



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:58 AM UTC

PDB ID : 8AJ8 / pdb_00008aj8
Title : Structure of p110 gamma bound to the p84 regulatory subunit
Authors : Burke, J.E.; Williams, R.L.; Zhang, X.
Deposited on : 2022-07-27
Resolution : 8.50 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
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

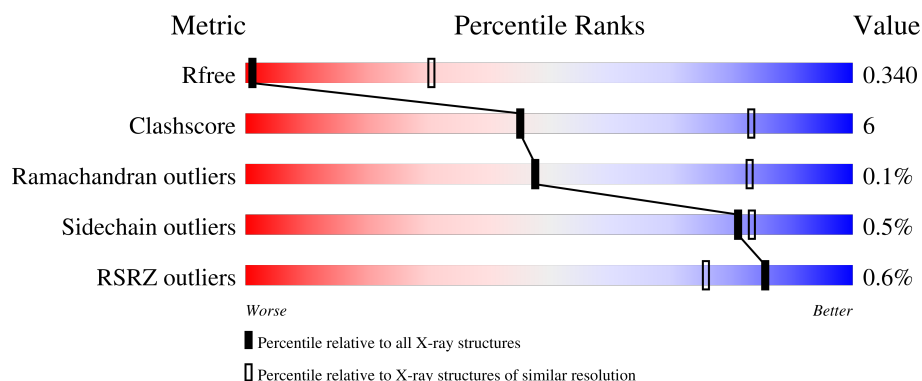
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 8.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1168 (11.50-4.00)
Clashscore	190562	1001 (11.50-4.06)
Ramachandran outliers	187476	1055 (11.50-4.00)
Sidechain outliers	187428	1018 (11.50-4.00)
RSRZ outliers	180081	1162 (11.50-4.00)

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	1102	% 79% 11% 10%
1	C	1102	% 80% 10% 10%
1	E	1102	81% 10% 10%
1	G	1102	80% 10% 10%
2	B	756	% 59% 15% 26%

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Mol	Chain	Length	Quality of chain
2	D	756	% 59% 15% 26%
2	F	756	% 60% 14% 26%
2	H	756	59% 15% 26%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 50008 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 Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit gamma isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	995	Total	C	N	O	S	0	0	0
			8066	5175	1380	1470	41			
1	C	995	Total	C	N	O	S	0	0	0
			8066	5175	1380	1470	41			
1	E	995	Total	C	N	O	S	0	0	0
			8066	5175	1380	1470	41			
1	G	995	Total	C	N	O	S	0	0	0
			8066	5175	1380	1470	41			

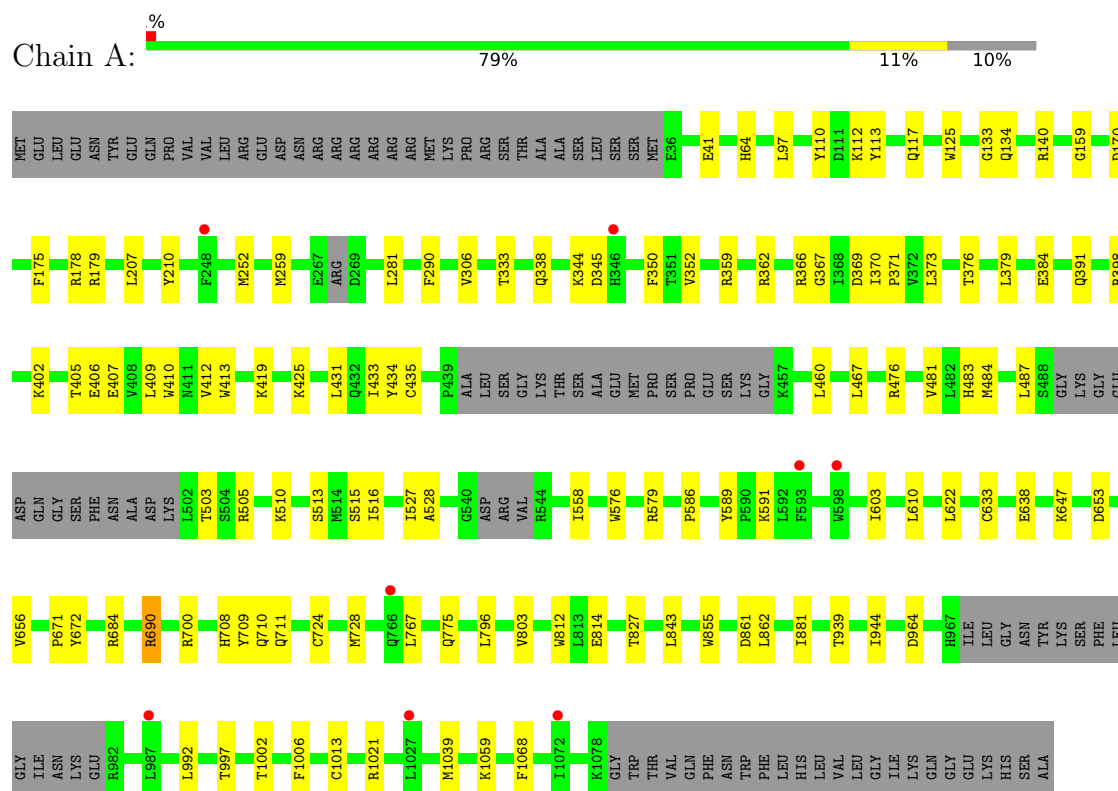
- Molecule 2 is a protein called Phosphoinositide 3-kinase regulatory subunit 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	558	Total	C	N	O	S	0	0	0
			4436	2831	765	818	22			
2	D	558	Total	C	N	O	S	0	0	0
			4436	2831	765	818	22			
2	F	558	Total	C	N	O	S	0	0	0
			4436	2831	765	818	22			
2	H	558	Total	C	N	O	S	0	0	0
			4436	2831	765	818	22			

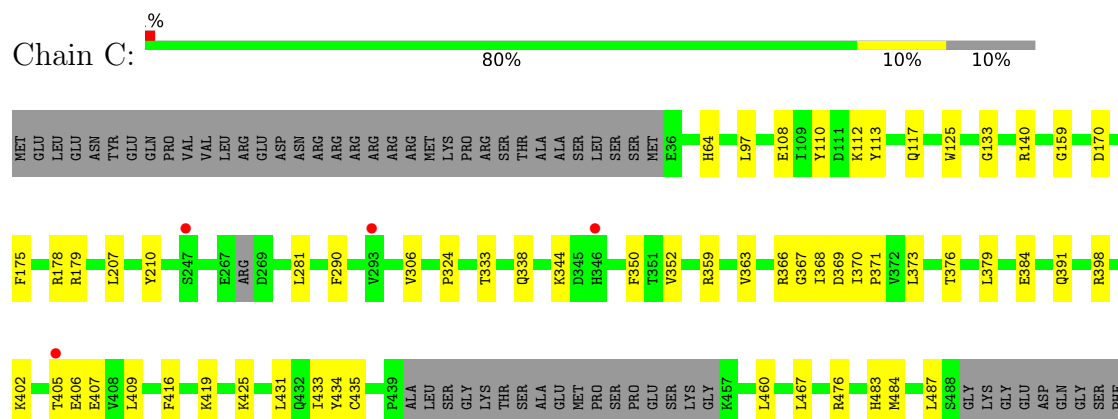
3 Residue-property plots

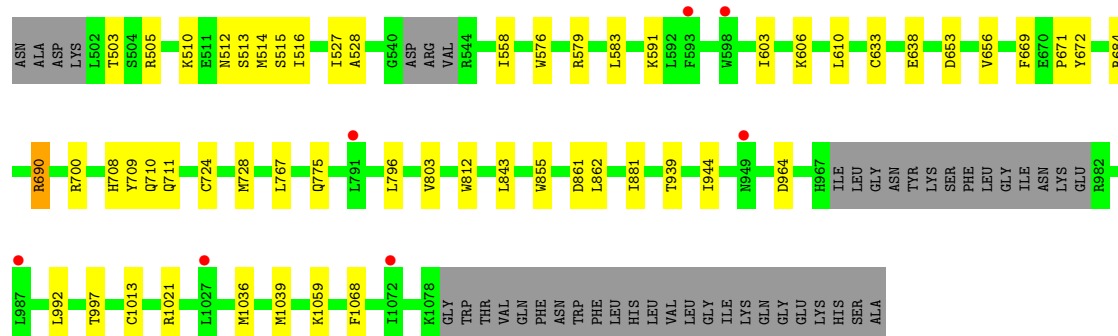
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit gamma isoform

