



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:57 PM UTC

PDB ID : 5U9O / pdb_00005u9o
Title : Cocrystal structure of the intermembrane space region of the plastid division proteins PARC6 and PDV1
Authors : Delmar, J.A.; Chou, T.H.
Deposited on : 2016-12-16
Resolution : 3.37 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:

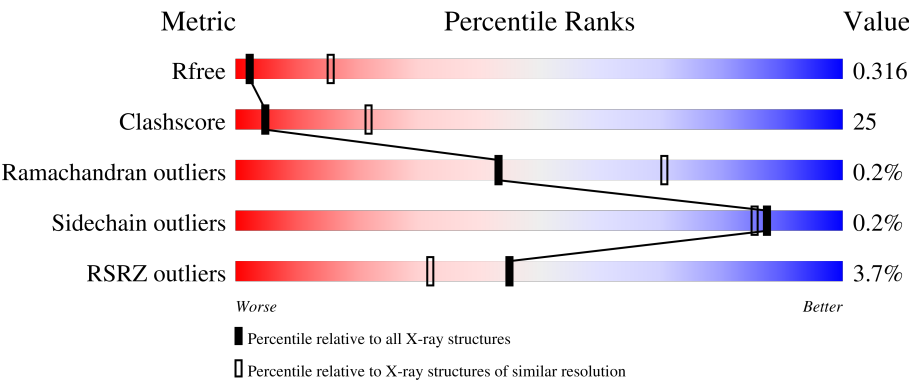
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.37 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.



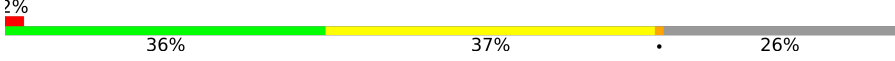
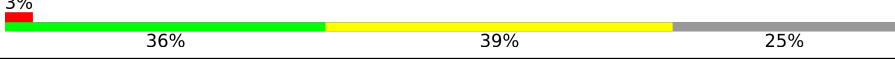
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1047 (3.42-3.34)
Clashscore	190562	1067 (3.42-3.34)
Ramachandran outliers	187476	1056 (3.42-3.34)
Sidechain outliers	187428	1056 (3.42-3.34)
RSRZ outliers	180081	1047 (3.42-3.34)

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	187	4% 35% 42% • 22%
1	B	187	% 39% 39% 23%
1	C	187	3% 38% 40% 22%
1	D	187	4% 40% 38% • 22%
1	E	187	2% 45% 32% 23%

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Mol	Chain	Length	Quality of chain
1	F	187	 3% 44% 32% 24%
1	G	187	 2% 36% 37% 26%
1	H	187	 3% 36% 39% 25%

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 9299 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 Plastid division protein CDP1, chloroplastic, Plastid division protein PDV1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	145	Total	C	N	O	S	0	0	0
			1174	745	195	228	6			
1	B	144	Total	C	N	O	S	0	0	0
			1173	745	195	227	6			
1	C	145	Total	C	N	O	S	0	0	0
			1178	747	195	230	6			
1	D	146	Total	C	N	O	S	0	0	0
			1188	755	196	231	6			
1	E	144	Total	C	N	O	S	0	0	0
			1170	744	192	228	6			
1	F	142	Total	C	N	O	S	0	0	0
			1156	734	192	224	6			
1	G	139	Total	C	N	O	S	0	0	0
			1127	716	184	221	6			
1	H	140	Total	C	N	O	S	0	0	0
			1133	721	183	223	6			

There are 208 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	670	MET	-	initiating methionine	UNP Q8VY16
A	671	GLY	-	expression tag	UNP Q8VY16
A	672	HIS	-	expression tag	UNP Q8VY16
A	673	HIS	-	expression tag	UNP Q8VY16
A	674	HIS	-	expression tag	UNP Q8VY16
A	675	HIS	-	expression tag	UNP Q8VY16
A	676	HIS	-	expression tag	UNP Q8VY16
A	677	HIS	-	expression tag	UNP Q8VY16
A	678	LEU	-	expression tag	UNP Q8VY16
A	679	VAL	-	expression tag	UNP Q8VY16
A	680	PRO	-	expression tag	UNP Q8VY16
A	681	ARG	-	expression tag	UNP Q8VY16

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Chain	Residue	Modelled	Actual	Comment	Reference
A	682	GLY	-	expression tag	UNP Q8VY16
A	683	SER	-	expression tag	UNP Q8VY16
A	820	GLY	-	linker	UNP Q8VY16
A	821	SER	-	linker	UNP Q8VY16
A	822	GLY	-	linker	UNP Q8VY16
A	823	SER	-	linker	UNP Q8VY16
A	824	GLY	-	linker	UNP Q8VY16
A	825	SER	-	linker	UNP Q8VY16
A	826	GLY	-	linker	UNP Q8VY16
A	827	SER	-	linker	UNP Q8VY16
A	828	GLY	-	linker	UNP Q8VY16
A	829	SER	-	linker	UNP Q8VY16
A	830	GLY	-	linker	UNP Q8VY16
A	831	SER	-	linker	UNP Q8VY16
B	670	MET	-	initiating methionine	UNP Q8VY16
B	671	GLY	-	expression tag	UNP Q8VY16
B	672	HIS	-	expression tag	UNP Q8VY16
B	673	HIS	-	expression tag	UNP Q8VY16
B	674	HIS	-	expression tag	UNP Q8VY16
B	675	HIS	-	expression tag	UNP Q8VY16
B	676	HIS	-	expression tag	UNP Q8VY16
B	677	HIS	-	expression tag	UNP Q8VY16
B	678	LEU	-	expression tag	UNP Q8VY16
B	679	VAL	-	expression tag	UNP Q8VY16
B	680	PRO	-	expression tag	UNP Q8VY16
B	681	ARG	-	expression tag	UNP Q8VY16
B	682	GLY	-	expression tag	UNP Q8VY16
B	683	SER	-	expression tag	UNP Q8VY16
B	820	GLY	-	linker	UNP Q8VY16
B	821	SER	-	linker	UNP Q8VY16
B	822	GLY	-	linker	UNP Q8VY16
B	823	SER	-	linker	UNP Q8VY16
B	824	GLY	-	linker	UNP Q8VY16
B	825	SER	-	linker	UNP Q8VY16
B	826	GLY	-	linker	UNP Q8VY16
B	827	SER	-	linker	UNP Q8VY16
B	828	GLY	-	linker	UNP Q8VY16
B	829	SER	-	linker	UNP Q8VY16
B	830	GLY	-	linker	UNP Q8VY16
B	831	SER	-	linker	UNP Q8VY16
C	670	MET	-	initiating methionine	UNP Q8VY16
C	671	GLY	-	expression tag	UNP Q8VY16

