



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 11:58 pm GMT

PDB ID : 2RD0
Title : Structure of a human p110alpha/p85alpha complex
Authors : Huang, C.; Gabelli, S.B.; Amzel, L.M.
Deposited on : 2007-09-20
Resolution : 3.05 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

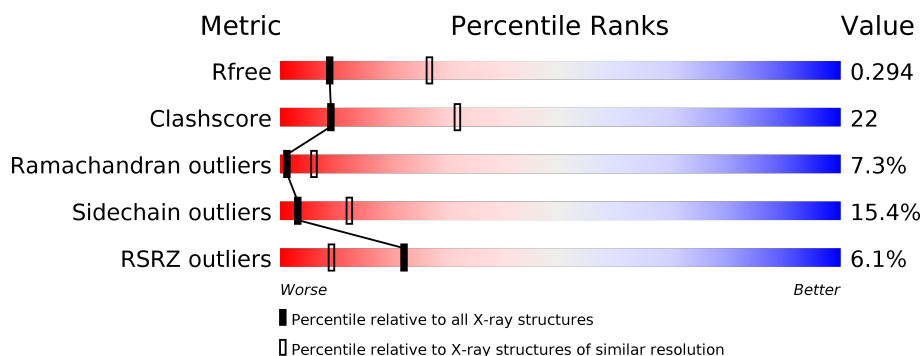
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.05 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}	100719	1348 (3.10-3.02)
Clashscore	112137	1462 (3.10-3.02)
Ramachandran outliers	110173	1410 (3.10-3.02)
Sidechain outliers	110143	1410 (3.10-3.02)
RSRZ outliers	101464	1355 (3.10-3.02)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	1096	
2	B	279	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9365 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 alpha isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	997	Total	C	N	O	S	0	0	0
			8154	5220	1396	1471	67			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-28	MET	-	EXPRESSION TAG	UNP P42336
A	-27	SER	-	EXPRESSION TAG	UNP P42336
A	-26	TYR	-	EXPRESSION TAG	UNP P42336
A	-25	TYR	-	EXPRESSION TAG	UNP P42336
A	-24	HIS	-	EXPRESSION TAG	UNP P42336
A	-23	HIS	-	EXPRESSION TAG	UNP P42336
A	-22	HIS	-	EXPRESSION TAG	UNP P42336
A	-21	HIS	-	EXPRESSION TAG	UNP P42336
A	-20	HIS	-	EXPRESSION TAG	UNP P42336
A	-19	HIS	-	EXPRESSION TAG	UNP P42336
A	-18	ASP	-	EXPRESSION TAG	UNP P42336
A	-17	TYR	-	EXPRESSION TAG	UNP P42336
A	-16	ASP	-	EXPRESSION TAG	UNP P42336
A	-15	ILE	-	EXPRESSION TAG	UNP P42336
A	-13	PRO	-	EXPRESSION TAG	UNP P42336
A	-12	THR	-	EXPRESSION TAG	UNP P42336
A	-11	THR	-	EXPRESSION TAG	UNP P42336
A	-10	GLU	-	EXPRESSION TAG	UNP P42336
A	-9	ASN	-	EXPRESSION TAG	UNP P42336
A	-8	LEU	-	EXPRESSION TAG	UNP P42336
A	-7	TYR	-	EXPRESSION TAG	UNP P42336
A	-6	PHE	-	EXPRESSION TAG	UNP P42336
A	-5	GLN	-	EXPRESSION TAG	UNP P42336
A	-4	GLY	-	EXPRESSION TAG	UNP P42336
A	-3	ALA	-	EXPRESSION TAG	UNP P42336
A	-2	MET	-	EXPRESSION TAG	UNP P42336

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP P42336
A	0	SER	-	EXPRESSION TAG	UNP P42336

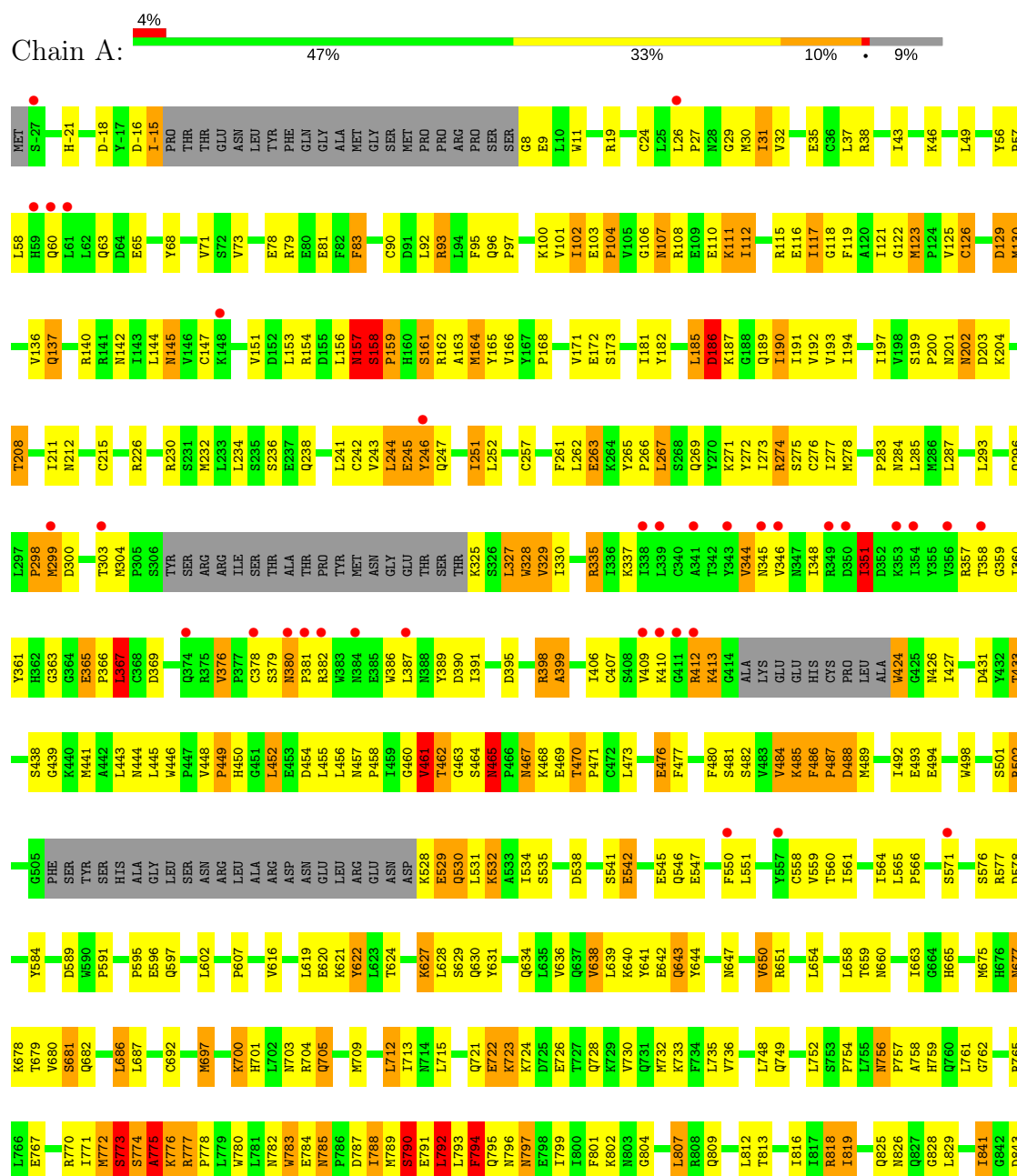
- Molecule 2 is a protein called Phosphatidylinositol 3-kinase regulatory subunit alpha.

