



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 07:45 PM UTC

PDB ID : 5K3H / pdb_00005k3h
Title : Crystals structure of Acyl-CoA oxidase-1 in Caenorhabditis elegans, Apo form-II
Authors : Zhang, X.; Li, K.; Jones, R.A.; Bruner, S.D.; Butcher, R.A.
Deposited on : 2016-05-19
Resolution : 2.48 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
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

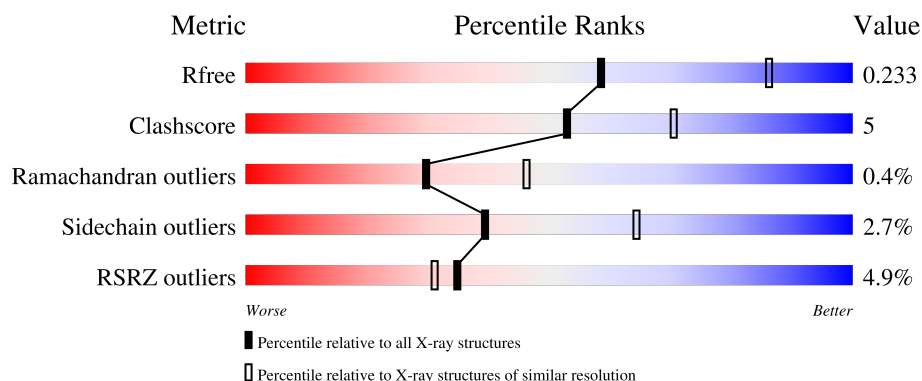
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.48 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	7589 (2.50-2.46)
Clashscore	190562	8295 (2.50-2.46)
Ramachandran outliers	187476	8164 (2.50-2.46)
Sidechain outliers	187428	8166 (2.50-2.46)
RSRZ outliers	180081	7593 (2.50-2.46)

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	684	6% 78% 13% 7%
1	B	684	3% 81% 10% 7%
1	C	684	3% 81% 11% 7%
1	D	684	4% 83% 8% 7%
1	E	684	4% 80% 11% 7%

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Mol	Chain	Length	Quality of chain
1	F	684	9% 78% 13% 7%
1	G	684	4% 82% 10% 7%
1	H	684	4% 81% 10% 7%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 41742 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 Acyl-coenzyme A oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	634	Total	C	N	O	S	0	0	0
			5036	3199	885	928	24			
1	B	635	Total	C	N	O	S	0	0	0
			5039	3198	887	931	23			
1	C	633	Total	C	N	O	S	0	0	0
			5023	3190	885	925	23			
1	D	634	Total	C	N	O	S	0	0	0
			5035	3196	886	930	23			
1	E	635	Total	C	N	O	S	0	0	0
			5036	3197	887	929	23			
1	F	633	Total	C	N	O	S	0	0	0
			5030	3193	885	929	23			
1	G	634	Total	C	N	O	S	0	0	0
			5032	3195	886	928	23			
1	H	634	Total	C	N	O	S	0	0	0
			5035	3196	886	930	23			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	675	HIS	-	expression tag	UNP O62140
A	676	HIS	-	expression tag	UNP O62140
A	677	HIS	-	expression tag	UNP O62140
A	678	HIS	-	expression tag	UNP O62140
A	679	HIS	-	expression tag	UNP O62140
A	680	HIS	-	expression tag	UNP O62140
A	681	HIS	-	expression tag	UNP O62140
A	682	HIS	-	expression tag	UNP O62140
A	683	HIS	-	expression tag	UNP O62140
A	684	HIS	-	expression tag	UNP O62140
B	675	HIS	-	expression tag	UNP O62140
B	676	HIS	-	expression tag	UNP O62140
B	677	HIS	-	expression tag	UNP O62140

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Chain	Residue	Modelled	Actual	Comment	Reference
B	678	HIS	-	expression tag	UNP O62140
B	679	HIS	-	expression tag	UNP O62140
B	680	HIS	-	expression tag	UNP O62140
B	681	HIS	-	expression tag	UNP O62140
B	682	HIS	-	expression tag	UNP O62140
B	683	HIS	-	expression tag	UNP O62140
B	684	HIS	-	expression tag	UNP O62140
C	675	HIS	-	expression tag	UNP O62140
C	676	HIS	-	expression tag	UNP O62140
C	677	HIS	-	expression tag	UNP O62140
C	678	HIS	-	expression tag	UNP O62140
C	679	HIS	-	expression tag	UNP O62140
C	680	HIS	-	expression tag	UNP O62140
C	681	HIS	-	expression tag	UNP O62140
C	682	HIS	-	expression tag	UNP O62140
C	683	HIS	-	expression tag	UNP O62140
C	684	HIS	-	expression tag	UNP O62140
D	675	HIS	-	expression tag	UNP O62140
D	676	HIS	-	expression tag	UNP O62140
D	677	HIS	-	expression tag	UNP O62140
D	678	HIS	-	expression tag	UNP O62140
D	679	HIS	-	expression tag	UNP O62140
D	680	HIS	-	expression tag	UNP O62140
D	681	HIS	-	expression tag	UNP O62140
D	682	HIS	-	expression tag	UNP O62140
D	683	HIS	-	expression tag	UNP O62140
D	684	HIS	-	expression tag	UNP O62140
E	675	HIS	-	expression tag	UNP O62140
E	676	HIS	-	expression tag	UNP O62140
E	677	HIS	-	expression tag	UNP O62140
E	678	HIS	-	expression tag	UNP O62140
E	679	HIS	-	expression tag	UNP O62140
E	680	HIS	-	expression tag	UNP O62140
E	681	HIS	-	expression tag	UNP O62140
E	682	HIS	-	expression tag	UNP O62140
E	683	HIS	-	expression tag	UNP O62140
E	684	HIS	-	expression tag	UNP O62140
F	675	HIS	-	expression tag	UNP O62140
F	676	HIS	-	expression tag	UNP O62140
F	677	HIS	-	expression tag	UNP O62140
F	678	HIS	-	expression tag	UNP O62140
F	679	HIS	-	expression tag	UNP O62140

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Chain	Residue	Modelled	Actual	Comment	Reference
F	680	HIS	-	expression tag	UNP O62140
F	681	HIS	-	expression tag	UNP O62140
F	682	HIS	-	expression tag	UNP O62140
F	683	HIS	-	expression tag	UNP O62140
F	684	HIS	-	expression tag	UNP O62140
G	675	HIS	-	expression tag	UNP O62140
G	676	HIS	-	expression tag	UNP O62140
G	677	HIS	-	expression tag	UNP O62140
G	678	HIS	-	expression tag	UNP O62140
G	679	HIS	-	expression tag	UNP O62140
G	680	HIS	-	expression tag	UNP O62140
G	681	HIS	-	expression tag	UNP O62140
G	682	HIS	-	expression tag	UNP O62140
G	683	HIS	-	expression tag	UNP O62140
G	684	HIS	-	expression tag	UNP O62140
H	675	HIS	-	expression tag	UNP O62140
H	676	HIS	-	expression tag	UNP O62140
H	677	HIS	-	expression tag	UNP O62140
H	678	HIS	-	expression tag	UNP O62140
H	679	HIS	-	expression tag	UNP O62140
H	680	HIS	-	expression tag	UNP O62140
H	681	HIS	-	expression tag	UNP O62140
H	682	HIS	-	expression tag	UNP O62140
H	683	HIS	-	expression tag	UNP O62140
H	684	HIS	-	expression tag	UNP O62140

- Molecule 2 is water.