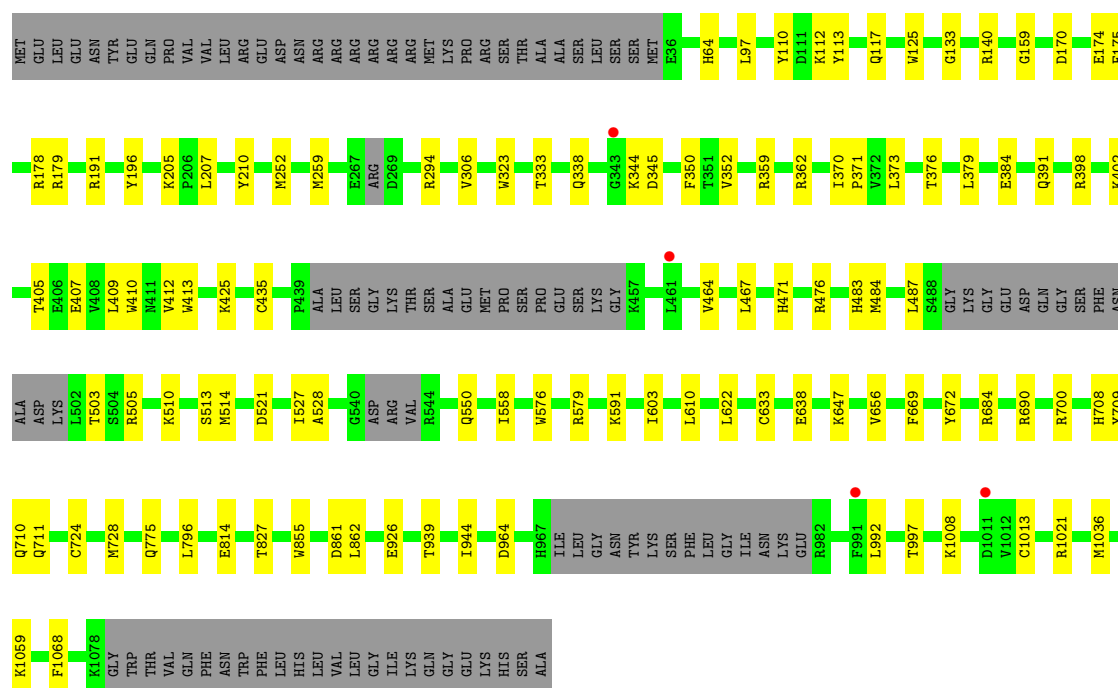
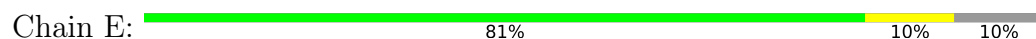


- Molecule 1: Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit gamma isoform

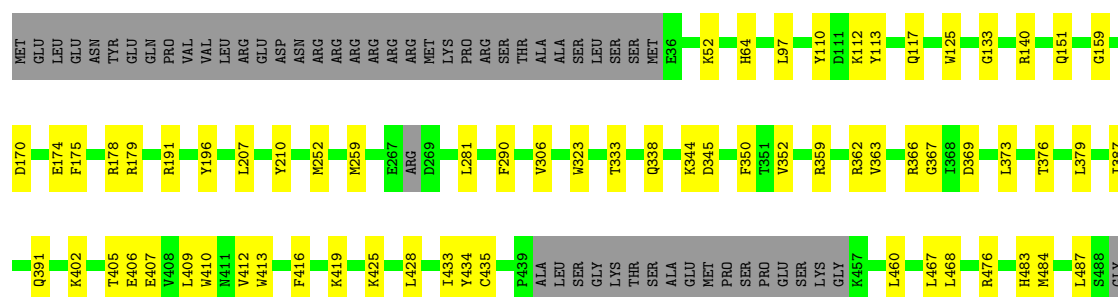
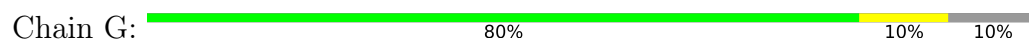


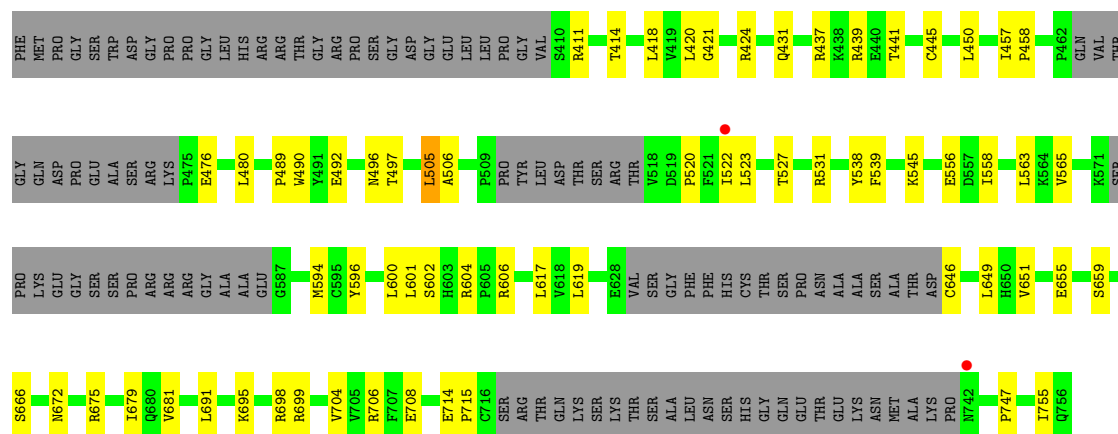


- Molecule 1: Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit gamma isoform

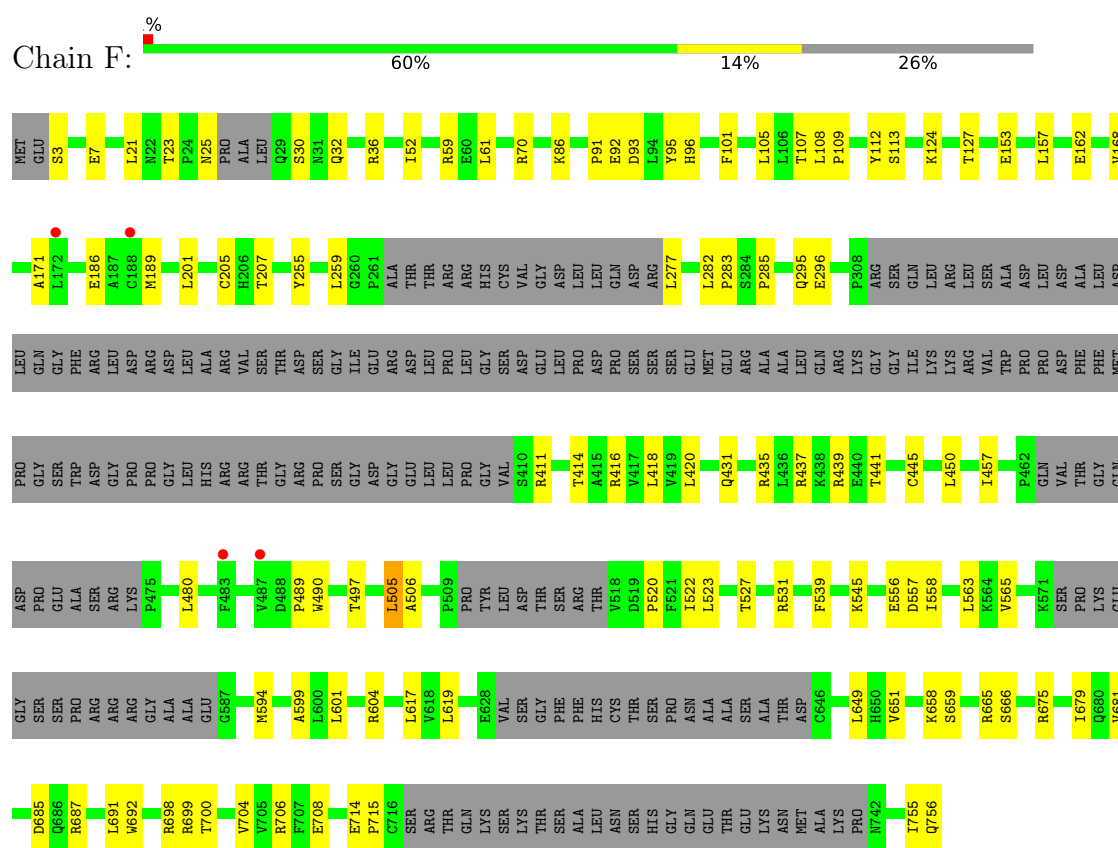


- Molecule 1: Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit gamma isoform

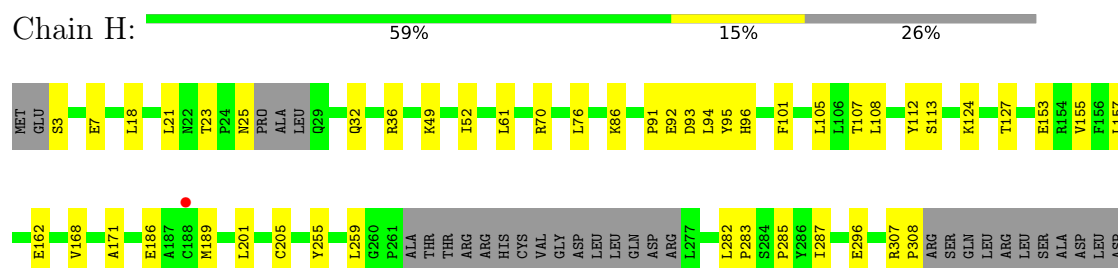




• Molecule 2: Phosphoinositide 3-kinase regulatory subunit 6



• Molecule 2: Phosphoinositide 3-kinase regulatory subunit 6



[illegible]

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	322.35Å 166.60Å 255.79Å 90.00° 114.02° 90.00°	Depositor
Resolution (Å)	90.29 – 8.50 90.29 – 8.50	Depositor EDS
% Data completeness (in resolution range)	97.6 (90.29-8.50) 93.9 (90.29-8.50)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.75 (at 8.41Å)	Xtrriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.280 , 0.340 0.280 , 0.340	Depositor DCC
R_{free} test set	1084 reflections (9.76%)	wwPDB-VP
Wilson B-factor (Å ²)	449.1	Xtrriage
Anisotropy	0.200	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 656.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.74	EDS
Total number of atoms	50008	wwPDB-VP
Average B, all atoms (Å ²)	545.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.07 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.8875e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.18	0/8247	0.35	0/11169
1	C	0.17	0/8247	0.35	0/11169
1	E	0.16	0/8247	0.34	0/11169
1	G	0.17	0/8247	0.34	0/11169
2	B	0.19	0/4522	0.37	0/6136
2	D	0.21	0/4522	0.38	0/6136
2	F	0.19	0/4522	0.37	0/6136
2	H	0.19	0/4522	0.38	0/6136
All	All	0.18	0/51076	0.36	0/69220

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8066	0	8121	92	0
1	C	8066	0	8121	88	0
1	E	8066	0	8121	72	0
1	G	8066	0	8121	83	0
2	B	4436	0	4519	94	1
2	D	4436	0	4519	90	0
2	F	4436	0	4519	76	1
2	H	4436	0	4519	88	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	50008	0	50560	590	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 6.

