



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:53 PM UTC

PDB ID : 6TC0 / pdb_00006tc0
Title : Crystal structure of MMS19-CIAO1-CIAO2B CIA targeting complex
Authors : Kassube, S.A.; Thoma, N.H.
Deposited on : 2019-11-04
Resolution : 3.60 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

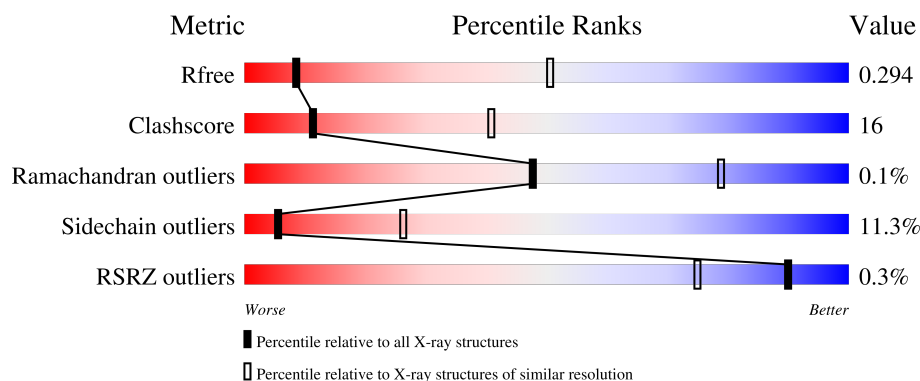
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

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

Mol	Chain	Length	Quality of chain
1	A	338	 82% 17% ..
1	D	338	 82% 17% ..
2	B	159	 70% 24% . .
2	E	159	 77% 18% . .
3	C	1035	 57% 33% 6% .

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Mol	Chain	Length	Quality of chain
3	F	1035	 A horizontal bar chart showing the quality of chain F. The bar is divided into three segments: green (58%), yellow (31%), and orange (6%). The segments are labeled with their respective percentages: 58%, 31%, and 6%. The bar ends with a small black dot.

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 22972 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 Probable cytosolic iron-sulfur protein assembly protein Ciao1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	336	Total	C	N	O	S	0	0	0
			2613	1629	455	516	13			
1	D	336	Total	C	N	O	S	0	0	0
			2613	1629	455	516	13			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q7K1Y4
A	-1	GLY	-	expression tag	UNP Q7K1Y4
A	0	GLY	-	expression tag	UNP Q7K1Y4
A	1	ARG	-	expression tag	UNP Q7K1Y4
D	-2	GLY	-	expression tag	UNP Q7K1Y4
D	-1	GLY	-	expression tag	UNP Q7K1Y4
D	0	GLY	-	expression tag	UNP Q7K1Y4
D	1	ARG	-	expression tag	UNP Q7K1Y4

- Molecule 2 is a protein called MIP18 family protein galla-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	154	Total	C	N	O	S	0	0	0
			1223	765	217	238	3			
2	E	154	Total	C	N	O	S	0	0	0
			1223	765	217	238	3			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	expression tag	UNP Q9VTC4
B	-1	GLY	-	expression tag	UNP Q9VTC4
B	0	GLY	-	expression tag	UNP Q9VTC4
B	1	ARG	-	expression tag	UNP Q9VTC4

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	GLY	-	expression tag	UNP Q9VTC4
E	-1	GLY	-	expression tag	UNP Q9VTC4
E	0	GLY	-	expression tag	UNP Q9VTC4
E	1	ARG	-	expression tag	UNP Q9VTC4

- Molecule 3 is a protein called MMS19 nucleotide excision repair protein homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	994	Total	C	N	O	S	0	0	0
			7669	4888	1311	1424	46			
3	F	989	Total	C	N	O	S	0	0	0
			7631	4862	1306	1418	45			

There are 8 discrepancies between the modelled and reference sequences:

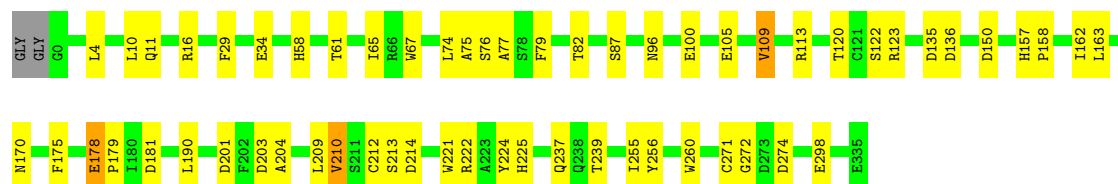
Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	GLY	-	expression tag	UNP Q9D071
C	-2	GLY	-	expression tag	UNP Q9D071
C	-1	GLY	-	expression tag	UNP Q9D071
C	0	ARG	-	expression tag	UNP Q9D071
F	-3	GLY	-	expression tag	UNP Q9D071
F	-2	GLY	-	expression tag	UNP Q9D071
F	-1	GLY	-	expression tag	UNP Q9D071
F	0	ARG	-	expression tag	UNP Q9D071

3 Residue-property plots

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

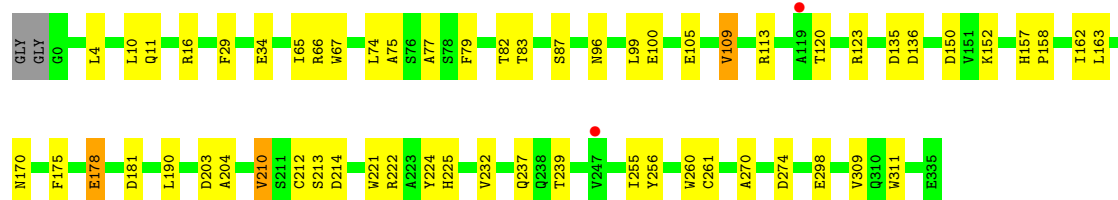
- Molecule 1: Probable cytosolic iron-sulfur protein assembly protein Ciaol

Chain A: 



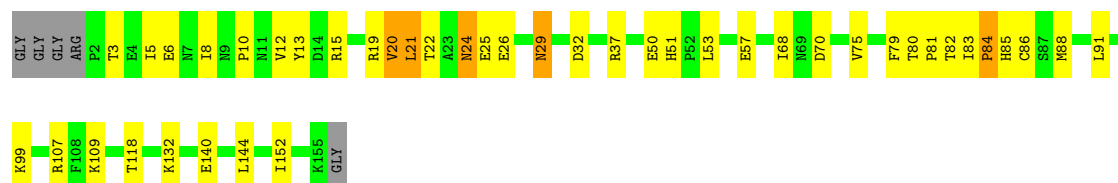
- Molecule 1: Probable cytosolic iron-sulfur protein assembly protein Ciaol

Chain D: 



- Molecule 2: MIP18 family protein galla-2

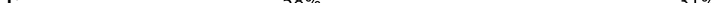
Chain B: 

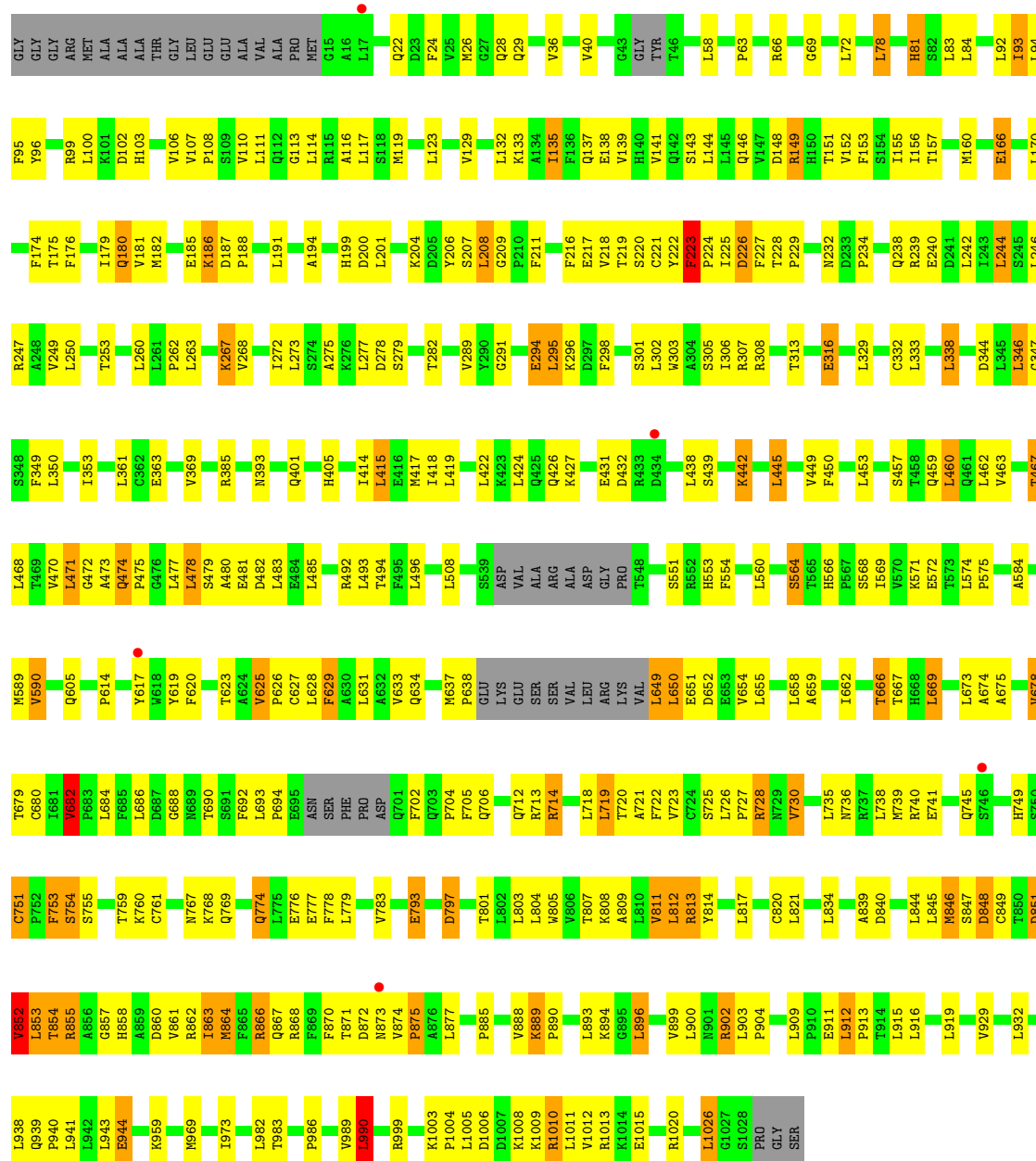


- Molecule 2: MIP18 family protein galla-2

Chain E: 