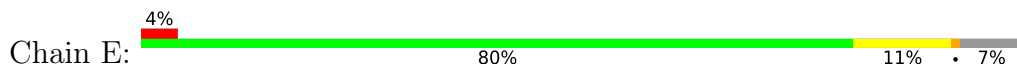
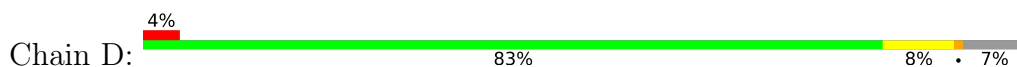
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	150	Total 150	O 150	0	0
2	B	180	Total 180	O 180	0	0
2	C	199	Total 199	O 199	0	0
2	D	215	Total 215	O 215	0	0
2	E	188	Total 188	O 188	0	0
2	F	156	Total 156	O 156	0	0
2	G	203	Total 203	O 203	0	0

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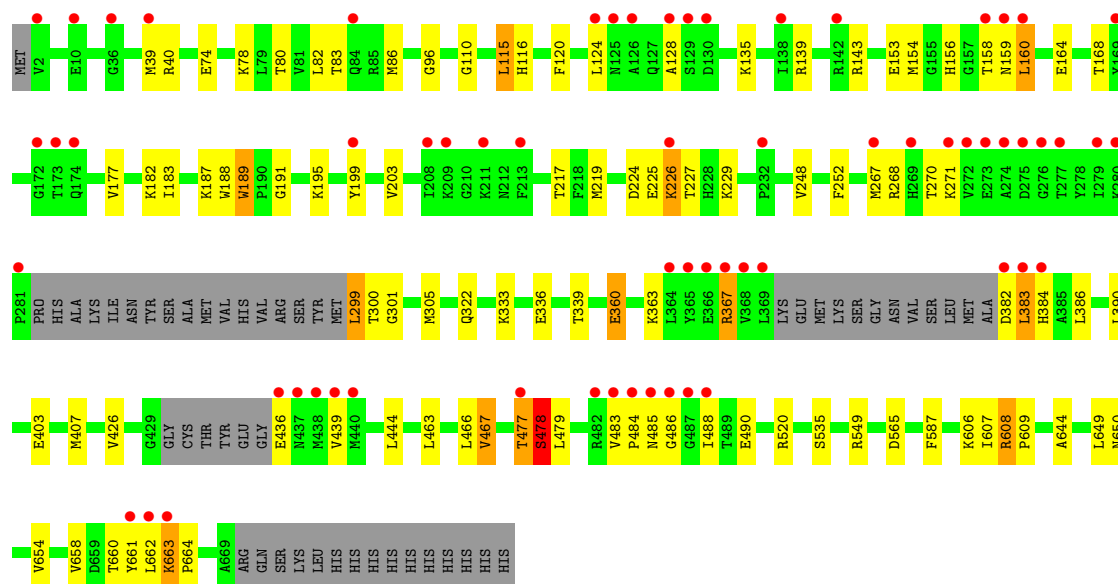
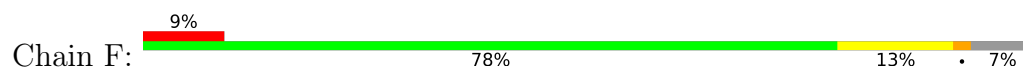
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	H	185	Total 185	O 185	0	0

Chain C: 3% 81% 11% 7%

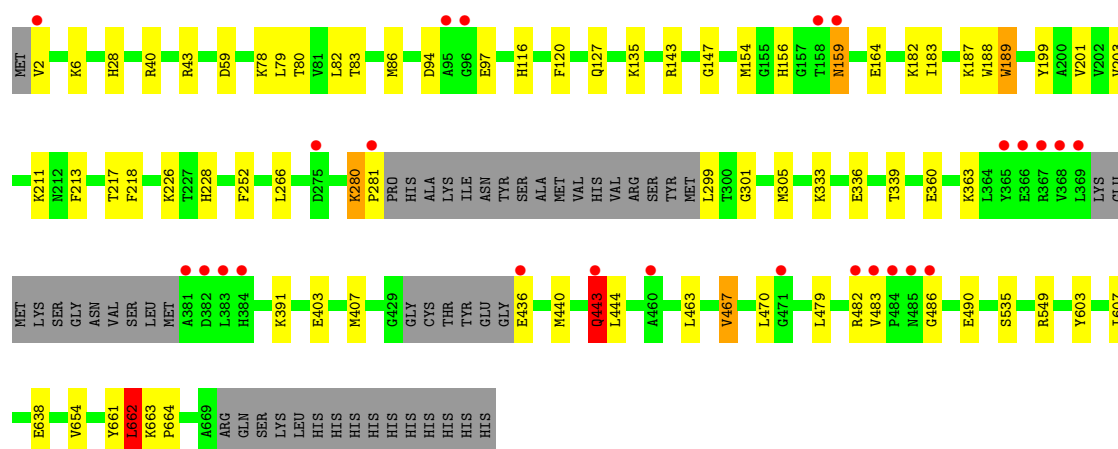
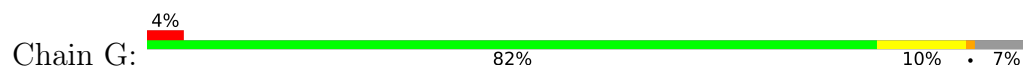




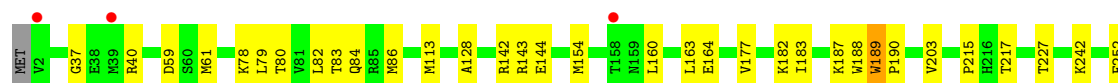
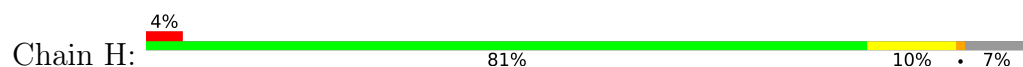
• Molecule 1: Acyl-coenzyme A oxidase

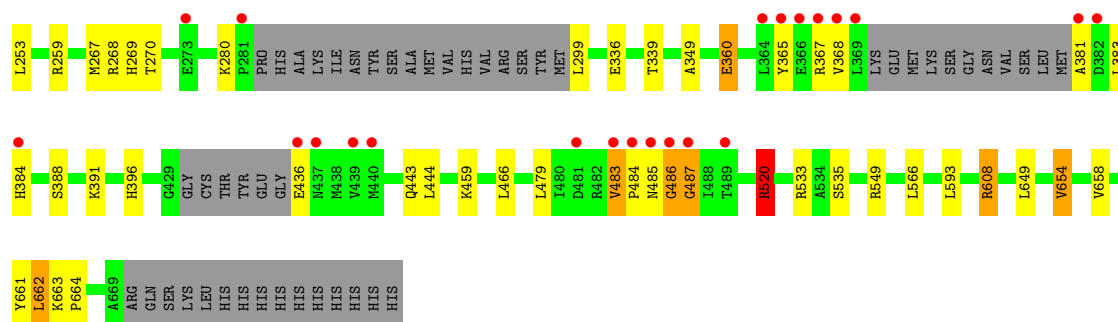


• Molecule 1: Acyl-coenzyme A oxidase



• Molecule 1: Acyl-coenzyme A oxidase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	153.07Å 140.79Å 154.93Å 90.00° 117.20° 90.00°	Depositor
Resolution (Å)	49.24 – 2.48 49.24 – 2.48	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.24-2.48) 99.7 (49.24-2.48)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.16 (at 2.48Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.191 , 0.232 0.194 , 0.233	Depositor DCC
R_{free} test set	10075 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	23.3	Xtriage
Anisotropy	0.331	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 42.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.074 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	41742	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 55.36 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.1995e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

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	0.38	0/5137	0.59	0/6943
1	B	0.39	0/5140	0.60	0/6949
1	C	0.41	0/5124	0.59	2/6928 (0.0%)
1	D	0.42	0/5136	0.62	2/6944 (0.0%)
1	E	0.40	0/5137	0.61	0/6945
1	F	0.38	0/5131	0.61	2/6937 (0.0%)
1	G	0.42	0/5133	0.62	2/6940 (0.0%)
1	H	0.41	0/5136	0.65	4/6944 (0.1%)
All	All	0.40	0/41074	0.61	12/55530 (0.0%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	483	VAL	CA-C-N	9.46	129.71	119.87
1	H	483	VAL	C-N-CA	9.46	129.71	119.87
1	H	484	PRO	N-CA-C	8.73	124.77	114.03
1	D	274	ALA	CA-C-N	5.99	130.19	120.60
1	D	274	ALA	C-N-CA	5.99	130.19	120.60
1	C	443	GLN	N-CA-C	-5.99	104.38	111.03
1	G	443	GLN	N-CA-C	-5.91	104.76	111.14
1	H	520	ARG	N-CA-C	5.35	117.80	111.33
1	G	159	ASN	N-CA-C	5.20	116.78	108.41
1	C	660	THR	N-CA-C	5.15	116.70	111.14
1	F	478	SER	N-CA-C	-5.08	99.98	110.80
1	F	660	THR	N-CA-C	5.00	116.54	111.14

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	5036	0	5056	63	0
1	B	5039	0	5058	51	0
1	C	5023	0	5047	47	0
1	D	5035	0	5055	40	0
1	E	5036	0	5056	52	0
1	F	5030	0	5050	80	0
1	G	5032	0	5053	48	0
1	H	5035	0	5055	55	0
2	A	150	0	0	5	0
2	B	180	0	0	3	0
2	C	199	0	0	3	0
2	D	215	0	0	2	0
2	E	188	0	0	1	0
2	F	156	0	0	2	0
2	G	203	0	0	1	0
2	H	185	0	0	5	0
All	All	41742	0	40430	405	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 5.