All (590) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:359:ARG:HH12	2:F:108:LEU:HG	1.10	1.15
1:C:359:ARG:HH12	2:D:108:LEU:HD23	1.22	1.04
1:C:513:SER:O	2:D:604:ARG:NH2	1.97	0.98
1:E:359:ARG:NH1	2:F:108:LEU:HG	1.85	0.92
1:E:505:ARG:HH12	1:E:710:GLN:HG2	1.36	0.90
1:A:505:ARG:HH12	1:A:710:GLN:HG2	1.35	0.90
1:A:513:SER:O	2:B:604:ARG:NH2	2.04	0.89
1:E:513:SER:O	2:F:604:ARG:NH2	2.07	0.88
1:C:505:ARG:HH12	1:C:710:GLN:HG2	1.37	0.87
1:G:505:ARG:HH12	1:G:710:GLN:HG2	1.42	0.85
1:G:391:GLN:NE2	1:G:633:CYS:SG	2.51	0.84
2:F:558:ILE:O	2:F:699:ARG:NH2	2.10	0.82
1:E:391:GLN:NE2	1:E:633:CYS:SG	2.51	0.82
1:C:391:GLN:NE2	1:C:633:CYS:SG	2.54	0.81
1:A:391:GLN:NE2	1:A:633:CYS:SG	2.55	0.80
1:G:406:GLU:OE1	2:H:606:ARG:NH1	2.13	0.80
1:A:369:ASP:OD1	2:B:602:SER:N	2.15	0.79
2:H:558:ILE:O	2:H:699:ARG:NH2	2.12	0.78
1:C:409:LEU:HD23	2:D:601:LEU:HD11	1.66	0.77
2:D:558:ILE:O	2:D:699:ARG:NH2	2.14	0.77
1:C:367:GLY:HA3	2:D:601:LEU:HD13	1.67	0.76
2:H:296:GLU:OE1	2:H:439:ARG:NH1	2.20	0.75
1:E:413:TRP:HE1	2:F:756:GLN:HB3	1.49	0.75
1:E:345:ASP:OD1	2:F:124:LYS:NZ	2.20	0.75
2:F:296:GLU:OE1	2:F:439:ARG:NH1	2.20	0.75
1:G:513:SER:O	2:H:604:ARG:NH2	2.20	0.74
1:G:425:LYS:NZ	1:G:638:GLU:OE1	2.19	0.74
1:C:369:ASP:O	2:D:604:ARG:NH1	2.20	0.73
1:C:359:ARG:HH22	2:D:108:LEU:HG	1.52	0.73
1:G:402:LYS:NZ	1:G:409:LEU:O	2.19	0.73
1:A:425:LYS:NZ	1:A:638:GLU:OE1	2.20	0.72
1:C:425:LYS:NZ	1:C:638:GLU:OE1	2.21	0.72
2:B:558:ILE:O	2:B:699:ARG:NH2	2.17	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:369:ASP:OD2	2:H:604:ARG:NH1	2.23	0.72
2:B:706:ARG:NH2	2:B:708:GLU:OE2	2.23	0.72
1:C:406:GLU:OE1	2:D:606:ARG:NH1	2.17	0.71
2:B:157:LEU:HD11	2:B:420:LEU:HD13	1.71	0.71
1:E:425:LYS:NZ	1:E:638:GLU:OE1	2.22	0.70
2:D:296:GLU:OE1	2:D:439:ARG:NH1	2.24	0.70
2:B:296:GLU:OE1	2:B:439:ARG:NH1	2.24	0.69
2:F:108:LEU:HD23	2:F:109:PRO:HD2	1.73	0.69
2:B:431:GLN:HA	2:B:558:ILE:HD11	1.75	0.69
2:D:418:LEU:HD11	2:D:457:ILE:HG13	1.75	0.69
2:H:706:ARG:NH2	2:H:708:GLU:OE2	2.26	0.69
2:B:418:LEU:HD11	2:B:457:ILE:HG13	1.74	0.69
1:G:345:ASP:OD1	2:H:124:LYS:NZ	2.26	0.69
1:E:359:ARG:NE	2:F:107:THR:OG1	2.26	0.68
1:A:376:THR:HB	1:A:379:LEU:HD11	1.75	0.68
2:D:157:LEU:HD11	2:D:420:LEU:HD13	1.73	0.68
2:D:706:ARG:NH2	2:D:708:GLU:OE2	2.26	0.68
1:C:366:ARG:NH2	2:D:646:CYS:SG	2.67	0.67
2:H:162:GLU:OE1	2:H:698:ARG:NH1	2.27	0.67
2:H:157:LEU:HD11	2:H:420:LEU:HD13	1.75	0.67
2:D:282:LEU:HD12	2:D:283:PRO:HD2	1.75	0.67
2:D:565:VAL:HG22	2:D:691:LEU:HG	1.77	0.67
2:F:157:LEU:HD11	2:F:420:LEU:HD13	1.75	0.67
1:A:413:TRP:HE1	2:B:756:GLN:HB3	1.60	0.67
2:H:431:GLN:HA	2:H:558:ILE:HD11	1.77	0.67
2:D:162:GLU:OE1	2:D:698:ARG:NH1	2.27	0.66
2:B:162:GLU:OE1	2:B:698:ARG:NH1	2.27	0.66
1:G:376:THR:HB	1:G:379:LEU:HD11	1.76	0.66
2:F:418:LEU:HD11	2:F:457:ILE:HG13	1.77	0.66
2:B:105:LEU:HD22	2:B:108:LEU:HD12	1.78	0.66
1:E:402:LYS:NZ	1:E:409:LEU:O	2.25	0.66
1:C:376:THR:HB	1:C:379:LEU:HD11	1.76	0.66
2:B:282:LEU:HD12	2:B:283:PRO:HD2	1.76	0.66
1:A:402:LYS:NZ	1:A:409:LEU:O	2.22	0.66
2:D:431:GLN:HA	2:D:558:ILE:HD11	1.78	0.65
1:A:481:VAL:HG21	2:B:603:HIS:CD2	2.30	0.65
1:G:579:ARG:HD2	1:G:610:LEU:HD11	1.76	0.65
1:A:406:GLU:OE1	2:B:606:ARG:NH1	2.24	0.65
2:B:153:GLU:HG2	2:B:414:THR:HB	1.78	0.65
1:E:345:ASP:CG	2:F:124:LYS:HZ1	2.04	0.65
2:F:706:ARG:NH2	2:F:708:GLU:OE2	2.28	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:579:ARG:HD2	1:A:610:LEU:HD11	1.78	0.65
1:C:579:ARG:HD2	1:C:610:LEU:HD11	1.77	0.65
1:E:376:THR:HB	1:E:379:LEU:HD11	1.80	0.64
2:F:565:VAL:HG22	2:F:691:LEU:HG	1.78	0.64
1:E:579:ARG:HD2	1:E:610:LEU:HD11	1.78	0.64
2:H:105:LEU:HD22	2:H:108:LEU:HD12	1.80	0.64
1:C:402:LYS:NZ	1:C:409:LEU:O	2.24	0.64
2:F:437:ARG:NH2	2:F:714:GLU:OE2	2.30	0.63
2:F:162:GLU:OE1	2:F:698:ARG:NH1	2.32	0.63
1:C:366:ARG:HH22	2:D:646:CYS:CB	2.11	0.63
2:H:282:LEU:HD12	2:H:283:PRO:HD2	1.79	0.63
1:C:210:TYR:CZ	1:C:861:ASP:HB2	2.34	0.62
1:G:366:ARG:NH2	2:H:646:CYS:SG	2.72	0.62
2:F:431:GLN:HA	2:F:558:ILE:HD11	1.82	0.61
1:A:210:TYR:CZ	1:A:861:ASP:HB2	2.35	0.61
2:F:282:LEU:HD12	2:F:283:PRO:HD2	1.81	0.61
2:H:153:GLU:HG2	2:H:414:THR:HB	1.81	0.61
2:H:418:LEU:HD11	2:H:457:ILE:HG13	1.81	0.61
2:H:565:VAL:HG22	2:H:691:LEU:HG	1.81	0.61
1:G:175:PHE:CE1	1:G:179:ARG:HD2	2.36	0.61
2:H:283:PRO:O	2:H:531:ARG:NH2	2.32	0.61
1:C:1013:CYS:HB3	1:C:1068:PHE:HE1	1.66	0.61
2:D:283:PRO:O	2:D:531:ARG:NH2	2.33	0.61
1:E:175:PHE:CE1	1:E:179:ARG:HD2	2.35	0.61
2:H:692:TRP:CD1	2:H:700:THR:HG1	2.18	0.60
2:H:437:ARG:NH2	2:H:714:GLU:OE2	2.33	0.60
1:A:159:GLY:HA3	1:A:700:ARG:HH12	1.67	0.60
1:G:379:LEU:HB3	1:G:435:CYS:SG	2.41	0.60
1:C:369:ASP:OD1	2:D:602:SER:N	2.30	0.60
1:G:700:ARG:HG3	1:G:700:ARG:HH11	1.67	0.60
1:E:210:TYR:CZ	1:E:861:ASP:HB2	2.36	0.60
1:G:338:GLN:O	1:G:344:LYS:NZ	2.35	0.60
1:G:939:THR:HG22	1:G:944:ILE:HD12	1.84	0.60
2:B:283:PRO:O	2:B:531:ARG:NH2	2.35	0.59
1:C:724:CYS:HB3	1:C:728:MET:HB2	1.83	0.59
1:G:210:TYR:CZ	1:G:861:ASP:HB2	2.37	0.59
2:F:692:TRP:CD1	2:F:700:THR:HG1	2.20	0.59
2:B:108:LEU:HD13	2:B:112:TYR:HB3	1.84	0.59
2:B:489:PRO:HD2	2:B:755:ILE:HD12	1.84	0.59
2:F:105:LEU:HD22	2:F:108:LEU:HD12	1.84	0.59
1:E:362:ARG:NH1	2:F:70:ARG:HH12	2.00	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:489:PRO:HD2	2:F:755:ILE:HD12	1.84	0.59
1:E:379:LEU:HB3	1:E:435:CYS:SG	2.43	0.59
1:G:366:ARG:HH22	2:H:646:CYS:CB	2.16	0.59
2:F:153:GLU:HG2	2:F:414:THR:HB	1.84	0.59
1:G:159:GLY:HA3	1:G:700:ARG:HH12	1.66	0.59
1:C:175:PHE:CE1	1:C:179:ARG:HD2	2.38	0.58
1:A:406:GLU:CD	2:B:606:ARG:HH12	2.10	0.58
1:C:700:ARG:HG3	1:C:700:ARG:HH11	1.69	0.58
1:G:345:ASP:CG	2:H:124:LYS:HZ1	2.11	0.58
1:C:515:SER:N	2:D:604:ARG:HH22	2.01	0.58
1:C:939:THR:HG22	1:C:944:ILE:HD12	1.85	0.58
1:A:175:PHE:CE1	1:A:179:ARG:HD2	2.39	0.58
1:A:700:ARG:HG3	1:A:700:ARG:HH11	1.69	0.58
1:A:481:VAL:HG21	2:B:603:HIS:HD2	1.69	0.58
1:A:379:LEU:HB3	1:A:435:CYS:SG	2.43	0.57
1:E:407:GLU:OE2	2:F:675:ARG:NH2	2.36	0.57
1:E:700:ARG:HH11	1:E:700:ARG:HG3	1.69	0.57
1:E:939:THR:HG22	1:E:944:ILE:HD12	1.85	0.57
1:A:370:ILE:HA	2:B:604:ARG:HH12	1.69	0.57
2:H:70:ARG:HB3	2:H:112:TYR:OH	2.04	0.57
1:C:159:GLY:HA3	1:C:700:ARG:HH12	1.68	0.57
1:E:159:GLY:HA3	1:E:700:ARG:HH12	1.68	0.57
2:B:619:LEU:HD23	2:B:649:LEU:HD13	1.86	0.57
2:F:619:LEU:HD23	2:F:649:LEU:HD13	1.87	0.57
1:E:407:GLU:OE2	2:F:601:LEU:HG	2.05	0.57
2:B:437:ARG:NH2	2:B:714:GLU:OE2	2.38	0.57
2:D:437:ARG:NH2	2:D:714:GLU:OE2	2.37	0.57
1:G:110:TYR:CZ	1:G:178:ARG:HG3	2.40	0.56
2:H:563:LEU:HD11	2:H:691:LEU:HD23	1.87	0.56
1:A:413:TRP:NE1	2:B:756:GLN:HB3	2.19	0.56
2:D:153:GLU:HG2	2:D:414:THR:HB	1.86	0.56
