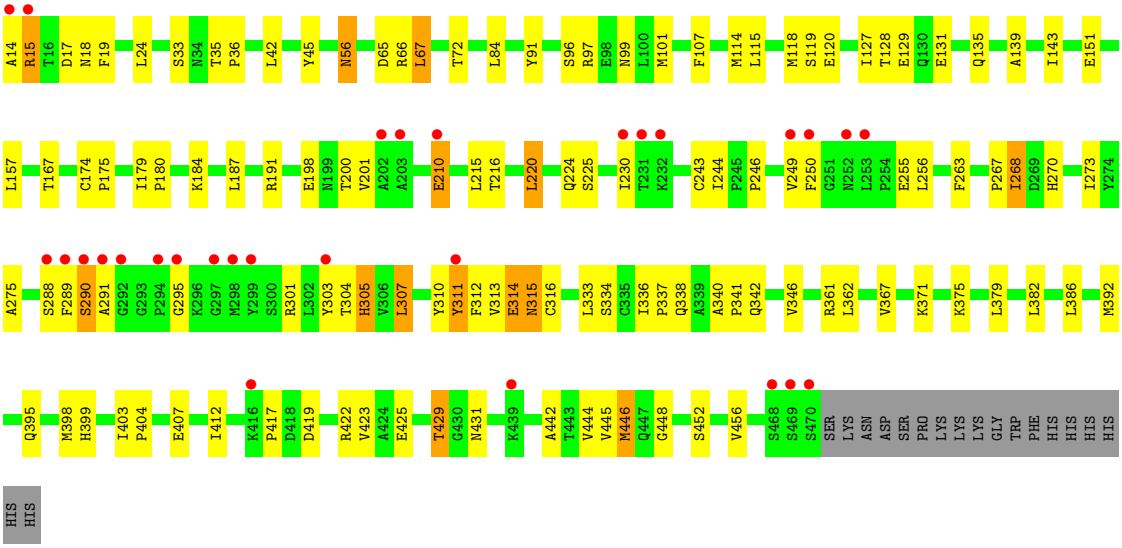
• Molecule 1: MITOCHONDRIAL PROCESSING PEPTIDASE ALPHA SUBUNIT

Chain E:



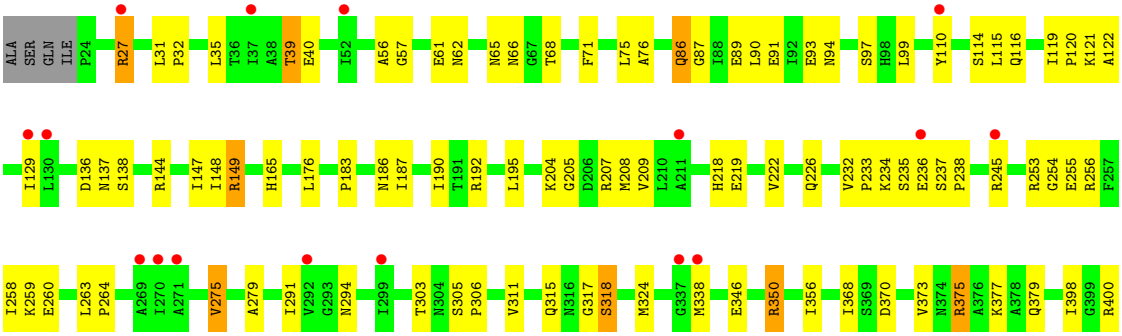
- Molecule 1: MITOCHONDRIAL PROCESSING PEPTIDASE ALPHA SUBUNIT

Chain G:



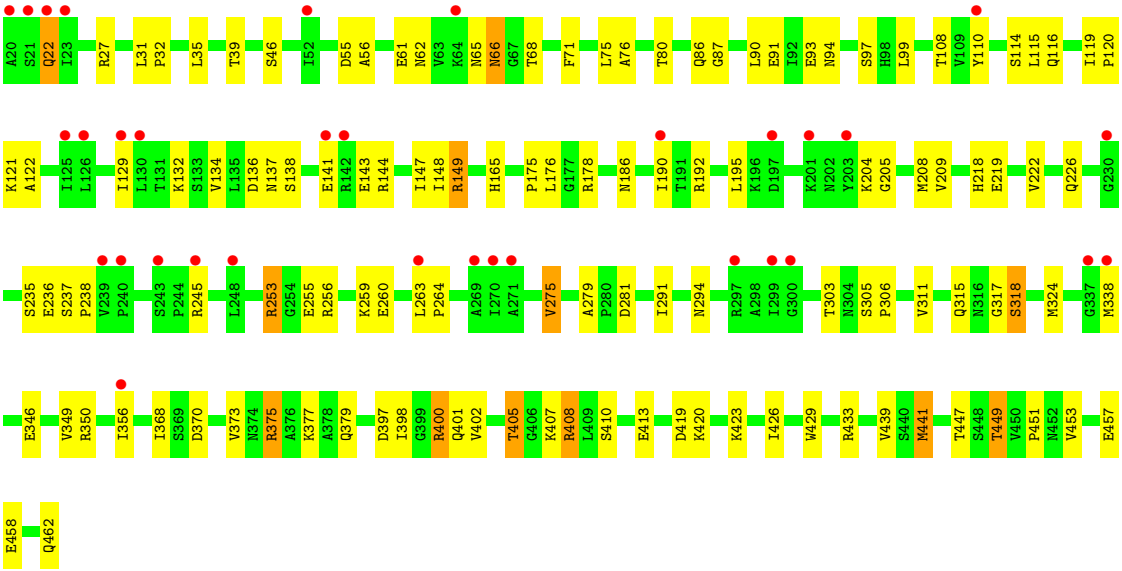
- Molecule 2: MITOCHONDRIAL PROCESSING PEPTIDASE BETA SUBUNIT