All (405) 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:A:658:VAL:HA	1:A:662:LEU:HB2	1.30	1.13
1:G:661:TYR:O	1:G:664:PRO:HD2	1.56	1.04
1:H:658:VAL:HA	1:H:662:LEU:HB2	1.36	1.03
1:F:658:VAL:HG22	1:F:662:LEU:HD12	1.44	0.99
1:F:658:VAL:HA	1:F:662:LEU:HB2	1.44	0.97
1:F:663:LYS:HB3	1:F:664:PRO:HD3	1.46	0.95
1:F:40:ARG:HH22	1:F:96:GLY:HA3	1.33	0.94
1:C:661:TYR:HB3	1:D:80:THR:HG21	1.50	0.94
1:A:382:ASP:N	1:A:447:TYR:HH	1.65	0.93
1:H:658:VAL:HG22	1:H:662:LEU:HD23	1.49	0.92
1:H:663:LYS:HB3	1:H:664:PRO:HD3	1.52	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:THR:HG22	1:A:143:ARG:HH11	1.35	0.88
1:B:83:THR:HG22	1:B:143:ARG:HH11	1.38	0.86
1:E:157:GLY:H	1:F:322:GLN:HE22	1.18	0.86
1:H:177:VAL:HG22	1:H:259:ARG:HG2	1.60	0.83
1:H:483:VAL:HG23	1:H:485:ASN:HB2	1.61	0.83
1:E:80:THR:HG21	1:F:661:TYR:HB3	1.63	0.80
1:F:227:THR:HG23	1:F:229:LYS:H	1.47	0.80
1:A:360:GLU:OE2	1:A:549:ARG:HD2	1.83	0.78
1:F:565:ASP:HB3	1:F:607:ILE:HD11	1.68	0.76
1:D:39:MET:HE1	1:D:42:ARG:NH2	2.00	0.76
1:C:360:GLU:OE2	1:C:549:ARG:HD2	1.86	0.75
1:C:83:THR:HG22	1:C:143:ARG:NH1	2.03	0.74
1:B:83:THR:HG22	1:B:143:ARG:NH1	2.03	0.73
1:C:661:TYR:HB3	1:D:80:THR:CG2	2.18	0.73
1:A:339:THR:HG21	1:B:438:MET:HG2	1.70	0.73
1:C:661:TYR:O	1:C:664:PRO:HD2	1.90	0.72
1:E:360:GLU:OE2	1:E:549:ARG:HD2	1.90	0.72
1:C:267:MET:HB3	1:C:271:LYS:HD3	1.72	0.71
1:E:83:THR:HG22	1:E:143:ARG:HH11	1.55	0.71
1:A:663:LYS:HB3	1:A:664:PRO:HD3	1.72	0.70
1:C:403:GLU:HG3	1:C:407:MET:HE3	1.74	0.70
1:F:40:ARG:NH2	1:F:96:GLY:HA3	2.06	0.70
1:D:83:THR:HG22	1:D:143:ARG:NH1	2.07	0.69
1:E:157:GLY:N	1:F:322:GLN:HE22	1.91	0.68
1:G:661:TYR:O	1:G:664:PRO:CD	2.36	0.68
1:F:83:THR:HG22	1:F:143:ARG:HH11	1.57	0.68
1:F:403:GLU:HG3	1:F:407:MET:HE3	1.76	0.67
1:A:177:VAL:HG22	1:A:259:ARG:HG2	1.74	0.67
1:B:203:VAL:HG22	1:B:217:THR:HG22	1.77	0.66
1:F:159:ASN:O	1:F:160:LEU:HB2	1.96	0.66
1:B:360:GLU:OE2	1:B:549:ARG:HD2	1.94	0.66
1:D:83:THR:HG22	1:D:143:ARG:HH11	1.60	0.66
1:A:83:THR:HG22	1:A:143:ARG:NH1	2.07	0.66
1:H:663:LYS:HB3	1:H:664:PRO:CD	2.26	0.65
1:F:224:ASP:HB3	1:F:227:THR:HG22	1.79	0.64
1:C:203:VAL:HG22	1:C:217:THR:HG22	1.79	0.64
1:G:80:THR:HG21	1:H:661:TYR:HB3	1.79	0.64
1:G:83:THR:HG22	1:G:143:ARG:NH1	2.12	0.64
1:H:83:THR:HG22	1:H:143:ARG:HH11	1.63	0.64
1:F:565:ASP:HB3	1:F:607:ILE:CD1	2.28	0.64
1:B:403:GLU:HG3	1:B:407:MET:HE3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:463:LEU:HD22	1:B:467:VAL:HG13	1.81	0.63
1:A:403:GLU:OE2	1:A:406:ARG:NH2	2.31	0.63
1:C:270:THR:HG22	1:C:281:PRO:HD3	1.81	0.62
1:G:86:MET:HE1	1:G:143:ARG:HH12	1.64	0.62
1:D:159:ASN:ND2	1:D:162:ASN:OD1	2.32	0.62
1:G:333:LYS:O	1:G:336:GLU:HB2	2.00	0.62
1:C:440:MET:HE2	1:C:443:GLN:OE1	2.00	0.62
1:F:115:LEU:HD13	1:F:191:GLY:HA3	1.81	0.62
1:A:403:GLU:HG3	1:A:407:MET:HE3	1.82	0.62
1:D:2:VAL:HG13	1:D:3:HIS:H	1.63	0.61
1:D:164:GLU:OE2	1:D:182:LYS:HE3	2.00	0.61
1:H:164:GLU:OE2	1:H:182:LYS:HE3	2.00	0.61
1:G:203:VAL:HG22	1:G:217:THR:HG22	1.81	0.61
1:A:403:GLU:OE2	1:A:406:ARG:NE	2.33	0.61
1:B:156:HIS:NE2	1:B:164:GLU:OE2	2.30	0.61
1:B:488:ILE:HD12	1:B:571:VAL:HG21	1.82	0.61
1:H:268:ARG:HG2	1:H:269:HIS:CD2	2.36	0.61
1:A:228:HIS:CD2	1:B:658:VAL:HG11	2.36	0.61
1:A:663:LYS:CB	1:A:664:PRO:HD3	2.30	0.61
1:A:661:TYR:O	1:A:664:PRO:HD2	2.00	0.61
1:H:658:VAL:HA	1:H:662:LEU:CB	2.23	0.60
1:A:42:ARG:HD2	1:A:46:GLU:OE2	2.00	0.60
1:E:83:THR:HG22	1:E:143:ARG:NH1	2.16	0.60
1:F:661:TYR:O	1:F:664:PRO:HD2	2.00	0.60
1:E:463:LEU:HD22	1:E:467:VAL:HG13	1.84	0.60
1:F:663:LYS:HB3	1:F:664:PRO:CD	2.27	0.59
1:H:142:ARG:NH1	1:H:144:GLU:OE2	2.35	0.59
1:C:403:GLU:OE2	1:C:406:ARG:NH2	2.32	0.59
1:A:533:ARG:NH2	2:A:704:HOH:O	2.35	0.59
1:F:565:ASP:CB	1:F:607:ILE:HD11	2.32	0.59
1:E:164:GLU:OE2	1:E:182:LYS:HE3	2.02	0.58
1:C:349:ALA:HB2	1:C:566:LEU:HD22	1.86	0.58
1:B:154:MET:HE3	1:B:183:ILE:HG12	1.86	0.58
1:E:203:VAL:HG22	1:E:217:THR:HG22	1.85	0.58
1:C:42:ARG:NH1	2:C:701:HOH:O	2.34	0.58
1:D:299:LEU:N	2:D:704:HOH:O	2.37	0.58
1:C:484:PRO:O	1:C:485:ASN:HB2	2.04	0.58
1:F:360:GLU:OE2	1:F:549:ARG:HD2	2.04	0.58
1:F:382:ASP:CG	1:F:383:LEU:H	2.12	0.58
1:A:39:MET:HE3	1:A:43:ARG:HG3	1.84	0.58
1:B:437:ASN:HA	1:B:440:MET:HE3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:444:LEU:HD23	1:E:535:SER:HB3	1.86	0.57
1:E:154:MET:HE3	1:E:183:ILE:HG12	1.87	0.57
1:C:42:ARG:HD2	2:C:701:HOH:O	2.03	0.57
1:F:305:MET:HE1	1:F:426:VAL:HG12	1.85	0.57
1:A:339:THR:CG2	1:B:438:MET:HG2	2.32	0.57
1:A:662:LEU:HD12	1:B:146:ILE:HD11	1.87	0.56
1:C:188:TRP:O	1:C:189:TRP:HB2	2.06	0.56
1:G:187:LYS:O	1:G:252:PHE:HA	2.05	0.56
1:H:154:MET:HE3	1:H:183:ILE:HG12	1.86	0.56
1:D:403:GLU:HG3	1:D:407:MET:HE3	1.87	0.56
1:D:270:THR:HG22	1:D:280:LYS:HD3	1.86	0.56
1:H:360:GLU:OE2	1:H:549:ARG:HD2	2.05	0.56
1:B:227:THR:HG23	1:B:229:LYS:H	1.70	0.56
1:H:83:THR:HG22	1:H:143:ARG:NH1	2.19	0.56
1:F:444:LEU:HD23	1:F:535:SER:HB3	1.87	0.55
1:G:116:HIS:O	1:G:120:PHE:HB3	2.07	0.55
1:G:59:ASP:OD1	1:G:78:LYS:NZ	2.39	0.55
1:G:479:LEU:HB3	1:G:483:VAL:HG13	1.88	0.55
1:A:115:LEU:HD13	1:A:191:GLY:HA3	1.87	0.55
1:D:86:MET:HE1	1:D:143:ARG:HH12	1.72	0.55
1:F:83:THR:HG22	1:F:143:ARG:NH1	2.22	0.55
1:F:663:LYS:CB	1:F:664:PRO:HD3	2.29	0.55
1:H:533:ARG:NH2	2:H:705:HOH:O	2.40	0.55
1:G:360:GLU:OE2	1:G:549:ARG:HD2	2.07	0.55
1:A:154:MET:HE3	1:A:183:ILE:HG12	1.89	0.54
1:E:403:GLU:HG3	1:E:407:MET:HE3	1.88	0.54
1:E:403:GLU:OE2	1:E:406:ARG:NE	2.32	0.54
1:H:203:VAL:HG22	1:H:217:THR:HG22	1.89	0.54
1:H:658:VAL:HG22	1:H:662:LEU:CD2	2.30	0.54
1:E:484:PRO:O	1:H:520:ARG:NH2	2.41	0.54
1:B:483:VAL:HG13	1:C:520:ARG:NH2	2.22	0.54
1:D:360:GLU:OE2	1:D:549:ARG:HD2	2.07	0.53
1:A:382:ASP:N	2:A:707:HOH:O	2.40	0.53
1:F:139:ARG:NH2	2:F:711:HOH:O	2.42	0.53
1:A:280:LYS:HD2	1:A:281:PRO:HD2	1.91	0.53
1:F:363:LYS:O	1:F:367:ARG:HB2	2.09	0.53
1:G:164:GLU:OE2	1:G:182:LYS:HE3	2.09	0.53
1:C:80:THR:HG21	1:D:661:TYR:HB3	1.89	0.53
1:B:301:GLY:O	1:B:305:MET:HG2	2.09	0.52
1:E:80:THR:CG2	1:F:661:TYR:HB3	2.37	0.52
1:F:383:LEU:HD13	1:F:384:HIS:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:403:GLU:HG3	1:G:407:MET:HE3	1.91	0.52
1:H:188:TRP:O	1:H:189:TRP:HB2	2.09	0.52