2:D:171:ALA:HB1	2:D:505:LEU:HD23	1.86	0.56
1:E:170:ASP:OD2	1:E:476:ARG:NH2	2.39	0.56
2:F:565:VAL:HB	2:F:617:LEU:HG	1.87	0.56
2:F:411:ARG:NH1	2:F:450:LEU:O	2.37	0.56
1:G:362:ARG:NH1	2:H:70:ARG:HH12	2.04	0.56
1:A:370:ILE:HA	2:B:604:ARG:NH1	2.21	0.56
1:A:515:SER:N	2:B:604:ARG:HH22	2.03	0.56
1:A:939:THR:HG22	1:A:944:ILE:HD12	1.88	0.56
1:E:110:TYR:CZ	1:E:178:ARG:HG3	2.40	0.56
1:E:117:GLN:NE2	1:E:338:GLN:HB3	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:97:LEU:HD21	1:G:140:ARG:HE	1.71	0.56
2:D:594:MET:HG2	2:D:681:VAL:HG22	1.86	0.55
2:H:565:VAL:HB	2:H:617:LEU:HG	1.87	0.55
1:C:359:ARG:NH1	2:D:108:LEU:HD23	2.06	0.55
2:D:105:LEU:HD22	2:D:108:LEU:CD1	2.36	0.55
2:D:563:LEU:HD11	2:D:691:LEU:HD23	1.88	0.55
2:D:565:VAL:HB	2:D:617:LEU:HG	1.87	0.55
2:F:108:LEU:HD13	2:F:112:TYR:CG	2.41	0.55
1:C:117:GLN:NE2	1:C:338:GLN:HB3	2.22	0.55
2:H:171:ALA:HB1	2:H:505:LEU:HD23	1.89	0.55
1:A:117:GLN:NE2	1:A:338:GLN:HB3	2.22	0.55
2:B:171:ALA:HB1	2:B:505:LEU:HD23	1.89	0.54
1:G:369:ASP:C	2:H:604:ARG:HH12	2.15	0.54
1:A:359:ARG:HE	2:B:107:THR:CB	2.20	0.54
1:G:407:GLU:OE1	2:H:675:ARG:NH2	2.41	0.54
1:G:117:GLN:NE2	1:G:338:GLN:HB3	2.22	0.54
1:C:110:TYR:CZ	1:C:178:ARG:HG3	2.43	0.54
1:C:373:LEU:HD21	1:C:405:THR:C	2.33	0.54
1:G:170:ASP:OD2	1:G:476:ARG:NH2	2.41	0.54
2:H:619:LEU:HD23	2:H:649:LEU:HD13	1.90	0.54
1:C:370:ILE:HA	2:D:604:ARG:NH1	2.22	0.54
2:H:489:PRO:HD2	2:H:755:ILE:HD12	1.90	0.54
2:D:619:LEU:HD23	2:D:649:LEU:HD13	1.88	0.54
2:B:505:LEU:HD22	2:B:522:ILE:HD12	1.88	0.54
1:G:775:GLN:OE1	1:G:796:LEU:N	2.40	0.54
1:A:112:LYS:HE3	1:A:113:TYR:CE2	2.43	0.54
1:C:371:PRO:HG3	2:D:604:ARG:HD3	1.88	0.54
1:G:1021:ARG:NH2	1:G:1059:LYS:O	2.40	0.54
1:A:367:GLY:HA3	2:B:601:LEU:HD13	1.89	0.53
1:A:503:THR:HG21	1:A:708:HIS:HB3	1.90	0.53
2:B:225:TYR:OH	2:B:258:LEU:HA	2.08	0.53
2:D:70:ARG:HB3	2:D:112:TYR:OH	2.08	0.53
2:D:105:LEU:HD22	2:D:108:LEU:HD12	1.89	0.53
1:E:338:GLN:O	1:E:344:LYS:NZ	2.42	0.53
2:B:594:MET:HG2	2:B:681:VAL:HG22	1.91	0.53
1:C:112:LYS:HE3	1:C:113:TYR:CE2	2.44	0.53
1:C:1013:CYS:HB3	1:C:1068:PHE:CE1	2.44	0.53
1:E:352:VAL:HB	1:E:527:ILE:HD13	1.90	0.53
1:G:373:LEU:HD21	1:G:405:THR:C	2.34	0.53
1:A:409:LEU:HD23	2:B:601:LEU:HD11	1.91	0.53
2:D:207:THR:HG21	2:D:277:LEU:HD23	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:283:PRO:O	2:F:531:ARG:NH2	2.40	0.53
1:G:112:LYS:HE3	1:G:113:TYR:CE2	2.44	0.53
1:A:992:LEU:HB3	1:A:997:THR:OG1	2.09	0.53
2:B:21:LEU:HD21	2:B:490:TRP:CE3	2.44	0.53
1:E:775:GLN:OE1	1:E:796:LEU:N	2.42	0.53
1:G:369:ASP:OD1	2:H:602:SER:HB3	2.09	0.53
1:C:379:LEU:HD13	1:C:435:CYS:SG	2.49	0.53
2:D:225:TYR:OH	2:D:258:LEU:HA	2.08	0.52
2:F:520:PRO:HB2	2:F:523:LEU:HB3	1.90	0.52
2:B:520:PRO:HB2	2:B:523:LEU:HB3	1.92	0.52
2:B:565:VAL:HG22	2:B:691:LEU:HG	1.91	0.52
2:B:565:VAL:HB	2:B:617:LEU:HG	1.90	0.52
1:C:503:THR:HG21	1:C:708:HIS:HB3	1.91	0.52
2:F:563:LEU:HD11	2:F:691:LEU:HD23	1.91	0.52
2:H:441:THR:HG21	2:H:715:PRO:HB2	1.92	0.52
1:G:409:LEU:HD21	2:H:601:LEU:HD21	1.91	0.52
1:A:407:GLU:OE2	2:B:601:LEU:HG	2.09	0.52
2:F:7:GLU:OE2	2:F:59:ARG:NH2	2.43	0.52
2:D:255:TYR:CZ	2:D:259:LEU:HD12	2.46	0.51
1:E:112:LYS:HE3	1:E:113:TYR:CE2	2.45	0.51
2:B:563:LEU:HD11	2:B:691:LEU:HD23	1.92	0.51
1:E:373:LEU:HD21	1:E:405:THR:C	2.35	0.51
1:A:467:LEU:HD21	1:A:672:TYR:CE1	2.46	0.51
2:D:441:THR:HG21	2:D:715:PRO:HB2	1.92	0.51
1:C:515:SER:OG	2:D:602:SER:HB3	2.11	0.51
1:G:558:ILE:O	1:G:591:LYS:NZ	2.42	0.51
2:F:171:ALA:HB1	2:F:505:LEU:HD23	1.93	0.51
1:E:550:GLN:CD	1:G:52:LYS:HG3	2.35	0.51
1:C:379:LEU:HB3	1:C:435:CYS:SG	2.50	0.51
2:F:659:SER:OG	2:F:666:SER:OG	2.27	0.51
1:G:505:ARG:NH1	1:G:711:GLN:H	2.08	0.51
2:H:411:ARG:NH1	2:H:450:LEU:O	2.40	0.51
2:D:520:PRO:HB2	2:D:523:LEU:HB3	1.93	0.50
2:F:599:ALA:O	2:F:675:ARG:NH2	2.45	0.50
2:H:21:LEU:HD21	2:H:490:TRP:CE3	2.46	0.50
2:B:659:SER:OG	2:B:666:SER:OG	2.29	0.50
2:F:441:THR:HG21	2:F:715:PRO:HB2	1.93	0.50
1:G:407:GLU:OE2	2:H:601:LEU:HG	2.11	0.50
1:A:1013:CYS:HB3	1:A:1068:PHE:HE1	1.76	0.50
1:C:505:ARG:HD3	1:C:708:HIS:O	2.11	0.50
2:D:489:PRO:HD2	2:D:755:ILE:HD12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:125:TRP:CE3	1:G:133:GLY:HA3	2.46	0.50
1:A:338:GLN:O	1:A:344:LYS:NZ	2.45	0.50
2:D:21:LEU:HD21	2:D:490:TRP:CE3	2.47	0.50
1:E:724:CYS:HB3	1:E:728:MET:HB2	1.94	0.50
2:D:659:SER:OG	2:D:666:SER:OG	2.29	0.50
1:A:97:LEU:HD21	1:A:140:ARG:HE	1.76	0.50
2:B:153:GLU:OE1	2:B:416:ARG:NH1	2.30	0.50
1:E:467:LEU:HD21	1:E:672:TYR:CE1	2.47	0.50
2:H:659:SER:OG	2:H:666:SER:OG	2.28	0.50
1:A:373:LEU:HD21	1:A:405:THR:C	2.36	0.50
2:B:70:ARG:HB3	2:B:112:TYR:OH	2.11	0.50
1:A:724:CYS:HB3	1:A:728:MET:HB2	1.92	0.50
1:E:1013:CYS:HB3	1:E:1068:PHE:HE1	1.76	0.50
2:H:520:PRO:HB2	2:H:523:LEU:HB3	1.93	0.50
1:C:467:LEU:HD21	1:C:672:TYR:CE1	2.47	0.49
1:G:367:GLY:HA3	2:H:601:LEU:HD13	1.94	0.49
1:G:724:CYS:HB3	1:G:728:MET:HB2	1.94	0.49
1:A:352:VAL:HB	1:A:527:ILE:HD13	1.94	0.49
1:E:125:TRP:CE3	1:E:133:GLY:HA3	2.48	0.49
1:E:521:ASP:CG	2:F:109:PRO:HB3	2.37	0.49
2:F:21:LEU:HD21	2:F:490:TRP:CE3	2.47	0.49
2:H:108:LEU:HD13	2:H:112:TYR:HB3	1.93	0.49
2:H:201:LEU:HB2	2:H:205:CYS:HB2	1.93	0.49
2:B:411:ARG:NH1	2:B:450:LEU:O	2.41	0.49
1:C:170:ASP:OD2	1:C:476:ARG:NH2	2.45	0.49
2:D:480:LEU:HD11	2:D:539:PHE:CE1	2.47	0.49
1:A:359:ARG:O	1:A:419:LYS:HA	2.13	0.49
1:A:431:LEU:HD13	1:A:516:ILE:HD13	1.94	0.49
1:A:1021:ARG:NH2	1:A:1059:LYS:O	2.45	0.49
1:C:992:LEU:HB3	1:C:997:THR:OG1	2.12	0.49
1:E:992:LEU:HB3	1:E:997:THR:OG1	2.13	0.49
1:G:359:ARG:O	1:G:419:LYS:HA	2.12	0.49
2:D:7:GLU:OE2	2:D:59:ARG:NH2	2.45	0.49
1:E:97:LEU:HD21	1:E:140:ARG:HE	1.78	0.49
1:E:413:TRP:HE1	2:F:756:GLN:CB	2.24	0.49
2:H:476:GLU:O	2:H:695:LYS:NZ	2.28	0.49
2:B:441:THR:HG21	2:B:715:PRO:HB2	1.95	0.49
1:A:170:ASP:OD2	1:A:476:ARG:NH2	2.46	0.49
1:A:366:ARG:NH2	2:B:646:CYS:SG	2.86	0.49
1:C:1021:ARG:NH2	1:C:1059:LYS:O	2.45	0.49
2:D:476:GLU:O	2:D:695:LYS:NZ	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:352:VAL:HB	1:G:527:ILE:HD13	1.93	0.49
2:B:108:LEU:O	2:B:113:SER:HB3	2.13	0.49
2:F:32:GLN:HB3	2:F:497:THR:HG21	1.95	0.49
2:F:505:LEU:HD22	2:F:522:ILE:HD12	1.95	0.48
1:E:505:ARG:NH1	1:E:711:GLN:H	2.10	0.48
2:F:108:LEU:O	2:F:113:SER:HB3	2.13	0.48
2:H:594:MET:HG2	2:H:681:VAL:HG22	1.94	0.48
2:F:594:MET:HG2	2:F:681:VAL:HG22	1.95	0.48
2:B:61:LEU:HB3	2:B:101:PHE:CZ	2.49	0.48
1:E:252:MET:HE2	1:E:259:MET:SD	2.53	0.48
1:G:359:ARG:HE	2:H:107:THR:CB	2.26	0.48
1:G:467:LEU:HD21	1:G:672:TYR:CE1	2.48	0.48
2:B:108:LEU:HB3	2:B:112:TYR:HB2	1.95	0.48
2:F:168:VAL:HG22	2:F:506:ALA:HB2	1.96	0.48
1:G:409:LEU:HD23	2:H:601:LEU:HD11	1.96	0.48