Chain B:



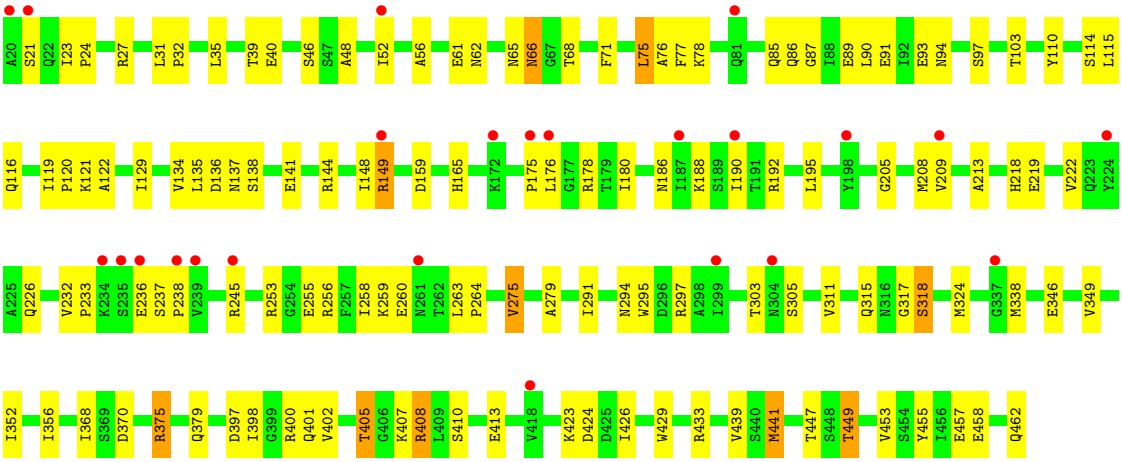
• Molecule 2: MITOCHONDRIAL PROCESSING PEPTIDASE BETA SUBUNIT

Chain D:



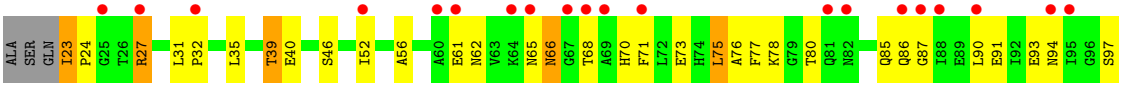
• Molecule 2: MITOCHONDRIAL PROCESSING PEPTIDASE BETA SUBUNIT

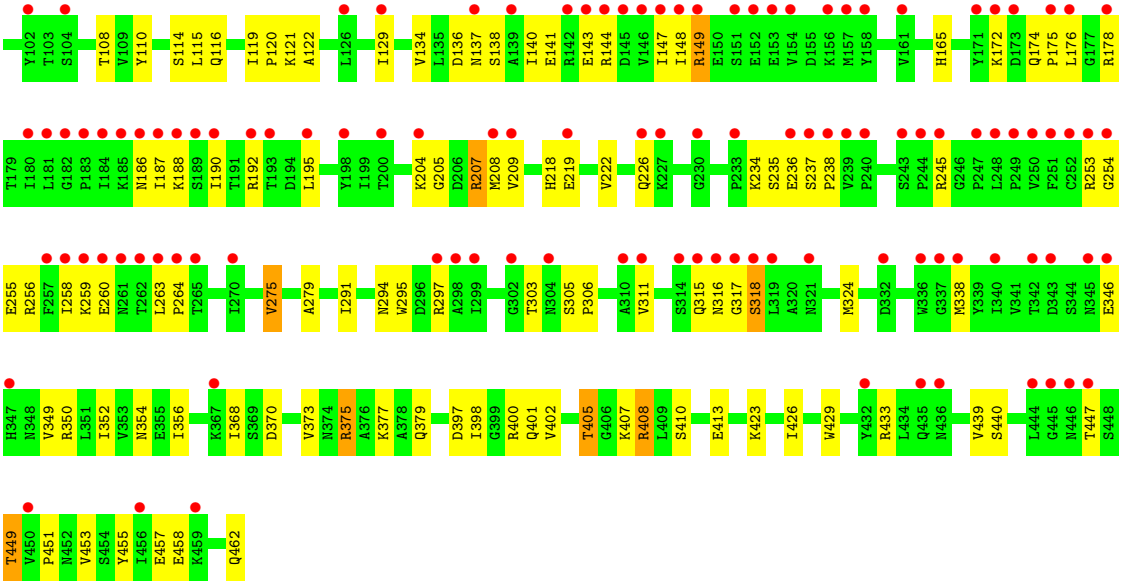
Chain F:



• Molecule 2: MITOCHONDRIAL PROCESSING PEPTIDASE BETA SUBUNIT

Chain H:




Y102 T103 S104 T108 V109 Y110 S114 L115 Q116 I119 P120 K121 A122 L126 I129 V134 L135 D136 N137 S138 A139 I140 E141 R142 E143 R144 D145 V146 I147 I148 R149 E150 S151 E152 E153 V154 D155 K156 M157 Y158 V161 H165 Y171 K172 D173 Q174 P175 L176 G177 R178
T179 I180 L181 G182 P183 I184 K185 N186 I187 K188 S189 I190 T191 R192 T193 D194 L195 Y198 I199 T200 K204 G205 D206 R207 M208 V209 H218 E219 V222 Q226 K227 G230 P233 K234 S235 E236 S237 P238 V239 P240 S243 P244 R245 G246 P247 L248 P249 V250 F251 C252 R253 G254
E255 R256 F257 I258 K259 E260 N261 T262 L263 P264 T265 I270 V275 A279 I291 N294 W295 D296 R297 A298 I299 G302 T303 N304 S305 P306 A310 V311 S314 Q315 N316 G317 S318 L319 A320 N321 M324 D332 W336 G337 M338 Y339 I340 V341 T342 D343 S344 N345 E346
H347 N348 V349 R350 L351 I352 V353 N354 E355 I356 K367 I368 S369 D370 V373 N374 R375 A376 K377 A378 Q379 D397 I398 G399 R400 Q401 V402 T405 G406 K407 R408 L409 S410 E413 K423 I426 W429 Y432 R433 L434 Q435 N436 V439 S440 L444 G445 N446 T447 S448
T449 V450 P451 N452 V453 S454 Y455 I456 E457 E458 K459 Q462

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	134.18Å 178.50Å 202.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.96 – 2.50 29.96 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.4 (29.96-2.50) 99.1 (29.96-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.68 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.245 , 0.279 0.234 , 0.264	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 , 44.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.70	4/3604 (0.1%)	0.77	3/4877 (0.1%)
1	C	0.66	1/3576 (0.0%)	0.76	1/4840 (0.0%)
1	E	0.63	2/3592 (0.1%)	0.83	4/4861 (0.1%)
1	G	0.62	0/3604	0.76	3/4877 (0.1%)
2	B	0.62	0/3478	0.80	5/4720 (0.1%)
2	D	0.57	0/3506	0.84	6/4759 (0.1%)
2	F	0.53	0/3506	0.75	4/4759 (0.1%)
2	H	0.56	2/3486 (0.1%)	0.87	7/4732 (0.1%)
All	All	0.61	9/28352 (0.0%)	0.80	33/38425 (0.1%)

All (9) bond length outliers are listed below:

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

All (33) bond angle outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	149	ARG	NE-CZ-NH1	16.11	128.35	120.30
2	H	207	ARG	NE-CZ-NH1	-15.68	112.46	120.30
1	E	422	ARG	NE-CZ-NH2	14.66	127.63	120.30
2	H	207	ARG	NE-CZ-NH2	14.49	127.55	120.30
2	B	350	ARG	NE-CZ-NH2	8.93	124.76	120.30
1	E	311	TYR	CB-CG-CD1	-8.77	115.74	121.00
2	D	253	ARG	CD-NE-CZ	8.43	135.41	123.60
2	H	149	ARG	CD-NE-CZ	7.92	134.69	123.60
2	B	350	ARG	NE-CZ-NH1	-7.47	116.56	120.30
1	E	422	ARG	CD-NE-CZ	7.26	133.76	123.60
2	H	207	ARG	CD-NE-CZ	6.66	132.93	123.60
1	G	422	ARG	NE-CZ-NH2	-6.55	117.02	120.30
2	B	253	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	G	97	ARG	NE-CZ-NH1	-6.49	117.06	120.30
1	G	422	ARG	NE-CZ-NH1	6.48	123.54	120.30
2	D	149	ARG	NE-CZ-NH2	6.20	123.40	120.30
2	H	253	ARG	NE-CZ-NH1	6.04	123.32	120.30
2	D	149	ARG	NE-CZ-NH1	-6.03	117.28	120.30
2	F	253	ARG	NE-CZ-NH1	6.01	123.30	120.30
1	C	422	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	A	422	ARG	NE-CZ-NH2	-5.90	117.35	120.30
2	F	149	ARG	NE-CZ-NH2	5.83	123.21	120.30
2	F	149	ARG	NE-CZ-NH1	-5.62	117.49	120.30
1	A	97	ARG	NE-CZ-NH1	-5.61	117.50	120.30
2	B	149	ARG	NE-CZ-NH2	5.52	123.06	120.30
2	F	253	ARG	NE-CZ-NH2	-5.36	117.62	120.30
2	B	408	ARG	NE-CZ-NH1	5.20	122.90	120.30
2	D	350	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	A	422	ARG	NE-CZ-NH1	5.03	122.81	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (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	3531	0	3488	85	0
1	C	3503	0	3460	84	0
1	E	3519	0	3478	70	0
1	G	3531	0	3488	97	0
2	B	3414	0	3412	97	0
2	D	3442	0	3440	92	0
2	F	3442	0	3440	90	0
2	H	3422	0	3422	113	0
3	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	703	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (703) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:230:ILE:HD12	1:E:230:ILE:H	1.51	0.76
1:C:425:GLU:O	1:C:429:THR:HB	1.87	0.75
1:G:96:SER:HB3	1:G:99:ASN:OD1	1.87	0.75
2:D:338:MET:HG2	2:D:356:ILE:HD13	1.69	0.74
1:E:295:GLY:HA2	2:F:93:GLU:HG2	1.69	0.74
1:G:230:ILE:HD12	1:G:230:ILE:N	2.02	0.74
2:B:294:ASN:HD22	2:B:324:MET:CA	1.99	0.73
2:D:144:ARG:O	2:D:148:ILE:HG12	1.87	0.73
2:F:144:ARG:O	2:F:148:ILE:HG12	1.87	0.73
2:H:76:ALA:HB1	2:H:129:ILE:CG2	2.19	0.73
2:H:294:ASN:HD22	2:H:324:MET:CA	1.96	0.73
2:B:458:GLU:O	2:B:462:GLN:HB2	1.89	0.72
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
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
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: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
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
2:F:256:ARG:HG3	2:F:256:ARG:NH1	2.05	0.67
1:G:14:ALA:N	1:G:17:ASP:OD2	2.27	0.67
2:D:458:GLU:O	2:D:462:GLN:HB2	1.94	0.67
2:H:119:ILE:O	2:H:122:ALA:HB3	1.95	0.67
1:G:429:THR:HG21	1:G:431:ASN:HD22	1.60	0.67
2:B:186:ASN:O	2:B:190:ILE:HG12	1.94	0.66
2:H:116:GLN:O	2:H:119:ILE:HG12	1.95	0.66