1:H:80:THR:O	1:H:84:GLN:HG2	2.09	0.52
1:B:211:LYS:NZ	2:B:709:HOH:O	2.43	0.52
1:C:154:MET:HE3	1:C:183:ILE:HG12	1.92	0.52
1:C:301:GLY:O	1:C:305:MET:HG2	2.09	0.52
1:F:608:ARG:HB3	1:F:609:PRO:HD3	1.91	0.52
1:G:80:THR:CG2	1:H:661:TYR:HB3	2.40	0.52
1:A:444:LEU:HD23	1:A:535:SER:HB3	1.92	0.52
1:F:382:ASP:OD1	1:F:382:ASP:N	2.43	0.52
1:E:40:ARG:NH2	1:E:94:ASP:OD1	2.43	0.52
1:G:40:ARG:NH2	1:G:94:ASP:OD2	2.36	0.52
1:C:661:TYR:O	1:C:664:PRO:CD	2.58	0.51
1:F:188:TRP:O	1:F:189:TRP:HB2	2.08	0.51
1:F:305:MET:HE1	1:F:426:VAL:CG1	2.40	0.51
1:D:467:VAL:HG22	1:D:470:LEU:HD12	1.92	0.51
1:F:156:HIS:NE2	1:F:164:GLU:OE1	2.33	0.51
1:B:62:PRO:HA	2:B:763:HOH:O	2.11	0.51
1:B:187:LYS:HB2	1:B:253:LEU:HB3	1.93	0.51
1:C:658:VAL:HA	1:C:662:LEU:HB2	1.91	0.51
1:D:484:PRO:O	1:F:520:ARG:NH2	2.44	0.51
1:E:110:GLY:HA3	1:E:248:VAL:HG23	1.93	0.51
1:E:381:ALA:N	2:E:709:HOH:O	2.42	0.51
1:C:110:GLY:HA3	1:C:248:VAL:HG23	1.93	0.51
1:D:444:LEU:HD23	1:D:535:SER:HB3	1.93	0.50
1:H:654:VAL:HA	2:H:774:HOH:O	2.10	0.50
1:D:82:LEU:O	1:D:86:MET:HB2	2.10	0.50
1:B:188:TRP:O	1:B:189:TRP:HB2	2.12	0.50
1:F:226:LYS:HG3	1:F:227:THR:N	2.27	0.50
1:G:661:TYR:O	1:G:663:LYS:N	2.44	0.50
1:A:188:TRP:O	1:A:189:TRP:HB2	2.10	0.50
1:E:2:VAL:HG13	1:E:3:HIS:H	1.76	0.50
1:F:479:LEU:HB2	1:F:490:GLU:OE2	2.12	0.50
1:E:479:LEU:HB2	1:E:490:GLU:OE2	2.12	0.49
1:F:483:VAL:HG23	1:F:486:GLY:CA	2.43	0.49
1:F:607:ILE:O	1:F:607:ILE:HG22	2.11	0.49
1:B:110:GLY:HA3	1:B:248:VAL:HG23	1.94	0.49
1:E:187:LYS:HB2	1:E:253:LEU:HB3	1.94	0.49
1:A:305:MET:HE1	1:A:426:VAL:HG12	1.95	0.49
1:D:39:MET:HE1	1:D:42:ARG:HH22	1.76	0.49
1:A:59:ASP:OD1	1:A:78:LYS:NZ	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:128:ALA:O	1:H:268:ARG:NH1	2.41	0.49
1:D:188:TRP:O	1:D:189:TRP:HB2	2.12	0.49
1:F:363:LYS:NZ	2:F:705:HOH:O	2.37	0.48
1:F:565:ASP:C	1:F:607:ILE:HD11	2.37	0.48
1:G:663:LYS:HB3	1:G:664:PRO:HD3	1.95	0.48
1:H:383:LEU:HD12	1:H:466:LEU:HD11	1.96	0.48
1:G:43:ARG:NH2	1:G:97:GLU:OE1	2.36	0.48
1:H:187:LYS:O	1:H:252:PHE:HA	2.12	0.48
1:H:658:VAL:O	1:H:663:LYS:HB2	2.13	0.48
1:A:663:LYS:CB	1:A:664:PRO:CD	2.91	0.48
1:C:479:LEU:HB2	1:C:490:GLU:OE2	2.12	0.48
1:E:599:GLN:OE1	1:H:459:LYS:NZ	2.35	0.48
1:G:154:MET:HE3	1:G:183:ILE:HG12	1.96	0.48
1:E:115:LEU:HD13	1:E:191:GLY:HA3	1.96	0.48
1:A:305:MET:HE1	1:A:426:VAL:CG1	2.44	0.48
1:C:33:GLN:OE1	1:C:550:ARG:HD2	2.13	0.48
1:D:203:VAL:HG22	1:D:217:THR:HG22	1.94	0.48
1:H:40:ARG:HG3	2:H:740:HOH:O	2.14	0.48
1:H:396:HIS:HB2	2:H:733:HOH:O	2.14	0.48
1:E:483:VAL:HG13	1:H:520:ARG:NH2	2.29	0.48
1:B:602:PHE:CE2	1:C:459:LYS:HG2	2.49	0.48
1:A:382:ASP:N	1:A:447:TYR:OH	2.39	0.47
1:E:187:LYS:O	1:E:252:PHE:HA	2.13	0.47
1:H:381:ALA:N	1:H:384:HIS:HB3	2.28	0.47
1:E:595:TYR:O	1:E:599:GLN:HG2	2.14	0.47
1:G:156:HIS:NE2	1:G:164:GLU:OE1	2.34	0.47
1:H:82:LEU:O	1:H:86:MET:HB2	2.14	0.47
1:F:187:LYS:O	1:F:252:PHE:HA	2.14	0.47
1:A:203:VAL:HG22	1:A:217:THR:HG22	1.95	0.47
1:E:364:LEU:HB3	1:E:383:LEU:HD11	1.96	0.47
1:G:479:LEU:HB2	1:G:490:GLU:OE1	2.15	0.47
1:C:265:LEU:O	1:C:267:MET:HG3	2.15	0.47
2:G:743:HOH:O	1:H:649:LEU:HB2	2.14	0.47
1:A:339:THR:HG23	1:B:438:MET:HE3	1.97	0.47
1:E:211:LYS:HD2	1:E:213:PHE:CZ	2.49	0.47
1:F:128:ALA:O	1:F:268:ARG:NH1	2.48	0.47
1:F:477:THR:OG1	1:F:478:SER:N	2.45	0.47
1:G:662:LEU:HD13	1:G:662:LEU:H	1.80	0.47
1:A:463:LEU:HD22	1:A:467:VAL:HG13	1.95	0.47
1:E:188:TRP:O	1:E:189:TRP:HB2	2.15	0.47
1:F:164:GLU:OE2	1:F:182:LYS:HD2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:VAL:HA	1:A:365:TYR:HB2	1.95	0.47
1:C:80:THR:CG2	1:D:661:TYR:HB3	2.44	0.47
1:D:479:LEU:HB2	1:D:490:GLU:OE2	2.14	0.47
1:F:124:LEU:HD21	1:F:219:MET:HE2	1.96	0.47
1:B:124:LEU:HD21	1:B:219:MET:CE	2.44	0.47
1:B:488:ILE:HG22	1:B:492:ILE:HG13	1.97	0.47
1:C:228:HIS:CD2	1:D:658:VAL:HG11	2.50	0.47
1:E:655:LEU:O	1:E:658:VAL:HG22	2.15	0.46
1:F:224:ASP:OD2	1:F:227:THR:HG22	2.15	0.46
1:G:79:LEU:O	1:G:83:THR:HG23	2.15	0.46
1:G:188:TRP:O	1:G:189:TRP:HB2	2.15	0.46
1:G:301:GLY:O	1:G:305:MET:HG2	2.14	0.46
1:A:226:LYS:HA	1:A:226:LYS:HD3	1.63	0.46
1:A:634:GLY:HA2	2:A:791:HOH:O	2.15	0.46
1:A:154:MET:HE2	1:A:186:LEU:HD12	1.97	0.46
1:A:224:ASP:O	1:A:228:HIS:N	2.48	0.46
1:B:56:GLU:H	1:B:56:GLU:CD	2.24	0.46
1:E:216:HIS:HD2	1:E:270:THR:HG21	1.80	0.46
1:H:479:LEU:O	1:H:483:VAL:HG22	2.15	0.46
1:A:25:PHE:HB2	1:A:559:ILE:HD13	1.96	0.46
1:A:40:ARG:NH2	1:A:94:ASP:OD1	2.48	0.46
1:A:207:TYR:CE2	1:A:212:ASN:HB2	2.49	0.46
1:D:382:ASP:HB2	1:D:447:TYR:CE1	2.51	0.46
1:G:226:LYS:HA	1:G:226:LYS:HD3	1.70	0.46
1:A:349:ALA:HB2	1:A:566:LEU:HD22	1.96	0.46
1:B:475:GLU:OE1	1:B:493:LYS:NZ	2.49	0.46
1:F:463:LEU:HD22	1:F:467:VAL:HG13	1.98	0.46
1:C:39:MET:SD	1:C:42:ARG:NH1	2.89	0.46
1:C:306:LEU:HB2	1:C:398:THR:HG23	1.98	0.46
1:G:467:VAL:HG22	1:G:470:LEU:HD12	1.98	0.45
1:H:59:ASP:OD1	1:H:78:LYS:NZ	2.49	0.45
1:F:203:VAL:HG22	1:F:217:THR:HG22	1.98	0.45
1:D:661:TYR:O	1:D:663:LYS:N	2.49	0.45
1:F:124:LEU:HD21	1:F:219:MET:CE	2.46	0.45
1:C:177:VAL:HG22	1:C:259:ARG:HG2	1.98	0.45
1:F:153:GLU:HG2	1:F:187:LYS:HD3	1.97	0.45
1:F:484:PRO:O	1:F:485:ASN:HB2	2.15	0.45
1:G:391:LYS:HD2	1:G:440:MET:SD	2.55	0.45
1:B:467:VAL:HG22	1:B:470:LEU:HD12	1.99	0.45
1:E:160:LEU:HB3	1:E:215:PRO:HG3	1.99	0.45
1:E:301:GLY:O	1:E:305:MET:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:ASP:HB3	1:B:227:THR:HG22	1.99	0.45
1:F:188:TRP:CE3	1:F:252:PHE:HB3	2.52	0.45
1:F:658:VAL:CG2	1:F:662:LEU:HD12	2.31	0.45
1:G:83:THR:HG22	1:G:143:ARG:HH11	1.81	0.45
1:G:443:GLN:HE21	1:G:443:GLN:HB2	1.59	0.45
1:F:154:MET:HE3	1:F:183:ILE:HG12	1.99	0.45
1:H:187:LYS:HB2	1:H:253:LEU:HB3	1.98	0.45
1:A:450:LYS:NZ	2:A:714:HOH:O	2.46	0.45
1:F:267:MET:HB3	1:F:271:LYS:HD3	1.99	0.45
1:E:436:GLU:O	1:E:439:VAL:HG12	2.16	0.45
1:A:265:LEU:O	1:A:267:MET:HG3	2.17	0.44
1:B:187:LYS:O	1:B:252:PHE:HA	2.17	0.44
1:D:663:LYS:HB3	1:D:664:PRO:HD3	1.99	0.44
1:E:86:MET:HE1	1:E:143:ARG:HH12	1.82	0.44
1:C:530:GLU:OE2	1:C:533:ARG:NH1	2.50	0.44
1:F:477:THR:O	1:F:587:PHE:O	2.35	0.44
1:B:382:ASP:OD2	1:B:447:TYR:OH	2.33	0.44
1:C:245:TYR:CE2	1:C:248:VAL:HG21	2.53	0.44
1:C:396:HIS:HB2	2:C:705:HOH:O	2.17	0.44
1:G:6:LYS:HG3	1:G:28:HIS:CD2	2.52	0.44