1:A:814:GLU:OE1	1:A:827:THR:OG1	2.23	0.48
1:C:503:THR:HB	1:C:709:TYR:CE1	2.49	0.48
1:G:843:LEU:HD22	1:G:1039:MET:HE1	1.95	0.48
1:A:505:ARG:NH1	1:A:710:GLN:HG2	2.16	0.48
1:A:656:VAL:HG21	1:A:684:ARG:HH21	1.79	0.48
1:C:338:GLN:O	1:C:344:LYS:NZ	2.47	0.48
2:D:91:PRO:HD2	2:D:94:LEU:HD12	1.94	0.48
1:A:690:ARG:HB2	1:A:690:ARG:HH11	1.79	0.48
2:B:105:LEU:HD22	2:B:108:LEU:CD1	2.44	0.47
1:C:367:GLY:CA	2:D:601:LEU:HD13	2.40	0.47
2:D:36:ARG:HD3	2:D:490:TRP:CZ2	2.49	0.47
2:H:285:PRO:HD3	2:H:527:THR:HG23	1.96	0.47
2:H:505:LEU:HD22	2:H:522:ILE:HD12	1.96	0.47
1:A:379:LEU:HD13	1:A:435:CYS:SG	2.54	0.47
1:A:505:ARG:HD3	1:A:708:HIS:O	2.14	0.47
2:D:538:TYR:CE2	2:D:747:PRO:HB3	2.48	0.47
1:E:558:ILE:O	1:E:591:LYS:NZ	2.44	0.47
1:A:775:GLN:OE1	1:A:796:LEU:N	2.48	0.47
1:C:352:VAL:HB	1:C:527:ILE:HD13	1.96	0.47
2:H:441:THR:HG21	2:H:715:PRO:O	2.14	0.47
2:F:207:THR:HG21	2:F:277:LEU:HD23	1.97	0.47
1:G:359:ARG:HH12	2:H:108:LEU:HG	1.79	0.47
1:C:371:PRO:HG2	1:C:512:ASN:HA	1.96	0.47
1:E:503:THR:HG21	1:E:708:HIS:HB3	1.96	0.47
1:G:407:GLU:OE2	2:H:601:LEU:N	2.48	0.47
1:G:1013:CYS:HB3	1:G:1068:PHE:HE1	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:480:LEU:HD11	2:H:539:PHE:CE1	2.49	0.47
1:C:406:GLU:CD	2:D:606:ARG:HH12	2.16	0.47
2:D:411:ARG:NH1	2:D:450:LEU:O	2.43	0.47
1:G:579:ARG:HH21	1:G:606:LYS:HE2	1.80	0.47
1:A:366:ARG:HH22	2:B:646:CYS:HB3	1.79	0.47
2:B:285:PRO:HD3	2:B:527:THR:HG23	1.97	0.47
2:F:285:PRO:HD3	2:F:527:THR:HG23	1.97	0.47
2:H:168:VAL:HG22	2:H:506:ALA:HB2	1.97	0.47
2:B:32:GLN:HB3	2:B:497:THR:HG21	1.96	0.47
1:G:505:ARG:HD3	1:G:708:HIS:O	2.14	0.47
1:A:384:GLU:OE1	1:A:398:ARG:NH2	2.48	0.46
2:D:49:LYS:O	2:D:52:ILE:HB	2.14	0.46
1:A:503:THR:HB	1:A:709:TYR:CE1	2.51	0.46
2:D:168:VAL:HG22	2:D:506:ALA:HB2	1.96	0.46
1:A:281:LEU:HA	1:A:290:PHE:CE2	2.50	0.46
1:C:369:ASP:CG	2:D:600:LEU:HB3	2.41	0.46
1:A:407:GLU:OE2	2:B:675:ARG:NH2	2.49	0.46
1:G:405:THR:OG1	1:G:407:GLU:O	2.33	0.46
1:G:64:HIS:HD2	1:G:350:PHE:CD2	2.33	0.46
1:G:151:GLN:OE1	1:G:722:ARG:NH2	2.49	0.46
1:A:515:SER:OG	2:B:602:SER:HB3	2.16	0.46
2:D:691:LEU:HD13	2:D:704:VAL:HG21	1.97	0.46
2:B:218:SER:OG	2:B:221:VAL:HG23	2.15	0.46
1:C:690:ARG:HH11	1:C:690:ARG:HB2	1.81	0.46
2:F:108:LEU:HB3	2:F:112:TYR:HB2	1.96	0.46
2:B:619:LEU:HG	2:B:651:VAL:HG22	1.98	0.46
1:C:97:LEU:HD21	1:C:140:ARG:HE	1.80	0.46
1:E:505:ARG:HD3	1:E:708:HIS:O	2.16	0.46
1:G:992:LEU:HB3	1:G:997:THR:OG1	2.16	0.46
1:C:483:HIS:CD2	1:C:510:LYS:HG2	2.51	0.45
1:C:505:ARG:NH1	1:C:711:GLN:H	2.14	0.45
1:C:505:ARG:NH1	1:C:710:GLN:HG2	2.18	0.45
2:H:91:PRO:HD2	2:H:94:LEU:HD12	1.98	0.45
2:H:155:VAL:HB	2:H:287:ILE:HG12	1.99	0.45
2:B:691:LEU:HD13	2:B:704:VAL:HG21	1.99	0.45
2:H:619:LEU:HG	2:H:651:VAL:HG22	1.97	0.45
2:H:691:LEU:HD13	2:H:704:VAL:HG21	1.99	0.45
2:D:505:LEU:HD22	2:D:522:ILE:HD12	1.96	0.45
2:F:186:GLU:HA	2:F:189:MET:HE3	1.98	0.45
2:F:441:THR:HG21	2:F:715:PRO:O	2.17	0.45
2:F:619:LEU:HD21	2:F:679:ILE:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:36:ARG:HD3	2:H:490:TRP:CZ2	2.51	0.45
2:H:61:LEU:HB3	2:H:101:PHE:CZ	2.51	0.45
2:B:91:PRO:HB2	2:B:93:ASP:OD1	2.16	0.45
2:F:23:THR:O	2:F:25:ASN:N	2.46	0.45
2:B:7:GLU:OE1	2:B:52:ILE:HG23	2.16	0.45
2:B:108:LEU:HD13	2:B:112:TYR:CB	2.46	0.45
1:E:64:HIS:HD2	1:E:350:PHE:CD2	2.35	0.45
2:F:619:LEU:HG	2:F:651:VAL:HG22	1.99	0.45
1:C:359:ARG:NH1	2:D:108:LEU:HA	2.32	0.45
1:E:191:ARG:HD2	1:E:196:TYR:CG	2.51	0.45
1:E:814:GLU:OE1	1:E:827:THR:OG1	2.27	0.45
2:F:480:LEU:HD11	2:F:539:PHE:CE1	2.51	0.45
1:G:333:THR:HG21	1:G:528:ALA:HB1	1.98	0.45
2:D:95:TYR:HB3	2:D:127:THR:OG1	2.17	0.45
1:E:669:PHE:CE1	1:E:1036:MET:HG3	2.52	0.45
2:F:36:ARG:HD3	2:F:490:TRP:CZ2	2.52	0.45
1:G:281:LEU:HA	1:G:290:PHE:CE2	2.52	0.45
2:B:619:LEU:HD21	2:B:679:ILE:HG21	1.99	0.45
1:C:653:ASP:OD1	1:C:684:ARG:NH2	2.50	0.45
1:E:1021:ARG:NH2	1:E:1059:LYS:O	2.49	0.45
2:F:691:LEU:HD13	2:F:704:VAL:HG21	1.99	0.45
1:G:369:ASP:HB2	1:G:406:GLU:O	2.16	0.45
1:G:379:LEU:HD13	1:G:435:CYS:SG	2.57	0.45
1:G:413:TRP:HE1	2:H:756:GLN:HB3	1.81	0.45
1:A:110:TYR:CZ	1:A:178:ARG:HG3	2.52	0.45
2:B:163:LEU:HD22	2:B:424:ARG:CZ	2.47	0.45
2:B:186:GLU:HA	2:B:189:MET:HE3	1.98	0.45
1:C:359:ARG:O	1:C:419:LYS:HA	2.17	0.45
1:E:410:TRP:HB3	1:E:412:VAL:HG22	1.99	0.45
1:A:558:ILE:O	1:A:591:LYS:NZ	2.43	0.45
2:F:70:ARG:HB3	2:F:112:TYR:OH	2.17	0.45
1:G:191:ARG:HD2	1:G:196:TYR:CG	2.52	0.45
2:B:545:LYS:HG2	2:B:556:GLU:HG2	1.99	0.44
2:D:7:GLU:OE1	2:D:52:ILE:HG23	2.17	0.44
2:F:108:LEU:HD13	2:F:112:TYR:CB	2.48	0.44
2:H:7:GLU:OE1	2:H:52:ILE:HG23	2.16	0.44
1:A:505:ARG:NH1	1:A:711:GLN:H	2.15	0.44
2:B:36:ARG:HD3	2:B:490:TRP:CZ2	2.53	0.44
1:C:333:THR:HG21	1:C:528:ALA:HB1	1.99	0.44
1:C:384:GLU:OE1	1:C:398:ARG:NH2	2.51	0.44
2:D:545:LYS:HG2	2:D:556:GLU:HG2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:576:TRP:CZ2	1:E:603:ILE:HG23	2.53	0.44
1:G:345:ASP:CG	2:H:124:LYS:NZ	2.73	0.44
1:G:503:THR:HB	1:G:709:TYR:CE1	2.52	0.44
2:B:201:LEU:HB2	2:B:205:CYS:HB2	1.99	0.44
1:C:576:TRP:CZ2	1:C:603:ILE:HG23	2.53	0.44
2:D:492:GLU:O	2:D:497:THR:HG23	2.16	0.44
1:G:483:HIS:CD2	1:G:510:LYS:HG2	2.52	0.44
2:B:441:THR:HG21	2:B:715:PRO:O	2.16	0.44
2:F:7:GLU:OE1	2:F:52:ILE:HG23	2.17	0.44
2:F:86:LYS:HE2	2:F:282:LEU:HD23	1.99	0.44
1:G:387:ILE:HD12	1:G:468:LEU:HD11	2.00	0.44
1:A:410:TRP:HB3	1:A:412:VAL:HG22	1.99	0.44
1:A:483:HIS:CD2	1:A:510:LYS:HG2	2.53	0.44
2:B:480:LEU:HD11	2:B:539:PHE:CE1	2.53	0.44
1:E:669:PHE:HE1	1:E:1036:MET:HG3	1.83	0.44
2:F:108:LEU:CD2	2:F:109:PRO:HD2	2.45	0.44
2:H:186:GLU:HA	2:H:189:MET:HE3	2.00	0.44
1:A:1013:CYS:HB3	1:A:1068:PHE:CE1	2.53	0.44
2:B:95:TYR:HB3	2:B:127:THR:OG1	2.18	0.44
2:B:168:VAL:HG22	2:B:506:ALA:HB2	1.99	0.44
2:B:255:TYR:CZ	2:B:259:LEU:HD12	2.53	0.44
1:C:108:GLU:HB2	1:C:324:PRO:HB2	1.99	0.44
1:C:370:ILE:HD12	1:C:514:MET:HE2	2.00	0.44
1:C:583:LEU:HD11	1:C:610:LEU:HB3	1.99	0.44
2:D:92:GLU:HG2	2:D:96:HIS:CD2	2.53	0.44
2:D:285:PRO:HD3	2:D:527:THR:HG23	2.00	0.44
1:A:366:ARG:HH22	2:B:646:CYS:CB	2.30	0.44
2:D:32:GLN:HB3	2:D:497:THR:HG21	1.99	0.44
2:H:49:LYS:O	2:H:52:ILE:HB	2.18	0.44
2:H:307:ARG:HA	2:H:308:PRO:HD3	1.71	0.44
2:D:20:GLU:OE2	2:D:33:GLY:N	2.48	0.43
1:E:656:VAL:HG21	1:E:684:ARG:HH21	1.82	0.43
2:F:255:TYR:CZ	2:F:259:LEU:HD12	2.53	0.43
1:A:371:PRO:HG3	2:B:604:ARG:HD3	2.00	0.43
1:A:653:ASP:OD1	1:A:684:ARG:NH2	2.51	0.43
2:D:619:LEU:HG	2:D:651:VAL:HG22	2.00	0.43
1:G:656:VAL:HG21	1:G:684:ARG:HH21	1.83	0.43
1:A:125:TRP:CE3	1:A:133:GLY:HA3	2.53	0.43
2:D:225:TYR:CE2	2:D:258:LEU:HD13	2.53	0.43
2:H:153:GLU:OE1	2:H:416:ARG:NH1	2.31	0.43
2:H:619:LEU:HD21	2:H:679:ILE:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:622:LEU:HD13	1:A:647:LYS:HG3	2.00	0.43
