



Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 09:36 AM EDT

PDB ID : 6QZV / pdb_00006qzv
Title : DPP9 bound to a dipeptide (MP) from the N-terminus of BRCA2
Authors : Ross, B.; Geiss-Friedlander, R.; Huber, R.
Deposited on : 2019-03-12
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

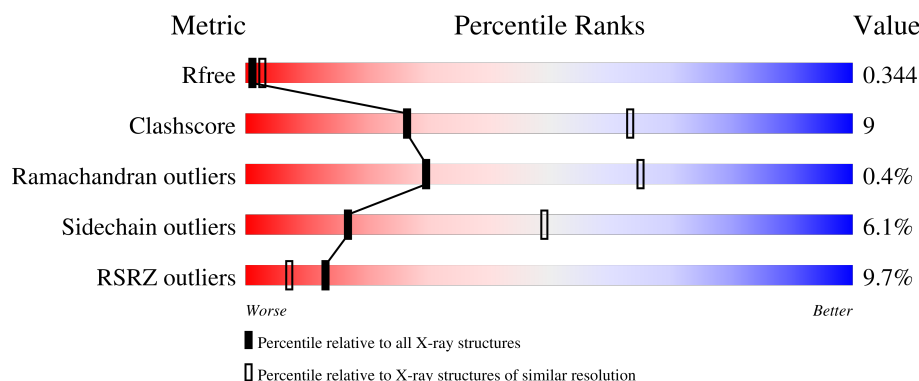
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	898	9% 70% 18% • 10%
1	B	898	6% 67% 21% • 10%
1	C	898	9% 68% 20% • 10%
1	D	898	10% 67% 22% • 10%
2	E	2	100% 50% 50%

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Mol	Chain	Length	Quality of chain
2	F	2	100% 50% 50%
2	G	2	100% 50% 50%
2	H	2	100% 50% 50%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 26316 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 Dipeptidyl peptidase 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	808	Total	C	N	O	S	0	0	0
			6563	4226	1123	1186	28			
1	B	805	Total	C	N	O	S	0	0	0
			6540	4213	1115	1184	28			
1	C	808	Total	C	N	O	S	0	0	0
			6560	4222	1118	1192	28			
1	D	812	Total	C	N	O	S	0	0	0
			6585	4236	1122	1199	28			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	864	HIS	-	expression tag	UNP Q86TI2
A	865	HIS	-	expression tag	UNP Q86TI2
A	866	HIS	-	expression tag	UNP Q86TI2
A	867	HIS	-	expression tag	UNP Q86TI2
A	868	HIS	-	expression tag	UNP Q86TI2
A	869	HIS	-	expression tag	UNP Q86TI2
B	864	HIS	-	expression tag	UNP Q86TI2
B	865	HIS	-	expression tag	UNP Q86TI2
B	866	HIS	-	expression tag	UNP Q86TI2
B	867	HIS	-	expression tag	UNP Q86TI2
B	868	HIS	-	expression tag	UNP Q86TI2
B	869	HIS	-	expression tag	UNP Q86TI2
C	864	HIS	-	expression tag	UNP Q86TI2
C	865	HIS	-	expression tag	UNP Q86TI2
C	866	HIS	-	expression tag	UNP Q86TI2
C	867	HIS	-	expression tag	UNP Q86TI2
C	868	HIS	-	expression tag	UNP Q86TI2
C	869	HIS	-	expression tag	UNP Q86TI2
D	864	HIS	-	expression tag	UNP Q86TI2
D	865	HIS	-	expression tag	UNP Q86TI2
D	866	HIS	-	expression tag	UNP Q86TI2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	867	HIS	-	expression tag	UNP Q86TI2
D	868	HIS	-	expression tag	UNP Q86TI2
D	869	HIS	-	expression tag	UNP Q86TI2

- Molecule 2 is a protein called MET-PRO.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	2	Total	C	N	O	S	0	0	0
			16	10	2	3	1			
2	F	2	Total	C	N	O	S	0	0	0
			16	10	2	3	1			
2	G	2	Total	C	N	O	S	0	0	0
			16	10	2	3	1			
2	H	2	Total	C	N	O	S	0	0	0
			16	10	2	3	1			