Chain F:  58% 31% 6% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	107.40Å 140.70Å 327.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.60 20.00 – 3.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-3.60) 99.3 (20.00-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 3.62Å)	Xtriage
Refinement program	CNS, PHENIX 1.16_3549	Depositor
R, R_{free}	0.258 , 0.277 0.278 , 0.294	Depositor DCC
R_{free} test set	2900 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	175.8	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 120.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	22972	wwPDB-VP
Average B, all atoms (Å ²)	211.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	0.33	0/2679	0.64	0/3649
1	D	0.40	0/2679	0.68	0/3649
2	B	0.55	0/1244	1.06	11/1694 (0.6%)
2	E	0.49	0/1244	0.92	6/1694 (0.4%)
3	C	0.42	1/7816 (0.0%)	0.79	14/10614 (0.1%)
3	F	0.44	1/7775 (0.0%)	0.78	6/10558 (0.1%)
All	All	0.43	2/23437 (0.0%)	0.78	37/31858 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	682	VAL	CA-CB	-8.03	1.50	1.54
3	C	187	ASP	CB-CG	-5.26	1.38	1.52

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	13	TYR	CA-C-N	11.02	135.05	120.28
2	B	13	TYR	C-N-CA	11.02	135.05	120.28
2	E	10	PRO	CA-C-N	9.60	134.10	120.28
2	E	10	PRO	C-N-CA	9.60	134.10	120.28
2	B	3	THR	CA-C-N	7.55	132.15	120.75
2	B	3	THR	C-N-CA	7.55	132.15	120.75
3	F	1026	LEU	CD1-CG-CD2	6.69	125.52	110.80
2	B	84	PRO	CA-C-N	-6.61	112.75	122.86
2	B	84	PRO	C-N-CA	-6.61	112.75	122.86
3	C	735	LEU	CB-CG-CD2	-6.45	91.34	110.70
2	B	6	GLU	CA-C-N	6.44	132.26	123.11
2	B	6	GLU	C-N-CA	6.44	132.26	123.11
3	C	684	LEU	CA-C-N	-6.33	111.83	120.44
3	C	684	LEU	C-N-CA	-6.33	111.83	120.44
2	E	83	ILE	CB-CA-C	6.31	115.52	109.33
3	C	136	PHE	CA-CB-CG	6.06	119.86	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	29	ASN	CA-C-N	6.04	131.27	120.59
2	E	29	ASN	C-N-CA	6.04	131.27	120.59
2	B	29	ASN	CA-C-N	6.03	131.26	120.59
2	B	29	ASN	C-N-CA	6.03	131.26	120.59
3	C	814	TYR	CA-CB-CG	5.96	124.62	113.90
3	F	135	ILE	CA-C-N	-5.96	111.18	121.66
3	F	135	ILE	C-N-CA	-5.96	111.18	121.66
2	B	20	VAL	N-CA-CB	-5.95	101.42	111.23
3	C	135	ILE	CA-C-N	-5.89	110.83	121.14
3	C	135	ILE	C-N-CA	-5.89	110.83	121.14
3	C	208	LEU	CA-CB-CG	5.68	136.20	116.30
3	C	804	LEU	CB-CG-CD1	-5.60	93.89	110.70
3	F	208	LEU	CA-CB-CG	5.59	135.86	116.30
3	F	852	VAL	CB-CA-C	-5.46	102.33	111.29
3	C	990	LEU	CA-CB-CG	5.33	134.94	116.30
3	C	852	VAL	CB-CA-C	-5.28	102.63	111.29
3	C	694	PRO	CA-C-N	5.20	127.97	120.38
3	C	694	PRO	C-N-CA	5.20	127.97	120.38
3	F	990	LEU	CA-CB-CG	5.13	134.25	116.30
3	C	712	GLN	CA-CB-CG	-5.09	103.91	114.10
2	E	107	ARG	NE-CZ-NH1	-5.01	116.49	121.50

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	2613	0	2480	39	0
1	D	2613	0	2480	33	0
2	B	1223	0	1230	56	0
2	E	1223	0	1230	41	0
3	C	7669	0	7810	311	0
3	F	7631	0	7774	316	0
All	All	22972	0	23004	743	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 16.