1:C:64:HIS:HD2	1:C:350:PHE:CD2	2.36	0.43
1:A:252:MET:HE2	1:A:259:MET:SD	2.58	0.43
1:A:407:GLU:CD	2:B:675:ARG:NH2	2.77	0.43
2:B:21:LEU:HD21	2:B:490:TRP:HE3	1.82	0.43
1:C:514:MET:C	2:D:604:ARG:HH22	2.27	0.43
2:D:86:LYS:HG2	2:D:282:LEU:HB2	2.01	0.43
2:D:655:GLU:OE1	2:D:672:ASN:ND2	2.52	0.43
1:G:252:MET:HE2	1:G:259:MET:SD	2.59	0.43
2:H:255:TYR:CZ	2:H:259:LEU:HD12	2.53	0.43
1:A:366:ARG:HH12	2:B:646:CYS:HB2	1.83	0.43
2:B:7:GLU:OE2	2:B:59:ARG:NH2	2.52	0.43
2:B:596:TYR:HB3	2:B:679:ILE:HG13	2.00	0.43
1:C:368:ILE:HG21	1:C:433:ILE:HD11	2.00	0.43
1:E:379:LEU:HD13	1:E:435:CYS:SG	2.59	0.43
1:E:503:THR:HB	1:E:709:TYR:CE1	2.53	0.43
2:F:201:LEU:HB2	2:F:205:CYS:HB2	1.99	0.43
2:F:545:LYS:HG2	2:F:556:GLU:HG2	1.99	0.43
1:A:369:ASP:O	2:B:604:ARG:NH1	2.50	0.43
1:A:812:TRP:CE2	1:A:881:ILE:HD13	2.53	0.43
2:B:91:PRO:HD2	2:B:94:LEU:HD12	2.00	0.43
1:E:333:THR:HG21	1:E:528:ALA:HB1	2.00	0.43
1:A:345:ASP:CG	2:B:124:LYS:HZ1	2.26	0.43
1:G:433:ILE:HG13	1:G:484:MET:HE1	2.01	0.43
1:G:812:TRP:CE2	1:G:881:ILE:HD13	2.54	0.43
2:H:108:LEU:O	2:H:113:SER:HB3	2.19	0.43
1:C:281:LEU:HA	1:C:290:PHE:CE2	2.53	0.43
1:G:428:LEU:HD23	1:G:467:LEU:HA	2.01	0.43
1:A:367:GLY:CA	2:B:601:LEU:HD13	2.49	0.42
1:E:174:GLU:O	1:E:178:ARG:HG2	2.19	0.42
2:H:23:THR:O	2:H:25:ASN:N	2.49	0.42
2:H:108:LEU:HD13	2:H:112:TYR:CB	2.49	0.42
2:B:49:LYS:O	2:B:52:ILE:HB	2.18	0.42
2:D:23:THR:O	2:D:25:ASN:N	2.47	0.42
2:D:225:TYR:CE1	2:D:258:LEU:HB2	2.54	0.42
1:E:205:LYS:O	1:E:294:ARG:NH2	2.37	0.42
2:H:92:GLU:HG2	2:H:96:HIS:CD2	2.54	0.42
1:A:41:GLU:O	1:A:134:GLN:HA	2.19	0.42
1:A:855:TRP:CE3	1:A:862:LEU:HD12	2.54	0.42
1:C:407:GLU:HB2	2:D:600:LEU:HD22	2.01	0.42
1:C:656:VAL:HG21	1:C:684:ARG:HH21	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:384:GLU:OE1	1:E:398:ARG:NH2	2.52	0.42
1:E:471:HIS:HA	1:E:672:TYR:CE1	2.54	0.42
1:G:434:TYR:CE2	1:G:460:LEU:HB2	2.55	0.42
2:H:32:GLN:HB3	2:H:497:THR:HG21	2.01	0.42
2:H:49:LYS:HD2	2:H:52:ILE:HD12	1.99	0.42
1:A:1002:THR:HG23	1:A:1006:PHE:HD2	1.83	0.42
2:F:91:PRO:HB2	2:F:93:ASP:OD1	2.18	0.42
2:B:86:LYS:HE2	2:B:282:LEU:HD23	2.00	0.42
2:B:421:GLY:O	2:B:458:PRO:HA	2.20	0.42
2:F:95:TYR:HB3	2:F:127:THR:OG1	2.19	0.42
2:B:129:VAL:HG13	2:B:247:HIS:CD2	2.55	0.42
1:C:579:ARG:HH21	1:C:606:LYS:HE2	1.84	0.42
1:C:671:PRO:HB2	1:C:672:TYR:CD2	2.55	0.42
1:C:855:TRP:CE3	1:C:862:LEU:HD12	2.54	0.42
2:D:421:GLY:O	2:D:458:PRO:HA	2.20	0.42
1:E:371:PRO:HG3	2:F:604:ARG:NH1	2.33	0.42
2:H:21:LEU:HD21	2:H:490:TRP:HE3	1.84	0.42
1:A:359:ARG:NH1	2:B:108:LEU:HG	2.35	0.42
1:C:434:TYR:CE2	1:C:460:LEU:HB2	2.55	0.42
1:G:855:TRP:CE3	1:G:862:LEU:HD12	2.55	0.42
2:H:685:ASP:C	2:H:687:ARG:H	2.28	0.42
1:A:433:ILE:HG13	1:A:484:MET:HE1	2.01	0.42
1:E:1013:CYS:HB3	1:E:1068:PHE:CE1	2.55	0.42
2:H:108:LEU:HB3	2:H:112:TYR:HB2	2.01	0.42
2:H:538:TYR:CE2	2:H:747:PRO:HB3	2.54	0.42
1:A:64:HIS:HD2	1:A:350:PHE:CD2	2.37	0.42
1:A:333:THR:HG21	1:A:528:ALA:HB1	2.01	0.42
1:C:515:SER:OG	2:D:602:SER:CB	2.68	0.42
2:D:225:TYR:CZ	2:D:258:LEU:HD13	2.54	0.42
2:F:153:GLU:OE1	2:F:416:ARG:NH1	2.35	0.42
1:G:174:GLU:O	1:G:178:ARG:HG2	2.19	0.42
1:A:843:LEU:HD22	1:A:1039:MET:HE1	2.02	0.42
2:B:23:THR:O	2:B:25:ASN:N	2.47	0.42
1:C:407:GLU:OE2	2:D:600:LEU:HA	2.19	0.41
2:D:91:PRO:HB2	2:D:93:ASP:OD1	2.19	0.41
1:E:483:HIS:CD2	1:E:510:LYS:HG2	2.54	0.41
2:F:658:LYS:HE3	2:F:665:ARG:HD3	2.01	0.41
1:G:363:VAL:HG12	1:G:416:PHE:HE1	1.85	0.41
1:C:125:TRP:CE3	1:C:133:GLY:HA3	2.55	0.41
1:C:359:ARG:CZ	2:D:108:LEU:HA	2.51	0.41
1:E:370:ILE:HD12	1:E:514:MET:HE2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:405:THR:OG1	1:E:407:GLU:O	2.38	0.41
2:F:21:LEU:HD21	2:F:490:TRP:HE3	1.84	0.41
1:A:586:PRO:HA	1:A:589:TYR:CD1	2.56	0.41
1:A:767:LEU:HD22	1:A:803:VAL:HG23	2.02	0.41
2:F:557:ASP:CG	2:F:699:ARG:HH21	2.28	0.41
1:G:359:ARG:NH1	2:H:108:LEU:HG	2.35	0.41
1:A:576:TRP:CZ2	1:A:603:ILE:HG23	2.55	0.41
1:C:407:GLU:OE2	2:D:601:LEU:HG	2.20	0.41
1:C:558:ILE:O	1:C:591:LYS:NZ	2.45	0.41
1:E:855:TRP:CE3	1:E:862:LEU:HD12	2.56	0.41
2:H:95:TYR:HB3	2:H:127:THR:OG1	2.21	0.41
2:D:108:LEU:HB3	2:D:112:TYR:HB2	2.01	0.41
1:E:926:GLU:OE2	1:E:1008:LYS:NZ	2.53	0.41
2:F:92:GLU:HG2	2:F:96:HIS:CD2	2.55	0.41
1:C:431:LEU:HD13	1:C:516:ILE:HD13	2.01	0.41
1:C:843:LEU:HD22	1:C:1039:MET:HE1	2.02	0.41
2:D:163:LEU:HD22	2:D:424:ARG:CZ	2.51	0.41
2:D:596:TYR:HB3	2:D:679:ILE:HG13	2.02	0.41
1:A:376:THR:HB	1:A:379:LEU:CD1	2.47	0.41
1:C:376:THR:HB	1:C:379:LEU:CD1	2.47	0.41
1:C:767:LEU:HD22	1:C:803:VAL:HG23	2.02	0.41
2:D:190:ARG:HG3	2:D:214:LEU:HB3	2.02	0.41
2:F:61:LEU:HB3	2:F:101:PHE:CZ	2.56	0.41
1:G:696:PHE:CD1	1:G:717:LEU:HD11	2.56	0.41
1:A:369:ASP:HB3	1:A:407:GLU:HG3	2.03	0.41
2:B:92:GLU:HG2	2:B:96:HIS:CD2	2.55	0.41
2:B:476:GLU:O	2:B:695:LYS:NZ	2.32	0.41
1:E:622:LEU:HD13	1:E:647:LYS:HG3	2.03	0.41
1:A:345:ASP:CG	2:B:124:LYS:NZ	2.79	0.41
1:A:362:ARG:NH1	2:B:70:ARG:HH12	2.19	0.41
1:A:671:PRO:HB2	1:A:672:TYR:CD2	2.56	0.41
1:C:363:VAL:HG12	1:C:416:PHE:HE1	1.86	0.41
1:E:464:VAL:HG12	1:E:484:MET:HE3	2.03	0.41
1:E:521:ASP:HB3	2:F:109:PRO:HB3	2.01	0.41
1:G:641:ARG:HE	1:G:670:GLU:CD	2.28	0.41
2:H:18:LEU:HD21	2:H:76:LEU:HD11	2.03	0.41
2:H:86:LYS:HE2	2:H:282:LEU:HD23	2.03	0.41
1:A:407:GLU:CD	2:B:675:ARG:HH21	2.29	0.41
1:C:407:GLU:CD	2:D:675:ARG:NH2	2.79	0.41
2:D:86:LYS:HE2	2:D:282:LEU:HD23	2.02	0.41
2:H:545:LYS:HG2	2:H:556:GLU:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:49:LYS:HD2	2:B:52:ILE:HD12	2.03	0.40
1:C:812:TRP:CE2	1:C:881:ILE:HD13	2.56	0.40
1:E:178:ARG:HH12	1:E:323:TRP:HB3	1.87	0.40
1:G:949:ASN:OD1	1:G:949:ASN:N	2.53	0.40
2:H:86:LYS:HG2	2:H:282:LEU:HB2	2.03	0.40
2:H:91:PRO:HB2	2:H:93:ASP:OD1	2.20	0.40
1:C:669:PHE:CE1	1:C:1036:MET:HG3	2.56	0.40
1:C:775:GLN:OE1	1:C:796:LEU:N	2.51	0.40
2:D:492:GLU:HA	2:D:496:ASN:HB2	2.02	0.40
2:F:295:GLN:OE1	2:F:435:ARG:NH2	2.54	0.40
2:H:296:GLU:CD	2:H:439:ARG:HH22	2.29	0.40
1:A:434:TYR:CE2	1:A:460:LEU:HB2	2.56	0.40
2:D:155:VAL:HB	2:D:287:ILE:HG12	2.03	0.40
1:G:410:TRP:HB3	1:G:412:VAL:HG22	2.04	0.40
1:G:503:THR:HG21	1:G:708:HIS:HB3	2.02	0.40
1:G:690:ARG:HH11	1:G:690:ARG:HB2	1.87	0.40
2:D:61:LEU:HB3	2:D:101:PHE:CZ	2.57	0.40
1:G:178:ARG:HH12	1:G:323:TRP:HB3	1.87	0.40
2:H:433:TYR:OH	2:H:437:ARG:NH1	2.54	0.40
2:H:655:GLU:OE1	2:H:672:ASN:ND2	2.55	0.40
1:C:433:ILE:HG13	1:C:484:MET:HE1	2.03	0.40
1:E:550:GLN:NE2	1:G:52:LYS:HG3	2.37	0.40
2:F:685:ASP:C	2:F:687:ARG:H	2.29	0.40
2:H:658:LYS:HE3	2:H:665:ARG:HD3	2.02	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)
2:B:30:SER:OG	2:F:30:SER:OG[2_555]	2.16	0.04