1:B:82:LEU:O	1:B:86:MET:HB2	2.18	0.44
1:D:301:GLY:O	1:D:305:MET:HG2	2.16	0.44
1:E:668:LYS:HE3	1:E:668:LYS:HB2	1.80	0.44
1:D:2:VAL:HG13	1:D:3:HIS:N	2.33	0.44
1:G:211:LYS:HE3	1:G:213:PHE:CE2	2.52	0.44
1:A:665:MET:HB2	1:B:80:THR:HG22	1.99	0.44
1:H:444:LEU:HD23	1:H:535:SER:HB3	2.00	0.44
1:F:158:THR:HG21	1:F:439:VAL:HG11	2.00	0.43
1:F:168:THR:O	1:F:177:VAL:HG12	2.17	0.43
1:C:493:LYS:HB2	1:C:493:LYS:HE3	1.90	0.43
1:F:267:MET:HG2	1:F:270:THR:O	2.18	0.43
1:H:349:ALA:HB2	1:H:566:LEU:HD22	2.00	0.43
1:A:195:LYS:HE3	1:B:649:LEU:O	2.18	0.43
1:D:164:GLU:OE2	1:D:182:LYS:CE	2.66	0.43
1:G:147:GLY:HA2	1:G:199:TYR:O	2.18	0.43
1:A:82:LEU:O	1:A:86:MET:HB2	2.18	0.43
1:E:661:TYR:HB3	1:F:80:THR:HG21	2.00	0.43
1:F:82:LEU:O	1:F:86:MET:HB2	2.18	0.43
1:F:135:LYS:O	1:F:139:ARG:HG3	2.18	0.43
1:B:86:MET:HE1	1:B:143:ARG:HH12	1.82	0.43
1:D:110:GLY:HA3	1:D:248:VAL:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:228:HIS:CD2	1:F:658:VAL:HG11	2.54	0.43
1:F:74:GLU:HG3	1:F:78:LYS:HE2	2.01	0.43
1:F:301:GLY:O	1:F:305:MET:HG2	2.17	0.43
1:B:224:ASP:OD1	1:B:227:THR:HG22	2.18	0.43
1:A:2:VAL:HG13	1:A:3:HIS:H	1.83	0.43
1:B:242:LYS:HB2	1:B:242:LYS:HE3	1.83	0.43
1:C:482:ARG:HD2	1:C:592:GLN:NE2	2.33	0.43
1:F:116:HIS:O	1:F:120:PHE:HB3	2.19	0.43
1:B:235:THR:O	1:B:253:LEU:HA	2.18	0.43
1:D:396:HIS:HB2	2:D:889:HOH:O	2.19	0.43
1:B:154:MET:HG2	1:B:184:THR:HA	2.01	0.42
1:A:236:ILE:HD12	1:A:253:LEU:HD13	2.00	0.42
1:B:661:TYR:O	1:B:663:LYS:N	2.52	0.42
1:D:124:LEU:HD21	1:D:219:MET:CE	2.48	0.42
1:E:43:ARG:NE	1:E:97:GLU:OE2	2.41	0.42
1:F:382:ASP:CG	1:F:383:LEU:N	2.78	0.42
1:H:160:LEU:HD23	1:H:163:LEU:HD11	1.99	0.42
1:H:663:LYS:CB	1:H:664:PRO:HD3	2.34	0.42
1:A:333:LYS:O	1:A:336:GLU:HB2	2.19	0.42
1:A:583:LEU:HD21	1:A:593:LEU:HD22	2.01	0.42
1:C:321:ARG:HA	1:C:332:VAL:O	2.19	0.42
1:G:201:VAL:HA	1:G:218:PHE:O	2.19	0.42
1:A:500:LYS:HB3	1:A:500:LYS:HE2	1.85	0.42
1:B:333:LYS:O	1:B:336:GLU:HB2	2.19	0.42
1:D:187:LYS:O	1:D:252:PHE:HA	2.19	0.42
1:F:110:GLY:HA3	1:F:248:VAL:HG23	2.00	0.42
1:F:135:LYS:HE3	1:F:135:LYS:HB2	1.88	0.42
1:A:23:ALA:HB2	1:A:613:SER:OG	2.20	0.42
1:A:51:LEU:HD11	1:A:101:LEU:HD12	2.01	0.42
1:B:660:THR:O	1:B:664:PRO:HG2	2.19	0.42
1:H:242:LYS:HB2	1:H:242:LYS:HE3	1.90	0.42
1:H:267:MET:HG2	1:H:270:THR:O	2.19	0.42
1:C:275:ASP:HB3	1:C:277:THR:OG1	2.20	0.42
1:E:59:ASP:OD1	1:E:78:LYS:NZ	2.53	0.42
1:E:349:ALA:HB2	1:E:566:LEU:HD22	2.02	0.42
1:H:483:VAL:O	1:H:485:ASN:HB3	2.19	0.42
1:H:486:GLY:HA3	1:H:487:GLY:HA2	1.82	0.42
1:C:187:LYS:O	1:C:252:PHE:HA	2.19	0.42
1:C:444:LEU:HD23	1:C:535:SER:HB3	2.02	0.42
1:E:178:LEU:HD23	1:E:255:PHE:CE1	2.54	0.42
1:E:644:ALA:O	1:E:650:ASN:ND2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:612:VAL:HG12	1:C:616:ASP:OD2	2.19	0.42
1:E:177:VAL:HG22	1:E:259:ARG:HG2	2.01	0.42
1:F:386:LEU:HD22	1:F:466:LEU:HD13	2.02	0.42
1:F:565:ASP:OD2	1:F:606:LYS:NZ	2.52	0.42
1:G:228:HIS:CD2	1:H:658:VAL:HG11	2.55	0.42
1:H:37:GLY:HA3	2:H:740:HOH:O	2.20	0.42
1:A:85:ARG:O	1:A:88:GLU:HG2	2.19	0.42
1:C:188:TRP:HD1	1:C:189:TRP:CD1	2.38	0.42
1:C:483:VAL:HG23	1:C:486:GLY:HA3	2.01	0.42
1:D:76:ALA:O	1:D:80:THR:HG23	2.19	0.42
1:G:86:MET:CE	1:G:143:ARG:HH12	2.31	0.42
1:E:216:HIS:CD2	1:E:270:THR:HG21	2.55	0.41
1:F:333:LYS:O	1:F:336:GLU:HB2	2.20	0.41
1:H:593:LEU:HD12	1:H:593:LEU:HA	1.89	0.41
1:B:305:MET:HE1	1:B:426:VAL:CG1	2.50	0.41
1:C:2:VAL:HG13	1:C:3:HIS:H	1.84	0.41
1:G:444:LEU:HD23	1:G:535:SER:HB3	2.01	0.41
1:G:661:TYR:HB3	1:H:80:THR:CG2	2.50	0.41
1:A:245:TYR:CE2	1:A:248:VAL:HG21	2.55	0.41
1:A:403:GLU:OE2	1:A:406:ARG:CZ	2.68	0.41
1:B:299:LEU:HD22	1:B:299:LEU:HA	1.94	0.41
1:E:663:LYS:HA	1:E:666:MET:HE3	2.02	0.41
1:G:483:VAL:HG21	1:G:486:GLY:HA3	2.01	0.41
1:E:412:HIS:CD2	1:F:189:TRP:HE1	2.39	0.41
1:G:603:TYR:O	1:G:607:ILE:HG12	2.21	0.41
1:A:603:TYR:HA	1:A:606:LYS:HB3	2.01	0.41
1:E:82:LEU:O	1:E:86:MET:HB2	2.21	0.41
1:A:402:ILE:HD13	1:A:423:ILE:HG22	2.02	0.41
1:B:118:VAL:O	1:B:122:PRO:HG2	2.19	0.41
1:B:306:LEU:HB2	1:B:398:THR:HG23	2.03	0.41
1:B:595:TYR:O	1:B:599:GLN:HG2	2.20	0.41
1:D:483:VAL:HB	1:F:520:ARG:NH2	2.36	0.41
1:F:661:TYR:C	1:F:664:PRO:HD2	2.45	0.41
1:G:483:VAL:HG21	1:G:490:GLU:HG3	2.02	0.41
1:H:160:LEU:HB3	1:H:215:PRO:HG3	2.03	0.41
1:A:383:LEU:HA	1:A:383:LEU:HD12	1.79	0.41
1:G:661:TYR:HB3	1:H:80:THR:HG21	2.03	0.41
1:H:79:LEU:HD21	1:H:113:MET:HG3	2.02	0.41
1:A:124:LEU:HD21	1:A:219:MET:CE	2.50	0.41
1:A:164:GLU:HB2	1:A:185:ALA:HB2	2.02	0.41
1:B:164:GLU:OE1	1:B:182:LYS:HE3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:VAL:HG22	1:B:259:ARG:HG2	2.03	0.41
1:E:661:TYR:O	1:E:663:LYS:N	2.54	0.41
1:F:195:LYS:HA	1:F:195:LYS:HD3	1.92	0.41
1:G:127:GLN:O	1:G:266:LEU:HB3	2.20	0.41
1:G:280:LYS:HA	1:G:281:PRO:HA	1.90	0.41
1:A:437:ASN:N	2:A:723:HOH:O	2.53	0.41
1:D:59:ASP:OD1	1:D:78:LYS:NZ	2.54	0.41
1:E:467:VAL:HG22	1:E:470:LEU:HD12	2.03	0.41
1:D:494:THR:O	1:D:498:ILE:HG23	2.22	0.40
1:D:563:LEU:HD23	1:D:563:LEU:HA	1.91	0.40
1:F:299:LEU:HD21	1:F:390:LEU:HD13	2.03	0.40
1:G:82:LEU:HD23	1:G:82:LEU:HA	1.93	0.40
1:C:82:LEU:HD23	1:C:82:LEU:HA	1.92	0.40
1:F:199:TYR:OH	1:F:225:GLU:OE2	2.33	0.40
1:H:336:GLU:OE2	1:H:608:ARG:NH2	2.53	0.40
1:E:124:LEU:HD21	1:E:219:MET:CE	2.51	0.40
1:E:268:ARG:HG2	1:E:269:HIS:CD2	2.56	0.40
1:F:644:ALA:O	1:F:650:ASN:ND2	2.54	0.40
1:G:463:LEU:HD22	1:G:467:VAL:HG13	2.03	0.40
1:H:189:TRP:N	1:H:190:PRO:CD	2.85	0.40
1:H:388:SER:OG	1:H:443:GLN:NE2	2.53	0.40
1:B:623:ARG:HD3	2:B:774:HOH:O	2.20	0.40
1:C:47:ILE:HG12	1:C:90:ILE:HG22	2.04	0.40
1:D:79:LEU:O	1:D:83:THR:HG23	2.22	0.40
1:G:662:LEU:H	1:G:662:LEU:CD1	2.34	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	624/684 (91%)	610 (98%)	13 (2%)	1 (0%)	43 61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	627/684 (92%)	613 (98%)	12 (2%)	2 (0%)	36	53
1	C	625/684 (91%)	609 (97%)	14 (2%)	2 (0%)	36	53
1	D	626/684 (92%)	613 (98%)	10 (2%)	3 (0%)	24	40
1	E	627/684 (92%)	614 (98%)	11 (2%)	2 (0%)	36	53
1	F	625/684 (91%)	607 (97%)	15 (2%)	3 (0%)	24	40
1	G	626/684 (92%)	617 (99%)	7 (1%)	2 (0%)	36	53
1	H	626/684 (92%)	609 (97%)	14 (2%)	3 (0%)	24	40
All	All	5006/5472 (92%)	4892 (98%)	96 (2%)	18 (0%)	30	46