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Chain	Residue	Modelled	Actual	Comment	Reference
C	672	HIS	-	expression tag	UNP Q8VY16
C	673	HIS	-	expression tag	UNP Q8VY16
C	674	HIS	-	expression tag	UNP Q8VY16
C	675	HIS	-	expression tag	UNP Q8VY16
C	676	HIS	-	expression tag	UNP Q8VY16
C	677	HIS	-	expression tag	UNP Q8VY16
C	678	LEU	-	expression tag	UNP Q8VY16
C	679	VAL	-	expression tag	UNP Q8VY16
C	680	PRO	-	expression tag	UNP Q8VY16
C	681	ARG	-	expression tag	UNP Q8VY16
C	682	GLY	-	expression tag	UNP Q8VY16
C	683	SER	-	expression tag	UNP Q8VY16
C	820	GLY	-	linker	UNP Q8VY16
C	821	SER	-	linker	UNP Q8VY16
C	822	GLY	-	linker	UNP Q8VY16
C	823	SER	-	linker	UNP Q8VY16
C	824	GLY	-	linker	UNP Q8VY16
C	825	SER	-	linker	UNP Q8VY16
C	826	GLY	-	linker	UNP Q8VY16
C	827	SER	-	linker	UNP Q8VY16
C	828	GLY	-	linker	UNP Q8VY16
C	829	SER	-	linker	UNP Q8VY16
C	830	GLY	-	linker	UNP Q8VY16
C	831	SER	-	linker	UNP Q8VY16
D	670	MET	-	initiating methionine	UNP Q8VY16
D	671	GLY	-	expression tag	UNP Q8VY16
D	672	HIS	-	expression tag	UNP Q8VY16
D	673	HIS	-	expression tag	UNP Q8VY16
D	674	HIS	-	expression tag	UNP Q8VY16
D	675	HIS	-	expression tag	UNP Q8VY16
D	676	HIS	-	expression tag	UNP Q8VY16
D	677	HIS	-	expression tag	UNP Q8VY16
D	678	LEU	-	expression tag	UNP Q8VY16
D	679	VAL	-	expression tag	UNP Q8VY16
D	680	PRO	-	expression tag	UNP Q8VY16
D	681	ARG	-	expression tag	UNP Q8VY16
D	682	GLY	-	expression tag	UNP Q8VY16
D	683	SER	-	expression tag	UNP Q8VY16
D	820	GLY	-	linker	UNP Q8VY16
D	821	SER	-	linker	UNP Q8VY16
D	822	GLY	-	linker	UNP Q8VY16
D	823	SER	-	linker	UNP Q8VY16

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Chain	Residue	Modelled	Actual	Comment	Reference
D	824	GLY	-	linker	UNP Q8VY16
D	825	SER	-	linker	UNP Q8VY16
D	826	GLY	-	linker	UNP Q8VY16
D	827	SER	-	linker	UNP Q8VY16
D	828	GLY	-	linker	UNP Q8VY16
D	829	SER	-	linker	UNP Q8VY16
D	830	GLY	-	linker	UNP Q8VY16
D	831	SER	-	linker	UNP Q8VY16
E	670	MET	-	initiating methionine	UNP Q8VY16
E	671	GLY	-	expression tag	UNP Q8VY16
E	672	HIS	-	expression tag	UNP Q8VY16
E	673	HIS	-	expression tag	UNP Q8VY16
E	674	HIS	-	expression tag	UNP Q8VY16
E	675	HIS	-	expression tag	UNP Q8VY16
E	676	HIS	-	expression tag	UNP Q8VY16
E	677	HIS	-	expression tag	UNP Q8VY16
E	678	LEU	-	expression tag	UNP Q8VY16
E	679	VAL	-	expression tag	UNP Q8VY16
E	680	PRO	-	expression tag	UNP Q8VY16
E	681	ARG	-	expression tag	UNP Q8VY16
E	682	GLY	-	expression tag	UNP Q8VY16
E	683	SER	-	expression tag	UNP Q8VY16
E	820	GLY	-	linker	UNP Q8VY16
E	821	SER	-	linker	UNP Q8VY16
E	822	GLY	-	linker	UNP Q8VY16
E	823	SER	-	linker	UNP Q8VY16
E	824	GLY	-	linker	UNP Q8VY16
E	825	SER	-	linker	UNP Q8VY16
E	826	GLY	-	linker	UNP Q8VY16
E	827	SER	-	linker	UNP Q8VY16
E	828	GLY	-	linker	UNP Q8VY16
E	829	SER	-	linker	UNP Q8VY16
E	830	GLY	-	linker	UNP Q8VY16
E	831	SER	-	linker	UNP Q8VY16
F	670	MET	-	initiating methionine	UNP Q8VY16
F	671	GLY	-	expression tag	UNP Q8VY16
F	672	HIS	-	expression tag	UNP Q8VY16
F	673	HIS	-	expression tag	UNP Q8VY16
F	674	HIS	-	expression tag	UNP Q8VY16
F	675	HIS	-	expression tag	UNP Q8VY16
F	676	HIS	-	expression tag	UNP Q8VY16
F	677	HIS	-	expression tag	UNP Q8VY16

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Chain	Residue	Modelled	Actual	Comment	Reference
F	678	LEU	-	expression tag	UNP Q8VY16
F	679	VAL	-	expression tag	UNP Q8VY16
F	680	PRO	-	expression tag	UNP Q8VY16
F	681	ARG	-	expression tag	UNP Q8VY16
F	682	GLY	-	expression tag	UNP Q8VY16
F	683	SER	-	expression tag	UNP Q8VY16
F	820	GLY	-	linker	UNP Q8VY16
F	821	SER	-	linker	UNP Q8VY16
F	822	GLY	-	linker	UNP Q8VY16
F	823	SER	-	linker	UNP Q8VY16
F	824	GLY	-	linker	UNP Q8VY16
F	825	SER	-	linker	UNP Q8VY16
F	826	GLY	-	linker	UNP Q8VY16
F	827	SER	-	linker	UNP Q8VY16
F	828	GLY	-	linker	UNP Q8VY16
F	829	SER	-	linker	UNP Q8VY16
F	830	GLY	-	linker	UNP Q8VY16
F	831	SER	-	linker	UNP Q8VY16
G	670	MET	-	initiating methionine	UNP Q8VY16
G	671	GLY	-	expression tag	UNP Q8VY16
G	672	HIS	-	expression tag	UNP Q8VY16
G	673	HIS	-	expression tag	UNP Q8VY16
G	674	HIS	-	expression tag	UNP Q8VY16
G	675	HIS	-	expression tag	UNP Q8VY16
G	676	HIS	-	expression tag	UNP Q8VY16
G	677	HIS	-	expression tag	UNP Q8VY16
G	678	LEU	-	expression tag	UNP Q8VY16
G	679	VAL	-	expression tag	UNP Q8VY16
G	680	PRO	-	expression tag	UNP Q8VY16
G	681	ARG	-	expression tag	UNP Q8VY16
G	682	GLY	-	expression tag	UNP Q8VY16
G	683	SER	-	expression tag	UNP Q8VY16
G	820	GLY	-	linker	UNP Q8VY16
G	821	SER	-	linker	UNP Q8VY16
G	822	GLY	-	linker	UNP Q8VY16
G	823	SER	-	linker	UNP Q8VY16
G	824	GLY	-	linker	UNP Q8VY16
G	825	SER	-	linker	UNP Q8VY16
G	826	GLY	-	linker	UNP Q8VY16
G	827	SER	-	linker	UNP Q8VY16
G	828	GLY	-	linker	UNP Q8VY16
G	829	SER	-	linker	UNP Q8VY16

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Chain	Residue	Modelled	Actual	Comment	Reference
G	830	GLY	-	linker	UNP Q8VY16
G	831	SER	-	linker	UNP Q8VY16
H	670	MET	-	initiating methionine	UNP Q8VY16
H	671	GLY	-	expression tag	UNP Q8VY16
H	672	HIS	-	expression tag	UNP Q8VY16
H	673	HIS	-	expression tag	UNP Q8VY16
H	674	HIS	-	expression tag	UNP Q8VY16
H	675	HIS	-	expression tag	UNP Q8VY16
H	676	HIS	-	expression tag	UNP Q8VY16
H	677	HIS	-	expression tag	UNP Q8VY16
H	678	LEU	-	expression tag	UNP Q8VY16
H	679	VAL	-	expression tag	UNP Q8VY16
H	680	PRO	-	expression tag	UNP Q8VY16
H	681	ARG	-	expression tag	UNP Q8VY16
H	682	GLY	-	expression tag	UNP Q8VY16
H	683	SER	-	expression tag	UNP Q8VY16
H	820	GLY	-	linker	UNP Q8VY16
H	821	SER	-	linker	UNP Q8VY16
H	822	GLY	-	linker	UNP Q8VY16
H	823	SER	-	linker	UNP Q8VY16
H	824	GLY	-	linker	UNP Q8VY16
H	825	SER	-	linker	UNP Q8VY16
H	826	GLY	-	linker	UNP Q8VY16
H	827	SER	-	linker	UNP Q8VY16
H	828	GLY	-	linker	UNP Q8VY16
H	829	SER	-	linker	UNP Q8VY16
H	830	GLY	-	linker	UNP Q8VY16
H	831	SER	-	linker	UNP Q8VY16