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	983/1102 (89%)	967 (98%)	15 (2%)	1 (0%)	48	83
1	C	983/1102 (89%)	967 (98%)	15 (2%)	1 (0%)	48	83
1	E	983/1102 (89%)	967 (98%)	15 (2%)	1 (0%)	48	83
1	G	983/1102 (89%)	967 (98%)	15 (2%)	1 (0%)	48	83
2	B	540/756 (71%)	530 (98%)	10 (2%)	0	100	100
2	D	540/756 (71%)	530 (98%)	10 (2%)	0	100	100
2	F	540/756 (71%)	530 (98%)	10 (2%)	0	100	100
2	H	540/756 (71%)	530 (98%)	10 (2%)	0	100	100
All	All	6092/7432 (82%)	5988 (98%)	100 (2%)	4 (0%)	48	83

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	964	ASP
1	C	964	ASP
1	E	964	ASP
1	G	964	ASP

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	897/988 (91%)	893 (100%)	4 (0%)	84	84
1	C	897/988 (91%)	893 (100%)	4 (0%)	84	84
1	E	897/988 (91%)	893 (100%)	4 (0%)	84	84
1	G	897/988 (91%)	893 (100%)	4 (0%)	84	84
2	B	500/665 (75%)	497 (99%)	3 (1%)	78	83
2	D	500/665 (75%)	497 (99%)	3 (1%)	78	83
2	F	500/665 (75%)	497 (99%)	3 (1%)	78	83
2	H	500/665 (75%)	497 (99%)	3 (1%)	78	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	5588/6612 (84%)	5560 (100%)	28 (0%)	81	83