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	189	TRP
1	B	189	TRP
1	C	189	TRP
1	D	189	TRP
1	D	488	ILE
1	E	189	TRP
1	E	488	ILE
1	F	160	LEU
1	F	189	TRP
1	F	478	SER
1	G	189	TRP
1	G	662	LEU
1	H	189	TRP
1	C	662	LEU
1	D	437	ASN
1	H	487	GLY
1	B	368	VAL
1	H	486	GLY

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	534/579 (92%)	517 (97%)	17 (3%)	34	58
1	B	534/579 (92%)	521 (98%)	13 (2%)	43	67
1	C	532/579 (92%)	520 (98%)	12 (2%)	44	69
1	D	534/579 (92%)	521 (98%)	13 (2%)	43	67
1	E	533/579 (92%)	519 (97%)	14 (3%)	40	65
1	F	534/579 (92%)	517 (97%)	17 (3%)	34	58
1	G	533/579 (92%)	519 (97%)	14 (3%)	40	65
1	H	534/579 (92%)	519 (97%)	15 (3%)	38	63
All	All	4268/4632 (92%)	4153 (97%)	115 (3%)	39	64

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	MET
1	A	42	ARG
1	A	61	MET
1	A	135	LYS
1	A	158	THR
1	A	280	LYS
1	A	298	MET
1	A	299	LEU
1	A	300	THR
1	A	339	THR
1	A	360	GLU
1	A	361	THR
1	A	364	LEU
1	A	365	TYR
1	A	439	VAL
1	A	467	VAL
1	A	662	LEU
1	B	56	GLU
1	B	280	LYS
1	B	299	LEU
1	B	339	THR
1	B	361	THR
1	B	382	ASP
1	B	436	GLU
1	B	438	MET
1	B	467	VAL
1	B	483	VAL