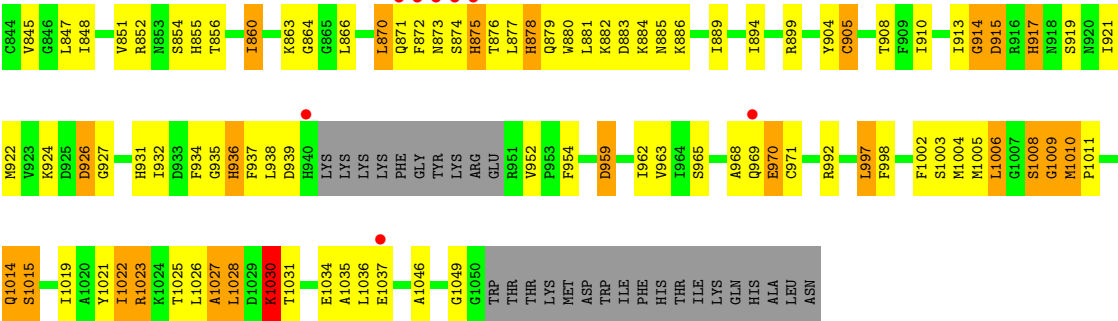
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	139	Total	C	N	O	S	0	0	0
			1211	757	218	231	5			

3 Residue-property plots

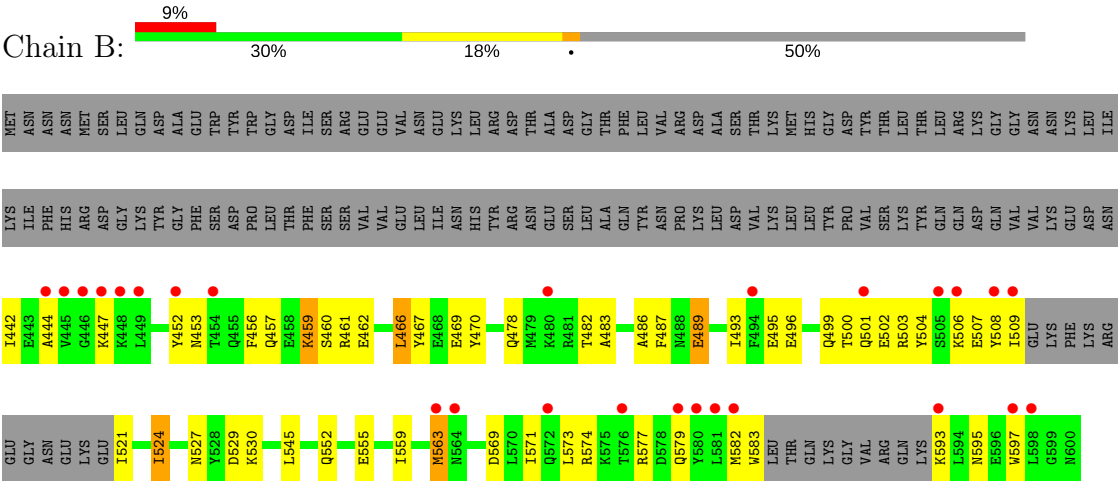
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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 alpha isoform





● Molecule 2: Phosphatidylinositol 3-kinase regulatory subunit alpha



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	115.06Å 117.05Å 151.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.37 – 3.05 46.39 – 3.07	Depositor EDS
% Data completeness (in resolution range)	98.0 (46.37-3.05) 98.0 (46.39-3.07)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.96 (at 3.06Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.263 , 0.323 0.254 , 0.294	Depositor DCC
R_{free} test set	1926 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	90.4	Xtriage
Anisotropy	0.382	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 90.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.011 for k,h,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	9365	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% 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	0.50	0/8339	0.72	2/11268 (0.0%)
2	B	0.37	0/1227	0.55	0/1635
All	All	0.49	0/9566	0.70	2/12903 (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	A	0	9
2	B	0	1
All	All	0	10

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	A	794	PHE	N-CA-C	6.97	129.82	111.00
1	A	465	ASN	N-CA-C	5.63	126.21	111.00

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	-18	ASP	Peptide
1	A	115	ARG	Peptide
1	A	185	LEU	Peptide
1	A	186	ASP	Peptide
1	A	452	LEU	Peptide
1	A	467	ASN	Peptide
1	A	773	SER	Peptide

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Mol	Chain	Res	Type	Group
1	A	775	ALA	Peptide
1	A	936	HIS	Peptide
2	B	524	ILE	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	8154	0	8154	397	0
2	B	1211	0	1205	27	0
All	All	9365	0	9359	417	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 22.