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	61.23Å 80.19Å 84.07Å 88.36° 80.99° 83.49°	Depositor
Resolution (Å)	38.23 – 3.37 38.23 – 3.37	Depositor EDS
% Data completeness (in resolution range)	97.7 (38.23-3.37) 97.7 (38.23-3.37)	Depositor EDS
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155, Coot	Depositor
R, R_{free}	0.250 , 0.318 0.248 , 0.316	Depositor DCC
R_{free} test set	1028 reflections (3.62%)	wwPDB-VP
Wilson B-factor (Å ²)	54.1	Xtriage
Anisotropy	0.515	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 27.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	9299	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.65% 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	0.32	0/1197	0.61	0/1617
1	B	0.28	0/1196	0.51	0/1616
1	C	0.30	0/1201	0.53	0/1623
1	D	0.29	0/1210	0.53	0/1634
1	E	0.26	0/1192	0.47	0/1611
1	F	0.23	0/1179	0.46	0/1593
1	G	0.25	0/1148	0.57	2/1552 (0.1%)
1	H	0.25	0/1154	0.47	0/1560
All	All	0.28	0/9477	0.52	2/12806 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	G	851	VAL	CA-C-N	-5.25	113.08	122.32
1	G	851	VAL	C-N-CA	-5.25	113.08	122.32

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	759	GLU	Peptide
1	D	761	GLY	Peptide

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	1174	0	1139	83	0
1	B	1173	0	1139	67	0
1	C	1178	0	1140	77	0
1	D	1188	0	1160	58	0
1	E	1170	0	1139	45	1
1	F	1156	0	1120	43	1
1	G	1127	0	1093	61	0
1	H	1133	0	1100	71	0
All	All	9299	0	9030	463	1

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 25.