All (743) 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)
3:F:226:ASP:HB3	3:F:239:ARG:HD3	1.20	1.19
3:C:226:ASP:HB2	3:C:239:ARG:HD2	1.21	1.12
3:F:751:CYS:SG	3:F:754:SER:N	2.26	1.09
3:F:769:GLN:O	3:F:813:ARG:NH2	1.83	1.09
3:F:474:GLN:H	3:F:474:GLN:CD	1.64	1.01
3:F:474:GLN:OE1	3:F:474:GLN:N	1.93	1.00
3:C:604:GLN:HB2	3:C:661:VAL:HG22	1.44	0.98
2:B:8:ILE:HG21	2:E:144:LEU:HD13	1.42	0.98
3:F:877:LEU:HD13	3:F:896:LEU:HG	1.47	0.97
3:C:629:PHE:HB2	3:C:693:LEU:HD22	1.43	0.96
3:F:846:MET:O	3:F:866:ARG:NH1	1.98	0.96
3:C:746:SER:HB2	3:C:759:THR:HG22	1.46	0.95
3:C:629:PHE:HE1	3:C:697:SER:HB3	1.32	0.94
3:F:760:LYS:NZ	3:F:851:ASP:OD1	2.01	0.94
3:C:685:PHE:C	3:C:705:PHE:HE2	1.74	0.93
3:F:751:CYS:SG	3:F:755:SER:N	2.41	0.93
1:D:113:ARG:HD3	1:D:158:PRO:O	1.71	0.90
3:C:760:LYS:NZ	3:C:851:ASP:OD1	2.05	0.89
2:B:26:GLU:HG2	3:C:1010:ARG:HB2	1.55	0.88
3:F:735:LEU:HD21	3:F:769:GLN:NE2	1.90	0.87
3:C:629:PHE:CE1	3:C:697:SER:HB3	2.10	0.86
1:A:113:ARG:HD3	1:A:158:PRO:O	1.75	0.86
3:C:247:ARG:HG2	3:C:282:THR:HG22	1.57	0.86
3:C:216:PHE:O	3:C:220:SER:OG	1.94	0.86
3:C:873:ASN:HD21	3:C:877:LEU:HD12	1.38	0.85
3:F:735:LEU:HD21	3:F:769:GLN:HE22	1.40	0.85
3:F:814:TYR:HD2	3:F:862:ARG:HG3	1.38	0.85
3:F:216:PHE:O	3:F:220:SER:OG	1.95	0.84
3:C:58:LEU:HD11	3:C:73:LEU:HD11	1.59	0.84
2:B:19:ARG:O	2:B:37:ARG:NH2	2.10	0.83
2:E:107:ARG:NH2	3:F:1006:ASP:OD1	2.12	0.83
3:F:426:GLN:HE22	3:F:474:GLN:HB3	1.43	0.83
3:C:862:ARG:HA	3:F:217:GLU:OE1	1.78	0.82
3:F:226:ASP:CB	3:F:239:ARG:HD3	2.05	0.82
3:F:720:THR:HG22	3:F:761:CYS:HB2	1.60	0.82
3:C:734:GLN:HE21	3:C:737:ARG:HD2	1.45	0.82
3:C:597:VAL:HG23	3:C:654:VAL:HG23	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:735:LEU:HD21	3:C:769:GLN:NE2	1.96	0.81
3:F:713:ARG:HE	3:F:749:HIS:HD2	1.28	0.81
3:C:702:PHE:CZ	3:C:712:GLN:HB3	2.15	0.81
2:B:53:LEU:HD11	2:E:53:LEU:HD11	1.63	0.80
3:F:846:MET:HE2	3:F:903:LEU:HD21	1.64	0.80
3:F:805:TRP:HZ3	3:F:852:VAL:HG21	1.45	0.79
3:C:659:ALA:HB1	3:C:721:ALA:HB2	1.65	0.78
3:F:871:THR:O	3:F:875:PRO:HD2	1.83	0.78
3:F:24:PHE:CE1	3:F:72:LEU:HD13	2.19	0.78
3:C:750:SER:HA	3:C:798:GLN:HG2	1.64	0.78
3:C:132:LEU:HD23	3:C:132:LEU:H	1.49	0.77
3:C:705:PHE:HD1	3:C:741:GLU:CD	1.91	0.77
3:C:178:PHE:HA	3:C:181:VAL:HG22	1.65	0.77
3:C:191:LEU:HD21	3:C:222:TYR:HE2	1.50	0.77
3:F:625:VAL:HG12	3:F:692:PHE:HE1	1.50	0.77
3:F:848:ASP:OD2	3:F:848:ASP:N	2.15	0.77
1:A:87:SER:OG	1:A:96:ASN:OD1	2.02	0.77
1:D:87:SER:OG	1:D:96:ASN:OD1	2.01	0.77
2:B:107:ARG:NH2	3:C:1006:ASP:OD1	2.17	0.77
3:F:625:VAL:HG23	3:F:626:PRO:HD3	1.67	0.76
3:C:199:HIS:HB2	3:C:249:VAL:HG12	1.67	0.76
3:C:291:GLY:N	3:C:294:GLU:OE2	2.17	0.76
3:F:474:GLN:CD	3:F:474:GLN:N	2.29	0.76
3:C:686:LEU:HA	3:C:705:PHE:CE2	2.20	0.75
3:C:855:ARG:H	3:C:855:ARG:HD2	1.51	0.75
3:F:704:PRO:HG3	3:F:712:GLN:HB3	1.68	0.75
1:D:225:HIS:HA	1:D:239:THR:HG22	1.67	0.74
3:F:199:HIS:HB2	3:F:249:VAL:HG12	1.68	0.74
3:C:191:LEU:HD21	3:C:222:TYR:CE2	2.23	0.74
2:E:22:THR:O	2:E:26:GLU:HG3	1.87	0.74
1:A:272:GLY:O	2:B:109:LYS:NZ	2.20	0.74
1:D:256:TYR:CZ	2:E:132:LYS:HE2	2.22	0.74
3:F:229:PRO:HG2	3:F:232:ASN:O	1.88	0.74
3:C:747:CYS:HA	3:C:798:GLN:HB3	1.70	0.73
1:A:225:HIS:HA	1:A:239:THR:HG22	1.70	0.73
3:F:247:ARG:HG2	3:F:282:THR:HG22	1.70	0.73
3:C:182:MET:SD	3:C:194:ALA:HB1	2.27	0.73
1:D:152:LYS:NZ	2:E:133:GLU:OE1	2.21	0.73
3:F:855:ARG:H	3:F:855:ARG:HD2	1.52	0.73
2:B:84:PRO:HG3	2:E:118:THR:HA	1.69	0.73
3:F:267:LYS:HE2	3:F:275:ALA:HA	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:726:LEU:HB3	3:F:730:VAL:HG11	1.71	0.72
3:C:797:ASP:OD1	3:C:797:ASP:N	2.22	0.72
3:F:473:ALA:N	3:F:474:GLN:OE1	2.23	0.72
2:B:32:ASP:HB2	3:C:1013:ARG:NH2	2.04	0.72
2:B:144:LEU:HD13	2:E:8:ILE:HG21	1.72	0.72
3:F:426:GLN:NE2	3:F:474:GLN:HB3	2.05	0.72
3:F:805:TRP:CZ3	3:F:852:VAL:HG21	2.24	0.72
3:F:457:SER:HB2	3:F:460:LEU:HB2	1.72	0.71
3:C:188:PRO:HG3	3:C:227:PHE:HZ	1.55	0.71
3:F:678:VAL:O	3:F:682:VAL:HG23	1.90	0.71
3:C:294:GLU:N	3:C:294:GLU:OE1	2.23	0.71
3:F:848:ASP:OD1	3:F:855:ARG:NH2	2.23	0.71
3:C:714:ARG:HG2	3:C:753:PHE:CZ	2.26	0.71
3:F:690:THR:HB	3:F:693:LEU:HD11	1.72	0.71
3:F:814:TYR:CD2	3:F:862:ARG:HG3	2.23	0.71
3:C:746:SER:O	3:C:755:SER:HB2	1.90	0.71
3:F:807:THR:HG22	3:F:821:LEU:HB3	1.73	0.71
3:C:457:SER:HB2	3:C:460:LEU:HB2	1.73	0.70
3:F:226:ASP:HB3	3:F:239:ARG:CD	2.12	0.70
3:C:685:PHE:C	3:C:705:PHE:CE2	2.65	0.70
3:F:702:PHE:HA	3:F:712:GLN:NE2	2.05	0.70
3:F:659:ALA:HB1	3:F:721:ALA:HB2	1.73	0.70
3:C:217:GLU:HG3	3:F:863:ILE:HD13	1.72	0.70
3:F:103:HIS:HB3	3:F:106:VAL:HB	1.74	0.70
2:B:12:VAL:HA	2:B:15:ARG:HD2	1.73	0.69
3:C:292:GLN:N	3:C:293:LYS:HZ3	1.90	0.69
3:F:81:HIS:CE1	3:F:119:MET:HB3	2.28	0.69
3:C:223:PHE:CE1	3:C:267:LYS:HG3	2.28	0.69
3:C:223:PHE:HE1	3:C:267:LYS:HG3	1.57	0.69
3:F:182:MET:HG3	3:F:194:ALA:HB1	1.75	0.69
3:C:559:ALA:O	3:C:563:VAL:HG12	1.93	0.68
3:C:751:CYS:SG	3:C:752:PRO:HD2	2.33	0.68
3:F:797:ASP:N	3:F:797:ASP:OD1	2.23	0.68
3:F:81:HIS:HE1	3:F:119:MET:HB3	1.58	0.68
3:C:735:LEU:HD21	3:C:769:GLN:HE22	1.56	0.67
3:F:24:PHE:CE1	3:F:29:GLN:HB2	2.29	0.67
3:F:650:LEU:HD12	3:F:654:VAL:HG13	1.75	0.67
3:F:713:ARG:NE	3:F:749:HIS:HD2	1.91	0.67
3:F:221:CYS:HG	3:F:222:TYR:HD1	1.42	0.67
3:C:629:PHE:HE1	3:C:697:SER:CB	2.05	0.67
3:C:807:THR:HG22	3:C:821:LEU:HB3	1.74	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:24:ASN:OD1	2:B:24:ASN:N	2.26	0.67
3:C:81:HIS:HE1	3:C:119:MET:HB3	1.60	0.67
3:F:560:LEU:O	3:F:564:SER:OG	2.14	0.66
3:F:188:PRO:HG3	3:F:227:PHE:HZ	1.59	0.66
3:C:81:HIS:CE1	3:C:119:MET:HB3	2.31	0.66
2:B:26:GLU:HG3	2:B:32:ASP:CG	2.20	0.66
3:C:229:PRO:HG2	3:C:232:ASN:O	1.95	0.66
3:C:808:LYS:HB2	3:C:845:LEU:CD2	2.25	0.66
3:C:866:ARG:HB3	3:C:903:LEU:HD22	1.78	0.65
3:F:714:ARG:HG2	3:F:753:PHE:HE1	1.62	0.65
3:F:191:LEU:HD21	3:F:222:TYR:HE2	1.62	0.65
3:C:803:LEU:O	3:C:807:THR:HG23	1.97	0.65
3:F:191:LEU:HD21	3:F:222:TYR:CE2	2.31	0.65
3:F:625:VAL:HG12	3:F:692:PHE:CE1	2.30	0.65
2:B:118:THR:HA	2:E:84:PRO:HG3	1.78	0.65
3:C:226:ASP:HB2	3:C:239:ARG:CD	2.12	0.65
3:F:107:VAL:HG23	3:F:108:PRO:HD3	1.79	0.65
3:C:812:LEU:HB3	3:C:861:VAL:HG23	1.77	0.65
2:B:118:THR:CA	2:E:84:PRO:HG3	2.27	0.65
3:C:625:VAL:HB	3:C:626:PRO:HD3	1.77	0.65
3:F:24:PHE:CG	3:F:72:LEU:HD22	2.32	0.64
1:A:61:THR:OG1	2:B:140:GLU:OE2	2.14	0.64
3:C:873:ASN:ND2	3:C:877:LEU:HD12	2.12	0.64
3:F:78:LEU:HD12	3:F:116:ALA:HB2	1.79	0.64
3:F:267:LYS:HD2	3:F:279:SER:HB3	1.78	0.64
3:C:727:PRO:HA	3:C:858:HIS:ND1	2.13	0.64
3:C:739:MET:HG3	3:C:778:PHE:HE1	1.63	0.64
2:B:8:ILE:O	2:B:10:PRO:HD3	1.97	0.64
3:C:103:HIS:HB3	3:C:106:VAL:HB	1.79	0.64
3:C:734:GLN:NE2	3:C:737:ARG:HD2	2.13	0.64
2:B:68:ILE:HG13	2:B:75:VAL:HG22	1.80	0.64
3:F:471:LEU:C	3:F:474:GLN:CD	2.66	0.64
2:B:57:GLU:O	2:E:51:HIS:HE1	1.81	0.63
3:F:240:GLU:HG3	3:F:244:LEU:HD12	1.80	0.63
3:C:54:LEU:HD13	3:C:73:LEU:CD2	2.29	0.63
3:C:720:THR:HG22	3:C:761:CYS:HB2	1.80	0.63
3:F:22:GLN:O	3:F:26:MET:HG2	1.98	0.63
3:F:675:ALA:O	3:F:678:VAL:HG23	1.98	0.63
3:C:132:LEU:HA	3:C:135:ILE:HG23	1.80	0.63
3:F:226:ASP:CG	3:F:239:ARG:HH11	2.07	0.62
2:B:32:ASP:HB2	3:C:1013:ARG:HH22	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:714:ARG:HG2	3:C:753:PHE:HZ	1.63	0.62
3:C:940:PRO:O	3:C:944:GLU:HG2	2.00	0.62
3:C:93:ILE:HG13	3:C:117:LEU:HD13	1.80	0.62
3:C:768:LYS:HD3	3:C:858:HIS:O	1.97	0.62
3:F:846:MET:HE2	3:F:903:LEU:CD2	2.30	0.62
2:E:83:ILE:HG23	2:E:84:PRO:HD2	1.82	0.62
3:F:626:PRO:HA	3:F:629:PHE:HD2	1.64	0.62
3:F:439:SER:HA	3:F:442:LYS:HD2	1.81	0.62
3:F:803:LEU:O	3:F:807:THR:HG23	2.00	0.62
3:C:299:LEU:HD21	3:C:349:PHE:CD1	2.34	0.62
3:C:127:LEU:O	3:C:131:VAL:HG23	2.00	0.61
3:F:415:LEU:HD22	3:F:463:VAL:HG12	1.82	0.61
2:E:99:LYS:HB2	2:E:152:ILE:HD12	1.83	0.61
3:F:768:LYS:HD3	3:F:858:HIS:O	1.99	0.61
2:B:83:ILE:HG12	2:E:81:PRO:O	2.01	0.61
3:C:652:ASP:HB3	3:C:714:ARG:NH2	2.15	0.61
3:F:226:ASP:OD2	3:F:239:ARG:NH1	2.34	0.61
3:C:713:ARG:NH1	3:C:749:HIS:HB2	2.16	0.61
2:B:26:GLU:HG3	2:B:32:ASP:OD2	2.00	0.61
3:C:211:PHE:HA	3:C:214:GLU:OE2	2.01	0.61
3:F:847:SER:HB2	3:F:902:ARG:HE	1.65	0.61
3:C:70:ALA:HA	3:C:73:LEU:HD12	1.83	0.61
2:E:32:ASP:HB2	3:F:1013:ARG:NH2	2.16	0.61
3:F:851:ASP:OD2	3:F:851:ASP:N	2.29	0.61
2:B:51:HIS:HE1	2:E:57:GLU:O	1.84	0.60
3:F:940:PRO:O	3:F:944:GLU:HG2	1.99	0.60
3:C:680:CYS:C	3:C:683:PRO:HD2	2.26	0.60
3:C:750:SER:HA	3:C:798:GLN:CG	2.32	0.60