All (417) 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:398:ARG:HG3	1:A:398:ARG:HH11	1.04	1.12
1:A:992:ARG:HH12	1:A:1027:ALA:HB3	1.03	1.12
1:A:772:MET:CE	1:A:772:MET:HA	1.80	1.11
1:A:634:GLN:HB3	1:A:1004:MET:HE2	1.22	1.11
1:A:367:LEU:HD11	1:A:389:TYR:HB3	1.33	1.10
1:A:470:THR:HB	1:A:471:PRO:HD2	1.37	1.04
1:A:776:LYS:O	1:A:778:PRO:HD3	1.56	1.03
1:A:299:MET:HG3	1:A:300:ASP:H	1.18	1.02
1:A:470:THR:HB	1:A:471:PRO:CD	1.86	1.02
1:A:913:ILE:HG22	1:A:914:GLY:H	1.27	1.00
1:A:748:LEU:O	1:A:783:TRP:HZ3	1.44	0.99
1:A:793:LEU:O	1:A:794:PHE:HB3	1.62	0.98
1:A:992:ARG:HH12	1:A:1027:ALA:CB	1.79	0.95
1:A:106:GLY:O	1:A:108:ARG:N	2.00	0.95
1:A:773:SER:OG	1:A:777:ARG:CZ	2.16	0.93
1:A:267:LEU:HD13	1:A:273:ILE:HG12	1.52	0.91
1:A:992:ARG:NH1	1:A:1027:ALA:HB3	1.85	0.90
1:A:860:ILE:HG21	1:A:877:LEU:HD23	1.52	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:772:MET:HE2	1:A:772:MET:HA	1.56	0.88
1:A:398:ARG:NH1	1:A:398:ARG:HG3	1.83	0.86
1:A:788:ILE:H	1:A:788:ILE:HD12	1.43	0.83
1:A:446:TRP:HE1	1:A:465:ASN:HD22	1.25	0.83
1:A:337:LYS:HB3	1:A:476:GLU:HB3	1.61	0.83
1:A:678:LYS:HA	1:A:681:SER:OG	1.80	0.82
1:A:164:MET:HE1	1:A:262:LEU:HB2	1.62	0.82
1:A:756:ASN:HD22	1:A:756:ASN:C	1.84	0.81
1:A:765:ARG:HG3	1:A:782:ASN:OD1	1.82	0.79
1:A:913:ILE:HG22	1:A:914:GLY:N	1.97	0.79
1:A:154:ARG:O	1:A:161:SER:HB3	1.83	0.79
1:A:771:ILE:C	1:A:773:SER:H	1.86	0.78
1:A:875:HIS:CE1	1:A:879:GLN:HG2	2.18	0.77
1:A:251:ILE:HD12	1:A:262:LEU:HD22	1.66	0.77
1:A:952:VAL:HG11	1:A:1046:ALA:HB2	1.67	0.77
1:A:502:ARG:NE	1:A:502:ARG:HA	1.98	0.76
1:A:532:LYS:HG2	1:A:561:ILE:HD13	1.65	0.76
1:A:709:MET:O	1:A:713:ILE:HG13	1.86	0.75
1:A:398:ARG:CG	1:A:398:ARG:HH11	1.93	0.75
1:A:799:ILE:HD11	1:A:847:LEU:HB3	1.69	0.75
1:A:446:TRP:HE1	1:A:465:ASN:ND2	1.86	0.73
1:A:299:MET:HG3	1:A:300:ASP:N	1.99	0.73
1:A:627:LYS:HB2	1:A:627:LYS:HZ3	1.52	0.73
1:A:748:LEU:O	1:A:783:TRP:CZ3	2.36	0.73
1:A:79:ARG:HH11	2:B:489:GLU:HG3	1.53	0.73
1:A:398:ARG:O	1:A:399:ALA:HB3	1.89	0.73
1:A:299:MET:CG	1:A:300:ASP:H	2.00	0.72
1:A:914:GLY:O	1:A:915:ASP:HB2	1.88	0.72
1:A:145:ASN:HD22	1:A:651:ARG:HH12	1.36	0.72
1:A:145:ASN:ND2	1:A:651:ARG:HH12	1.87	0.72
1:A:327:LEU:HD11	1:A:486:PHE:HB3	1.71	0.71
1:A:71:VAL:HG22	1:A:81:GLU:HA	1.72	0.71
1:A:756:ASN:ND2	1:A:758:ALA:H	1.88	0.71
1:A:328:TRP:CE3	1:A:486:PHE:CZ	2.79	0.71
1:A:171:VAL:HG13	1:A:172:GLU:O	1.89	0.71
1:A:939:ASP:HB3	1:A:1021:TYR:CE1	2.26	0.70
1:A:885:ASN:HB3	1:A:889:ILE:HG22	1.75	0.69
1:A:913:ILE:HG21	1:A:934:PHE:HB3	1.73	0.69
1:A:182:TYR:O	1:A:185:LEU:HB2	1.92	0.69
1:A:192:VAL:HG13	1:A:283:PRO:HB2	1.75	0.68
2:B:467:TYR:HD2	2:B:563:MET:SD	2.16	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:913:ILE:CG2	1:A:914:GLY:H	2.05	0.68
1:A:873:ASN:HD22	1:A:876:THR:HB	1.58	0.68
1:A:212:ASN:HB2	1:A:215:CYS:HB2	1.76	0.68
1:A:772:MET:HG2	1:A:780:TRP:HB2	1.76	0.68
1:A:29:GLY:HA3	2:B:501:GLN:HB3	1.76	0.67
1:A:164:MET:CE	1:A:262:LEU:HB2	2.25	0.67
1:A:772:MET:HE3	1:A:772:MET:HA	1.71	0.67
1:A:794:PHE:O	1:A:795:GLN:HB3	1.95	0.67
1:A:267:LEU:CD1	1:A:273:ILE:HG12	2.25	0.67
1:A:426:ASN:H	1:A:462:THR:HG22	1.59	0.66
1:A:937:PHE:CZ	1:A:1002:PHE:HE2	2.13	0.66
1:A:360:ILE:O	1:A:366:PRO:HD2	1.96	0.66
1:A:709:MET:HE1	1:A:847:LEU:HD21	1.78	0.66
1:A:752:LEU:O	1:A:754:PRO:HD3	1.96	0.66
1:A:296:GLN:O	1:A:298:PRO:HD3	1.95	0.65
1:A:303:THR:HG22	1:A:304:MET:H	1.61	0.65
1:A:284:ASN:ND2	1:A:793:LEU:HD22	2.11	0.65
2:B:462:GLU:O	2:B:466:LEU:HB2	1.97	0.65
1:A:705:GLN:HG2	1:A:754:PRO:HG3	1.79	0.65
1:A:445:LEU:HD11	1:A:473:LEU:HD23	1.78	0.65
2:B:499:GLN:HA	2:B:502:GLU:HG2	1.78	0.65
1:A:529:GLU:HG2	1:A:529:GLU:O	1.97	0.64
1:A:194:ILE:HD11	1:A:287:LEU:HD21	1.79	0.64
1:A:470:THR:CB	1:A:471:PRO:CD	2.72	0.64
1:A:57:PRO:O	1:A:58:LEU:HB2	1.98	0.63
1:A:773:SER:OG	1:A:777:ARG:NE	2.30	0.63
1:A:1023:ARG:HH12	1:A:1028:LEU:HD23	1.63	0.63
1:A:677:ASN:C	1:A:677:ASN:HD22	2.02	0.62
1:A:627:LYS:H	1:A:627:LYS:HZ3	1.45	0.62
1:A:791:GLU:O	1:A:792:LEU:C	2.37	0.62
1:A:1027:ALA:HB2	1:A:1035:ALA:HB1	1.81	0.62
1:A:357:ARG:HG2	1:A:456:LEU:HD13	1.80	0.62
1:A:103:GLU:HG3	1:A:104:PRO:HD2	1.82	0.62
1:A:163:ALA:O	1:A:166:VAL:O	2.17	0.62
1:A:426:ASN:N	1:A:462:THR:HG22	2.14	0.62
1:A:185:LEU:O	1:A:187:LYS:N	2.29	0.62
1:A:461:VAL:O	1:A:463:GLY:N	2.33	0.61
1:A:792:LEU:CD2	1:A:793:LEU:HG	2.30	0.61
1:A:770:ARG:HG3	1:A:772:MET:HE3	1.82	0.61
1:A:634:GLN:CB	1:A:1004:MET:HE2	2.13	0.61
1:A:642:GLU:O	1:A:644:TYR:N	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:732:MET:O	1:A:736:VAL:HG23	2.00	0.61
1:A:910:ILE:HA	1:A:1025:THR:HG21	1.81	0.61