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
2:B:165:HIS:CD2	2:B:258:ILE:HD11	2.36	0.60
1:A:139:ALA:O	1:A:143:ILE:HD13	2.01	0.60
1:G:315:ASN:HD22	1:G:315:ASN:C	2.04	0.60
1:E:243:CYS:HA	1:E:446:MET:O	2.02	0.60
1:A:224:GLN:CD	1:G:129:GLU:HG3	2.22	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:G:311:TYR:C	1:G:313:VAL:H	2.06	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
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
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: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:236:GLU:C	2:D:238:PRO:HD3	2.25	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:G:19:PHE:HD1	1:G:392:MET:HE1	1.68	0.56
1:E:268:ILE:HD13	1:E:268:ILE:N	2.20	0.56
1:E:311:TYR:C	1:E:313:VAL:H	2.09	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:F:291:ILE:HD12	2:F:426:ILE:HD13	1.88	0.56
1:G:311:TYR:C	1:G:313:VAL:N	2.55	0.56
2:D:405:THR:HG22	2:D:407:LYS:H	1.70	0.56
1:A:99:ASN:HB2	1:A:101:MET:HE3	1.88	0.56
1:A:336:ILE:HG22	1:A:338:GLN:OE1	2.04	0.56
1:E:333:LEU:HD13	1:E:334:SER:N	2.20	0.56
1:E:311:TYR:C	1:E:313:VAL:N	2.58	0.56
2:F:218:HIS:O	2:F:222:VAL:HG23	2.06	0.56
1:A: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
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:A:311:TYR:C	1:A:313:VAL:H	2.08	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
1:C:19:PHE:HD1	1:C:392:MET:HE1	1.72	0.54
2:F:119:ILE:N	2:F:120:PRO:HD2	2.22	0.54
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:A:99:ASN:HB2	1:A:101:MET:CE	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1: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
1:A:311:TYR:C	1:A:313:VAL:N	2.60	0.53
2:B:90:LEU:HD13	2:B:94:ASN:ND2	2.22	0.53
1:G:403:ILE:HG23	1:G:403:ILE:O	2.07	0.53
2:H:237:SER:N	2:H:238:PRO:HD3	2.23	0.53
2:H:303:THR:HG22	2:H:305:SER:N	2.24	0.53
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:C:311:TYR:C	1:C:313:VAL:H	2.11	0.53
1:E:429:THR:HG22	1:E:431:ASN:HD22	1.74	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
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
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:19:PHE:HD1	1:A:392:MET:HE1	1.75	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:THR:HG22	1:A:431:ASN:HD22	1.73	0.52
2: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
2:D:76:ALA:O	2:D:129:ILE:HG23	2.10	0.51
1:C:33:SER:HB3	1:C:392:MET:HE3	1.90	0.51
2: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
1:C:311:TYR:C	1:C:313:VAL:N	2.60	0.51
2:D:115:LEU:HD12	2:D:115:LEU:H	1.75	0.51
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:99:ASN:HB2	1:E:101:MET:CE	2.42	0.50
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
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
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
2:D:62:ASN:CG	2:D:65:ASN:HB2	2.32	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:62:ASN:CG	2:B:65:ASN:HB2	2.33	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
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
1:A:176:ARG:NH2	1:E:242:SER:OG	2.46	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: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
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: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
1:C:403:ILE:O	1:C:403:ILE:HG23	2.13	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
2:H:62:ASN:CG	2:H:65:ASN:HB2	2.33	0.48
1:A:67:LEU:HD13	1:A:135:GLN:HG3	1.95	0.48
2:F:62:ASN:CG	2:F:65:ASN:HB2	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
2:F:75:LEU:HA	2:F:78:LYS:HG2	1.96	0.47
1:G:210:GLU:OE1	1:G:210:GLU:HA	2.14	0.47
1:A:336:ILE:HG22	1:A:337:PRO:HD2	1.97	0.47
1:G:157:LEU:HD11	1:G:244:ILE:HD13	1.95	0.47
2:B:90:LEU:CD1	2:B:94:ASN:HD21	2.28	0.47
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: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
1:G:99:ASN:HB2	1:G:101:MET:CE	2.44	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
2:F:236:GLU:C	2:F:238:PRO:HD3	2.34	0.47
1:G:119:SER:HB2	1:G:220:LEU:CD1	2.45	0.47
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
2:H:204:LYS:HG3	2:H:235:SER:OG	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:99:ASN:HB2	1:C:101:MET:CE	2.45	0.46
2:H:317:GLY:O	2:H:318:SER:CB	2.62	0.46
1:E:467:ASN:O	1:E:468:SER:HB2	2.15	0.46
1:G:114:MET:HE2	1:G:118:MET:HG3	1.96	0.46
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:253:ARG:HH21	2:D:457:GLU:CD	2.19	0.46
2:D:263:LEU:HA	2:D:264:PRO:HD3	1.79	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:C:315:ASN:C	1:C:315:ASN:ND2	2.68	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
1:A:371:LYS:HE3	1:A:412:ILE:O	2.17	0.45