3:F:675:ALA:O	3:F:679:THR:HG23	2.01	0.60
3:C:807:THR:HG22	3:C:821:LEU:CB	2.30	0.60
3:F:631:LEU:HD23	3:F:718:LEU:CD1	2.31	0.60
3:C:217:GLU:HG3	3:F:863:ILE:CD1	2.31	0.60
3:F:471:LEU:O	3:F:474:GLN:NE2	2.35	0.60
3:F:807:THR:HG22	3:F:821:LEU:CB	2.31	0.60
1:D:190:LEU:HD23	1:D:221:TRP:CD2	2.37	0.59
3:C:107:VAL:HG23	3:C:108:PRO:HD3	1.84	0.59
3:C:146:GLN:NE2	3:C:187:ASP:HB2	2.17	0.59
3:C:623:THR:HA	3:C:626:PRO:HD2	1.83	0.59
3:F:740:ARG:NH2	3:F:777:GLU:OE2	2.35	0.59
3:C:709:SER:HB2	3:C:712:GLN:CD	2.28	0.59
3:C:739:MET:HG3	3:C:778:PHE:CE1	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:717:ALA:O	3:C:720:THR:OG1	2.14	0.59
3:C:969:MET:HE2	3:C:1009:LYS:HE2	1.83	0.59
3:F:650:LEU:HD11	3:F:655:LEU:HG	1.84	0.59
3:F:470:VAL:O	3:F:474:GLN:HG3	2.02	0.59
3:F:899:VAL:O	3:F:903:LEU:HG	2.02	0.59
3:F:631:LEU:HD23	3:F:718:LEU:HD11	1.85	0.59
3:C:78:LEU:HD12	3:C:116:ALA:HB2	1.83	0.59
3:C:234:PRO:HD3	3:F:427:LYS:HG2	1.85	0.59
3:C:938:LEU:HA	3:C:941:LEU:HD12	1.85	0.59
3:C:415:LEU:HD22	3:C:463:VAL:HG12	1.85	0.58
3:F:674:ALA:O	3:F:678:VAL:HG22	2.03	0.58
3:C:69:GLY:O	3:C:73:LEU:HG	2.03	0.58
3:C:182:MET:HG3	3:C:194:ALA:HB1	1.84	0.58
2:E:81:PRO:HG2	2:E:119:HIS:HB2	1.85	0.58
3:F:93:ILE:HG13	3:F:117:LEU:HD13	1.85	0.58
3:F:739:MET:HG3	3:F:778:PHE:HE1	1.68	0.58
1:A:203:ASP:OD2	1:A:204:ALA:N	2.32	0.58
3:C:808:LYS:NZ	3:C:847:SER:O	2.36	0.58
3:F:714:ARG:HG2	3:F:753:PHE:CE1	2.38	0.58
1:A:222:ARG:HG2	1:A:224:TYR:CE1	2.38	0.58
3:C:560:LEU:O	3:C:564:SER:OG	2.22	0.58
3:F:793:GLU:N	3:F:793:GLU:OE2	2.37	0.58
3:C:240:GLU:HG3	3:C:244:LEU:HD12	1.85	0.58
2:B:84:PRO:CG	2:E:118:THR:HA	2.34	0.57
3:F:182:MET:SD	3:F:194:ALA:HB1	2.44	0.57
2:B:99:LYS:HB2	2:B:152:ILE:HD12	1.86	0.57
2:E:9:ASN:OD1	2:E:11:ASN:HB2	2.04	0.57
3:F:751:CYS:SG	3:F:753:PHE:N	2.77	0.57
1:D:210:VAL:HG22	1:D:260:TRP:CE3	2.40	0.57
3:F:938:LEU:HA	3:F:941:LEU:HD12	1.85	0.57
1:A:190:LEU:HD23	1:A:221:TRP:CD2	2.40	0.57
2:B:22:THR:O	2:B:26:GLU:OE1	2.23	0.57
2:E:68:ILE:HG13	2:E:75:VAL:HG22	1.86	0.57
3:F:267:LYS:HD3	3:F:275:ALA:O	2.05	0.57
2:B:29:ASN:HA	3:C:1009:LYS:HE3	1.86	0.57
3:C:728:ARG:NE	3:F:180:GLN:HE21	2.02	0.57
3:C:854:THR:HG23	3:C:857:GLY:HA3	1.87	0.57
3:F:111:LEU:HD22	3:F:152:VAL:HG22	1.87	0.57
3:F:226:ASP:CB	3:F:239:ARG:HH11	2.17	0.57
3:F:854:THR:HG23	3:F:857:GLY:HA3	1.86	0.57
2:B:19:ARG:C	2:B:37:ARG:HH22	2.10	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:24:PHE:CE2	3:C:72:LEU:HB2	2.40	0.56
3:F:623:THR:C	3:F:626:PRO:HD2	2.30	0.56
2:B:29:ASN:HA	3:C:1009:LYS:CE	2.34	0.56
3:F:751:CYS:SG	3:F:754:SER:CA	2.93	0.56
3:C:713:ARG:HH12	3:C:749:HIS:HB2	1.70	0.56
3:C:727:PRO:HA	3:C:858:HIS:HD1	1.70	0.56
3:F:902:ARG:C	3:F:904:PRO:HD3	2.31	0.56
1:A:256:TYR:CZ	2:B:132:LYS:HE2	2.41	0.56
3:C:422:LEU:HD21	3:C:445:LEU:HD11	1.88	0.56
3:F:422:LEU:HD21	3:F:445:LEU:HD11	1.87	0.56
3:C:738:LEU:O	3:C:742:LEU:HG	2.06	0.56
3:F:247:ARG:HH11	3:F:282:THR:HG23	1.71	0.56
3:C:1008:LYS:HG3	3:C:1009:LYS:HD2	1.87	0.56
3:C:153:PHE:HA	3:C:156:ILE:HD12	1.88	0.56
3:F:129:VAL:HG23	3:F:166:GLU:HG2	1.87	0.56
3:F:839:ALA:HB1	3:F:894:LYS:HB3	1.88	0.56
3:C:969:MET:HG3	3:C:1009:LYS:HD3	1.88	0.55
3:C:563:VAL:HG22	3:C:569:ILE:HG21	1.88	0.55
3:C:146:GLN:HE21	3:C:187:ASP:HB2	1.70	0.55
3:C:151:THR:O	3:C:155:ILE:HG13	2.05	0.55
3:C:805:TRP:HZ3	3:C:852:VAL:HG21	1.71	0.55
3:F:471:LEU:C	3:F:474:GLN:NE2	2.64	0.55
2:B:8:ILE:HD11	2:E:91:LEU:HD22	1.87	0.55
3:C:482:ASP:OD1	3:C:482:ASP:N	2.40	0.55
3:C:627:CYS:O	3:C:631:LEU:HD12	2.06	0.55
3:F:682:VAL:HG12	3:F:738:LEU:HD12	1.88	0.55
3:F:704:PRO:HB3	3:F:712:GLN:HB3	1.88	0.55
3:C:211:PHE:HD1	3:C:214:GLU:OE1	1.90	0.55
3:C:333:LEU:HB3	3:C:346:LEU:HB3	1.89	0.55
3:C:973:ILE:HG23	3:C:1015:GLU:HG3	1.88	0.55
3:C:736:ASN:O	3:C:740:ARG:HG3	2.06	0.55
3:F:361:LEU:HA	3:F:369:VAL:HG23	1.88	0.55
3:C:299:LEU:C	3:C:299:LEU:HD23	2.32	0.55
3:F:704:PRO:CG	3:F:712:GLN:HB3	2.36	0.55
3:C:727:PRO:O	3:C:730:VAL:HG13	2.07	0.55
1:A:11:GLN:HE21	3:C:999:ARG:NH2	2.05	0.55
3:C:96:TYR:HD1	3:C:110:VAL:HG13	1.72	0.55
1:A:190:LEU:HD23	1:A:221:TRP:CE3	2.43	0.54
1:A:210:VAL:HG22	1:A:260:TRP:CE3	2.43	0.54
3:F:153:PHE:CE1	3:F:185:GLU:HG3	2.42	0.54
3:F:713:ARG:HE	3:F:749:HIS:CD2	2.18	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:ALA:HB2	1:A:109:VAL:HG22	1.89	0.54
3:F:574:LEU:HD13	3:F:623:THR:HG21	1.89	0.54
3:C:72:LEU:O	3:C:72:LEU:HG	2.07	0.54
1:D:212:CYS:HB2	1:D:255:ILE:HB	1.90	0.54
1:A:212:CYS:HB2	1:A:255:ILE:HB	1.88	0.54
3:C:50:VAL:O	3:C:54:LEU:HD12	2.06	0.54
3:F:426:GLN:HE22	3:F:475:PRO:HD2	1.73	0.54
3:C:247:ARG:NH1	3:C:281:GLN:HB3	2.23	0.54
3:C:680:CYS:HB3	3:C:692:PHE:CD1	2.43	0.54
1:A:271:CYS:SG	1:A:272:GLY:N	2.80	0.54
2:B:26:GLU:OE1	2:B:26:GLU:N	2.39	0.54
3:C:226:ASP:CB	3:C:239:ARG:HD2	2.15	0.54
3:C:349:PHE:CZ	3:C:353:ILE:HD11	2.43	0.54
3:C:695:GLU:HA	3:C:698:PHE:CZ	2.43	0.54
3:C:702:PHE:CE1	3:C:712:GLN:HB3	2.42	0.54
3:C:902:ARG:C	3:C:904:PRO:HD3	2.31	0.54
3:C:401:GLN:HE21	3:C:405:HIS:HE1	1.56	0.54
3:C:188:PRO:HG3	3:C:227:PHE:CZ	2.39	0.54
3:F:1008:LYS:HG3	3:F:1009:LYS:HD2	1.89	0.54
3:F:153:PHE:HA	3:F:156:ILE:HD12	1.89	0.53
3:C:684:LEU:HD13	3:C:690:THR:HG22	1.89	0.53
1:D:77:ALA:HB2	1:D:109:VAL:HG22	1.90	0.53
2:E:22:THR:HG21	3:F:1010:ARG:NH1	2.24	0.53
3:F:873:ASN:ND2	3:F:899:VAL:HG11	2.24	0.53
3:F:973:ILE:HG23	3:F:1015:GLU:HG3	1.91	0.53
3:C:790:LEU:O	3:C:796:ARG:NE	2.42	0.53
3:C:846:MET:HE2	3:C:903:LEU:CD2	2.38	0.53
1:D:222:ARG:HG2	1:D:224:TYR:CE1	2.43	0.53
3:C:614:PRO:HA	3:C:617:TYR:CE2	2.44	0.53
3:C:1005:LEU:HD11	3:C:1020:ARG:HD2	1.91	0.53
1:A:109:VAL:HG13	1:A:120:THR:HG22	1.90	0.52
3:C:338:LEU:HG	3:C:385:ARG:HH12	1.73	0.52
3:C:705:PHE:CD1	3:C:741:GLU:CD	2.81	0.52
3:F:96:TYR:HD1	3:F:110:VAL:HG13	1.74	0.52
3:C:182:MET:CG	3:C:194:ALA:HB1	2.39	0.52
2:B:84:PRO:HG3	2:E:118:THR:CA	2.38	0.52
3:F:779:LEU:HD22	3:F:817:LEU:HD23	1.91	0.52
3:F:779:LEU:O	3:F:783:VAL:HG23	2.09	0.52
1:A:82:THR:HG22	1:A:100:GLU:HG2	1.89	0.52
3:C:153:PHE:HE1	3:C:185:GLU:HG2	1.74	0.52
3:C:659:ALA:HB2	3:C:718:LEU:HD23	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:855:ARG:H	3:F:855:ARG:CD	2.19	0.52
2:E:32:ASP:HB2	3:F:1013:ARG:HH22	1.74	0.52
3:F:450:PHE:HA	3:F:453:LEU:HD12	1.91	0.52
3:C:347:GLY:HA2	3:C:350:LEU:HD12	1.91	0.52
3:C:808:LYS:HG2	3:C:812:LEU:HD11	1.92	0.52
3:C:1023:TRP:CE3	3:C:1026:LEU:HD11	2.45	0.52
1:D:190:LEU:HD23	1:D:221:TRP:CE3	2.45	0.52
3:F:182:MET:CG	3:F:194:ALA:HB1	2.40	0.52
3:F:442:LYS:HD3	3:F:477:LEU:O	2.09	0.52
3:F:132:LEU:HD21	3:F:174:PHE:CD1	2.44	0.52
3:F:333:LEU:HB3	3:F:346:LEU:HB3	1.92	0.52
2:B:5:ILE:HD12	2:E:128:GLN:HB3	1.91	0.51
3:C:415:LEU:HA	3:C:418:ILE:HD12	1.92	0.51
3:F:678:VAL:HG13	3:F:722:PHE:HE2	1.76	0.51
2:B:118:THR:HA	2:E:84:PRO:CG	2.40	0.51
3:C:695:GLU:HA	3:C:698:PHE:CE1	2.46	0.51
3:F:151:THR:O	3:F:155:ILE:HG13	2.10	0.51
3:F:726:LEU:HB3	3:F:730:VAL:CG1	2.38	0.51
3:C:188:PRO:CG	3:C:227:PHE:HZ	2.21	0.51
3:C:867:GLN:O	3:C:871:THR:HG23	2.10	0.51
3:F:338:LEU:HG	3:F:385:ARG:HH12	1.76	0.51
3:F:551:SER:HA	3:F:554:PHE:HD2	1.75	0.51
1:D:237:GLN:H	1:D:237:GLN:CD	2.19	0.51
2:B:82:THR:O	2:B:83:ILE:HB	2.10	0.51
3:C:92:LEU:HB3	3:C:117:LEU:HD11	1.92	0.51
3:C:361:LEU:HA	3:C:369:VAL:HG23	1.93	0.51
3:C:774:GLN:O	3:C:778:PHE:HD2	1.93	0.51
3:C:779:LEU:O	3:C:783:VAL:HG23	2.11	0.51
3:C:851:ASP:OD2	3:C:851:ASP:N	2.28	0.51
3:C:890:PRO:HA	3:C:893:LEU:HD12	1.93	0.51
3:F:896:LEU:HD22	3:F:900:LEU:HD11	1.92	0.51
3:C:779:LEU:HD22	3:C:817:LEU:HD23	1.91	0.50
1:A:157:HIS:HB2	1:A:162:ILE:HB	1.93	0.50
3:C:28:GLN:O	3:C:32:PRO:HD2	2.11	0.50
3:C:776:GLU:HA	3:C:779:LEU:HD12	1.93	0.50
1:D:82:THR:HG22	1:D:100:GLU:HG2	1.93	0.50
3:F:736:ASN:OD1	3:F:740:ARG:NE	2.44	0.50
3:C:666:THR:HG21	3:C:722:PHE:CD1	2.46	0.50
3:C:767:ASN:HB2	3:C:809:ALA:HB1	1.94	0.50
3:F:424:LEU:HD23	3:F:427:LYS:HD2	1.93	0.50
3:F:625:VAL:HG23	3:F:626:PRO:CD	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:669:LEU:HD23	3:F:674:ALA:HA	1.93	0.50
3:C:24:PHE:CZ	3:C:72:LEU:HB2	2.47	0.50
3:C:24:PHE:CE1	3:C:72:LEU:HD13	2.47	0.50
3:F:141:VAL:HG21	3:F:181:VAL:HG22	1.94	0.50
3:F:774:GLN:O	3:F:778:PHE:HD2	1.95	0.50
3:C:360:HIS:NE2	3:C:368:LEU:HB3	2.27	0.50
3:C:40:VAL:HG11	3:C:80:CYS:SG	2.52	0.50
3:C:769:GLN:HB3	3:C:775:LEU:HD12	1.94	0.50
3:F:808:LYS:HB2	3:F:845:LEU:CD2	2.42	0.50
3:C:180:GLN:NE2	3:F:728:ARG:HH11	2.09	0.49