1:A:194:ILE:HD11	1:A:287:LEU:CD2	2.30	0.61
1:A:730:VAL:O	1:A:733:LYS:HB2	2.01	0.61
1:A:630:GLN:HE21	1:A:819:ILE:HG13	1.66	0.61
1:A:771:ILE:C	1:A:773:SER:N	2.53	0.60
1:A:278:MET:HA	1:A:278:MET:HE2	1.82	0.60
2:B:447:LYS:HA	2:B:597:TRP:HZ2	1.66	0.60
1:A:776:LYS:O	1:A:778:PRO:CD	2.42	0.60
1:A:24:CYS:HB2	1:A:32:VAL:HG23	1.84	0.60
1:A:636:VAL:O	1:A:639:LEU:HB2	2.02	0.60
1:A:399:ALA:HA	1:A:643:GLN:HE22	1.66	0.60
1:A:728:GLN:NE2	1:A:773:SER:HB3	2.16	0.60
1:A:1027:ALA:HB2	1:A:1035:ALA:CB	2.32	0.59
1:A:125:VAL:O	1:A:125:VAL:HG12	2.01	0.59
1:A:502:ARG:HA	1:A:502:ARG:HE	1.65	0.59
1:A:756:ASN:C	1:A:756:ASN:ND2	2.56	0.59
1:A:785:ASN:C	1:A:785:ASN:HD22	2.06	0.59
1:A:398:ARG:O	1:A:399:ALA:CB	2.49	0.59
1:A:11:TRP:HB3	1:A:95:PHE:HA	1.85	0.59
1:A:682:GLN:O	1:A:686:LEU:HB2	2.04	0.58
1:A:634:GLN:HB3	1:A:1004:MET:CE	2.15	0.58
1:A:870:LEU:C	1:A:872:PHE:H	2.07	0.58
1:A:93:ARG:HD3	1:A:93:ARG:H	1.68	0.58
1:A:908:THR:HG21	1:A:954:PHE:CB	2.34	0.58
1:A:398:ARG:HD2	1:A:485:LYS:HD2	1.86	0.58
1:A:424:TRP:CZ2	1:A:462:THR:OG1	2.54	0.57
1:A:547:GLU:O	1:A:551:LEU:HG	2.03	0.57
1:A:855:HIS:HB2	1:A:860:ILE:HD12	1.86	0.57
1:A:550:PHE:HD2	1:A:551:LEU:HD23	1.69	0.57
1:A:874:SER:HB3	1:A:962:ILE:HD13	1.85	0.57
1:A:535:SER:OG	1:A:564:ILE:HG22	2.04	0.57
1:A:790:SER:O	1:A:792:LEU:O	2.21	0.57
1:A:756:ASN:HD22	1:A:758:ALA:H	1.51	0.57
1:A:269:GLN:HA	1:A:274:ARG:HH21	1.68	0.57
1:A:367:LEU:HD11	1:A:389:TYR:CB	2.23	0.57
1:A:194:ILE:HD12	1:A:252:LEU:HD21	1.85	0.57
1:A:96:GLN:HG3	1:A:97:PRO:HD2	1.87	0.57
1:A:284:ASN:HD22	1:A:793:LEU:HD13	1.69	0.57
1:A:721:GLN:O	1:A:722:GLU:C	2.44	0.57
1:A:778:PRO:HB3	1:A:802:LYS:HG3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:883:ASP:OD1	1:A:884:LYS:N	2.31	0.56
1:A:278:MET:HA	1:A:278:MET:CE	2.34	0.56
1:A:785:ASN:C	1:A:785:ASN:ND2	2.57	0.56
1:A:785:ASN:HD21	1:A:787:ASP:HB2	1.69	0.56
1:A:770:ARG:HG3	1:A:772:MET:CE	2.36	0.56
1:A:908:THR:HG21	1:A:954:PHE:HB2	1.86	0.56
1:A:190:ILE:HG12	1:A:191:ILE:N	2.19	0.56
1:A:735:LEU:HD22	1:A:771:ILE:HG13	1.87	0.56
1:A:789:MET:O	1:A:792:LEU:O	2.24	0.56
1:A:785:ASN:ND2	1:A:787:ASP:H	2.03	0.56
1:A:118:GLY:O	1:A:122:GLY:N	2.37	0.55
1:A:19:ARG:HD2	1:A:35:GLU:OE2	2.04	0.55
1:A:344:VAL:HG13	1:A:345:ASN:N	2.20	0.55
1:A:876:THR:HA	1:A:879:GLN:HB3	1.89	0.55
1:A:284:ASN:HD22	1:A:793:LEU:HD22	1.71	0.55
1:A:771:ILE:O	1:A:773:SER:N	2.40	0.55
1:A:773:SER:O	1:A:774:SER:OG	2.16	0.55
1:A:1014:GLN:O	1:A:1015:SER:HB3	2.07	0.55
1:A:263:GLU:HB3	1:A:265:TYR:CD1	2.40	0.55
1:A:344:VAL:HG13	1:A:345:ASN:H	1.70	0.55
2:B:457:GLN:HA	2:B:460:SER:HB3	1.89	0.55
1:A:529:GLU:O	1:A:531:LEU:N	2.40	0.55
1:A:640:LYS:HG2	1:A:680:VAL:HG11	1.87	0.55
1:A:32:VAL:HG21	1:A:49:LEU:HD11	1.88	0.55
1:A:773:SER:O	1:A:774:SER:CB	2.55	0.55
1:A:774:SER:O	1:A:775:ALA:CB	2.55	0.55
1:A:337:LYS:HD2	1:A:386:TRP:CE2	2.42	0.54
1:A:785:ASN:O	1:A:790:SER:HB2	2.07	0.54
1:A:335:ARG:HA	1:A:387:LEU:O	2.06	0.54
1:A:722:GLU:O	1:A:724:LYS:N	2.40	0.54
1:A:126:CYS:HA	1:A:129:ASP:HB2	1.89	0.54
1:A:793:LEU:O	1:A:794:PHE:CB	2.44	0.54
1:A:843:ASP:O	1:A:845:VAL:HG23	2.07	0.54
1:A:879:GLN:HA	1:A:882:LYS:HD2	1.89	0.54
1:A:460:GLY:C	1:A:462:THR:N	2.60	0.54
1:A:486:PHE:N	1:A:486:PHE:CD2	2.75	0.54
1:A:528:LYS:HB3	1:A:530:GLN:HG3	1.90	0.54
1:A:137:GLN:HE22	1:A:140:ARG:HH11	1.56	0.54
1:A:774:SER:O	1:A:775:ALA:HB2	2.07	0.54
1:A:11:TRP:CB	1:A:95:PHE:HA	2.38	0.54
1:A:83:PHE:CZ	1:A:112:ILE:HB	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:SER:CB	1:A:159:PRO:HD3	2.37	0.53
1:A:713:ILE:HG12	1:A:801:PHE:HZ	1.74	0.53
1:A:790:SER:OG	1:A:791:GLU:N	2.40	0.53
1:A:103:GLU:HG3	1:A:104:PRO:CD	2.37	0.53
1:A:854:SER:HB3	1:A:924:LYS:HG2	1.89	0.53
1:A:484:VAL:HG13	1:A:485:LYS:O	2.08	0.53
1:A:905:CYS:HA	1:A:954:PHE:HD2	1.73	0.53
1:A:1014:GLN:O	1:A:1015:SER:CB	2.56	0.53
2:B:555:GLU:O	2:B:559:ILE:HG12	2.09	0.53
1:A:462:THR:HG23	1:A:465:ASN:HD22	1.74	0.53
1:A:876:THR:HG22	1:A:880:TRP:HB2	1.90	0.52
1:A:57:PRO:HG2	2:B:524:ILE:HG23	1.90	0.52
2:B:467:TYR:O	2:B:470:TYR:HB3	2.09	0.52
1:A:701:HIS:HD2	1:A:704:ARG:HH21	1.57	0.52
1:A:705:GLN:O	1:A:709:MET:HG2	2.10	0.52
1:A:359:GLY:HA2	1:A:369:ASP:HB2	1.92	0.52
1:A:772:MET:O	1:A:773:SER:O	2.28	0.52
1:A:792:LEU:HD22	1:A:793:LEU:HG	1.91	0.52
1:A:765:ARG:NE	1:A:796:ASN:HD21	2.08	0.52
1:A:876:THR:HA	1:A:880:TRP:H	1.75	0.52
1:A:244:LEU:HA	1:A:247:GLN:HG3	1.90	0.52
1:A:722:GLU:O	1:A:723:LYS:C	2.49	0.51
1:A:856:THR:HG23	1:A:922:MET:CE	2.41	0.51
1:A:200:PRO:C	1:A:202:ASN:H	2.13	0.51
1:A:772:MET:O	1:A:773:SER:C	2.48	0.51