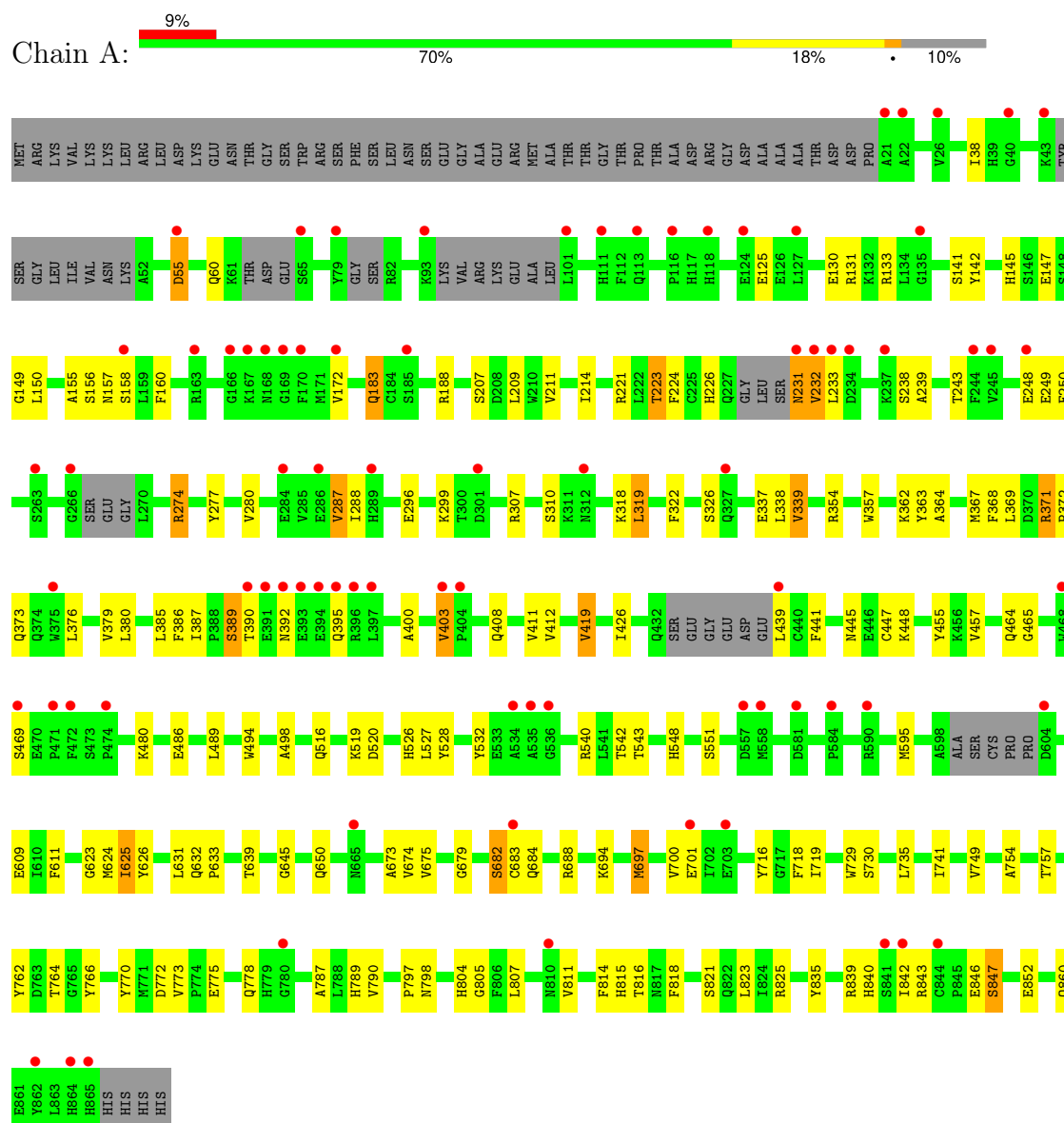
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	2	Total	O	0	0
			2	2		
3	D	2	Total	O	0	0
			2	2		

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.