3:F:58:LEU:HD21	3:F:69:GLY:HA3	1.94	0.49
3:F:209:GLY:C	3:F:211:PHE:H	2.20	0.49
3:F:566:HIS:HD2	3:F:568:SER:H	1.60	0.49
1:A:237:GLN:CD	1:A:237:GLN:H	2.20	0.49
2:B:25:GLU:H	2:B:25:GLU:CD	2.20	0.49
3:C:566:HIS:HB3	3:C:569:ILE:HD12	1.93	0.49
3:F:223:PHE:HB3	3:F:224:PRO:CD	2.42	0.49
3:C:211:PHE:HD1	3:C:214:GLU:CD	2.20	0.49
3:F:414:ILE:HA	3:F:417:MET:HE3	1.95	0.49
3:F:614:PRO:HA	3:F:617:TYR:CE2	2.45	0.49
3:F:303:TRP:CZ2	3:F:307:ARG:HD3	2.48	0.49
3:F:401:GLN:HE21	3:F:405:HIS:HE1	1.60	0.49
3:F:808:LYS:HB2	3:F:845:LEU:HD23	1.94	0.49
3:F:1005:LEU:HD11	3:F:1020:ARG:HD2	1.94	0.49
2:B:12:VAL:HG22	2:B:15:ARG:CZ	2.42	0.49
1:D:135:ASP:OD2	1:D:136:ASP:N	2.45	0.49
3:F:713:ARG:NE	3:F:749:HIS:CD2	2.76	0.49
2:B:80:THR:HG21	2:E:83:ILE:HG23	1.95	0.49
2:B:85:HIS:CD2	2:E:118:THR:HG22	2.48	0.49
3:F:141:VAL:HG21	3:F:181:VAL:HG13	1.94	0.49
1:A:213:SER:OG	1:A:214:ASP:N	2.46	0.49
3:C:650:LEU:C	3:C:650:LEU:HD12	2.37	0.49
3:F:634:GLN:OE1	3:F:650:LEU:HD22	2.12	0.49
3:F:983:THR:HA	3:F:990:LEU:HD11	1.95	0.49
3:C:414:ILE:HA	3:C:417:MET:HE3	1.95	0.48
3:C:709:SER:HB2	3:C:712:GLN:HG3	1.95	0.48
3:C:801:THR:O	3:C:805:TRP:HD1	1.95	0.48
3:F:739:MET:HG3	3:F:778:PHE:CE1	2.47	0.48
2:E:83:ILE:H	2:E:86:CYS:HB2	1.77	0.48
3:F:590:VAL:HG11	3:F:649:LEU:HD13	1.95	0.48
3:C:899:VAL:O	3:C:903:LEU:HG	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:228:THR:HG22	3:F:229:PRO:HD2	1.95	0.48
3:F:862:ARG:HA	3:F:862:ARG:HD3	1.51	0.48
3:F:478:LEU:CD2	3:F:482:ASP:HB2	2.44	0.48
3:C:735:LEU:HD23	3:C:774:GLN:HE22	1.78	0.48
3:C:983:THR:HA	3:C:990:LEU:HD11	1.95	0.48
1:D:4:LEU:HD23	1:D:298:GLU:HB2	1.95	0.48
3:F:684:LEU:HD12	3:F:692:PHE:CZ	2.49	0.48
3:C:149:ARG:NE	3:C:185:GLU:OE1	2.47	0.48
3:C:209:GLY:C	3:C:211:PHE:H	2.20	0.48
3:F:874:VAL:HG11	3:F:915:LEU:HD21	1.94	0.48
2:B:70:ASP:OD2	2:B:107:ARG:NH1	2.46	0.48
3:F:751:CYS:SG	3:F:753:PHE:C	2.96	0.48
3:C:131:VAL:O	3:C:135:ILE:HG22	2.13	0.48
3:C:292:GLN:N	3:C:293:LYS:NZ	2.60	0.48
3:C:551:SER:HA	3:C:554:PHE:HD2	1.79	0.48
1:A:163:LEU:HB3	1:A:175:PHE:HB2	1.95	0.48
3:C:129:VAL:HG23	3:C:166:GLU:HB3	1.96	0.48
3:C:566:HIS:HD2	3:C:568:SER:H	1.61	0.48
3:F:267:LYS:CD	3:F:279:SER:HB3	2.44	0.48
3:F:793:GLU:CD	3:F:793:GLU:H	2.22	0.48
3:F:969:MET:HE2	3:F:1009:LYS:HE2	1.96	0.48
3:F:63:PRO:HA	3:F:66:ARG:HD2	1.96	0.47
1:D:163:LEU:HB3	1:D:175:PHE:HB2	1.96	0.47
3:F:132:LEU:HD21	3:F:174:PHE:CE1	2.49	0.47
3:C:100:LEU:HB2	3:C:110:VAL:HG11	1.96	0.47
3:C:187:ASP:CG	3:C:190:ASN:H	2.22	0.47
1:D:157:HIS:HB2	1:D:162:ILE:HB	1.96	0.47
3:F:221:CYS:SG	3:F:222:TYR:HD1	2.38	0.47
3:F:571:LYS:HA	3:F:619:TYR:CE2	2.49	0.47
3:C:111:LEU:HD22	3:C:152:VAL:HG22	1.95	0.47
3:C:634:GLN:NE2	3:C:650:LEU:HD23	2.29	0.47
3:F:188:PRO:HB3	3:F:242:LEU:HD11	1.95	0.47
3:C:96:TYR:CD1	3:C:110:VAL:HG13	2.49	0.47
3:F:153:PHE:HE1	3:F:185:GLU:HG3	1.79	0.47
3:F:704:PRO:CB	3:F:712:GLN:HB3	2.43	0.47
3:F:705:PHE:CD1	3:F:741:GLU:HB3	2.49	0.47
3:F:864:MET:O	3:F:867:GLN:HG2	2.14	0.47
3:C:804:LEU:HD21	3:C:841:GLY:HA3	1.95	0.47
2:E:25:GLU:HB3	2:E:32:ASP:OD1	2.15	0.47
3:F:95:PHE:CZ	3:F:99:ARG:HG3	2.50	0.47
3:F:149:ARG:NE	3:F:185:GLU:OE1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:267:LYS:NZ	3:F:278:ASP:HB2	2.30	0.47
3:F:650:LEU:HD12	3:F:654:VAL:CG1	2.41	0.47
1:A:16:ARG:HG2	1:A:34:GLU:HB2	1.95	0.47
3:C:58:LEU:HD21	3:C:69:GLY:HA3	1.96	0.47
3:C:625:VAL:HG13	3:C:692:PHE:CE1	2.50	0.47
1:D:16:ARG:HG2	1:D:34:GLU:HB2	1.97	0.47
2:E:70:ASP:OD2	2:E:107:ARG:NH1	2.47	0.47
3:F:291:GLY:H	3:F:294:GLU:HG2	1.78	0.47
3:F:574:LEU:HD11	3:F:620:PHE:CD1	2.50	0.47
3:C:450:PHE:HA	3:C:453:LEU:HD12	1.96	0.47
3:F:629:PHE:O	3:F:633:VAL:HG23	2.14	0.47
3:F:767:ASN:HB2	3:F:809:ALA:HB1	1.96	0.47
3:F:854:THR:OG1	3:F:857:GLY:N	2.48	0.47
3:C:424:LEU:HD23	3:C:427:LYS:HD2	1.96	0.47
3:C:571:LYS:HA	3:C:619:TYR:CE2	2.50	0.47
1:D:109:VAL:HG13	1:D:120:THR:HG22	1.96	0.47
3:C:426:GLN:NE2	3:C:474:GLN:HG2	2.30	0.47
3:C:679:THR:O	3:C:683:PRO:HG2	2.15	0.47
1:D:261:CYS:HB2	1:D:311:TRP:CG	2.50	0.47
1:A:4:LEU:HD23	1:A:298:GLU:HB2	1.97	0.46
3:C:795:SER:HB3	3:C:798:GLN:OE1	2.15	0.46
3:C:24:PHE:CD1	3:C:29:GLN:HA	2.49	0.46
3:C:750:SER:HA	3:C:798:GLN:CD	2.39	0.46
1:D:203:ASP:OD2	1:D:204:ALA:N	2.41	0.46
3:C:617:TYR:OH	3:F:143:SER:HB2	2.15	0.46
2:E:99:LYS:HD3	2:E:152:ILE:HG23	1.96	0.46
3:C:63:PRO:HA	3:C:66:ARG:HD2	1.97	0.46
3:C:479:SER:HB3	3:C:482:ASP:CG	2.41	0.46
2:B:79:PHE:CE2	2:B:81:PRO:HG3	2.51	0.46
3:C:182:MET:HE2	3:C:218:VAL:CG1	2.46	0.46
2:E:26:GLU:OE2	3:F:1011:LEU:HG	2.15	0.46
3:F:626:PRO:HA	3:F:629:PHE:CD2	2.48	0.46
3:F:678:VAL:HG13	3:F:722:PHE:CE2	2.50	0.46
3:F:753:PHE:C	3:F:753:PHE:CD2	2.93	0.46
3:C:221:CYS:HG	3:C:222:TYR:HD1	1.63	0.46
3:F:714:ARG:HD3	3:F:753:PHE:HE1	1.81	0.46
3:F:813:ARG:O	3:F:813:ARG:HG2	2.15	0.46
3:F:188:PRO:HG3	3:F:227:PHE:CZ	2.46	0.46
3:F:866:ARG:HB3	3:F:903:LEU:HD22	1.97	0.46
3:C:625:VAL:HG12	3:C:693:LEU:HD23	1.97	0.46
3:C:739:MET:HA	3:C:742:LEU:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:99:LYS:HD3	2:B:152:ILE:HG23	1.98	0.46
3:C:480:ALA:HA	3:C:483:LEU:CD1	2.46	0.45
3:F:678:VAL:CG1	3:F:722:PHE:HE2	2.29	0.45
3:F:804:LEU:HD13	3:F:844:LEU:HD23	1.98	0.45
1:A:135:ASP:OD2	1:A:136:ASP:N	2.49	0.45
3:F:81:HIS:CE1	3:F:119:MET:CB	2.99	0.45
3:F:96:TYR:CD1	3:F:110:VAL:HG13	2.51	0.45
3:F:492:ARG:HH21	3:F:493:LEU:HD21	1.81	0.45
3:F:755:SER:O	3:F:759:THR:HG23	2.16	0.45
2:B:5:ILE:HB	2:E:128:GLN:OE1	2.16	0.45
3:C:43:GLY:O	3:C:46:THR:HG23	2.16	0.45
3:C:863:ILE:HG22	3:C:864:MET:SD	2.56	0.45
1:D:10:LEU:HD12	1:D:29:PHE:HZ	1.81	0.45
3:F:24:PHE:CD1	3:F:72:LEU:HD22	2.51	0.45
3:C:826:MET:HE1	3:C:877:LEU:HD23	1.98	0.45
3:F:347:GLY:HA2	3:F:350:LEU:HD12	1.97	0.45
3:C:36:VAL:O	3:C:40:VAL:HG23	2.17	0.45
3:C:685:PHE:HB3	3:C:705:PHE:CZ	2.51	0.45
3:C:685:PHE:CD2	3:C:719:LEU:HD22	2.51	0.45
3:F:24:PHE:CD2	3:F:72:LEU:HD22	2.52	0.45
3:C:709:SER:HB2	3:C:712:GLN:CG	2.46	0.45
3:C:712:GLN:HA	3:C:715:LEU:HD12	1.98	0.45
3:C:713:ARG:NH1	3:C:745:GLN:NE2	2.65	0.45
3:F:426:GLN:NE2	3:F:475:PRO:HD2	2.32	0.45
3:C:188:PRO:HB3	3:C:242:LEU:HD11	1.98	0.45
3:C:214:GLU:CG	3:F:862:ARG:HH12	2.30	0.45
3:F:221:CYS:SG	3:F:222:TYR:CD1	3.10	0.45
1:A:178:GLU:OE1	1:A:181:ASP:HB2	2.17	0.45
3:C:24:PHE:CE1	3:C:29:GLN:HB3	2.52	0.45
3:C:729:ASN:N	3:C:729:ASN:OD1	2.50	0.45
2:E:9:ASN:HD21	2:E:11:ASN:HD22	1.65	0.45
3:F:650:LEU:HD11	3:F:655:LEU:CG	2.47	0.45
3:F:675:ALA:HA	3:F:678:VAL:CG2	2.47	0.45
3:C:221:CYS:SG	3:C:222:TYR:HD1	2.40	0.45
3:C:426:GLN:CD	3:C:474:GLN:HG2	2.43	0.45
3:C:649:LEU:HB2	3:C:650:LEU:H	1.60	0.45
3:F:566:HIS:HB3	3:F:569:ILE:HD12	1.99	0.45
3:C:574:LEU:HD11	3:C:620:PHE:CD1	2.52	0.44
3:F:182:MET:O	3:F:182:MET:HG2	2.17	0.44
3:F:619:TYR:O	3:F:623:THR:HG23	2.17	0.44
3:F:688:GLY:O	3:F:690:THR:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:713:ARG:HD2	3:F:745:GLN:NE2	2.31	0.44
3:C:650:LEU:HD12	3:C:650:LEU:O	2.17	0.44
3:C:728:ARG:HH12	3:C:860:ASP:HB2	1.83	0.44
2:E:28:GLU:HB3	2:E:30:VAL:HG23	1.99	0.44
3:F:480:ALA:HA	3:F:483:LEU:HD12	2.00	0.44
1:A:10:LEU:HD12	1:A:29:PHE:HZ	1.83	0.44
3:C:805:TRP:CZ3	3:C:852:VAL:HG21	2.50	0.44
1:D:123:ARG:HA	1:D:150:ASP:OD1	2.17	0.44
3:F:223:PHE:HB3	3:F:224:PRO:HD3	2.00	0.44
1:A:79:PHE:HA	1:A:105:GLU:HB3	2.00	0.44
2:B:25:GLU:OE1	2:B:25:GLU:N	2.40	0.44
2:B:91:LEU:HD22	2:E:8:ILE:HD11	1.99	0.44
3:F:846:MET:HE3	3:F:846:MET:HA	1.98	0.44
3:C:479:SER:HB3	3:C:482:ASP:OD2	2.18	0.44
3:F:349:PHE:CZ	3:F:353:ILE:HD11	2.53	0.44
3:C:22:GLN:C	3:C:26:MET:HE2	2.43	0.44
3:F:415:LEU:HA	3:F:418:ILE:HD12	1.99	0.44
3:C:745:GLN:HG2	3:C:758:ALA:HB2	1.99	0.44
3:C:855:ARG:H	3:C:855:ARG:CD	2.19	0.44
3:F:308:ARG:HH11	3:F:308:ARG:HG3	1.83	0.44
3:F:727:PRO:O	3:F:730:VAL:HG13	2.17	0.44
2:B:82:THR:O	2:B:86:CYS:HB2	2.18	0.44
3:C:674:ALA:O	3:C:678:VAL:HG23	2.17	0.44
3:F:267:LYS:HG2	3:F:275:ALA:HB1	2.00	0.44
3:F:625:VAL:CG1	3:F:692:PHE:CE1	3.00	0.44
3:F:627:CYS:O	3:F:631:LEU:HD13	2.17	0.44
3:F:637:MET:HB3	3:F:638:PRO:HD3	2.00	0.44
1:A:11:GLN:HE21	3:C:999:ARG:CZ	2.30	0.43
1:A:256:TYR:CE1	2:B:132:LYS:HE2	2.53	0.43
3:C:153:PHE:CE1	3:C:185:GLU:HG2	2.53	0.43
3:C:160:MET:HE1	3:C:200:ASP:HB2	2.00	0.43
3:C:516:THR:HG23	3:C:565:THR:HB	2.00	0.43
1:D:79:PHE:HA	1:D:105:GLU:HB3	2.01	0.43
3:C:89:VAL:HG11	3:C:123:LEU:HB3	2.00	0.43
3:C:221:CYS:SG	3:C:222:TYR:CD1	3.11	0.43