1:A:11:TRP:H	1:A:95:PHE:HA	1.76	0.51
1:A:701:HIS:CD2	1:A:704:ARG:NH2	2.79	0.50
1:A:189:GLN:HB2	1:A:211:ILE:O	2.12	0.50
1:A:376:VAL:HG21	1:A:379:SER:HB2	1.93	0.50
1:A:462:THR:HG23	1:A:465:ASN:ND2	2.27	0.50
1:A:910:ILE:HA	1:A:1025:THR:CG2	2.41	0.50
2:B:467:TYR:CD2	2:B:563:MET:SD	3.01	0.50
1:A:172:GLU:HG2	1:A:271:LYS:HG2	1.94	0.50
2:B:453:ASN:O	2:B:456:PHE:HB3	2.12	0.50
1:A:532:LYS:N	1:A:532:LYS:HD2	2.26	0.50
1:A:-21:HIS:CD2	1:A:-21:HIS:N	2.80	0.49
1:A:462:THR:O	1:A:465:ASN:CG	2.50	0.49
1:A:640:LYS:HE2	1:A:680:VAL:HG11	1.94	0.49
1:A:917:HIS:O	1:A:921:ILE:HD12	2.12	0.49
1:A:26:LEU:HB3	1:A:27:PRO:HD2	1.93	0.49
1:A:327:LEU:CD1	1:A:486:PHE:HB3	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:771:ILE:HG22	1:A:773:SER:HB2	1.94	0.49
1:A:791:GLU:HA	1:A:791:GLU:OE1	2.11	0.49
1:A:199:SER:HB2	1:A:200:PRO:HA	1.93	0.49
1:A:538:ASP:O	1:A:541:SER:HB2	2.12	0.49
1:A:412:ARG:HD3	1:A:413:LYS:HG2	1.94	0.49
1:A:826:ASN:C	1:A:828:GLY:H	2.15	0.49
1:A:136:VAL:HG13	1:A:686:LEU:HD21	1.95	0.49
1:A:938:LEU:HD21	1:A:1022:ILE:HG22	1.95	0.49
2:B:506:LYS:HA	2:B:509:ILE:HG22	1.95	0.49
1:A:63:GLN:HB2	1:A:68:TYR:CE2	2.47	0.49
1:A:728:GLN:HE21	1:A:773:SER:HB3	1.77	0.49
1:A:873:ASN:O	1:A:877:LEU:N	2.46	0.49
1:A:1008:SER:O	1:A:1009:GLY:C	2.51	0.48
1:A:57:PRO:HB2	2:B:524:ILE:HD12	1.94	0.48
1:A:565:LEU:N	1:A:566:PRO:HD2	2.28	0.48
1:A:-15:ILE:HG23	1:A:187:LYS:HG3	1.95	0.48
1:A:455:LEU:HB3	1:A:457:ASN:H	1.77	0.48
2:B:496:GLU:O	2:B:500:THR:OG1	2.31	0.48
1:A:771:ILE:HG21	1:A:777:ARG:HH21	1.79	0.48
1:A:450:HIS:HD2	1:A:1014:GLN:HE22	1.61	0.48
1:A:263:GLU:HB3	1:A:265:TYR:CE1	2.49	0.48
1:A:123:MET:HE1	1:A:675:MET:HE1	1.96	0.48
2:B:456:PHE:HA	2:B:459:LYS:HE2	1.96	0.48
1:A:257:CYS:HB3	1:A:794:PHE:HZ	1.79	0.47
1:A:616:VAL:O	1:A:620:GLU:HG3	2.12	0.47
1:A:1026:LEU:O	1:A:1027:ALA:HB3	2.14	0.47
1:A:558:CYS:C	1:A:560:THR:H	2.16	0.47
1:A:238:GLN:HA	1:A:238:GLN:OE1	2.14	0.47
1:A:327:LEU:HD23	1:A:328:TRP:CD1	2.49	0.47
1:A:142:ASN:O	1:A:145:ASN:ND2	2.47	0.47
1:A:470:THR:CB	1:A:471:PRO:HD2	2.26	0.47
1:A:531:LEU:O	1:A:534:ILE:HG12	2.15	0.47
1:A:201:ASN:O	1:A:203:ASP:N	2.48	0.47
1:A:621:LYS:HE3	1:A:622:TYR:CE2	2.49	0.47
1:A:158:SER:HB2	1:A:159:PRO:HD3	1.96	0.47
1:A:328:TRP:CD1	1:A:328:TRP:C	2.88	0.47
1:A:438:SER:HA	1:A:477:PHE:HB2	1.97	0.47
1:A:700:LYS:HD2	1:A:700:LYS:HA	1.47	0.47
1:A:462:THR:O	1:A:465:ASN:ND2	2.47	0.47
1:A:788:ILE:H	1:A:788:ILE:CD1	2.13	0.47
1:A:701:HIS:CD2	1:A:704:ARG:HH21	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:CYS:O	1:A:244:LEU:N	2.46	0.46
1:A:123:MET:CE	1:A:675:MET:CE	2.93	0.46
1:A:848:ILE:N	1:A:848:ILE:HD12	2.30	0.46
2:B:487:PHE:HE2	2:B:545:LEU:HD22	1.80	0.46
1:A:-21:HIS:CD2	1:A:926:ASP:OD2	2.68	0.46
1:A:665:HIS:CE1	1:A:754:PRO:HA	2.49	0.46
1:A:791:GLU:O	1:A:793:LEU:N	2.48	0.46
1:A:361:TYR:HA	1:A:366:PRO:HD2	1.98	0.46
1:A:410:LYS:HB3	1:A:413:LYS:O	2.15	0.46
1:A:558:CYS:C	1:A:560:THR:N	2.68	0.46
1:A:119:PHE:HD2	1:A:703:ASN:OD1	1.99	0.46
1:A:870:LEU:C	1:A:872:PHE:N	2.69	0.46
1:A:640:LYS:HG2	1:A:680:VAL:CG1	2.45	0.46
1:A:266:PRO:HD2	1:A:269:GLN:NE2	2.30	0.46
1:A:701:HIS:HD2	1:A:704:ARG:NH2	2.14	0.46
1:A:794:PHE:CD1	1:A:794:PHE:C	2.86	0.46
1:A:904:TYR:CD2	1:A:931:HIS:CD2	3.03	0.46
1:A:756:ASN:HD22	1:A:757:PRO:N	2.13	0.46
1:A:351:ILE:HB	1:A:410:LYS:HD3	1.97	0.46
1:A:367:LEU:HB2	1:A:391:ILE:HG23	1.97	0.46
1:A:864:GLY:O	1:A:873:ASN:ND2	2.42	0.46
1:A:439:GLY:O	1:A:476:GLU:HA	2.16	0.46
1:A:818:ARG:HB2	1:A:818:ARG:HE	1.38	0.46
1:A:117:ILE:HG12	1:A:692:CYS:HB3	1.97	0.45
1:A:461:VAL:C	1:A:463:GLY:N	2.69	0.45
1:A:812:LEU:HD23	1:A:937:PHE:CZ	2.51	0.45
1:A:351:ILE:HD13	1:A:413:LYS:O	2.16	0.45
1:A:856:THR:HG23	1:A:922:MET:HE2	1.98	0.45
1:A:199:SER:HA	1:A:202:ASN:N	2.32	0.45
1:A:337:LYS:HD2	1:A:386:TRP:NE1	2.31	0.45
1:A:642:GLU:HG2	1:A:647:ASN:CG	2.37	0.45
2:B:571:ILE:O	2:B:574:ARG:HB2	2.17	0.45
1:A:-21:HIS:H	1:A:-21:HIS:CD2	2.35	0.45
1:A:872:PHE:HB2	1:A:874:SER:OG	2.16	0.45
1:A:913:ILE:CG2	1:A:914:GLY:N	2.68	0.45
1:A:992:ARG:NH1	1:A:1026:LEU:O	2.50	0.45
1:A:1030:LYS:HB3	1:A:1034:GLU:HB3	1.99	0.45
1:A:1027:ALA:CB	1:A:1035:ALA:HB2	2.47	0.45
1:A:761:LEU:HD22	1:A:783:TRP:CD1	2.52	0.45
1:A:32:VAL:CG2	1:A:49:LEU:HD11	2.46	0.44
1:A:181:ILE:HG12	1:A:278:MET:SD	2.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:GLU:O	1:A:246:TYR:HB3	2.18	0.44
1:A:529:GLU:O	1:A:529:GLU:CG	2.65	0.44
1:A:602:LEU:HB3	1:A:638:VAL:HG11	1.99	0.44
1:A:721:GLN:O	1:A:723:LYS:N	2.51	0.44
1:A:57:PRO:CB	2:B:524:ILE:HD12	2.47	0.44
1:A:878:HIS:O	1:A:882:LYS:N	2.49	0.44
1:A:147:CYS:O	1:A:151:VAL:HG23	2.17	0.44