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Mol	Chain	Res	Type
1	B	519	LYS
1	B	649	LEU
1	B	654	VAL
1	C	61	MET
1	C	154	MET
1	C	280	LYS
1	C	299	LEU
1	C	361	THR
1	C	367	ARG
1	C	443	GLN
1	C	520	ARG
1	C	605	GLN
1	C	649	LEU
1	C	654	VAL
1	C	662	LEU
1	D	39	MET
1	D	135	LYS
1	D	280	LYS
1	D	299	LEU
1	D	339	THR
1	D	364	LEU
1	D	367	ARG
1	D	382	ASP
1	D	467	VAL
1	D	475	GLU
1	D	488	ILE
1	D	638	GLU
1	D	662	LEU
1	E	40	ARG
1	E	56	GLU
1	E	299	LEU
1	E	339	THR
1	E	363	LYS
1	E	364	LEU
1	E	383	LEU
1	E	391	LYS
1	E	436	GLU
1	E	467	VAL
1	E	482	ARG
1	E	483	VAL
1	E	649	LEU
1	E	658	VAL

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Mol	Chain	Res	Type
1	F	39	MET
1	F	115	LEU
1	F	226	LYS
1	F	299	LEU
1	F	300	THR
1	F	339	THR
1	F	360	GLU
1	F	367	ARG
1	F	383	LEU
1	F	436	GLU
1	F	467	VAL
1	F	477	THR
1	F	488	ILE
1	F	608	ARG
1	F	649	LEU
1	F	654	VAL
1	F	663	LYS
1	G	2	VAL
1	G	135	LYS
1	G	159	ASN
1	G	280	LYS
1	G	299	LEU
1	G	339	THR
1	G	363	LYS
1	G	436	GLU
1	G	443	GLN
1	G	467	VAL
1	G	482	ARG
1	G	638	GLU
1	G	654	VAL
1	G	662	LEU
1	H	61	MET
1	H	227	THR
1	H	280	LYS
1	H	299	LEU
1	H	339	THR
1	H	360	GLU
1	H	365	TYR
1	H	367	ARG
1	H	368	VAL
1	H	391	LYS
1	H	436	GLU

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Mol	Chain	Res	Type
1	H	520	ARG
1	H	608	ARG
1	H	654	VAL
1	H	662	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	HIS
1	A	228	HIS
1	A	257	ASN
1	B	257	ASN
1	B	639	ASN
1	C	151	GLN
1	C	174	GLN
1	C	257	ASN
1	C	302	GLN
1	C	311	ASN
1	D	151	GLN
1	D	159	ASN
1	D	162	ASN
1	D	174	GLN
1	D	302	GLN
1	D	311	ASN
1	D	328	ASN
1	E	151	GLN
1	E	302	GLN
1	E	311	ASN
1	E	384	HIS
1	E	552	ASN
1	F	302	GLN
1	F	311	ASN
1	F	322	GLN
1	F	341	GLN
1	F	443	GLN
1	F	496	GLN
1	G	174	GLN
1	G	257	ASN
1	G	302	GLN
1	G	311	ASN
1	G	443	GLN
1	G	552	ASN

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Mol	Chain	Res	Type
1	H	151	GLN
1	H	162	ASN
1	H	174	GLN
1	H	269	HIS
1	H	311	ASN
1	H	443	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	634/684 (92%)	0.38	42 (6%) 24 21	18, 30, 55, 71	0
1	B	635/684 (92%)	0.12	21 (3%) 49 45	15, 26, 46, 67	0
1	C	633/684 (92%)	0.15	23 (3%) 46 42	15, 26, 43, 63	0
1	D	634/684 (92%)	-0.05	24 (3%) 44 40	12, 22, 41, 64	0
1	E	635/684 (92%)	0.13	25 (3%) 43 39	14, 26, 46, 65	0
1	F	633/684 (92%)	0.51	64 (10%) 12 10	18, 30, 58, 71	0
1	G	634/684 (92%)	0.03	25 (3%) 43 39	13, 23, 44, 69	0
1	H	634/684 (92%)	0.19	25 (3%) 43 39	15, 27, 45, 81	0
All	All	5072/5472 (92%)	0.18	249 (4%) 35 31	12, 26, 48, 81	0