3:C:911:GLU:HB3	3:C:915:LEU:HD23	1.99	0.43
3:F:262:PRO:HG3	3:F:298:PHE:CE1	2.53	0.43
3:C:152:VAL:HA	3:C:155:ILE:HD12	1.99	0.43
3:C:182:MET:HG3	3:C:194:ALA:CB	2.48	0.43
3:C:257:ALA:C	3:C:259:PHE:H	2.26	0.43
1:D:83:THR:HB	1:D:99:LEU:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:631:LEU:HD23	3:F:718:LEU:HD13	2.00	0.43
3:F:713:ARG:C	3:F:754:SER:OG	2.62	0.43
3:F:808:LYS:HE2	3:F:812:LEU:HD21	2.00	0.43
3:F:890:PRO:HA	3:F:893:LEU:HD12	1.99	0.43
1:A:178:GLU:HA	1:A:179:PRO:HD3	1.82	0.43
3:C:885:PRO:O	3:C:889:LYS:HB2	2.19	0.43
3:F:877:LEU:HD13	3:F:896:LEU:CG	2.34	0.43
1:A:58:HIS:NE2	1:A:76:SER:OG	2.38	0.43
3:C:743:LEU:HB3	3:C:785:THR:HG21	2.00	0.43
3:C:912:LEU:N	3:C:913:PRO:HD2	2.33	0.43
3:F:188:PRO:CG	3:F:227:PHE:HZ	2.29	0.43
3:F:969:MET:HG3	3:F:1009:LYS:HD3	1.99	0.43
3:F:1003:LYS:HB3	3:F:1004:PRO:HD3	2.01	0.43
1:A:178:GLU:CD	1:A:181:ASP:HB2	2.44	0.43
3:C:227:PHE:N	3:C:227:PHE:CD2	2.86	0.43
3:C:299:LEU:HD21	3:C:349:PHE:CG	2.53	0.43
3:C:749:HIS:HD1	3:C:749:HIS:C	2.27	0.43
3:F:227:PHE:CD2	3:F:227:PHE:N	2.86	0.43
3:F:361:LEU:HD23	3:F:369:VAL:HG22	2.00	0.43
3:C:178:PHE:HE2	3:C:198:VAL:HG23	1.84	0.43
3:C:693:LEU:HD23	3:C:693:LEU:HA	1.74	0.43
3:C:854:THR:OG1	3:C:857:GLY:N	2.51	0.43
3:C:361:LEU:HD11	3:C:376:LEU:HD11	2.01	0.43
3:F:36:VAL:O	3:F:40:VAL:HG23	2.19	0.43
3:C:81:HIS:CE1	3:C:119:MET:CB	3.01	0.43
3:C:214:GLU:CD	3:F:862:ARG:HH12	2.27	0.43
3:C:360:HIS:CD2	3:C:368:LEU:HB3	2.54	0.43
1:D:11:GLN:HE21	3:F:999:ARG:HH22	1.67	0.43
1:A:122:SER:OG	1:A:123:ARG:N	2.52	0.43
2:B:32:ASP:CB	3:C:1013:ARG:HH22	2.29	0.43
3:C:483:LEU:O	3:C:487:VAL:HG23	2.19	0.43
3:C:637:MET:HB3	3:C:638:PRO:HD3	2.01	0.43
3:C:659:ALA:HB1	3:C:721:ALA:CB	2.42	0.43
3:C:712:GLN:H	3:C:712:GLN:HG2	0.88	0.42
3:C:848:ASP:OD2	3:C:848:ASP:N	2.51	0.42
3:F:152:VAL:HA	3:F:155:ILE:HD12	2.01	0.42
3:F:808:LYS:O	3:F:811:VAL:N	2.47	0.42
3:F:911:GLU:HB3	3:F:915:LEU:HD23	2.01	0.42
3:C:260:LEU:HD13	3:C:264:LEU:HD11	2.01	0.42
3:C:308:ARG:HG3	3:C:308:ARG:HH11	1.84	0.42
3:C:597:VAL:HG23	3:C:654:VAL:CG2	2.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:625:VAL:HG12	3:C:693:LEU:CD2	2.49	0.42
3:F:459:GLN:HA	3:F:462:LEU:HD12	2.01	0.42
3:F:590:VAL:HG21	3:F:649:LEU:HD13	2.02	0.42
3:F:680:CYS:HB3	3:F:692:PHE:CD1	2.54	0.42
2:B:25:GLU:CD	2:B:25:GLU:N	2.77	0.42
3:C:872:ASP:O	3:C:875:PRO:HD2	2.19	0.42
3:F:92:LEU:HB3	3:F:117:LEU:HD11	2.00	0.42
3:F:107:VAL:CG2	3:F:108:PRO:HD3	2.48	0.42
3:F:182:MET:HG3	3:F:194:ALA:CB	2.46	0.42
3:F:714:ARG:CG	3:F:753:PHE:HE1	2.28	0.42
3:F:719:LEU:O	3:F:720:THR:C	2.62	0.42
3:F:298:PHE:CD2	3:F:298:PHE:N	2.88	0.42
3:F:847:SER:HB2	3:F:902:ARG:NE	2.34	0.42
3:C:492:ARG:HH21	3:C:493:LEU:HD21	1.82	0.42
3:C:572:GLU:O	3:C:575:PRO:HD2	2.20	0.42
3:C:628:LEU:HD23	3:C:718:LEU:HD13	2.01	0.42
3:C:719:LEU:O	3:C:723:VAL:HG23	2.19	0.42
1:D:224:TYR:CE2	1:D:232:VAL:HG21	2.55	0.42
2:E:29:ASN:HA	3:F:1009:LYS:HE3	2.02	0.42
3:F:986:PRO:O	3:F:989:VAL:HG22	2.19	0.42
3:C:176:PHE:HA	3:C:179:ILE:HD12	2.02	0.42
3:C:182:MET:HE2	3:C:218:VAL:HG11	2.01	0.42
3:C:187:ASP:OD1	3:C:189:ARG:HB3	2.19	0.42
3:C:804:LEU:HA	3:C:804:LEU:HD23	1.55	0.42
3:F:584:ALA:HA	3:F:589:MET:HB2	2.00	0.42
3:C:216:PHE:CE2	3:C:259:PHE:HB3	2.54	0.42
3:C:296:LYS:HD2	3:C:296:LYS:C	2.45	0.42
3:C:600:CYS:SG	3:C:658:LEU:HD22	2.60	0.42
3:F:176:PHE:HA	3:F:179:ILE:HD12	2.00	0.42
3:F:182:MET:HE1	3:F:219:THR:HG23	2.02	0.42
2:B:5:ILE:HB	2:E:128:GLN:CD	2.45	0.42
3:C:459:GLN:HA	3:C:462:LEU:HD12	2.02	0.42
3:C:625:VAL:HB	3:C:626:PRO:CD	2.46	0.42
3:C:661:VAL:O	3:C:664:THR:OG1	2.32	0.42
3:C:986:PRO:O	3:C:989:VAL:HG22	2.20	0.42
3:F:472:GLY:C	3:F:474:GLN:OE1	2.63	0.42
3:F:650:LEU:O	3:F:650:LEU:HG	2.14	0.42
3:F:662:ILE:O	3:F:666:THR:OG1	2.37	0.42
3:F:713:ARG:HD2	3:F:745:GLN:HE21	1.84	0.42
3:F:721:ALA:O	3:F:725:SER:OG	2.32	0.42
3:F:912:LEU:N	3:F:913:PRO:HD2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:ARG:HA	1:A:150:ASP:OD1	2.20	0.42
3:F:719:LEU:HD11	3:F:738:LEU:HD21	2.01	0.42
3:C:846:MET:HE2	3:C:903:LEU:HD23	2.01	0.42
3:C:1003:LYS:HB3	3:C:1004:PRO:HD3	2.02	0.42
2:B:118:THR:O	2:E:84:PRO:HG3	2.20	0.41
3:C:187:ASP:HA	3:C:188:PRO:HD3	1.83	0.41
3:C:201:LEU:O	3:C:206:TYR:HB2	2.20	0.41
3:F:96:TYR:CE1	3:F:113:GLY:HA3	2.56	0.41
3:F:201:LEU:O	3:F:206:TYR:HB2	2.20	0.41
3:F:684:LEU:C	3:F:684:LEU:HD23	2.45	0.41
3:F:909:LEU:O	3:F:912:LEU:HB2	2.19	0.41
3:C:749:HIS:O	3:C:749:HIS:ND1	2.52	0.41
3:C:894:LYS:HG2	3:C:930:VAL:HG21	2.02	0.41
3:F:896:LEU:HD22	3:F:900:LEU:CD1	2.50	0.41
3:F:160:MET:HE1	3:F:200:ASP:HB2	2.02	0.41
3:F:692:PHE:H	3:F:692:PHE:HD2	1.67	0.41
3:C:187:ASP:OD2	3:C:190:ASN:CG	2.63	0.41
3:C:702:PHE:HZ	3:C:712:GLN:HB3	1.77	0.41
3:C:853:LEU:H	3:C:853:LEU:HD22	1.85	0.41
1:D:178:GLU:CD	1:D:181:ASP:HB2	2.45	0.41
1:A:65:ILE:HA	1:A:75:ALA:O	2.20	0.41
3:C:741:GLU:OE1	3:C:741:GLU:C	2.63	0.41
3:F:467:THR:O	3:F:471:LEU:HB2	2.21	0.41
3:F:702:PHE:HA	3:F:712:GLN:HE22	1.83	0.41
3:F:720:THR:HG22	3:F:761:CYS:CB	2.41	0.41
3:C:223:PHE:CD1	3:C:224:PRO:HD3	2.56	0.41
3:C:293:LYS:NZ	3:C:293:LYS:H	2.18	0.41
3:C:439:SER:HA	3:C:442:LYS:HD2	2.03	0.41
3:C:889:LYS:N	3:C:890:PRO:CD	2.84	0.41
1:D:65:ILE:HA	1:D:75:ALA:O	2.21	0.41
1:D:270:ALA:HB2	1:D:309:VAL:HG13	2.02	0.41
3:F:24:PHE:CD1	3:F:29:GLN:HA	2.56	0.41
3:F:572:GLU:O	3:F:575:PRO:HD2	2.21	0.41
3:F:885:PRO:O	3:F:889:LYS:HB2	2.20	0.41
3:F:939:GLN:HB3	3:F:940:PRO:HD3	2.01	0.41
3:C:629:PHE:HZ	3:C:696:ASN:HB2	1.86	0.41
3:C:749:HIS:C	3:C:749:HIS:ND1	2.78	0.41
3:F:303:TRP:CH2	3:F:307:ARG:HD3	2.56	0.41
3:F:736:ASN:O	3:F:740:ARG:HG3	2.20	0.41
3:C:695:GLU:OE1	3:C:695:GLU:N	2.53	0.41
3:F:246:LEU:HD22	3:F:250:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:713:ARG:O	3:F:754:SER:OG	2.36	0.41
3:F:870:PHE:HB2	3:F:903:LEU:HD13	2.02	0.41
1:A:190:LEU:HD12	1:A:190:LEU:N	2.35	0.41
3:C:187:ASP:OD2	3:C:190:ASN:CB	2.69	0.41
3:C:246:LEU:HD22	3:C:250:LEU:HD11	2.02	0.41
3:C:427:LYS:HG2	3:F:234:PRO:HD3	2.03	0.41
1:D:213:SER:OG	1:D:214:ASP:N	2.54	0.41
3:F:186:LYS:HD2	3:F:186:LYS:N	2.35	0.41
3:F:449:VAL:O	3:F:453:LEU:HG	2.20	0.41
3:F:651:GLU:H	3:F:654:VAL:HG11	1.86	0.41
3:F:714:ARG:HD3	3:F:753:PHE:CE1	2.55	0.41
3:F:751:CYS:HG	3:F:755:SER:H	1.56	0.41
3:F:776:GLU:HA	3:F:779:LEU:HD12	2.02	0.41
3:F:801:THR:O	3:F:805:TRP:HD1	2.04	0.41
3:F:814:TYR:HE1	3:F:868:ARG:CG	2.34	0.41
1:A:201:ASP:C	1:A:209:LEU:HD12	2.46	0.41
2:B:20:VAL:C	2:B:21:LEU:HD23	2.45	0.41
3:C:735:LEU:HG	3:C:778:PHE:CZ	2.55	0.41
3:F:191:LEU:HA	3:F:191:LEU:HD23	1.85	0.41
3:F:678:VAL:O	3:F:680:CYS:N	2.54	0.41
3:F:889:LYS:N	3:F:890:PRO:CD	2.84	0.41
3:C:261:LEU:O	3:C:265:ILE:HG13	2.22	0.40
3:F:629:PHE:CD2	3:F:694:PRO:HD2	2.56	0.40
3:F:846:MET:HA	3:F:846:MET:CE	2.51	0.40
1:A:67:TRP:CD2	1:A:74:LEU:HD13	2.56	0.40
2:B:12:VAL:HG22	2:B:15:ARG:NH1	2.37	0.40
3:C:214:GLU:HG3	3:F:862:ARG:HH12	1.85	0.40
3:C:909:LEU:O	3:C:912:LEU:HB2	2.20	0.40
3:F:182:MET:O	3:F:218:VAL:HG11	2.21	0.40
3:F:294:GLU:CD	3:F:294:GLU:H	2.29	0.40
3:F:494:THR:HG22	3:F:508:LEU:HG	2.01	0.40
3:F:690:THR:HB	3:F:693:LEU:CD1	2.47	0.40
3:F:809:ALA:HA	3:F:812:LEU:CD1	2.52	0.40
1:A:201:ASP:O	1:A:209:LEU:HD12	2.21	0.40
2:B:50:GLU:OE2	2:B:88:MET:HE3	2.21	0.40
2:B:83:ILE:HG22	2:B:85:HIS:H	1.87	0.40
1:D:66:ARG:HA	1:D:66:ARG:HD3	1.81	0.40
3:F:295:LEU:N	3:F:295:LEU:HD23	2.36	0.40
3:F:629:PHE:CD1	3:F:629:PHE:C	2.98	0.40
2:B:20:VAL:O	2:B:20:VAL:HG13	2.21	0.40
3:C:530:LEU:HD13	3:C:560:LEU:HG	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:652:ASP:HB3	3:C:714:ARG:HH21	1.82	0.40
3:C:657:ALA:O	3:C:661:VAL:HG23	2.22	0.40
3:C:848:ASP:HB3	3:C:855:ARG:HH21	1.87	0.40
1:D:67:TRP:CD2	1:D:74:LEU:HD13	2.56	0.40
2:E:9:ASN:CG	2:E:11:ASN:HB2	2.46	0.40
3:F:108:PRO:HB3	3:F:148:ASP:CG	2.46	0.40
3:F:316:GLU:H	3:F:316:GLU:HG3	1.67	0.40
3:C:625:VAL:HG13	3:C:692:PHE:CD1	2.57	0.40
3:F:853:LEU:HD22	3:F:853:LEU:H	1.86	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	334/338 (99%)	320 (96%)	14 (4%)	0	100	100
1	D	334/338 (99%)	322 (96%)	12 (4%)	0	100	100
2	B	152/159 (96%)	148 (97%)	4 (3%)	0	100	100
2	E	152/159 (96%)	148 (97%)	4 (3%)	0	100	100
3	C	984/1035 (95%)	936 (95%)	47 (5%)	1 (0%)	48	79
3	F	979/1035 (95%)	930 (95%)	48 (5%)	1 (0%)	48	79
All	All	2935/3064 (96%)	2804 (96%)	129 (4%)	2 (0%)	48	79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	223	PHE
3	F	223	PHE