All (463) 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:684:HIS:HB3	1:A:686:ARG:HH12	1.26	1.00
1:G:796:ILE:HG13	1:G:815:ILE:HG12	1.47	0.96
1:A:684:HIS:HB3	1:A:686:ARG:NH1	1.88	0.87
1:A:789:LYS:HG3	1:G:748:LEU:HA	1.59	0.85
1:H:725:MET:HE1	1:H:813:SER:HB3	1.60	0.84
1:E:745:PHE:HB3	1:E:777:ALA:HB2	1.59	0.83
1:C:765:GLU:HG2	1:C:802:LYS:HE2	1.61	0.82
1:B:701:GLU:HG2	1:B:747:LEU:HD22	1.64	0.79
1:B:745:PHE:HZ	1:B:854:ALA:HB1	1.46	0.79
1:A:706:GLU:HB3	1:A:713:GLN:HG3	1.65	0.78
1:A:691:GLU:O	1:A:695:GLU:HG2	1.84	0.77
1:H:815:ILE:HD12	1:H:855:ARG:NH1	1.98	0.77
1:A:692:GLU:O	1:A:696:LEU:HB2	1.85	0.77
1:C:725:MET:SD	1:C:813:SER:OG	2.42	0.77
1:E:701:GLU:HG2	1:E:747:LEU:HD22	1.66	0.76
1:B:792:SER:OG	1:B:855:ARG:NH1	2.19	0.76
1:A:700:TRP:NE1	1:A:856:GLY:O	2.19	0.75
1:B:779:LEU:HB2	1:B:851:VAL:HG13	1.69	0.75
1:F:850:ASP:HB3	1:F:853:MET:HG3	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:787:ASN:ND2	1:C:702:ASN:OD1	2.18	0.74
1:C:769:ILE:HD13	1:C:800:LEU:HD13	1.70	0.73
1:B:710:PRO:HB2	1:C:711:THR:HG23	1.70	0.73
1:C:775:GLU:OE2	1:C:794:TYR:OH	2.06	0.73
1:A:689:ASP:HB3	1:A:692:GLU:HB2	1.71	0.73
1:C:702:ASN:ND2	1:C:706:GLU:OE1	2.21	0.72
1:D:759:GLU:HB3	1:D:765:GLU:HA	1.71	0.72
1:D:717:LEU:HB3	1:D:721:LEU:HD12	1.70	0.72
1:H:744:ARG:HH12	1:H:780:VAL:HG21	1.54	0.72
1:C:725:MET:HA	1:C:728:GLN:HG3	1.72	0.72
1:H:815:ILE:HD12	1:H:855:ARG:HH11	1.54	0.72
1:C:725:MET:HA	1:C:728:GLN:CG	2.20	0.71
1:G:700:TRP:NE1	1:G:856:GLY:O	2.17	0.71
1:B:763:ALA:HA	1:G:710:PRO:HG2	1.73	0.71
1:G:760:ASP:OD1	1:G:761:GLY:N	2.24	0.70
1:D:773:LEU:HD22	1:D:856:GLY:HA2	1.74	0.70
1:A:713:GLN:OE1	1:A:715:TYR:OH	2.03	0.69
1:A:808:TRP:HB2	1:H:805:ASP:OD2	1.93	0.69
1:B:754:GLN:H	1:B:770:GLU:HB3	1.57	0.69
1:F:714:VAL:HG11	1:F:734:GLN:HG3	1.74	0.69
1:C:725:MET:HE2	1:C:810:PHE:HB3	1.73	0.69
1:H:700:TRP:CZ3	1:H:721:LEU:HD21	2.29	0.68
1:H:701:GLU:OE2	1:H:704:LYS:NZ	2.22	0.68
1:A:765:GLU:HB3	1:A:802:LYS:HB2	1.76	0.68
1:F:757:ILE:HG22	1:F:759:GLU:OE2	1.94	0.68
1:G:725:MET:HE3	1:G:810:PHE:HB3	1.75	0.68
1:G:796:ILE:HG23	1:G:798:TYR:CE1	2.29	0.68
1:A:796:ILE:HD11	1:A:813:SER:HB2	1.75	0.67
1:A:802:LYS:NZ	1:H:719:GLU:OE1	2.17	0.67
1:E:794:TYR:OH	1:E:856:GLY:N	2.27	0.67
1:H:691:GLU:HA	1:H:694:GLU:HG2	1.76	0.67
1:D:796:ILE:HD11	1:D:813:SER:HB2	1.75	0.67
1:E:711:THR:HG23	1:H:710:PRO:HB2	1.78	0.66
1:A:762:ILE:HG22	1:A:763:ALA:H	1.61	0.66
1:D:817:ILE:HD13	1:D:819:LYS:HD2	1.77	0.66
1:C:800:LEU:HD11	1:C:810:PHE:CD2	2.31	0.65
1:B:697:VAL:O	1:B:700:TRP:N	2.27	0.65
1:G:773:LEU:HD22	1:G:856:GLY:HA2	1.78	0.65
1:A:745:PHE:O	1:G:744:ARG:NH2	2.29	0.65
1:F:754:GLN:NE2	1:F:768:GLU:OE2	2.28	0.65
1:D:688:MET:HB2	1:D:757:ILE:HG13	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:701:GLU:HG2	1:D:747:LEU:HD22	1.78	0.65
1:A:802:LYS:HA	1:A:807:LEU:O	1.97	0.65
1:B:748:LEU:O	1:C:789:LYS:HD3	1.98	0.64
1:B:781:ASP:OD1	1:B:782:GLU:N	2.30	0.64
1:A:712:HIS:CD2	1:A:737:GLU:HA	2.33	0.64
1:F:698:ARG:HG2	1:F:750:LEU:HD23	1.79	0.63
1:H:744:ARG:NH1	1:H:780:VAL:HG21	2.13	0.63
1:E:689:ASP:HB3	1:E:692:GLU:HB3	1.80	0.63
1:G:686:ARG:NH1	1:G:758:PHE:HD1	1.96	0.63
1:H:717:LEU:HA	1:H:721:LEU:HD23	1.80	0.63
1:D:725:MET:CE	1:D:810:PHE:HB3	2.28	0.62
1:D:698:ARG:HH22	1:F:786:LYS:NZ	1.97	0.62
1:B:779:LEU:HD12	1:B:851:VAL:HA	1.81	0.62
1:H:800:LEU:HB3	1:H:810:PHE:HA	1.82	0.62
1:B:778:GLU:HA	1:B:789:LYS:HA	1.82	0.62
1:G:766:ALA:HA	1:G:801:LYS:HA	1.82	0.62
1:B:694:GLU:HG3	1:B:750:LEU:HD11	1.81	0.61
1:D:725:MET:HE1	1:D:810:PHE:HB3	1.83	0.61
1:C:698:ARG:HH11	1:C:749:HIS:CE1	2.18	0.61
1:F:765:GLU:OE2	1:F:802:LYS:HB2	2.00	0.61
1:A:807:LEU:HD23	1:A:808:TRP:H	1.65	0.61
1:A:850:ASP:OD1	1:A:851:VAL:N	2.34	0.61
1:H:714:VAL:HG11	1:H:734:GLN:HG3	1.80	0.61
1:H:788:ALA:HB1	1:H:851:VAL:HG11	1.81	0.61
1:C:721:LEU:HD23	1:C:810:PHE:HB2	1.82	0.61
1:E:777:ALA:HB3	1:E:790:TYR:CE2	2.36	0.61
1:G:749:HIS:NE2	1:G:751:GLU:HB2	2.15	0.61
1:C:770:GLU:HG3	1:C:797:ARG:HG2	1.82	0.61
1:A:791:TYR:HB2	1:G:748:LEU:HD21	1.82	0.61
1:D:794:TYR:OH	1:D:856:GLY:N	2.33	0.61
1:A:709:GLY:O	1:A:712:HIS:ND1	2.34	0.60
1:F:699:GLN:O	1:F:703:VAL:N	2.34	0.60
1:D:708:LEU:HB3	1:D:743:TRP:HB2	1.84	0.60
1:A:712:HIS:HD2	1:A:737:GLU:HA	1.67	0.59
1:C:768:GLU:OE2	1:C:797:ARG:HD3	2.03	0.59
1:G:756:HIS:C	1:G:757:ILE:HD12	2.27	0.59
1:B:849:LEU:HD22	1:B:853:MET:HE2	1.84	0.59
1:C:852:MET:SD	1:C:855:ARG:HD2	2.42	0.59
1:C:717:LEU:HB3	1:C:721:LEU:HD12	1.84	0.58
1:C:745:PHE:CZ	1:C:854:ALA:HB1	2.37	0.58
1:E:786:LYS:HA	1:H:698:ARG:HD2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:805:ASP:OD1	1:D:806:GLY:N	2.36	0.58
1:B:710:PRO:HG2	1:C:710:PRO:HG2	1.86	0.58
1:A:800:LEU:O	1:A:801:LYS:HD3	2.02	0.58
1:B:711:THR:HB	1:B:713:GLN:HG3	1.85	0.58
1:C:707:ALA:HA	1:C:713:GLN:O	2.03	0.58
1:G:688:MET:HB2	1:G:757:ILE:HD11	1.85	0.58
1:A:699:GLN:HG3	1:H:806:GLY:HA3	1.86	0.58
1:A:744:ARG:HH21	1:B:762:ILE:HG22	1.69	0.58
1:D:774:GLU:OE2	1:D:791:TYR:OH	2.22	0.57
1:B:701:GLU:N	1:B:701:GLU:OE1	2.37	0.57
1:G:777:ALA:HB3	1:G:790:TYR:CE2	2.40	0.57
1:B:739:LYS:HB3	1:B:741:CYS:SG	2.45	0.57
1:B:770:GLU:OE2	1:B:797:ARG:HG2	2.05	0.57