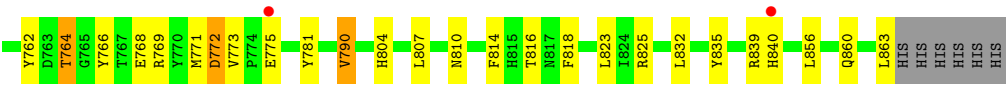
• Molecule 1: Dipeptidyl peptidase 9



• Molecule 1: Dipeptidyl peptidase 9







● Molecule 2: MET-PRO



● Molecule 2: MET-PRO



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● Molecule 2: MET-PRO



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	119.52Å 117.22Å 163.40Å 90.00° 105.72° 90.00°	Depositor
Resolution (Å)	43.47 – 3.00 43.47 – 3.00	Depositor EDS
% Data completeness (in resolution range)	88.1 (43.47-3.00) 88.0 (43.47-3.00)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.90 (at 3.01Å)	Xtrriage
Refinement program	REFMAC 5.8.0232	Depositor
R, R_{free}	0.286 , 0.345 0.287 , 0.344	Depositor DCC
R_{free} test set	3827 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	31.9	Xtrriage
Anisotropy	0.892	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 33.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	26316	wwPDB-VP
Average B, all atoms (Å ²)	27.0	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 59.79 % 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 1.6741e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.03	0/6759	1.12	0/9165
1	B	1.03	0/6733	1.13	0/9128
1	C	1.03	0/6754	1.14	2/9159 (0.0%)
1	D	1.03	0/6779	1.14	2/9192 (0.0%)
2	E	0.93	0/16	1.51	0/19
2	F	0.70	0/16	0.76	0/19
2	G	0.72	0/16	0.92	0/19
2	H	0.70	0/16	0.94	0/19
All	All	1.03	0/27089	1.13	4/36720 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	835	TYR	CB-CA-C	8.45	119.44	110.65
1	D	169	GLY	CA-C-O	-5.61	118.09	122.52
1	D	835	TYR	CB-CA-C	5.56	119.75	110.97
1	C	494	TRP	CA-C-O	-5.04	115.95	121.14

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	6563	0	6348	108	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	6540	0	6340	137	0
1	C	6560	0	6347	123	0
1	D	6585	0	6365	119	0
2	E	16	0	15	4	0
2	F	16	0	15	3	0
2	G	16	0	15	1	0
2	H	16	0	15	3	0
3	C	2	0	0	1	0
3	D	2	0	0	0	0
All	All	26316	0	25460	479	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 9.