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	284/284 (100%)	279 (98%)	5 (2%)	51	68
1	D	284/284 (100%)	279 (98%)	5 (2%)	51	68
2	B	141/142 (99%)	139 (99%)	2 (1%)	59	71
2	E	141/142 (99%)	141 (100%)	0	100	100
3	C	859/887 (97%)	725 (84%)	134 (16%)	2	16
3	F	854/887 (96%)	710 (83%)	144 (17%)	2	13
All	All	2563/2626 (98%)	2273 (89%)	290 (11%)	5	26

All (290) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	109	VAL
1	A	170	ASN
1	A	178	GLU
1	A	210	VAL
1	A	274	ASP
2	B	21	LEU
2	B	24	ASN
3	C	78	LEU
3	C	81	HIS
3	C	83	LEU
3	C	84	LEU
3	C	93	ILE
3	C	94	LEU
3	C	100	LEU
3	C	114	LEU
3	C	123	LEU
3	C	135	ILE
3	C	136	PHE
3	C	137	GLN
3	C	138	GLU
3	C	144	LEU
3	C	149	ARG

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Mol	Chain	Res	Type
3	C	157	THR
3	C	170	LEU
3	C	175	THR
3	C	187	ASP
3	C	204	LYS
3	C	207	SER
3	C	208	LEU
3	C	214	GLU
3	C	225	ILE
3	C	238	GLN
3	C	244	LEU
3	C	253	THR
3	C	260	LEU
3	C	263	LEU
3	C	268	VAL
3	C	272	ILE
3	C	273	LEU
3	C	277	LEU
3	C	289	VAL
3	C	293	LYS
3	C	294	GLU
3	C	295	LEU
3	C	296	LYS
3	C	301	SER
3	C	305	SER
3	C	306	ILE
3	C	313	THR
3	C	316	GLU
3	C	329	LEU
3	C	332	CYS
3	C	338	LEU
3	C	344	ASP
3	C	346	LEU
3	C	363	GLU
3	C	393	ASN
3	C	415	LEU
3	C	419	LEU
3	C	431	GLU
3	C	432	ASP
3	C	438	LEU
3	C	442	LYS
3	C	445	LEU