1:H:794:TYR:OH	1:H:855:ARG:O	2.18	0.57
1:A:799:ILE:O	1:A:811:CYS:N	2.29	0.57
1:B:728:GLN:HG2	1:H:759:GLU:HB2	1.85	0.57
1:G:803:GLN:N	1:G:807:LEU:O	2.38	0.57
1:D:803:GLN:HG3	1:D:804:GLU:N	2.20	0.57
1:A:794:TYR:OH	1:A:856:GLY:N	2.26	0.56
1:C:701:GLU:OE2	1:C:704:LYS:NZ	2.24	0.56
1:A:748:LEU:HD23	1:G:789:LYS:HB3	1.88	0.56
1:G:752:VAL:HG12	1:G:753:LEU:O	2.06	0.56
1:C:725:MET:HG3	1:C:728:GLN:HG3	1.87	0.56
1:C:688:MET:HE2	1:C:692:GLU:HG2	1.88	0.56
1:E:792:SER:HG	1:E:855:ARG:HH21	1.49	0.56
1:H:696:LEU:HD11	1:H:808:TRP:HB3	1.88	0.56
1:B:697:VAL:O	1:B:701:GLU:OE1	2.24	0.55
1:C:686:ARG:HB3	1:C:687:PRO:HD2	1.87	0.55
1:F:694:GLU:HB3	1:F:752:VAL:HG21	1.87	0.55
1:H:770:GLU:HG2	1:H:797:ARG:HG2	1.89	0.55
1:B:729:TRP:CZ2	1:H:762:ILE:HB	2.42	0.55
1:F:721:LEU:HB2	1:F:726:LEU:HD13	1.88	0.55
1:E:708:LEU:HB3	1:E:743:TRP:HB2	1.87	0.55
1:E:697:VAL:HB	1:E:750:LEU:HD11	1.89	0.55
1:B:702:ASN:O	1:B:706:GLU:HG3	2.07	0.55
1:B:728:GLN:HB3	1:H:761:GLY:O	2.06	0.55
1:B:815:ILE:HD11	1:H:762:ILE:HD13	1.89	0.55
1:D:698:ARG:HH22	1:F:786:LYS:HZ1	1.54	0.55
1:A:712:HIS:HE1	1:A:742:TYR:HB3	1.71	0.55
1:D:748:LEU:HD23	1:F:791:TYR:HB2	1.89	0.55
1:G:712:HIS:HB3	1:G:737:GLU:HG3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:805:ASP:HB3	1:H:807:LEU:HG	1.89	0.55
1:C:723:GLU:HB2	1:C:811:CYS:HB2	1.89	0.55
1:A:722:ASP:OD1	1:A:723:GLU:N	2.36	0.54
1:G:796:ILE:HD11	1:G:813:SER:OG	2.06	0.54
1:C:770:GLU:OE2	1:C:797:ARG:NH1	2.40	0.54
1:C:721:LEU:HB3	1:C:726:LEU:HA	1.90	0.54
1:G:781:ASP:HB3	1:G:783:SER:O	2.08	0.54
1:A:687:PRO:HD2	1:E:782:GLU:HB2	1.88	0.54
1:G:721:LEU:HD22	1:G:725:MET:HB3	1.89	0.54
1:F:779:LEU:HB3	1:F:851:VAL:HG22	1.90	0.54
1:A:713:GLN:HB2	1:A:716:SER:HB3	1.89	0.53
1:F:767:ALA:HB3	1:F:800:LEU:HB2	1.89	0.53
1:G:747:LEU:HD13	1:G:775:GLU:HB3	1.91	0.53
1:A:710:PRO:HD3	1:A:742:TYR:CD1	2.44	0.53
1:B:776:ALA:O	1:C:746:VAL:HG21	2.09	0.53
1:G:686:ARG:HB2	1:G:757:ILE:O	2.09	0.53
1:A:799:ILE:HB	1:A:812:GLN:HG2	1.89	0.53
1:C:725:MET:HA	1:C:728:GLN:HG2	1.91	0.53
1:F:805:ASP:OD1	1:F:806:GLY:N	2.36	0.53
1:A:688:MET:HG3	1:A:757:ILE:HD11	1.90	0.53
1:B:803:GLN:HB3	1:B:805:ASP:OD1	2.08	0.53
1:E:704:LYS:HD2	1:E:854:ALA:HB1	1.89	0.53
1:G:760:ASP:H	1:G:765:GLU:HA	1.73	0.53
1:A:801:LYS:O	1:A:808:TRP:HA	2.09	0.53
1:G:853:MET:HA	1:G:855:ARG:NH1	2.23	0.53
1:C:799:ILE:C	1:C:800:LEU:HD12	2.34	0.52
1:C:849:LEU:HD22	1:C:853:MET:HG3	1.92	0.52
1:A:799:ILE:HG22	1:A:811:CYS:HB3	1.91	0.52
1:F:701:GLU:OE2	1:F:773:LEU:HD22	2.09	0.52
1:F:736:ALA:HB1	1:F:741:CYS:O	2.10	0.52
1:G:688:MET:HE3	1:G:757:ILE:HD11	1.90	0.52
1:H:720:VAL:HG22	1:H:810:PHE:HD1	1.75	0.52
1:D:790:TYR:HD2	1:D:851:VAL:HB	1.74	0.52
1:E:805:ASP:OD1	1:E:805:ASP:N	2.41	0.52
1:G:703:VAL:HG21	1:G:720:VAL:HG11	1.90	0.52
1:G:801:LYS:HG2	1:G:811:CYS:SG	2.49	0.52
1:C:762:ILE:HG23	1:C:763:ALA:H	1.73	0.52
1:C:784:GLN:NE2	1:C:786:LYS:O	2.43	0.52
1:H:802:LYS:HZ3	1:H:808:TRP:NE1	2.08	0.52
1:E:688:MET:HB3	1:E:755:ALA:C	2.34	0.52
1:E:850:ASP:O	1:E:853:MET:HG2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:758:PHE:HE2	1:C:768:GLU:HB2	1.75	0.51
1:D:710:PRO:HD3	1:D:742:TYR:CD2	2.46	0.51
1:E:710:PRO:HG2	1:H:710:PRO:HG2	1.91	0.51
1:H:741:CYS:HB3	1:H:779:LEU:HD11	1.91	0.51
1:G:699:GLN:O	1:G:703:VAL:HG23	2.11	0.51
1:D:713:GLN:O	1:D:716:SER:OG	2.27	0.51
1:H:812:GLN:HG2	1:H:813:SER:N	2.24	0.51
1:F:689:ASP:HB3	1:F:692:GLU:HB3	1.93	0.51
1:C:700:TRP:NE1	1:C:856:GLY:O	2.44	0.51
1:A:744:ARG:NH2	1:B:762:ILE:HG22	2.25	0.51
1:C:790:TYR:OH	1:C:855:ARG:HG3	2.11	0.51
1:D:793:THR:HG22	1:D:818:GLN:OE1	2.10	0.50
1:A:708:LEU:HD23	1:A:854:ALA:HB2	1.93	0.50
1:D:807:LEU:HD23	1:D:807:LEU:H	1.75	0.50
1:D:777:ALA:HB3	1:D:790:TYR:CE2	2.45	0.50
1:D:797:ARG:NH1	1:D:812:GLN:OE1	2.44	0.50
1:F:797:ARG:CZ	1:F:799:ILE:HD11	2.41	0.50
1:A:717:LEU:HD13	1:A:730:GLN:HA	1.92	0.50
1:A:778:GLU:HA	1:A:789:LYS:HA	1.92	0.50
1:G:742:TYR:CZ	1:G:780:VAL:HG11	2.46	0.50
1:B:722:ASP:O	1:B:811:CYS:HA	2.10	0.50
1:F:803:GLN:HG2	1:F:804:GLU:OE1	2.11	0.50
1:B:777:ALA:HB3	1:B:790:TYR:CE2	2.46	0.50
1:G:703:VAL:HG13	1:G:716:SER:HB3	1.93	0.50
1:B:779:LEU:HD11	1:B:849:LEU:CD1	2.42	0.50
1:D:691:GLU:OE2	1:D:691:GLU:N	2.44	0.50
1:D:796:ILE:HD13	1:D:856:GLY:HA3	1.94	0.50
1:G:853:MET:HA	1:G:855:ARG:HH12	1.76	0.50
1:F:739:LYS:NZ	1:F:848:HIS:HB2	2.27	0.49
1:B:751:GLU:HG2	1:B:753:LEU:HD23	1.94	0.49
1:B:796:ILE:HD13	1:B:798:TYR:CZ	2.47	0.49
1:D:803:GLN:HG3	1:D:804:GLU:H	1.77	0.49
1:A:697:VAL:O	1:A:700:TRP:N	2.45	0.49
1:E:686:ARG:HB3	1:E:757:ILE:O	2.13	0.49
1:H:802:LYS:HB2	1:H:808:TRP:CZ3	2.47	0.49
1:A:755:ALA:HA	1:A:769:ILE:HG22	1.94	0.49
1:D:805:ASP:CG	1:D:806:GLY:H	2.20	0.49
1:H:688:MET:HE1	1:H:767:ALA:HB1	1.93	0.49
1:D:776:ALA:HB2	1:D:791:TYR:HD1	1.77	0.49
1:G:762:ILE:HG22	1:G:763:ALA:N	2.27	0.49
1:A:702:ASN:O	1:A:706:GLU:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:743:TRP:NE1	1:C:854:ALA:HB2	2.28	0.49
1:G:742:TYR:O	1:G:780:VAL:HG12	2.13	0.49
1:C:698:ARG:NH1	1:C:749:HIS:CE1	2.81	0.49
1:C:790:TYR:CZ	1:C:855:ARG:HG3	2.48	0.49
1:H:726:LEU:O	1:H:730:GLN:HB2	2.12	0.49
1:B:695:GLU:O	1:B:699:GLN:HB2	2.12	0.49
1:B:728:GLN:HA	1:H:759:GLU:O	2.13	0.49