All (479) 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:B:420:TRP:HZ3	1:B:694:LYS:HB2	1.26	0.97
1:A:307:ARG:O	1:A:310:SER:HB3	1.68	0.92
1:D:223:THR:HG21	1:D:239:ALA:HB3	1.54	0.87
1:B:420:TRP:CZ3	1:B:694:LYS:HB2	2.13	0.84
1:B:307:ARG:O	1:B:310:SER:HB3	1.78	0.81
1:A:729:TRP:CZ3	1:A:754:ALA:HB2	2.17	0.79
1:D:367:MET:HE1	1:D:423:VAL:HG13	1.65	0.78
1:D:307:ARG:O	1:D:310:SER:HB3	1.83	0.77
1:D:697:MET:HG3	1:D:771:MET:SD	2.26	0.75
1:A:223:THR:HG21	1:A:239:ALA:HB3	1.69	0.74
1:B:371:ARG:NH1	1:B:768:GLU:OE2	2.20	0.74
1:B:362:LYS:HE3	1:B:432:GLN:HE22	1.53	0.72
1:C:307:ARG:O	1:C:310:SER:HB3	1.90	0.71
1:A:339:VAL:HG13	1:A:387:ILE:HG21	1.72	0.71
1:B:362:LYS:HG2	1:B:363:TYR:CD2	2.26	0.70
1:A:762:TYR:OH	2:E:233:PRO:HA	1.92	0.70
1:D:494:TRP:CG	1:D:519:LYS:HA	2.27	0.70
1:C:367:MET:HE1	1:C:423:VAL:HG13	1.73	0.69
1:D:762:TYR:OH	2:H:233:PRO:HA	1.92	0.69
1:A:133:ARG:NH1	1:A:248:GLU:OE1	2.26	0.69
1:B:494:TRP:CG	1:B:519:LYS:HA	2.27	0.68
1:C:420:TRP:CZ3	1:C:694:LYS:HB2	2.29	0.68
1:C:371:ARG:NH1	1:C:768:GLU:OE2	2.25	0.68
1:B:810:ASN:C	1:B:810:ASN:HD22	1.99	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:641:LEU:HD13	1:C:709:LEU:HD13	1.75	0.67
1:B:54:HIS:HE1	1:B:84:ASN:HD21	1.41	0.66
1:A:339:VAL:HG13	1:A:387:ILE:CG2	2.25	0.66
1:A:392:ASN:ND2	1:A:395:GLN:OE1	2.30	0.65
1:C:223:THR:HG21	1:C:239:ALA:HB3	1.79	0.64
1:C:373:GLN:NE2	1:C:769:ARG:HB2	2.12	0.64
1:A:371:ARG:HH11	1:A:371:ARG:CG	2.11	0.62
1:A:729:TRP:HZ3	1:A:754:ALA:HB2	1.63	0.62
1:D:339:VAL:HG23	1:D:385:LEU:O	2.00	0.62
1:A:233:LEU:HD11	1:A:287:VAL:HG11	1.82	0.62
1:D:494:TRP:CB	1:D:519:LYS:HA	2.29	0.62
1:C:209:LEU:H	1:C:223:THR:HG22	1.65	0.61
1:B:620:ARG:O	1:B:685:ARG:NH1	2.33	0.61
1:C:362:LYS:HD3	1:C:363:TYR:CE1	2.36	0.61
1:D:74:TYR:HH	1:D:105:TRP:CD1	2.20	0.60
1:C:411:VAL:HG22	1:C:480:LYS:HA	1.84	0.60
1:C:420:TRP:HZ3	1:C:694:LYS:HB2	1.65	0.60
1:C:767:THR:HG22	1:C:771:MET:HB2	1.84	0.60
1:B:286:GLU:OE2	1:B:307:ARG:HD3	2.01	0.60
1:B:376:LEU:C	1:B:376:LEU:HD13	2.27	0.59
1:B:362:LYS:O	1:B:383:PRO:CD	2.50	0.59
1:C:644:TYR:HD2	1:C:646:GLY:H	1.49	0.59
1:C:712:VAL:HG12	1:C:719:ILE:HG13	1.84	0.59
1:C:60:GLN:NE2	1:C:557:ASP:OD2	2.36	0.59
1:C:347:PRO:O	1:C:348:LYS:HB2	2.00	0.59
1:A:379:VAL:HG12	1:A:411:VAL:HG22	1.83	0.59
1:B:709:LEU:HD21	1:B:724:VAL:HG11	1.85	0.59