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Mol	Chain	Res	Type
3	C	460	LEU
3	C	467	THR
3	C	468	LEU
3	C	469	THR
3	C	471	LEU
3	C	482	ASP
3	C	483	LEU
3	C	485	LEU
3	C	496	LEU
3	C	553	HIS
3	C	564	SER
3	C	590	VAL
3	C	597	VAL
3	C	605	GLN
3	C	649	LEU
3	C	653	GLU
3	C	654	VAL
3	C	658	LEU
3	C	666	THR
3	C	667	THR
3	C	669	LEU
3	C	673	LEU
3	C	686	LEU
3	C	692	PHE
3	C	695	GLU
3	C	709	SER
3	C	712	GLN
3	C	714	ARG
3	C	723	VAL
3	C	729	ASN
3	C	730	VAL
3	C	738	LEU
3	C	745	GLN
3	C	753	PHE
3	C	754	SER
3	C	759	THR
3	C	774	GLN
3	C	794	SER
3	C	795	SER
3	C	797	ASP
3	C	811	VAL
3	C	812	LEU

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Mol	Chain	Res	Type
3	C	814	TYR
3	C	820	CYS
3	C	842	PHE
3	C	843	SER
3	C	846	MET
3	C	847	SER
3	C	848	ASP
3	C	849	CYS
3	C	851	ASP
3	C	852	VAL
3	C	853	LEU
3	C	854	THR
3	C	855	ARG
3	C	860	ASP
3	C	861	VAL
3	C	863	ILE
3	C	864	MET
3	C	868	ARG
3	C	872	ASP
3	C	888	VAL
3	C	889	LYS
3	C	896	LEU
3	C	902	ARG
3	C	912	LEU
3	C	916	LEU
3	C	919	LEU
3	C	929	VAL
3	C	932	LEU
3	C	943	LEU
3	C	944	GLU
3	C	959	LYS
3	C	982	LEU
3	C	990	LEU
3	C	1010	ARG
3	C	1012	VAL
1	D	109	VAL
1	D	170	ASN
1	D	178	GLU
1	D	210	VAL
1	D	274	ASP
3	F	28	GLN
3	F	78	LEU

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Mol	Chain	Res	Type
3	F	81	HIS
3	F	83	LEU
3	F	84	LEU
3	F	93	ILE
3	F	94	LEU
3	F	100	LEU
3	F	102	ASP
3	F	114	LEU
3	F	123	LEU
3	F	133	LYS
3	F	135	ILE
3	F	137	GLN
3	F	138	GLU
3	F	139	VAL
3	F	144	LEU
3	F	146	GLN
3	F	149	ARG
3	F	157	THR
3	F	166	GLU
3	F	170	LEU
3	F	175	THR
3	F	180	GLN
3	F	186	LYS
3	F	187	ASP
3	F	204	LYS
3	F	207	SER
3	F	208	LEU
3	F	223	PHE
3	F	225	ILE
3	F	226	ASP
3	F	238	GLN
3	F	244	LEU
3	F	253	THR
3	F	260	LEU
3	F	263	LEU
3	F	267	LYS
3	F	268	VAL
3	F	272	ILE
3	F	273	LEU
3	F	277	LEU
3	F	289	VAL
3	F	294	GLU

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Mol	Chain	Res	Type
3	F	295	LEU
3	F	296	LYS
3	F	301	SER
3	F	302	LEU
3	F	305	SER
3	F	306	ILE
3	F	313	THR
3	F	316	GLU
3	F	329	LEU
3	F	332	CYS
3	F	338	LEU
3	F	344	ASP
3	F	346	LEU
3	F	363	GLU
3	F	393	ASN
3	F	415	LEU
3	F	419	LEU
3	F	431	GLU
3	F	432	ASP
3	F	438	LEU
3	F	442	LYS
3	F	445	LEU
3	F	460	LEU
3	F	467	THR
3	F	468	LEU
3	F	471	LEU
3	F	474	GLN
3	F	478	LEU
3	F	479	SER
3	F	481	GLU
3	F	485	LEU
3	F	496	LEU
3	F	553	HIS
3	F	564	SER
3	F	590	VAL
3	F	605	GLN
3	F	625	VAL
3	F	628	LEU
3	F	629	PHE
3	F	649	LEU
3	F	650	LEU
3	F	652	ASP

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Mol	Chain	Res	Type
3	F	658	LEU
3	F	666	THR
3	F	667	THR
3	F	669	LEU
3	F	673	LEU
3	F	678	VAL
3	F	682	VAL
3	F	686	LEU
3	F	706	GLN
3	F	714	ARG
3	F	719	LEU
3	F	723	VAL
3	F	728	ARG
3	F	730	VAL
3	F	751	CYS
3	F	753	PHE
3	F	754	SER
3	F	774	GLN
3	F	793	GLU
3	F	797	ASP
3	F	811	VAL
3	F	812	LEU
3	F	813	ARG
3	F	820	CYS
3	F	834	LEU
3	F	840	ASP
3	F	846	MET
3	F	848	ASP
3	F	849	CYS
3	F	851	ASP
3	F	852	VAL
3	F	853	LEU
3	F	854	THR
3	F	855	ARG
3	F	860	ASP
3	F	861	VAL
3	F	863	ILE
3	F	864	MET
3	F	866	ARG
3	F	872	ASP
3	F	875	PRO
3	F	888	VAL

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Mol	Chain	Res	Type
3	F	889	LYS
3	F	896	LEU
3	F	902	ARG
3	F	912	LEU
3	F	916	LEU
3	F	919	LEU
3	F	929	VAL
3	F	932	LEU
3	F	943	LEU
3	F	944	GLU
3	F	959	LYS
3	F	982	LEU
3	F	990	LEU
3	F	1010	ARG
3	F	1012	VAL
3	F	1026	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	228	ASN
1	A	310	GLN
2	B	9	ASN
2	B	51	HIS
2	B	76	HIS
2	B	85	HIS
3	C	29	GLN
3	C	75	GLN
3	C	81	HIS
3	C	103	HIS
3	C	137	GLN
3	C	146	GLN
3	C	180	GLN
3	C	199	HIS
3	C	312	GLN
3	C	389	HIS
3	C	401	GLN
3	C	410	GLN
3	C	461	GLN
3	C	489	HIS
3	C	535	HIS

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Mol	Chain	Res	Type
3	C	558	GLN
3	C	566	HIS
3	C	579	GLN
3	C	583	GLN
3	C	588	ASN
3	C	734	GLN
3	C	745	GLN
3	C	769	GLN
3	C	873	ASN
3	C	901	ASN
3	C	980	HIS
1	D	11	GLN
1	D	228	ASN
1	D	310	GLN
2	E	11	ASN
2	E	51	HIS
3	F	75	GLN
3	F	81	HIS
3	F	137	GLN
3	F	180	GLN
3	F	284	ASN
3	F	312	GLN
3	F	401	GLN
3	F	410	GLN
3	F	461	GLN
3	F	489	HIS
3	F	535	HIS
3	F	558	GLN
3	F	566	HIS
3	F	583	GLN
3	F	588	ASN
3	F	769	GLN
3	F	873	ASN
3	F	901	ASN
3	F	980	HIS

5.3.3 RNA ⓘ

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 [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	336/338 (99%)	-0.64	0 100 100	148, 195, 264, 303	0
1	D	336/338 (99%)	-0.30	2 (0%) 85 64	314, 381, 426, 449	0
2	B	154/159 (96%)	-0.37	0 100 100	164, 192, 281, 306	0
2	E	154/159 (96%)	-0.35	0 100 100	220, 249, 307, 323	0
3	C	994/1035 (96%)	-0.43	2 (0%) 91 80	118, 184, 263, 377	0
3	F	989/1035 (95%)	-0.45	5 (0%) 87 66	111, 167, 234, 375	0
All	All	2963/3064 (96%)	-0.44	9 (0%) 90 75	111, 189, 385, 449	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	873	ASN	5.9
3	F	434	ASP	4.2
1	D	247	VAL	3.5
3	C	617	TYR	3.4
3	F	617	TYR	3.1
3	C	873	ASN	2.6
1	D	119	ALA	2.3
3	F	17	LEU	2.2
3	F	746	SER	2.2

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.