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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: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:A:315:ASN:C	1:A:315:ASN:ND2	2.69	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
2:B:441:MET:HE1	2:B:451:PRO:O	2.17	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
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: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:F:165:HIS:CD2	2:F:258:ILE:HD11	2.52	0.45
2:H:144:ARG:HH21	2:H:188:LYS:C	2.21	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
1:G:115:LEU:HD23	1:G:215:LEU:HB3	1.98	0.45
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:80:THR:C	2:H:134:VAL:HG23	2.37	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:C:151:GLU:CD	1:C:151:GLU:H	2.20	0.44
1:G:99:ASN:HB2	1:G:101:MET:HE2	1.98	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: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
1:E:267:PRO:HA	1:E:323:TYR:O	2.17	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
1:C:467:ASN:CG	1:C:468:SER:N	2.71	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
2:B:236:GLU:C	2:B:238:PRO:HD3	2.38	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
1:E:263:PHE:CE2	1:E:442:ALA:HB2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:87:GLY:O	2:F:91:GLU:HB2	2.18	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
1:E:99:ASN:HB2	1:E:101:MET:HE3	2.00	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:87:GLY:O	2:D:91:GLU:HB2	2.18	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
1:C:304:THR:HG22	1:C:305:HIS:ND1	2.33	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
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
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:19:PHE:CD1	1:G:392:MET:CE	3.01	0.43
1:G:200:THR:HG22	1:G:201:VAL:N	2.34	0.43
1:G:315:ASN:C	1:G:315:ASN:ND2	2.69	0.43
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:455:TYR:CD1	2:F:455:TYR:C	2.92	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
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:C:19:PHE:CD1	1:C:392:MET:CE	3.02	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
2:H:455:TYR:CD1	2:H:455:TYR:C	2.92	0.42
1:A:333:LEU:HD13	1:A:334:SER:N	2.34	0.42
2:B:147:ILE:HG22	2:B:187:ILE:HD13	2.00	0.42
1:G:72:THR:HG21	1:G:120:GLU:HB3	2.00	0.42
2:H:209:VAL:HG21	2:H:402:VAL:HG12	2.00	0.42
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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:114:MET:HE2	1:A:118:MET:HG3	2.01	0.41
1:C:253:LEU:HA	1:C:254:PRO:HD3	1.87	0.41
2:H: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
2:F:144:ARG:HH21	2:F:188:LYS:C	2.24	0.41
1:G:289:PHE:HE2	1:G:291:ALA:HB2	1.79	0.41
2:H:172:LYS:O	2:H:174:GLN:HG3	2.20	0.41
1:A:122:VAL:O	1:A:191:ARG:NH2	2.54	0.41
1:C:72:THR:HG21	1:C:120:GLU:HB3	2.03	0.41
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
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: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:19:PHE:CD1	1:C:392:MET:HE2	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:114:MET:HE2	1:E:118:MET:HG3	2.02	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
2:B:97:SER:CB	2:B:114:SER:HB3	2.50	0.40
1:G:119:SER:HB2	1:G:220:LEU:HD13	2.02	0.40
1:G:174:CYS:O	1:G:175:PRO:C	2.60	0.40
2:H:350:ARG:HG3	2:H:451:PRO:HB3	2.02	0.40
1:A: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:429:THR:CG2	1:A:429:THR:O	2.70	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
2:D:55:ASP:OD1	2:D:55:ASP:C	2.59	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: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:80:THR:C	2:D:134:VAL:HG23	2.41	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:HG23	2:H:52:ILE:O	2.20	0.40
1:A:17:ASP:O	1:A:18:ASN:HB3	2.22	0.40
2:B:234:LYS:HB2	2:B:234:LYS:HE3	1.82	0.40
2:D:279:ALA:HB1	2:D:281:ASP:OD1	2.21	0.40
2:D:441:MET:HE1	2:D:451:PRO:O	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
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%)	34	54
1	C	451/475 (95%)	433 (96%)	16 (4%)	2 (0%)	34	54
1	E	453/475 (95%)	435 (96%)	16 (4%)	2 (0%)	34	54
1	G	455/475 (96%)	434 (95%)	17 (4%)	4 (1%)	17	31
2	B	437/443 (99%)	423 (97%)	11 (2%)	3 (1%)	22	39
2	D	441/443 (100%)	426 (97%)	12 (3%)	3 (1%)	22	39
2	F	441/443 (100%)	425 (96%)	13 (3%)	3 (1%)	22	39
2	H	438/443 (99%)	423 (97%)	11 (2%)	4 (1%)	17	31
All	All	3571/3672 (97%)	3435 (96%)	113 (3%)	23 (1%)	25	43