1:B:762:TYR:OH	2:F:233:PRO:HA	2.02	0.59
1:C:413:TYR:OH	1:C:445:ASN:ND2	2.36	0.59
1:D:766:TYR:CE2	2:H:233:PRO:HD3	2.38	0.59
1:A:408:GLN:HE22	1:A:464:GLN:H	1.50	0.58
1:C:358:THR:HG23	3:C:902:HOH:O	2.02	0.58
1:A:232:VAL:HG13	1:A:233:LEU:H	1.68	0.58
1:A:371:ARG:HH11	1:A:371:ARG:HG2	1.68	0.58
1:B:369:LEU:HD12	1:B:375:TRP:O	2.03	0.58
1:B:233:LEU:HD12	1:B:287:VAL:HG11	1.85	0.58
1:C:108:MET:SD	1:C:171:MET:HE1	2.44	0.58
1:A:367:MET:HE3	1:A:376:LEU:HD11	1.86	0.58
1:A:494:TRP:CG	1:A:519:LYS:HA	2.39	0.58
1:D:362:LYS:HD2	1:D:432:GLN:HE22	1.69	0.58
1:B:357:TRP:HZ3	1:B:383:PRO:HG3	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:840:HIS:NE2	2:E:233:PRO:OXT	2.36	0.57
1:A:133:ARG:NH2	2:E:233:PRO:O	2.37	0.57
1:A:419:VAL:O	1:A:694:LYS:HE2	2.04	0.57
1:A:338:LEU:HD21	1:A:386:PHE:CZ	2.40	0.57
1:A:842:ILE:CG2	1:A:847:SER:HB2	2.35	0.57
1:B:362:LYS:HE3	1:B:432:GLN:NE2	2.19	0.57
1:D:451:PHE:CE1	1:D:493:GLU:HA	2.40	0.57
1:D:410:TYR:HB3	1:D:481:CYS:SG	2.45	0.57
1:B:440:CYS:SG	1:B:456:LYS:NZ	2.64	0.56
1:B:129:ARG:O	1:B:134:LEU:N	2.38	0.56
1:B:378:LEU:HD13	1:B:427:PHE:CD1	2.41	0.56
1:D:411:VAL:HG23	1:D:479:PHE:HB2	1.86	0.56
1:D:773:VAL:HG12	1:D:775:GLU:H	1.69	0.56
1:C:846:GLU:OE2	1:D:825:ARG:NH1	2.38	0.56
1:A:804:HIS:HD2	1:A:816:THR:OG1	1.88	0.56
1:A:287:VAL:O	1:B:299:LYS:HE2	2.06	0.56
1:C:359:ARG:NH2	1:C:508:GLU:OE2	2.38	0.56
1:C:375:TRP:CD1	1:C:375:TRP:C	2.83	0.56
1:C:243:THR:CG2	1:C:280:VAL:HG11	2.36	0.56
1:D:91:ILE:HG21	1:D:558:MET:HE2	1.86	0.56
1:A:156:SER:OG	1:A:157:ASN:N	2.38	0.56
1:D:427:PHE:O	1:D:429:PRO:HD3	2.05	0.55
1:A:757:THR:HB	1:A:787:ALA:HB2	1.88	0.55
1:C:29:HIS:H	1:C:860:GLN:NE2	2.05	0.55
1:D:156:SER:OG	1:D:157:ASN:N	2.36	0.55
1:D:243:THR:CG2	1:D:280:VAL:HG11	2.36	0.55
1:B:201:PHE:CZ	1:B:212:ALA:HB3	2.41	0.55
1:A:489:LEU:HD22	1:A:532:TYR:HA	1.88	0.55
1:B:767:THR:HG22	1:B:771:MET:HB2	1.88	0.55
1:D:615:THR:HG1	1:D:617:SER:HG	1.55	0.55
1:B:697:MET:HE3	1:B:770:TYR:CB	2.37	0.55
1:D:511:LYS:HA	1:D:532:TYR:CE2	2.42	0.55
1:C:566:VAL:HG23	1:C:654:ASN:HA	1.89	0.55
1:C:208:ASP:OD1	1:C:223:THR:HG23	2.06	0.55
1:C:151:PHE:O	1:C:161:HIS:HA	2.07	0.55
1:A:249:GLU:OE1	1:A:249:GLU:HA	2.07	0.54
1:D:804:HIS:HD2	1:D:816:THR:OG1	1.89	0.54
1:A:133:ARG:HH12	1:A:248:GLU:CD	2.14	0.54