1:A:328:TRP:CE3	1:A:486:PHE:HZ	2.29	0.44
1:A:665:HIS:HE1	1:A:705:GLN:OE1	2.01	0.44
1:A:765:ARG:NE	1:A:784:GLU:HG2	2.32	0.44
1:A:11:TRP:HB3	1:A:95:PHE:O	2.18	0.44
1:A:467:ASN:O	1:A:468:LYS:HD3	2.18	0.44
1:A:712:LEU:HD12	1:A:712:LEU:HA	1.74	0.44
2:B:487:PHE:CE2	2:B:545:LEU:HD22	2.53	0.44
1:A:137:GLN:NE2	1:A:140:ARG:HH11	2.15	0.44
1:A:261:PHE:CE1	1:A:285:LEU:HD22	2.52	0.44
1:A:628:LEU:HD23	1:A:663:ILE:HD13	2.00	0.44
1:A:792:LEU:HD23	1:A:793:LEU:HG	2.00	0.44
1:A:123:MET:HE1	1:A:675:MET:CE	2.48	0.44
1:A:709:MET:CE	1:A:841:ILE:HD13	2.48	0.44
1:A:765:ARG:O	1:A:767:GLU:N	2.51	0.44
2:B:483:ALA:O	2:B:486:ALA:HB3	2.18	0.44
1:A:108:ARG:HB3	1:A:111:LYS:HB2	2.00	0.44
1:A:677:ASN:C	1:A:677:ASN:ND2	2.68	0.44
1:A:959:ASP:OD1	1:A:959:ASP:N	2.51	0.43
1:A:100:LYS:HE2	2:B:493:ILE:HG23	1.99	0.43
1:A:877:LEU:O	1:A:878:HIS:HB2	2.17	0.43
1:A:71:VAL:HG21	1:A:102:ILE:HD11	1.99	0.43
1:A:73:VAL:HA	1:A:78:GLU:O	2.18	0.43
1:A:399:ALA:HA	1:A:643:GLN:NE2	2.32	0.43
1:A:439:GLY:H	1:A:477:PHE:HB2	1.84	0.43
1:A:272:TYR:CZ	1:A:276:CYS:SG	3.12	0.43
1:A:398:ARG:CG	1:A:398:ARG:NH1	2.61	0.43
1:A:190:ILE:CG1	1:A:191:ILE:N	2.81	0.43
1:A:446:TRP:HE1	1:A:465:ASN:HB2	1.83	0.43
1:A:492:ILE:O	1:A:494:GLU:N	2.52	0.43
1:A:162:ARG:O	1:A:165:TYR:N	2.52	0.43
2:B:506:LYS:C	2:B:508:TYR:H	2.21	0.43
1:A:1019:ILE:O	1:A:1022:ILE:HG23	2.19	0.42
1:A:449:PRO:HG2	1:A:452:LEU:HD12	2.01	0.42
1:A:998:PHE:O	1:A:1002:PHE:HD1	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:500:THR:O	2:B:504:TYR:HB2	2.19	0.42
1:A:328:TRP:HD1	1:A:329:VAL:N	2.16	0.42
1:A:881:LEU:HD21	1:A:927:GLY:HA2	2.00	0.42
1:A:1028:LEU:H	1:A:1028:LEU:HD12	1.85	0.42
1:A:263:GLU:HB3	1:A:265:TYR:HD1	1.84	0.42
1:A:621:LYS:HG3	1:A:622:TYR:CD2	2.54	0.42
1:A:759:HIS:HB3	1:A:797:ASN:HD21	1.84	0.42
1:A:358:THR:O	1:A:369:ASP:HB2	2.20	0.42
1:A:712:LEU:HB3	1:A:801:PHE:CZ	2.55	0.42
1:A:266:PRO:HD2	1:A:269:GLN:HE21	1.84	0.42
1:A:1010:MET:HA	1:A:1011:PRO:HD2	1.62	0.42
1:A:181:ILE:HG12	1:A:278:MET:CE	2.49	0.42
1:A:379:SER:O	1:A:380:ASN:C	2.56	0.42
1:A:1006:LEU:HD11	1:A:1015:SER:O	2.20	0.42
1:A:226:ARG:O	1:A:230:ARG:HG3	2.20	0.42
1:A:365:GLU:HG3	1:A:365:GLU:O	2.20	0.42
1:A:576:SER:C	1:A:578:ASP:H	2.23	0.42
1:A:749:GLN:O	1:A:762:GLY:O	2.38	0.42
1:A:855:HIS:HB2	1:A:860:ILE:CD1	2.48	0.42
1:A:-15:ILE:HD13	1:A:-15:ILE:HA	1.63	0.42
1:A:201:ASN:C	1:A:203:ASP:H	2.23	0.42
1:A:193:VAL:HG22	1:A:208:THR:HG23	2.01	0.42
1:A:487:PRO:C	1:A:489:MET:H	2.23	0.42
1:A:1003:SER:C	1:A:1005:MET:H	2.23	0.42
1:A:444:ASN:HB2	1:A:467:ASN:H	1.85	0.41
1:A:328:TRP:CZ3	1:A:577:ARG:HB2	2.55	0.41
1:A:165:TYR:HD1	1:A:659:THR:O	2.03	0.41
1:A:771:ILE:HG22	1:A:773:SER:H	1.85	0.41
1:A:789:MET:HG2	1:A:792:LEU:HD13	2.00	0.41
1:A:807:LEU:HD13	1:A:807:LEU:HA	1.91	0.41
1:A:894:ILE:HD12	1:A:963:VAL:O	2.20	0.41
1:A:406:ILE:HD11	1:A:473:LEU:HD21	2.03	0.41
1:A:56:TYR:HA	1:A:57:PRO:HD2	1.82	0.41
1:A:908:THR:HG21	1:A:954:PHE:HB3	2.02	0.41
1:A:380:ASN:HA	1:A:381:PRO:HD3	1.71	0.41
1:A:486:PHE:HA	1:A:487:PRO:HD2	1.77	0.41
1:A:992:ARG:HG3	1:A:992:ARG:HH11	1.86	0.41
1:A:173:SER:OG	1:A:627:LYS:HE3	2.21	0.41
1:A:728:GLN:NE2	1:A:773:SER:CB	2.83	0.41
1:A:26:LEU:HD23	1:A:101:VAL:HG21	2.02	0.41
1:A:299:MET:HB3	1:A:697:MET:HG2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:THR:HB	1:A:471:PRO:HD3	1.90	0.41
1:A:244:LEU:C	1:A:246:TYR:N	2.73	0.41
1:A:492:ILE:C	1:A:494:GLU:H	2.23	0.41
1:A:46:LYS:HE3	1:A:65:GLU:HG2	2.02	0.41
1:A:431:ASP:HB3	1:A:433:THR:H	1.85	0.41
1:A:427:ILE:HD11	1:A:443:LEU:HD13	2.02	0.41
1:A:446:TRP:CZ2	1:A:465:ASN:HB2	2.56	0.41
1:A:395:ASP:HA	1:A:577:ARG:HB3	2.03	0.41
1:A:468:LYS:HA	1:A:468:LYS:HD3	1.78	0.41
1:A:595:PRO:HG2	1:A:622:TYR:O	2.20	0.41
1:A:826:ASN:C	1:A:828:GLY:N	2.74	0.41
1:A:627:LYS:H	1:A:627:LYS:NZ	2.16	0.41
1:A:772:MET:CG	1:A:780:TRP:HB2	2.48	0.41
1:A:874:SER:HB3	1:A:962:ILE:CD1	2.51	0.41
1:A:8:GLY:HA2	1:A:90:CYS:O	2.20	0.41
1:A:596:GLU:HG3	1:A:997:LEU:HG	2.03	0.41
1:A:121:ILE:HD13	1:A:121:ILE:HG21	1.86	0.40
1:A:168:PRO:HG2	1:A:660:ASN:OD1	2.21	0.40
1:A:32:VAL:HG12	1:A:56:TYR:CZ	2.57	0.40
1:A:647:ASN:OD1	1:A:650:VAL:CG2	2.69	0.40
1:A:156:LEU:O	1:A:157:ASN:CB	2.69	0.40
1:A:559:VAL:HG13	1:A:591:PRO:HD3	2.03	0.40
1:A:627:LYS:O	1:A:631:TYR:CD1	2.75	0.40
2:B:569:ASP:O	2:B:573:LEU:HG	2.22	0.40
1:A:244:LEU:HB3	1:A:245:GLU:H	1.69	0.40
1:A:31:ILE:O	2:B:527:ASN:ND2	2.54	0.40
1:A:144:LEU:HD13	1:A:304:MET:HB2	2.03	0.40
1:A:642:GLU:HG2	1:A:647:ASN:ND2	2.36	0.40
1:A:654:LEU:HG	1:A:658:LEU:HD12	2.02	0.40
2:B:579:GLN:HB2	2:B:579:GLN:HE21	1.71	0.40