All (23) Ramachandran outliers are listed below:

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

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

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	384/401 (96%)	364 (95%)	20 (5%)	23	44
1	C	381/401 (95%)	360 (94%)	21 (6%)	21	41
1	E	382/401 (95%)	360 (94%)	22 (6%)	20	38
1	G	384/401 (96%)	361 (94%)	23 (6%)	19	37
2	B	376/379 (99%)	359 (96%)	17 (4%)	27	51
2	D	379/379 (100%)	362 (96%)	17 (4%)	27	51
2	F	379/379 (100%)	361 (95%)	18 (5%)	26	49
2	H	377/379 (100%)	360 (96%)	17 (4%)	27	51
All	All	3042/3120 (98%)	2887 (95%)	155 (5%)	24	45

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

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

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

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Mol	Chain	Res	Type
1	C	361	ARG
1	C	382	LEU
1	C	386	LEU
1	C	399	HIS
1	C	429	THR
1	C	445	VAL
1	C	446	MET
2	D	27	ARG
2	D	39	THR
2	D	66	ASN
2	D	71	PHE
2	D	75	LEU
2	D	86	GLN
2	D	149	ARG
2	D	176	LEU
2	D	219	GLU
2	D	275	VAL
2	D	346	GLU
2	D	375	ARG
2	D	400	ARG
2	D	405	THR
2	D	408	ARG
2	D	441	MET
2	D	449	THR
1	E	56	ASN
1	E	65	ASP
1	E	66	ARG
1	E	67	LEU
1	E	151	GLU
1	E	210	GLU
1	E	220	LEU
1	E	268	ILE
1	E	273	ILE
1	E	288	SER
1	E	305	HIS
1	E	311	TYR
1	E	314	GLU
1	E	320	ASN
1	E	361	ARG
1	E	382	LEU
1	E	386	LEU
1	E	399	HIS

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

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

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

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

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides 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	$\#\|Z\| > 2$
3	EPE	G	489	-	15,15,15	1.40	2 (13%)	18,20,20	1.02	0
3	EPE	A	489	-	15,15,15	1.27	2 (13%)	18,20,20	1.03	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
3	EPE	G	489	-	-	2/9/19/19	0/1/1/1
3	EPE	A	489	-	-	2/9/19/19	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	489	EPE	C10-S	2.97	1.81	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	489	EPE	C10-S	2.50	1.81	1.77
3	G	489	EPE	C6-N1	2.36	1.53	1.46
3	A	489	EPE	C6-N1	2.01	1.52	1.46

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	489	EPE	C7-N4-C5	-2.08	105.91	111.23

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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	0.21	28 (6%)	21	22	30, 46, 85, 101	0
1	C	453/475 (95%)	0.15	17 (3%)	40	43	31, 49, 82, 101	0
1	E	455/475 (95%)	0.34	30 (6%)	18	19	33, 53, 85, 101	0
1	G	457/475 (96%)	0.33	29 (6%)	20	21	35, 54, 89, 101	0
2	B	439/443 (99%)	0.13	16 (3%)	42	46	28, 49, 75, 96	0
2	D	443/443 (100%)	0.38	33 (7%)	14	15	34, 58, 84, 101	0
2	F	443/443 (100%)	0.47	24 (5%)	25	27	45, 68, 88, 100	0
2	H	440/443 (99%)	1.49	133 (30%)	0	0	54, 78, 93, 100	0
All	All	3587/3672 (97%)	0.43	310 (8%)	10	10	28, 58, 88, 101	0

All (310) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	187	ILE	8.9
2	H	184	ILE	8.7
1	C	289	PHE	8.1
2	F	21	SER	7.9
1	C	290	SER	7.7
2	H	71	PHE	7.5
1	E	289	PHE	7.5
2	H	181	LEU	7.4
1	E	292	GLY	7.1
2	H	188	LYS	7.0
1	E	293	GLY	6.8
2	D	20	ALA	6.7
2	H	171	TYR	6.5
1	G	470	SER	6.4
1	G	311	TYR	6.2
2	D	21	SER	6.1