1:C:739:LYS:NZ	1:C:847:ASP:HB2	2.28	0.49
1:G:704:LYS:NZ	1:G:745:PHE:CZ	2.81	0.49
1:C:736:ALA:HB1	1:C:741:CYS:O	2.13	0.48
1:G:790:TYR:OH	1:G:854:ALA:O	2.25	0.48
1:H:774:GLU:HG3	1:H:793:THR:HB	1.95	0.48
1:C:772:LEU:HD21	1:C:793:THR:HG22	1.94	0.48
1:H:775:GLU:OE2	1:H:794:TYR:OH	2.32	0.48
1:H:798:TYR:HA	1:H:813:SER:HB2	1.96	0.48
1:D:699:GLN:O	1:D:703:VAL:HG13	2.13	0.48
1:G:725:MET:HE2	1:G:812:GLN:O	2.13	0.48
1:D:748:LEU:CD2	1:F:791:TYR:HB2	2.44	0.48
1:E:691:GLU:O	1:E:695:GLU:HG2	2.13	0.48
1:G:700:TRP:CZ3	1:G:721:LEU:HD11	2.49	0.48
1:A:748:LEU:HB2	1:A:774:GLU:HG2	1.95	0.48
1:D:690:THR:OG1	1:D:691:GLU:OE2	2.32	0.48
1:E:803:GLN:CD	1:E:809:LYS:HZ2	2.21	0.48
1:B:688:MET:HB3	1:B:755:ALA:HB1	1.95	0.48
1:E:743:TRP:CZ2	1:E:853:MET:HB2	2.48	0.48
1:E:767:ALA:O	1:E:799:ILE:HA	2.13	0.48
1:C:709:GLY:O	1:C:712:HIS:N	2.31	0.48
1:B:745:PHE:CZ	1:B:854:ALA:HB1	2.37	0.47
1:E:799:ILE:HD11	1:E:812:GLN:HB3	1.96	0.47
1:G:692:GLU:O	1:G:696:LEU:HG	2.14	0.47
1:H:707:ALA:HA	1:H:713:GLN:O	2.14	0.47
1:E:719:GLU:O	1:E:809:LYS:HE2	2.14	0.47
1:G:757:ILE:HG13	1:G:767:ALA:CB	2.44	0.47
1:D:710:PRO:HA	1:D:712:HIS:CE1	2.49	0.47
1:F:803:GLN:OE1	1:F:805:ASP:HB3	2.13	0.47
1:A:747:LEU:HD13	1:A:775:GLU:HB3	1.97	0.47
1:C:688:MET:HB3	1:C:755:ALA:HB1	1.96	0.47
1:D:704:LYS:HE3	1:D:745:PHE:CZ	2.48	0.47
1:D:720:VAL:HG12	1:D:810:PHE:CD1	2.50	0.47
1:D:748:LEU:HD22	1:D:791:TYR:HE1	1.80	0.47
1:A:804:GLU:N	1:A:804:GLU:OE1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:800:LEU:HG	1:B:810:PHE:HA	1.97	0.47
1:D:787:ASN:OD1	1:D:789:LYS:HE2	2.15	0.47
1:F:694:GLU:HB3	1:F:752:VAL:CG2	2.45	0.47
1:B:724:SER:OG	1:B:811:CYS:O	2.32	0.47
1:D:742:TYR:OH	1:D:744:ARG:NH2	2.47	0.47
1:A:717:LEU:O	1:A:721:LEU:HB2	2.14	0.47
1:A:790:TYR:OH	1:A:854:ALA:O	2.24	0.47
1:B:699:GLN:O	1:B:703:VAL:HG23	2.15	0.47
1:E:802:LYS:HD2	1:E:808:TRP:CZ2	2.49	0.47
1:H:731:THR:O	1:H:735:THR:N	2.47	0.47
1:H:746:VAL:HG12	1:H:748:LEU:HD12	1.97	0.47
1:E:724:SER:O	1:E:728:GLN:HG3	2.15	0.47
1:F:704:LYS:HZ1	1:F:856:GLY:C	2.22	0.47
1:A:711:THR:HB	1:A:713:GLN:NE2	2.31	0.46
1:C:739:LYS:HZ1	1:C:847:ASP:HB2	1.81	0.46
1:C:763:ALA:HB1	1:C:801:LYS:HE3	1.98	0.46
1:D:748:LEU:N	1:D:774:GLU:O	2.43	0.46
1:D:817:ILE:O	1:D:817:ILE:HD12	2.15	0.46
1:C:767:ALA:O	1:C:799:ILE:HA	2.15	0.46
1:A:854:ALA:O	1:A:855:ARG:HG3	2.15	0.46
1:E:694:GLU:OE1	1:E:698:ARG:HG3	2.16	0.46
1:H:781:ASP:OD1	1:H:783:SER:OG	2.30	0.46
1:D:723:GLU:HB2	1:D:811:CYS:HB3	1.97	0.46
1:A:800:LEU:C	1:A:801:LYS:HD3	2.40	0.46
1:C:773:LEU:HD12	1:C:796:ILE:HG21	1.98	0.46
1:D:698:ARG:HG3	1:D:750:LEU:HD23	1.96	0.46
1:G:722:ASP:O	1:G:811:CYS:HA	2.16	0.46
1:H:802:LYS:NZ	1:H:808:TRP:NE1	2.64	0.46
1:B:724:SER:O	1:B:728:GLN:HG3	2.16	0.46
1:E:725:MET:O	1:E:729:TRP:HD1	1.99	0.46
1:H:700:TRP:CH2	1:H:704:LYS:HB2	2.51	0.46
1:B:709:GLY:HA2	1:B:742:TYR:HB2	1.98	0.46
1:F:790:TYR:HD2	1:F:851:VAL:HG12	1.81	0.46
1:G:712:HIS:CE1	1:G:742:TYR:HB3	2.51	0.46
1:H:792:SER:HB3	1:H:794:TYR:CD1	2.51	0.46
1:C:702:ASN:O	1:C:706:GLU:HG3	2.15	0.46
1:D:704:LYS:HD2	1:D:729:TRP:CZ3	2.51	0.46
1:D:720:VAL:HG12	1:D:810:PHE:HD1	1.81	0.46
1:G:706:GLU:HB3	1:G:713:GLN:OE1	2.15	0.46
1:F:750:LEU:HD13	1:F:773:LEU:HD23	1.98	0.45
1:F:723:GLU:OE2	1:F:801:LYS:HE3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:708:LEU:HB3	1:G:743:TRP:HB2	1.98	0.45
1:A:720:VAL:HG23	1:A:721:LEU:HD13	1.98	0.45
1:E:748:LEU:HD12	1:E:791:TYR:HE1	1.82	0.45
1:F:795:LYS:HE2	1:F:816:GLN:HG3	1.99	0.45
1:A:779:LEU:HB3	1:A:851:VAL:HG22	1.98	0.45
1:H:802:LYS:HB2	1:H:808:TRP:CH2	2.52	0.45
1:C:850:ASP:OD1	1:C:851:VAL:N	2.47	0.45
1:E:721:LEU:HD23	1:E:810:PHE:HB2	1.97	0.45
1:F:790:TYR:OH	1:F:854:ALA:O	2.23	0.45
1:C:725:MET:N	1:C:811:CYS:O	2.49	0.45
1:F:756:HIS:HB2	1:F:758:PHE:HE1	1.81	0.45
1:H:850:ASP:OD1	1:H:851:VAL:N	2.50	0.45
1:H:852:MET:O	1:H:855:ARG:HG3	2.16	0.45
1:B:849:LEU:HD13	1:B:850:ASP:N	2.32	0.45
1:C:686:ARG:HB3	1:C:687:PRO:CD	2.46	0.45
1:C:755:ALA:HA	1:C:768:GLU:O	2.16	0.45
1:A:789:LYS:HG3	1:G:748:LEU:CA	2.38	0.45
1:C:758:PHE:CE2	1:C:768:GLU:HB2	2.52	0.45
1:A:715:TYR:CE2	1:B:797:ARG:HD2	2.52	0.45
1:C:812:GLN:HG2	1:C:813:SER:N	2.32	0.45
1:D:722:ASP:O	1:D:811:CYS:HA	2.17	0.45
1:E:698:ARG:HG2	1:E:750:LEU:HD13	1.98	0.44
1:E:703:VAL:HG11	1:E:720:VAL:HG22	1.99	0.44
1:A:720:VAL:O	1:A:810:PHE:N	2.44	0.44
1:D:770:GLU:HA	1:D:797:ARG:HA	1.99	0.44
1:D:805:ASP:CG	1:D:806:GLY:N	2.75	0.44
1:B:721:LEU:HD22	1:B:725:MET:HG2	1.99	0.44
1:F:722:ASP:OD1	1:F:723:GLU:N	2.50	0.44
1:F:750:LEU:HD12	1:F:751:GLU:N	2.32	0.44
1:A:710:PRO:HG3	1:B:761:GLY:N	2.33	0.44
1:B:686:ARG:O	1:B:756:HIS:HA	2.18	0.44
1:B:686:ARG:HB3	1:B:687:PRO:HD3	2.00	0.44
1:H:721:LEU:HD13	1:H:810:PHE:HB2	1.98	0.44
1:B:801:LYS:HG3	1:B:811:CYS:SG	2.58	0.44
1:F:719:GLU:O	1:F:809:LYS:NZ	2.46	0.44
1:H:777:ALA:HB3	1:H:790:TYR:CE2	2.52	0.44
1:A:777:ALA:HB3	1:A:790:TYR:CE2	2.52	0.44
1:A:794:TYR:HH	1:A:856:GLY:H	1.56	0.44
1:B:853:MET:H	1:B:853:MET:HG2	1.56	0.44
1:E:723:GLU:OE2	1:E:801:LYS:HD2	2.18	0.44
1:H:688:MET:HB3	1:H:755:ALA:HB1	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:736:ALA:HB1	1:A:741:CYS:O	2.18	0.43