There are no symmetry-related clashes.

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	985/1096 (90%)	767 (78%)	139 (14%)	79 (8%)	1	5
2	B	133/279 (48%)	110 (83%)	20 (15%)	3 (2%)	7	30
All	All	1118/1375 (81%)	877 (78%)	159 (14%)	82 (7%)	1	6

All (82) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	107	ASN
1	A	117	ILE
1	A	157	ASN
1	A	158	SER
1	A	186	ASP
1	A	202	ASN
1	A	299	MET
1	A	348	ILE
1	A	407	CYS
1	A	449	PRO
1	A	462	THR
1	A	470	THR
1	A	530	GLN
1	A	643	GLN
1	A	723	LYS
1	A	773	SER
1	A	774	SER
1	A	775	ALA
1	A	875	HIS
1	A	914	GLY
1	A	915	ASP
1	A	926	ASP
1	A	965	SER
1	A	968	ALA
1	A	1028	LEU
1	A	1030	LYS
1	A	116	GLU
1	A	126	CYS
1	A	129	ASP
1	A	159	PRO
1	A	244	LEU
1	A	454	ASP
1	A	461	VAL

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Mol	Chain	Res	Type
1	A	464	SER
1	A	493	GLU
1	A	542	GLU
1	A	722	GLU
1	A	790	SER
1	A	794	PHE
1	A	878	HIS
1	A	1015	SER
2	B	444	ALA
1	A	104	PRO
1	A	243	VAL
1	A	245	GLU
1	A	399	ALA
1	A	481	SER
1	A	487	PRO
1	A	777	ARG
1	A	1009	GLY
2	B	507	GLU
1	A	130	MET
1	A	277	ILE
1	A	344	VAL
1	A	378	CYS
1	A	482	SER
1	A	772	MET
1	A	792	LEU
1	A	1027	ALA
1	A	351	ILE
1	A	363	GLY
1	A	367	LEU
1	A	376	VAL
1	A	409	VAL
1	A	488	ASP
1	A	726	GLU
1	A	970	GLU
1	A	1010	MET
2	B	595	ASN
1	A	380	ASN
1	A	413	LYS
1	A	465	ASN
1	A	469	GLU
1	A	584	TYR
1	A	607	PRO

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Mol	Chain	Res	Type
1	A	329	VAL
1	A	935	GLY
1	A	365	GLU
1	A	804	GLY
1	A	1049	GLY
1	A	298	PRO
1	A	458	PRO

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	912/999 (91%)	771 (84%)	141 (16%)	3	12
2	B	132/259 (51%)	112 (85%)	20 (15%)	3	13
All	All	1044/1258 (83%)	883 (85%)	161 (15%)	3	12

All (161) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-16	ASP
1	A	-15	ILE
1	A	9	GLU
1	A	30	MET
1	A	31	ILE
1	A	37	LEU
1	A	38	ARG
1	A	43	ILE
1	A	60	GLN
1	A	83	PHE
1	A	92	LEU
1	A	93	ARG
1	A	102	ILE
1	A	107	ASN
1	A	110	GLU
1	A	111	LYS