1:B:412:VAL:HG21	1:B:439:LEU:CD2	2.37	0.54
1:D:417:THR:HG21	1:D:420:TRP:O	2.08	0.54
1:A:243:THR:CG2	1:A:280:VAL:HG11	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:234:ASP:O	1:C:236:PRO:HD3	2.08	0.54
1:B:380:LEU:HB2	1:B:410:TYR:HB2	1.90	0.54
1:A:825:ARG:HH22	1:B:837:ASN:HD22	1.56	0.54
1:D:354:ARG:NH1	1:D:425:ASP:OD1	2.41	0.54
1:B:554:GLN:CD	1:B:554:GLN:H	2.16	0.54
1:D:133:ARG:NH2	1:D:248:GLU:OE2	2.41	0.54
1:D:412:VAL:CG1	1:D:441:PHE:CE2	2.90	0.54
1:D:641:LEU:HD21	1:D:705:GLN:HB3	1.90	0.54
1:A:277:TYR:CZ	1:A:318:LYS:HB2	2.43	0.53
1:D:712:VAL:HG12	1:D:719:ILE:HG13	1.90	0.53
1:B:645:GLY:HA3	1:B:735:LEU:HD12	1.89	0.53
1:A:55:ASP:HB3	1:A:142:TYR:HE1	1.73	0.53
1:A:155:ALA:HB3	1:A:160:PHE:CD1	2.42	0.53
1:B:243:THR:CG2	1:B:280:VAL:HG11	2.38	0.53
1:A:805:GLY:HA2	1:A:835:TYR:HB2	1.90	0.53
1:D:234:ASP:C	1:D:236:PRO:HD3	2.33	0.53
1:D:367:MET:HE3	1:D:376:LEU:HD11	1.91	0.53
1:A:318:LYS:HD2	1:A:337:GLU:HB3	1.91	0.53
1:B:233:LEU:CD1	1:B:287:VAL:HG11	2.38	0.53
1:D:412:VAL:CG1	1:D:441:PHE:CZ	2.92	0.53
1:B:380:LEU:HD11	1:B:439:LEU:HD22	1.91	0.53
1:B:639:THR:OG1	1:B:719:ILE:HG23	2.09	0.53
1:C:201:PHE:CZ	1:C:212:ALA:HB3	2.43	0.53
1:D:377:GLN:NE2	1:D:414:GLU:OE2	2.42	0.53
1:C:417:THR:HG21	1:C:420:TRP:C	2.33	0.52
1:D:339:VAL:HG11	1:D:468:TRP:HB3	1.90	0.52
1:C:460:VAL:HB	1:C:482:PRO:HG2	1.90	0.52
1:B:802:ILE:HG21	1:B:816:THR:HG23	1.90	0.52
1:C:419:VAL:HG21	1:C:687:LEU:HD23	1.92	0.52
1:B:409:PRO:HD2	1:B:479:PHE:CE1	2.45	0.52
1:A:730:SER:OG	2:E:233:PRO:OXT	2.24	0.52
1:A:790:VAL:HG11	1:A:823:LEU:HA	1.91	0.52
1:B:642:PHE:HB3	1:B:676:VAL:HG22	1.91	0.52
1:A:221:ARG:HH21	1:A:224:PHE:HA	1.73	0.52
1:A:611:PHE:CZ	1:A:623:GLY:HA3	2.44	0.52
1:B:54:HIS:CE1	1:B:84:ASN:HD21	2.25	0.52
1:B:376:LEU:HD13	1:B:377:GLN:N	2.24	0.52
1:B:379:VAL:HG12	1:B:411:VAL:HG22	1.92	0.52
1:D:131:ARG:HG3	1:D:247:GLN:HE21	1.75	0.52
1:D:756:VAL:HG11	1:D:759:TRP:CE3	2.44	0.52
1:B:370:ASP:HB3	1:B:375:TRP:CE3	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:652:VAL:HB	1:B:678:ASP:OD2	2.10	0.52
1:A:519:LYS:HB3	1:A:528:TYR:CZ	2.45	0.51
1:B:56:PHE:CD1	1:B:72:LEU:HD12	2.45	0.51
1:B:298:ARG:HH11	1:B:298:ARG:HB2	1.74	0.51
1:C:762:TYR:OH	2:G:233:PRO:HA	2.09	0.51
1:C:334:GLN:NE2	1:C:336:LYS:HE3	2.25	0.51
1:C:773:VAL:HG13	1:C:775:GLU:CD	2.35	0.51