1:F:712:HIS:CE1	1:F:742:TYR:HB3	2.53	0.43
1:A:788:ALA:HB3	1:A:851:VAL:HG21	1.99	0.43
1:F:704:LYS:HZ3	1:F:856:GLY:N	2.16	0.43
1:G:739:LYS:HB3	1:G:741:CYS:SG	2.58	0.43
1:G:756:HIS:N	1:G:768:GLU:O	2.50	0.43
1:B:753:LEU:HD12	1:B:770:GLU:HG3	1.99	0.43
1:F:759:GLU:OE1	1:F:765:GLU:HG2	2.18	0.43
1:F:701:GLU:OE1	1:F:747:LEU:HB2	2.18	0.43
1:A:699:GLN:CG	1:H:806:GLY:HA3	2.49	0.43
1:A:744:ARG:NH1	1:B:761:GLY:HA3	2.33	0.43
1:A:849:LEU:HD23	1:A:853:MET:HE2	2.01	0.43
1:C:698:ARG:HH12	1:C:749:HIS:CD2	2.36	0.43
1:D:812:GLN:HG2	1:D:813:SER:N	2.33	0.43
1:G:709:GLY:C	1:G:742:TYR:HB2	2.44	0.43
1:G:757:ILE:HG13	1:G:767:ALA:HB2	1.99	0.43
1:G:774:GLU:HB2	1:G:793:THR:HG23	2.00	0.43
1:H:767:ALA:HB3	1:H:800:LEU:HD11	1.99	0.43
1:E:745:PHE:HB3	1:E:777:ALA:CB	2.38	0.43
1:C:748:LEU:HD23	1:C:748:LEU:HA	1.71	0.43
1:C:758:PHE:N	1:C:766:ALA:O	2.33	0.43
1:H:694:GLU:HG3	1:H:695:GLU:N	2.34	0.43
1:B:709:GLY:CA	1:B:742:TYR:HB2	2.49	0.43
1:C:783:SER:HA	1:D:687:PRO:HG2	2.01	0.43
1:E:799:ILE:HG13	1:E:811:CYS:SG	2.58	0.43
1:G:851:VAL:HG12	1:G:852:MET:N	2.34	0.43
1:H:725:MET:HG3	1:H:729:TRP:CD1	2.54	0.43
1:B:707:ALA:HA	1:B:713:GLN:O	2.19	0.43
1:H:697:VAL:HG22	1:H:810:PHE:HZ	1.82	0.43
1:A:725:MET:HB2	1:A:812:GLN:HA	2.01	0.43
1:B:700:TRP:HA	1:B:720:VAL:HG21	2.00	0.43
1:B:770:GLU:CD	1:B:797:ARG:HG2	2.43	0.43
1:E:751:GLU:HB3	1:E:772:LEU:HB3	2.01	0.43
1:F:750:LEU:HD13	1:F:773:LEU:CD2	2.49	0.43
1:B:731:THR:HG21	1:H:758:PHE:HB2	2.01	0.42
1:B:732:LEU:HB2	1:H:761:GLY:N	2.33	0.42
1:A:808:TRP:CB	1:H:805:ASP:OD2	2.63	0.42
1:C:767:ALA:HB3	1:C:800:LEU:HB2	2.00	0.42
1:E:773:LEU:HD13	1:E:856:GLY:HA2	2.00	0.42
1:F:803:GLN:OE1	1:F:807:LEU:HD23	2.18	0.42
1:B:697:VAL:O	1:B:698:ARG:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:717:LEU:HB3	1:H:726:LEU:HD13	2.02	0.42
1:H:743:TRP:HD1	1:H:777:ALA:HB1	1.84	0.42
1:H:769:ILE:HD11	1:H:800:LEU:HD21	2.01	0.42
1:H:796:ILE:HD12	1:H:815:ILE:HG22	2.02	0.42
1:A:786:LYS:HA	1:A:786:LYS:HD2	1.89	0.42
1:C:705:ALA:O	1:C:709:GLY:N	2.52	0.42
1:A:701:GLU:OE2	1:A:856:GLY:O	2.37	0.42
1:A:741:CYS:SG	1:A:849:LEU:HD12	2.60	0.42
1:B:784:GLN:OE1	1:B:784:GLN:N	2.38	0.42
1:A:774:GLU:HG3	1:A:793:THR:HG22	2.02	0.42
1:C:698:ARG:NH1	1:C:749:HIS:NE2	2.67	0.42
1:C:745:PHE:CE1	1:C:854:ALA:HB1	2.54	0.42
1:D:725:MET:HE2	1:D:812:GLN:C	2.45	0.42
1:D:753:LEU:HD21	1:D:772:LEU:HB2	2.01	0.42
1:A:709:GLY:C	1:A:742:TYR:HB2	2.44	0.42
1:C:772:LEU:HD23	1:C:795:LYS:HG3	2.00	0.42
1:D:726:LEU:O	1:D:730:GLN:N	2.50	0.42
1:F:748:LEU:HD23	1:F:748:LEU:HA	1.82	0.42
1:A:708:LEU:HD12	1:A:733:ALA:HB2	2.02	0.42
1:C:721:LEU:HD22	1:C:725:MET:HG2	2.01	0.42
1:C:800:LEU:HD11	1:C:810:PHE:CE2	2.54	0.42
1:D:694:GLU:OE2	1:D:698:ARG:NE	2.53	0.42
1:E:722:ASP:OD1	1:E:723:GLU:N	2.52	0.42
1:F:694:GLU:O	1:F:698:ARG:N	2.34	0.42
1:F:704:LYS:NZ	1:F:856:GLY:C	2.78	0.42
1:H:721:LEU:HD12	1:H:725:MET:HG2	2.00	0.42
1:C:688:MET:HE1	1:C:696:LEU:HD11	2.01	0.42
1:C:701:GLU:OE2	1:C:856:GLY:C	2.62	0.42
1:B:729:TRP:HZ2	1:H:762:ILE:HB	1.82	0.41
1:B:791:TYR:HB2	1:C:748:LEU:HD21	2.02	0.41
1:E:739:LYS:HE2	1:E:739:LYS:HB3	1.79	0.41
1:H:800:LEU:HD13	1:H:808:TRP:CE3	2.55	0.41
1:B:746:VAL:HG21	1:C:777:ALA:HA	2.01	0.41
1:E:722:ASP:O	1:E:811:CYS:HA	2.20	0.41
1:G:757:ILE:HD12	1:G:757:ILE:N	2.35	0.41
1:G:688:MET:HB2	1:G:757:ILE:CD1	2.50	0.41
1:A:807:LEU:HD23	1:A:808:TRP:N	2.32	0.41
1:D:739:LYS:HG2	1:D:849:LEU:HD23	2.03	0.41
1:G:753:LEU:HB2	1:G:770:GLU:HB3	2.03	0.41
1:A:759:GLU:OE2	1:A:762:ILE:O	2.37	0.41
1:C:790:TYR:OH	1:C:855:ARG:CG	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:729:TRP:HH2	1:D:855:ARG:H	1.68	0.41
1:E:802:LYS:NZ	1:E:808:TRP:HE1	2.19	0.41
1:E:803:GLN:HE22	1:E:809:LYS:NZ	2.18	0.41
1:G:698:ARG:HG2	1:G:750:LEU:HD13	2.03	0.41
1:G:721:LEU:HD13	1:G:725:MET:O	2.21	0.41
1:C:713:GLN:OE1	1:C:715:TYR:OH	2.31	0.41
1:A:732:LEU:HD11	1:A:743:TRP:CH2	2.56	0.41
1:A:777:ALA:O	1:A:790:TYR:N	2.54	0.41
1:E:686:ARG:HA	1:E:686:ARG:HD3	1.66	0.41
1:E:701:GLU:OE2	1:E:856:GLY:C	2.63	0.41
1:G:790:TYR:CD2	1:G:852:MET:HB3	2.56	0.41
1:B:746:VAL:HG23	1:C:746:VAL:HG23	2.02	0.41
1:C:743:TRP:CD1	1:C:854:ALA:HB2	2.56	0.41
1:E:802:LYS:HB2	1:E:808:TRP:CH2	2.56	0.41
1:C:796:ILE:HD12	1:C:856:GLY:HA2	2.02	0.40
1:H:709:GLY:C	1:H:742:TYR:HB2	2.46	0.40
1:A:712:HIS:HD2	1:A:737:GLU:CA	2.33	0.40
1:A:725:MET:O	1:A:729:TRP:HD1	2.04	0.40
1:B:754:GLN:N	1:B:770:GLU:HB3	2.30	0.40
1:E:802:LYS:HG2	1:E:806:GLY:HA2	2.02	0.40
1:A:688:MET:HG2	1:A:692:GLU:OE1	2.21	0.40
1:A:696:LEU:O	1:A:699:GLN:HB2	2.22	0.40
1:D:700:TRP:NE1	1:D:856:GLY:O	2.46	0.40
1:H:718:SER:O	1:H:809:LYS:NZ	2.54	0.40
1:A:791:TYR:HB2	1:G:748:LEU:CD2	2.50	0.40
1:C:745:PHE:HZ	1:C:854:ALA:HB1	1.86	0.40
1:G:686:ARG:NH1	1:G:686:ARG:HB3	2.37	0.40
1:H:696:LEU:HD22	1:H:810:PHE:CE1	2.56	0.40
1:H:788:ALA:CB	1:H:851:VAL:HG21	2.51	0.40
1:H:800:LEU:HD23	1:H:810:PHE:CE2	2.57	0.40
1:A:759:GLU:CD	1:A:763:ALA:HA	2.47	0.40
1:D:769:ILE:O	1:D:798:TYR:N	2.45	0.40
1:D:788:ALA:C	1:D:851:VAL:HG11	2.47	0.40
1:H:813:SER:OG	1:H:814:ASP:N	2.54	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:719:GLU:OE2	1:F:686:ARG:NH1[1_664]	2.11	0.09