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Mol	Chain	Res	Type
1	A	112	ILE
1	A	123	MET
1	A	130	MET
1	A	137	GLN
1	A	145	ASN
1	A	153	LEU
1	A	157	ASN
1	A	158	SER
1	A	161	SER
1	A	164	MET
1	A	186	ASP
1	A	190	ILE
1	A	197	ILE
1	A	204	LYS
1	A	208	THR
1	A	232	MET
1	A	234	LEU
1	A	236	SER
1	A	241	LEU
1	A	246	TYR
1	A	251	ILE
1	A	263	GLU
1	A	267	LEU
1	A	274	ARG
1	A	275	SER
1	A	293	LEU
1	A	325	LYS
1	A	327	LEU
1	A	328	TRP
1	A	330	ILE
1	A	335	ARG
1	A	346	VAL
1	A	351	ILE
1	A	367	LEU
1	A	382	ARG
1	A	390	ASP
1	A	398	ARG
1	A	412	ARG
1	A	424	TRP
1	A	433	THR
1	A	441	MET
1	A	448	VAL

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Mol	Chain	Res	Type
1	A	461	VAL
1	A	476	GLU
1	A	480	PHE
1	A	484	VAL
1	A	485	LYS
1	A	486	PHE
1	A	488	ASP
1	A	498	TRP
1	A	501	SER
1	A	502	ARG
1	A	529	GLU
1	A	532	LYS
1	A	542	GLU
1	A	545	GLU
1	A	546	GLN
1	A	571	SER
1	A	589	ASP
1	A	597	GLN
1	A	619	LEU
1	A	622	TYR
1	A	624	THR
1	A	627	LYS
1	A	629	SER
1	A	638	VAL
1	A	641	TYR
1	A	650	VAL
1	A	677	ASN
1	A	679	THR
1	A	681	SER
1	A	686	LEU
1	A	687	LEU
1	A	697	MET
1	A	700	LYS
1	A	705	GLN
1	A	712	LEU
1	A	715	LEU
1	A	756	ASN
1	A	773	SER
1	A	776	LYS
1	A	783	TRP
1	A	785	ASN
1	A	788	ILE

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Mol	Chain	Res	Type
1	A	790	SER
1	A	792	LEU
1	A	794	PHE
1	A	797	ASN
1	A	807	LEU
1	A	809	GLN
1	A	813	THR
1	A	816	ILE
1	A	818	ARG
1	A	819	ILE
1	A	825	GLN
1	A	829	LEU
1	A	841	ILE
1	A	851	VAL
1	A	852	ARG
1	A	860	ILE
1	A	863	LYS
1	A	866	LEU
1	A	870	LEU
1	A	871	GLN
1	A	886	LYS
1	A	899	ARG
1	A	905	CYS
1	A	917	HIS
1	A	919	SER
1	A	932	ILE
1	A	936	HIS
1	A	959	ASP
1	A	969	GLN
1	A	970	GLU
1	A	971	CYS
1	A	997	LEU
1	A	1006	LEU
1	A	1008	SER
1	A	1014	GLN
1	A	1022	ILE
1	A	1023	ARG
1	A	1030	LYS
1	A	1031	THR
1	A	1036	LEU
1	A	1037	GLU
2	B	442	ILE

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Mol	Chain	Res	Type
2	B	452	TYR
2	B	459	LYS
2	B	461	ARG
2	B	466	LEU
2	B	469	GLU
2	B	478	GLN
2	B	482	THR
2	B	489	GLU
2	B	495	GLU
2	B	503	ARG
2	B	521	ILE
2	B	529	ASP
2	B	530	LYS
2	B	552	GLN
2	B	563	MET
2	B	577	ARG
2	B	582	MET
2	B	583	TRP
2	B	593	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	-21	HIS
1	A	59	HIS
1	A	60	GLN
1	A	107	ASN
1	A	137	GLN
1	A	145	ASN
1	A	157	ASN
1	A	180	HIS
1	A	213	HIS
1	A	269	GLN
1	A	444	ASN
1	A	465	ASN
1	A	467	ASN
1	A	530	GLN
1	A	605	ASN
1	A	630	GLN
1	A	643	GLN
1	A	647	ASN
1	A	677	ASN

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Mol	Chain	Res	Type
1	A	701	HIS
1	A	728	GLN
1	A	756	ASN
1	A	759	HIS
1	A	763	ASN
1	A	785	ASN
1	A	795	GLN
1	A	797	ASN
1	A	825	GLN
1	A	826	ASN
1	A	861	GLN
1	A	871	GLN
1	A	873	ASN
1	A	875	HIS
1	A	879	GLN
1	A	931	HIS
1	A	1014	GLN
2	B	478	GLN
2	B	526	HIS
2	B	579	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	997/1096 (90%)	0.25	43 (4%) 36 17	54, 83, 114, 141	0
2	B	139/279 (49%)	0.98	26 (18%) 1 0	70, 86, 102, 108	0
All	All	1136/1375 (82%)	0.34	69 (6%) 22 9	54, 84, 112, 141	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	579	GLN	7.3
1	A	381	PRO	7.0
2	B	597	TRP	6.2
1	A	349	ARG	5.8
2	B	593	LYS	5.1
1	A	872	PHE	5.1
1	A	59	HIS	5.0
2	B	445	VAL	5.0
1	A	350	ASP	4.9
1	A	341	ALA	4.4
2	B	444	ALA	4.3
2	B	580	TYR	4.2
1	A	354	ILE	4.1
2	B	446	GLY	3.9
2	B	447	LYS	3.8
1	A	353	LYS	3.7
1	A	557	TYR	3.7
2	B	508	TYR	3.7
2	B	505	SER	3.5
1	A	378	CYS	3.5
1	A	412	ARG	3.2
1	A	345	ASN	3.1
1	A	343	TYR	3.0
2	B	576	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	374	GLN	3.0
1	A	384	ASN	3.0
1	A	382	ARG	2.9
1	A	60	GLN	2.9
1	A	338	ILE	2.8
1	A	411	GLY	2.8
2	B	564	ASN	2.7
2	B	506	LYS	2.7
2	B	572	GLN	2.7
1	A	61	LEU	2.7
1	A	380	ASN	2.7
2	B	509	ILE	2.7
1	A	346	VAL	2.6
2	B	452	TYR	2.6
2	B	598	LEU	2.5
2	B	449	LEU	2.4
1	A	356	VAL	2.4
1	A	26	LEU	2.4
1	A	303	THR	2.4
1	A	875	HIS	2.4
1	A	339	LEU	2.3
1	A	873	ASN	2.3
1	A	246	TYR	2.3
1	A	299	MET	2.3
2	B	454	THR	2.3
2	B	563	MET	2.3
2	B	480	LYS	2.3
1	A	969	GLN	2.2
1	A	1037	GLU	2.2
2	B	448	LYS	2.2
1	A	-27	SER	2.2
1	A	874	SER	2.2
2	B	582	MET	2.2
2	B	581	LEU	2.2
1	A	148	LYS	2.2
1	A	550	PHE	2.2
1	A	387	LEU	2.2
2	B	494	PHE	2.1
1	A	940	HIS	2.1
1	A	410	LYS	2.1
1	A	871	GLN	2.1
2	B	501	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	358	THR	2.0
1	A	409	VAL	2.0
1	A	571	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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.