1:D:234:ASP:O	1:D:236:PRO:HD3	2.10	0.51
1:A:223:THR:CG2	1:A:239:ALA:HB3	2.39	0.51
1:A:250:PHE:O	1:A:354:ARG:NH1	2.35	0.51
1:A:339:VAL:HG22	1:A:385:LEU:O	2.10	0.51
1:D:371:ARG:HB2	1:D:372:PRO:HD3	1.92	0.51
1:A:411:VAL:HB	1:A:480:LYS:HA	1.93	0.51
1:A:697:MET:HE1	1:A:770:TYR:CG	2.45	0.51
1:B:559:PHE:CZ	1:B:575:TYR:HB2	2.46	0.50
1:D:519:LYS:HB3	1:D:528:TYR:CZ	2.47	0.50
1:B:768:GLU:HA	1:B:772:ASP:O	2.12	0.50
1:D:201:PHE:CZ	1:D:212:ALA:HB3	2.47	0.50
1:D:623:GLY:HA2	1:D:652:VAL:HG21	1.92	0.50
1:A:395:GLN:HE22	1:C:404:PRO:HD3	1.76	0.50
1:B:371:ARG:C	1:B:373:GLN:H	2.20	0.50
1:A:412:VAL:CG1	1:A:441:PHE:CE2	2.95	0.50
1:A:729:TRP:CZ3	1:A:754:ALA:CB	2.93	0.50
1:B:368:PHE:CE2	1:B:379:VAL:HG21	2.46	0.50
1:A:38:ILE:HD12	1:A:852:GLU:HB3	1.93	0.50
1:A:412:VAL:HG13	1:A:441:PHE:CE2	2.47	0.50
1:B:223:THR:HG21	1:B:239:ALA:HB3	1.94	0.50
1:C:319:LEU:O	1:C:336:LYS:HB2	2.12	0.50
1:D:709:LEU:HD21	1:D:724:VAL:HG11	1.94	0.50
1:B:801:LEU:HD12	1:B:831:GLN:HB2	1.94	0.50
1:A:274:ARG:HB3	1:A:319:LEU:HD21	1.94	0.49
1:A:773:VAL:HG12	1:A:775:GLU:CD	2.37	0.49
1:B:201:PHE:CE1	1:B:214:ILE:HG23	2.47	0.49
1:B:362:LYS:CE	1:B:432:GLN:NE2	2.74	0.49
1:A:299:LYS:HE2	1:B:289:HIS:NE2	2.27	0.49
1:B:775:GLU:OE1	1:B:775:GLU:N	2.41	0.49
1:C:359:ARG:HH22	1:C:508:GLU:CD	2.20	0.49
1:A:516:GLN:HA	1:A:526:HIS:O	2.12	0.49
1:A:362:LYS:HG2	1:A:363:TYR:CE1	2.47	0.49
1:C:613:PHE:CZ	1:C:621:LEU:HD12	2.48	0.49
1:C:768:GLU:HA	1:C:772:ASP:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:766:TYR:CZ	2:F:233:PRO:HD3	2.47	0.49
1:B:807:LEU:O	1:B:839:ARG:NH1	2.45	0.49
1:B:362:LYS:O	1:B:383:PRO:HD3	2.12	0.49
1:B:773:VAL:HG13	1:B:775:GLU:CD	2.38	0.49
1:C:410:TYR:HB3	1:C:481:CYS:SG	2.53	0.49
1:A:338:LEU:CD2	1:A:386:PHE:CZ	2.96	0.49
1:B:740:LEU:HD23	1:B:793:LEU:CD2	2.43	0.48
1:B:778:GLN:HE21	1:B:778:GLN:HA	1.78	0.48
1:D:363:TYR:HB2	1:D:380:LEU:HD22	1.94	0.48
1:B:131:ARG:HG3	1:B:247:GLN:HE21	1.77	0.48
1:C:681:GLY:HA2	1:C:690:GLU:HA	1.95	0.48
1:C:767:THR:O	1:C:771:MET:N	2.32	0.48
1:D:693:LEU:HD13	1:D:697:MET:HE3	1.96	0.48
1:D:840:HIS:NE2	2:H:233:PRO:O	2.46	0.48
1:A:371:ARG:HB3	1:A:372:PRO:CD	2.44	0.48
1:A:626:TYR:HB2	1:A:674:VAL:HB	1.96	0.48
1:A:650:GLN:NE2	1:A:684:GLN:HG3	2.28	0.48
1:D:29:HIS:H	1:D:860:GLN:NE2	2.11	0.48