5.3 Torsion angles

5.3.1 Protein backbone

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	141/187 (75%)	133 (94%)	7 (5%)	1 (1%)	18	46
1	B	140/187 (75%)	138 (99%)	2 (1%)	0	100	100
1	C	141/187 (75%)	136 (96%)	5 (4%)	0	100	100
1	D	142/187 (76%)	136 (96%)	6 (4%)	0	100	100
1	E	140/187 (75%)	137 (98%)	3 (2%)	0	100	100
1	F	138/187 (74%)	134 (97%)	4 (3%)	0	100	100
1	G	135/187 (72%)	129 (96%)	5 (4%)	1 (1%)	18	46
1	H	136/187 (73%)	131 (96%)	5 (4%)	0	100	100
All	All	1113/1496 (74%)	1074 (96%)	37 (3%)	2 (0%)	43	70

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	762	ILE
1	G	762	ILE

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	124/157 (79%)	124 (100%)	0	100	100
1	B	124/157 (79%)	124 (100%)	0	100	100
1	C	125/157 (80%)	125 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	126/157 (80%)	125 (99%)	1 (1%)	73	77
1	E	124/157 (79%)	124 (100%)	0	100	100
1	F	122/157 (78%)	121 (99%)	1 (1%)	73	77
1	G	119/157 (76%)	119 (100%)	0	100	100
1	H	120/157 (76%)	120 (100%)	0	100	100
All	All	984/1256 (78%)	982 (100%)	2 (0%)	87	85

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	786	LYS
1	F	735	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	699	GLN
1	A	848	HIS
1	D	734	GLN
1	D	756	HIS
1	D	784	GLN
1	E	702	ASN
1	F	684	HIS
1	H	784	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	145/187 (77%)	0.50	8 (5%) 30 23	28, 48, 99, 134	0
1	B	144/187 (77%)	0.34	1 (0%) 84 72	30, 45, 77, 98	0
1	C	145/187 (77%)	0.43	6 (4%) 41 29	34, 48, 66, 88	0
1	D	146/187 (78%)	0.45	7 (4%) 35 26	30, 52, 86, 106	0
1	E	144/187 (77%)	0.41	4 (2%) 55 40	44, 58, 82, 97	0
1	F	142/187 (75%)	0.51	6 (4%) 40 29	32, 58, 86, 115	0
1	G	139/187 (74%)	0.51	4 (2%) 53 39	39, 64, 91, 122	0
1	H	140/187 (74%)	0.47	6 (4%) 40 29	39, 55, 84, 103	0
All	All	1145/1496 (76%)	0.45	42 (3%) 45 32	28, 54, 86, 134	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	701	GLU	3.6
1	A	763	ALA	3.4
1	H	778	GLU	3.4
1	G	795	LYS	3.4
1	H	687	PRO	3.2
1	D	760	ASP	3.2
1	A	764	GLY	3.2
1	F	762	ILE	3.0
1	F	748	LEU	2.7
1	G	849	LEU	2.7
1	F	758	PHE	2.6
1	C	728	GLN	2.6
1	H	786	LYS	2.6
1	C	766	ALA	2.5
1	G	758	PHE	2.5
1	A	762	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	685	LYS	2.3
1	F	816	GLN	2.3
1	A	760	ASP	2.3
1	A	805	ASP	2.3
1	F	786	LYS	2.3
1	C	738	ALA	2.2
1	D	733	ALA	2.2
1	E	688	MET	2.2
1	D	817	ILE	2.2
1	D	763	ALA	2.2
1	E	705	ALA	2.2
1	D	782	GLU	2.1
1	B	785	PRO	2.1
1	A	761	GLY	2.1
1	H	787	ASN	2.1
1	H	800	LEU	2.1
1	D	755	ALA	2.1
1	C	785	PRO	2.1
1	H	759	GLU	2.1
1	E	785	PRO	2.1
1	A	685	LYS	2.1
1	C	685	LYS	2.1
1	A	769	ILE	2.0
1	C	716	SER	2.0
1	G	766	ALA	2.0
1	E	759	GLU	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 ⓘ

There are no such residues in this entry.