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Mol	Chain	Res	Type	RSRZ
1	C	291	ALA	6.1
2	F	245	ARG	6.0
1	E	288	SER	6.0
1	G	250	PHE	6.0
1	G	291	ALA	5.9
2	H	149	ARG	5.9
1	G	252	ASN	5.9
1	E	291	ALA	5.7
1	A	469	SER	5.7
2	H	90	LEU	5.7
2	H	445	GLY	5.6
1	C	288	SER	5.6
2	H	245	ARG	5.6
2	H	190	ILE	5.6
1	A	470	SER	5.5
1	G	290	SER	5.4
2	H	251	PHE	5.3
1	E	311	TYR	5.3
1	E	312	PHE	5.3
2	H	226	GLN	5.3
1	A	252	ASN	5.2
1	A	289	PHE	5.2
1	E	14	ALA	5.2
1	G	289	PHE	5.2
2	H	86	GLN	5.2
2	F	20	ALA	5.2
2	H	185	LYS	5.2
1	C	311	TYR	5.1
1	E	252	ASN	5.1
2	H	238	PRO	5.0
2	H	148	ILE	5.0
1	G	469	SER	4.9
1	A	311	TYR	4.9
1	A	14	ALA	4.9
1	C	252	ASN	4.9
1	G	230	ILE	4.8
2	H	367	LYS	4.7
2	H	298	ALA	4.7
1	G	295	GLY	4.6
1	C	312	PHE	4.6
2	H	262	THR	4.6
2	H	145	ASP	4.6

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Mol	Chain	Res	Type	RSRZ
2	H	248	LEU	4.6
2	H	157	MET	4.5
2	H	432	TYR	4.5
2	H	189	SER	4.5
2	D	270	ILE	4.4
2	H	236	GLU	4.4
2	H	65	ASN	4.4
1	G	299	TYR	4.3
2	H	297	ARG	4.3
2	H	198	TYR	4.3
2	H	239	VAL	4.3
2	H	237	SER	4.2
2	D	337	GLY	4.2
1	E	290	SER	4.2
1	C	292	GLY	4.1
2	H	146	VAL	4.1
1	A	250	PHE	4.1
1	E	250	PHE	4.1
2	H	180	ILE	4.0
1	E	468	SER	4.0
1	G	294	PRO	4.0
2	H	258	ILE	4.0
2	B	299	ILE	4.0
1	A	312	PHE	3.9
2	H	249	PRO	3.9
2	H	147	ILE	3.9
1	A	253	LEU	3.9
2	H	299	ILE	3.9
1	E	295	GLY	3.9
2	D	126	LEU	3.8
2	H	317	GLY	3.8
2	H	195	LEU	3.8
2	H	263	LEU	3.8
2	H	126	LEU	3.8
1	E	296	LYS	3.8
2	H	347	HIS	3.8
1	A	290	SER	3.8
1	E	287	GLY	3.8
2	H	68	THR	3.8
1	A	291	ALA	3.7
1	G	14	ALA	3.7
2	H	64	LYS	3.7