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	207	LEU
1	A	306	VAL
1	A	487	LEU
1	A	690	ARG
2	B	3	SER
2	B	445	CYS
2	B	505	LEU
1	C	207	LEU
1	C	306	VAL
1	C	487	LEU
1	C	690	ARG
2	D	3	SER
2	D	445	CYS
2	D	505	LEU
1	E	207	LEU
1	E	306	VAL
1	E	487	LEU
1	E	690	ARG
2	F	3	SER
2	F	445	CYS
2	F	505	LEU
1	G	207	LEU
1	G	306	VAL
1	G	487	LEU
1	G	690	ARG
2	H	3	SER
2	H	445	CYS
2	H	505	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
1	A	95	HIS
1	A	117	GLN
1	A	386	ASN

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Mol	Chain	Res	Type
1	A	391	GLN
1	A	483	HIS
1	A	734	GLN
1	A	735	GLN
1	A	1010	GLN
2	B	142	GLN
2	B	453	GLN
2	B	603	HIS
2	B	680	GLN
2	B	684	GLN
1	C	60	HIS
1	C	89	HIS
1	C	95	HIS
1	C	117	GLN
1	C	199	HIS
1	C	391	GLN
1	C	512	ASN
1	C	734	GLN
1	C	1010	GLN
2	D	142	GLN
2	D	198	GLN
1	E	60	HIS
1	E	95	HIS
1	E	117	GLN
1	E	386	ASN
1	E	391	GLN
1	E	609	GLN
1	E	734	GLN
1	E	735	GLN
1	E	1010	GLN
2	F	183	GLN
2	F	650	HIS
1	G	60	HIS
1	G	95	HIS
1	G	117	GLN
1	G	386	ASN
1	G	391	GLN
1	G	734	GLN
1	G	735	GLN
1	G	1010	GLN
2	H	142	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	995/1102 (90%)	-0.32	8 (0%) 82 72	423, 476, 613, 741	0
1	C	995/1102 (90%)	-0.32	11 (1%) 78 67	427, 490, 635, 774	0
1	E	995/1102 (90%)	-0.42	4 (0%) 88 79	428, 571, 734, 866	0
1	G	995/1102 (90%)	-0.42	3 (0%) 90 82	486, 605, 754, 914	0
2	B	558/756 (73%)	-0.35	4 (0%) 84 74	452, 516, 654, 749	0
2	D	558/756 (73%)	-0.34	4 (0%) 84 74	413, 539, 657, 794	0
2	F	558/756 (73%)	-0.39	4 (0%) 84 74	423, 544, 662, 780	0
2	H	558/756 (73%)	-0.40	1 (0%) 91 84	424, 521, 659, 828	0
All	All	6212/7432 (83%)	-0.37	39 (0%) 85 76	413, 532, 702, 914	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1027	LEU	4.0
1	G	581	GLU	3.7
1	C	598	TRP	3.4
1	A	1072	ILE	3.2
2	D	172	LEU	3.2
1	A	593	PHE	3.1
1	A	987	LEU	3.1
2	B	480	LEU	3.1
1	A	598	TRP	3.0
2	B	560	LEU	2.9
1	E	343	GLY	2.7
2	F	487	VAL	2.6
1	A	766	GLN	2.6
2	D	182	GLN	2.6
1	G	551	LEU	2.5
1	C	1072	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	G	583	LEU	2.5
2	F	172	LEU	2.5
1	A	248	PHE	2.4
1	C	247	SER	2.4
1	C	405	THR	2.4
1	A	346	HIS	2.4
1	A	1027	LEU	2.4
1	E	461	LEU	2.4
2	F	188	CYS	2.4
2	D	742	ASN	2.3
2	B	429	LEU	2.3
2	H	188	CYS	2.3
1	C	346	HIS	2.3
1	E	1011	ASP	2.3
2	F	483	PHE	2.2
1	C	293	VAL	2.2
1	C	593	PHE	2.2
1	C	987	LEU	2.2
1	C	791	LEU	2.2
1	E	991	PHE	2.2
2	B	483	PHE	2.1
1	C	949	ASN	2.1
2	D	522	ILE	2.1

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.