All (249) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	369	LEU	5.5
1	F	159	ASN	5.3
1	C	486	GLY	5.1
1	H	483	VAL	5.0
1	B	369	LEU	5.0
1	B	487	GLY	5.0
1	F	486	GLY	5.0
1	A	368	VAL	4.9
1	H	368	VAL	4.8
1	C	382	ASP	4.7
1	F	281	PRO	4.7
1	E	369	LEU	4.7
1	G	159	ASN	4.6
1	C	437	ASN	4.5
1	F	439	VAL	4.4
1	D	369	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
1	F	368	VAL	4.2
1	G	382	ASP	4.1
1	H	382	ASP	4.0
1	H	486	GLY	4.0
1	F	383	LEU	4.0
1	A	281	PRO	3.9
1	G	484	PRO	3.9
1	E	485	ASN	3.9
1	H	437	ASN	3.8
1	D	381	ALA	3.8
1	B	435	GLY	3.8
1	F	279	ILE	3.7
1	D	158	THR	3.7
1	A	171	ILE	3.7
1	F	39	MET	3.7
1	F	272	VAL	3.7
1	A	365	TYR	3.7
1	H	281	PRO	3.6
1	C	439	VAL	3.6
1	B	486	GLY	3.6
1	F	484	PRO	3.6
1	H	365	TYR	3.6
1	B	365	TYR	3.5
1	E	437	ASN	3.5
1	C	2	VAL	3.5
1	G	158	THR	3.5
1	E	382	ASP	3.5
1	A	662	LEU	3.5
1	C	365	TYR	3.4
1	G	483	VAL	3.4
1	B	436	GLU	3.4
1	A	440	MET	3.4
1	F	158	THR	3.4
1	G	281	PRO	3.4
1	A	437	ASN	3.3
1	D	159	ASN	3.3
1	A	272	VAL	3.3
1	A	273	GLU	3.3
1	C	443	GLN	3.3
1	F	2	VAL	3.3
1	F	267	MET	3.2
1	F	277	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	F	437	ASN	3.2
1	A	369	LEU	3.2
1	B	437	ASN	3.2
1	F	369	LEU	3.2
1	B	439	VAL	3.2
1	E	487	GLY	3.2
1	H	158	THR	3.2
1	F	485	ASN	3.1
1	A	486	GLY	3.1
1	A	297	TYR	3.1
1	C	484	PRO	3.1
1	D	2	VAL	3.1
1	A	263	THR	3.0
1	A	274	ALA	3.0
1	F	169	TYR	3.0
1	H	381	ALA	3.0
1	E	281	PRO	3.0
1	F	275	ASP	3.0
1	G	482	ARG	3.0
1	C	364	LEU	3.0
1	C	383	LEU	3.0
1	F	84	GLN	3.0
1	F	130	ASP	3.0
1	G	443	GLN	3.0
1	F	138	ILE	2.9
1	D	366	GLU	2.9
1	A	277	THR	2.9
1	C	158	THR	2.9
1	B	95	ALA	2.9
1	C	281	PRO	2.9
1	D	368	VAL	2.9
1	E	381	ALA	2.9
1	B	281	PRO	2.9
1	F	477	THR	2.9
1	F	271	LYS	2.9
1	A	382	ASP	2.9
1	A	485	ASN	2.9
1	B	159	ASN	2.9
1	G	485	ASN	2.9
1	C	368	VAL	2.8
1	A	298	MET	2.8
1	D	382	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	142	ARG	2.8
1	G	486	GLY	2.8
1	F	208	ILE	2.8
1	G	460	ALA	2.8
1	F	213	PHE	2.8
1	F	226	LYS	2.8
1	E	365	TYR	2.8
1	F	160	LEU	2.8
1	D	38	GLU	2.8
1	F	280	LYS	2.8
1	C	384	HIS	2.8
1	F	276	GLY	2.8
1	C	485	ASN	2.8
1	F	364	LEU	2.8
1	H	364	LEU	2.8
1	H	384	HIS	2.8
1	D	486	GLY	2.7
1	F	483	VAL	2.7
1	A	442	LEU	2.7
1	A	2	VAL	2.7
1	F	436	GLU	2.7
1	H	481	ASP	2.7
1	A	172	GLY	2.7
1	G	369	LEU	2.7
1	D	436	GLU	2.7
1	E	435	GLY	2.7
1	E	158	THR	2.7
1	F	173	THR	2.7
1	E	84	GLN	2.7
1	G	384	HIS	2.6
1	E	659	ASP	2.6
1	F	10	GLU	2.6
1	H	485	ASN	2.6
1	G	365	TYR	2.6
1	A	275	ASP	2.6
1	F	382	ASP	2.6
1	F	274	ALA	2.6
1	D	281	PRO	2.5
1	F	662	LEU	2.5
1	C	483	VAL	2.5
1	F	269	HIS	2.5
1	A	169	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	440	MET	2.5
1	H	39	MET	2.5
1	E	486	GLY	2.5
1	H	366	GLU	2.5
1	B	485	ASN	2.5
1	E	159	ASN	2.5
1	E	669	ALA	2.5
1	B	158	THR	2.5
1	F	438	MET	2.5
1	D	365	TYR	2.5
1	D	487	GLY	2.5
1	G	96	GLY	2.5
1	E	481	ASP	2.5
1	B	2	VAL	2.5
1	B	368	VAL	2.5
1	H	2	VAL	2.5
1	A	364	LEU	2.5
1	G	381	ALA	2.5
1	C	300	THR	2.5
1	G	275	ASP	2.4
1	E	383	LEU	2.4
1	F	174	GLN	2.4
1	B	440	MET	2.4
1	B	667	GLU	2.4
1	G	471	GLY	2.4
1	B	382	ASP	2.4
1	G	383	LEU	2.4
1	H	439	VAL	2.4
1	F	487	GLY	2.4
1	H	484	PRO	2.4
1	F	172	GLY	2.4
1	F	365	TYR	2.4
1	G	368	VAL	2.4
1	F	128	ALA	2.4
1	D	56	GLU	2.4
1	E	666	MET	2.3
1	F	366	GLU	2.3
1	A	484	PRO	2.3
1	F	209	LYS	2.3
1	F	273	GLU	2.3
1	H	273	GLU	2.3
1	E	125	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	669	ALA	2.3
1	H	489	THR	2.3
1	C	39	MET	2.3
1	F	663	LYS	2.3
1	A	482	ARG	2.3
1	D	87	SER	2.3
1	A	438	MET	2.3
1	H	436	GLU	2.3
1	B	669	ALA	2.2
1	C	36	GLY	2.2
1	D	383	LEU	2.2
1	E	138	ILE	2.2
1	A	38	GLU	2.2
1	A	177	VAL	2.2
1	C	446	ARG	2.2
1	G	367	ARG	2.2
1	A	552	ASN	2.2
1	A	669	ALA	2.2
1	D	384	HIS	2.2
1	C	440	MET	2.2
1	A	483	VAL	2.2
1	E	2	VAL	2.2
1	G	95	ALA	2.2
1	A	39	MET	2.2
1	F	488	ILE	2.2
1	A	366	GLU	2.2
1	E	436	GLU	2.2
1	F	482	ARG	2.2
1	H	367	ARG	2.2
1	E	368	VAL	2.2
1	F	126	ALA	2.2
1	F	384	HIS	2.2
1	E	160	LEU	2.2
1	F	129	SER	2.2
1	B	134	ALA	2.1
1	D	437	ASN	2.1
1	F	367	ARG	2.1
1	A	167	ALA	2.1
1	F	125	ASN	2.1
1	D	157	GLY	2.1
1	A	279	ILE	2.1
1	F	661	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	2	VAL	2.1
1	A	158	THR	2.1
1	A	430	GLY	2.1
1	F	36	GLY	2.1
1	F	211	LYS	2.1
1	F	124	LEU	2.1
1	H	487	GLY	2.1
1	A	131	GLU	2.1
1	C	275	ASP	2.1
1	F	199	TYR	2.1
1	D	84	GLN	2.0
1	D	485	ASN	2.0
1	G	366	GLU	2.0
1	A	278	TYR	2.0
1	F	232	PRO	2.0
1	B	384	HIS	2.0
1	A	134	ALA	2.0
1	C	369	LEU	2.0
1	A	363	LYS	2.0
1	D	667	GLU	2.0
1	G	436	GLU	2.0
1	H	440	MET	2.0
1	E	87	SER	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.