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Mol	Chain	Res	Type	RSRZ
2	H	144	ARG	3.7
2	H	153	GLU	3.6
1	E	251	GLY	3.6
2	H	233	PRO	3.6
1	G	249	VAL	3.6
2	H	60	ALA	3.6
1	A	358	LYS	3.6
2	F	190	ILE	3.6
2	H	314	SER	3.6
1	A	15	ARG	3.6
2	H	315	GLN	3.6
1	E	249	VAL	3.5
2	H	137	ASN	3.5
1	G	298	MET	3.5
2	H	173	ASP	3.5
2	F	187	ILE	3.5
2	H	182	GLY	3.5
2	H	337	GLY	3.5
2	H	152	GLU	3.5
2	H	154	VAL	3.5
2	H	32	PRO	3.5
1	G	292	GLY	3.5
1	G	253	LEU	3.4
2	H	25	GLY	3.4
2	F	239	VAL	3.4
1	G	231	THR	3.4
2	D	338	MET	3.4
1	C	250	PHE	3.4
2	D	245	ARG	3.4
2	H	193	THR	3.3
2	H	447	THR	3.3
1	C	468	SER	3.3
2	H	436	ASN	3.3
2	D	129	ILE	3.3
2	H	259	LYS	3.3
2	H	82	ASN	3.3
1	G	297	GLY	3.3
2	H	250	VAL	3.3
2	H	161	VAL	3.2
2	H	311	VAL	3.2
2	H	176	LEU	3.2
2	D	23	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
2	D	248	LEU	3.2
2	H	342	THR	3.2
1	G	203	ALA	3.1
2	H	260	GLU	3.1
2	H	304	ASN	3.1
2	H	446	ASN	3.1
2	H	346	GLU	3.1
1	A	468	SER	3.1
2	H	321	ASN	3.1
2	F	235	SER	3.1
2	H	318	SER	3.1
2	F	81	GLN	3.1
1	G	468	SER	3.1
2	D	130	LEU	3.1
2	H	265	THR	3.0
2	D	52	ILE	3.0
2	H	338	MET	3.0
1	E	358	LYS	3.0
2	H	252	CYS	3.0
2	D	197	ASP	3.0
2	H	192	ARG	3.0
2	F	236	GLU	2.9
1	A	331	ILE	2.9
2	H	158	TYR	2.9
2	H	319	LEU	2.9
1	C	338	GLN	2.9
2	F	149	ARG	2.9
2	H	88	ILE	2.9
2	H	456	ILE	2.9
1	C	299	TYR	2.9
2	H	219	GLU	2.9
2	D	271	ALA	2.8
2	H	444	LEU	2.8
1	E	253	LEU	2.8
2	B	236	GLU	2.8
2	D	110	TYR	2.8
2	D	240	PRO	2.8
1	C	249	VAL	2.8
2	H	264	PRO	2.8
2	D	190	ILE	2.8
2	H	208	MET	2.8
2	H	257	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
2	H	69	ALA	2.7
2	B	27	ARG	2.7
1	G	288	SER	2.7
2	H	156	LYS	2.7
2	F	304	ASN	2.7
1	A	283	LEU	2.7
1	E	15	ARG	2.7
2	B	52	ILE	2.7
2	D	125	ILE	2.7
1	G	439	LYS	2.7
2	H	94	ASN	2.7
2	B	338	MET	2.7
1	A	44	LEU	2.6
2	B	130	LEU	2.6
2	H	240	PRO	2.6
2	F	299	ILE	2.6
2	B	245	ARG	2.6
2	H	332	ASP	2.6
1	A	329	PHE	2.6
1	A	330	GLY	2.6
2	H	253	ARG	2.6
2	H	200	THR	2.5
2	H	310	ALA	2.5
1	C	296	LYS	2.5
2	H	261	ASN	2.5
2	H	244	PRO	2.5
2	H	52	ILE	2.5
2	D	201	LYS	2.5
2	F	234	LYS	2.5
1	E	303	TYR	2.5
2	D	269	ALA	2.5
1	A	254	PRO	2.5
2	H	175	PRO	2.5
2	F	52	ILE	2.5
2	H	270	ILE	2.5
2	F	238	PRO	2.5
1	G	210	GLU	2.5
2	D	356	ILE	2.5
2	H	95	ILE	2.5
2	H	435	GLN	2.4
2	B	271	ALA	2.4
1	A	303	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	303	TYR	2.4
1	A	288	SER	2.4
2	H	243	SER	2.4
2	D	203	TYR	2.4
2	H	102	TYR	2.4
2	D	142	ARG	2.4
2	H	142	ARG	2.4
1	A	201	VAL	2.4
2	F	172	LYS	2.4
2	D	297	ARG	2.4
2	H	227	LYS	2.4
2	D	239	VAL	2.4
2	H	143	GLU	2.4
1	G	15	ARG	2.4
1	G	202	ALA	2.4
2	H	27	ARG	2.4
2	B	292	VAL	2.3
1	A	338	GLN	2.3
2	H	81	GLN	2.3
2	D	141	GLU	2.3
2	D	243	SER	2.3
1	A	262	GLY	2.3
2	H	450	VAL	2.3
2	B	270	ILE	2.3
2	H	209	VAL	2.3
2	H	316	ASN	2.3
2	H	345	ASN	2.3
1	A	231	THR	2.3
2	H	302	GLY	2.3
1	C	230	ILE	2.3
2	H	340	ILE	2.3
2	H	343	ASP	2.3
2	D	263	LEU	2.3
1	G	416	LYS	2.2
2	F	418	VAL	2.2
2	H	87	GLY	2.2
2	H	61	GLU	2.2
1	G	303	TYR	2.2
2	B	337	GLY	2.2
2	F	337	GLY	2.2
1	E	298	MET	2.2
2	H	139	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	269	ALA	2.2
2	F	261	ASN	2.2
2	H	183	PRO	2.2
2	D	299	ILE	2.2
1	E	467	ASN	2.2
2	F	209	VAL	2.2
1	A	336	ILE	2.2
2	H	67	GLY	2.2
2	D	22	GLN	2.1
2	H	172	LYS	2.1
1	C	435	ALA	2.1
2	H	247	PRO	2.1
2	H	104	SER	2.1
2	H	186	ASN	2.1
2	F	224	TYR	2.1
2	H	254	GLY	2.1
1	E	435	ALA	2.1
2	B	211	ALA	2.1
2	H	459	LYS	2.1
1	E	19	PHE	2.1
2	D	230	GLY	2.1
2	B	37	ILE	2.1
2	B	129	ILE	2.1
2	F	176	LEU	2.1
2	H	204	LYS	2.1
1	E	356	ALA	2.1
1	E	254	PRO	2.1
1	E	233	LYS	2.1
2	H	336	TRP	2.1
2	H	129	ILE	2.1
1	A	43	GLY	2.1
1	E	330	GLY	2.1
2	H	230	GLY	2.0
2	H	178	ARG	2.0
2	D	64	LYS	2.0
2	H	151	SER	2.0
2	D	300	GLY	2.0
2	F	198	TYR	2.0
1	G	232	LYS	2.0
2	B	110	TYR	2.0
1	E	294	PRO	2.0
2	F	175	PRO	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	ZN	F	503	1/1	0.83	0.06	84,84,84,84	0
3	EPE	G	489	15/15	0.91	0.26	70,78,84,85	0
4	ZN	H	504	1/1	0.94	0.13	101,101,101,101	0
4	ZN	D	502	1/1	0.95	0.06	79,79,79,79	0
3	EPE	A	489	15/15	0.96	0.22	68,73,80,81	0
4	ZN	B	501	1/1	0.98	0.04	62,62,62,62	0

6.5 Other polymers (i)

There are no such residues in this entry.