1:D:495:GLU:OE2	1:D:684:GLN:HA	2.14	0.48
1:A:448:LYS:HD3	1:A:455:TYR:CE2	2.49	0.48
1:B:357:TRP:CZ3	1:B:383:PRO:HG3	2.47	0.48
1:C:201:PHE:CD1	1:C:214:ILE:HG23	2.48	0.48
1:D:516:GLN:NE2	1:D:550:CYS:SG	2.87	0.48
1:C:511:LYS:HA	1:C:532:TYR:CE2	2.49	0.48
1:A:390:THR:HG21	1:A:395:GLN:NE2	2.29	0.47
1:A:697:MET:HE1	1:A:770:TYR:CD2	2.49	0.47
1:B:810:ASN:C	1:B:810:ASN:ND2	2.71	0.47
1:B:307:ARG:O	1:B:310:SER:CB	2.57	0.47
1:B:240:GLY:HA2	1:B:255:GLY:O	2.14	0.47
1:B:340:GLN:HB3	1:B:345:LEU:HG	1.96	0.47
1:D:373:GLN:OE1	1:D:769:ARG:HD3	2.14	0.47
1:D:494:TRP:HB2	1:D:519:LYS:HA	1.96	0.47
1:D:540:ARG:NH1	1:D:542:THR:O	2.47	0.47
1:D:542:THR:HB	1:D:548:HIS:CD2	2.49	0.47
1:C:410:TYR:CB	1:C:461:LEU:HD22	2.45	0.47
1:A:183:GLN:HE21	1:A:183:GLN:HA	1.78	0.47
1:B:809:GLU:HG3	1:B:839:ARG:NH1	2.29	0.47
1:C:339:VAL:CG1	1:C:403:VAL:HG21	2.45	0.47
1:D:209:LEU:H	1:D:223:THR:HG22	1.79	0.47
1:B:757:THR:HA	1:B:786:VAL:HG22	1.97	0.47
1:D:548:HIS:ND1	1:D:563:TYR:HB3	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:PRO:O	1:A:373:GLN:HB2	2.14	0.47
1:C:605:TYR:CE1	1:C:658:GLY:HA2	2.50	0.47
1:D:223:THR:CG2	1:D:239:ALA:HB3	2.37	0.47
1:A:543:THR:O	1:A:548:HIS:HE1	1.98	0.47
1:B:362:LYS:O	1:B:383:PRO:HD2	2.13	0.47
1:C:58:PHE:CD1	1:C:553:SER:HA	2.50	0.47
1:C:494:TRP:CG	1:C:519:LYS:HA	2.49	0.47
1:A:679:GLY:O	1:A:682:SER:HB2	2.15	0.47
1:A:716:TYR:HB3	1:A:718:PHE:CE2	2.50	0.47
1:D:494:TRP:CD2	1:D:519:LYS:HB2	2.50	0.47
1:C:405:ARG:HA	1:C:466:TYR:O	2.15	0.46
1:D:223:THR:HG21	1:D:239:ALA:CB	2.37	0.46
1:D:716:TYR:HB3	1:D:718:PHE:CE2	2.50	0.46
1:B:362:LYS:HG2	1:B:363:TYR:CE2	2.49	0.46
1:C:367:MET:HE3	1:C:376:LEU:HD11	1.97	0.46
1:C:681:GLY:O	1:C:690:GLU:HG3	2.15	0.46
1:D:617:SER:O	1:D:618:ASP:HB2	2.16	0.46
1:B:151:PHE:O	1:B:161:HIS:HA	2.15	0.46
1:C:24:PHE:O	1:C:723:ARG:NH1	2.46	0.46
1:D:417:THR:HG21	1:D:420:TRP:C	2.40	0.46
1:B:201:PHE:CD1	1:B:214:ILE:HG23	2.51	0.46
1:B:643:VAL:HG21	1:B:726:ILE:CG1	2.46	0.46
1:C:203:PHE:CE1	1:C:210:TRP:HB2	2.50	0.46
1:B:68:HIS:CE1	1:B:90:GLU:HB3	2.50	0.46
1:B:412:VAL:HG21	1:B:439:LEU:HD23	1.97	0.46
1:D:412:VAL:HG11	1:D:441:PHE:CE2	2.50	0.46
1:C:188:ARG:HG2	1:C:203:PHE:CD1	2.51	0.46
1:C:281:ASP:CG	1:C:283:SER:HG	2.23	0.46
1:C:751:ILE:HD13	1:C:855:LEU:HD13	1.98	0.46
1:B:773:VAL:HG12	1:B:775:GLU:HB2	1.98	0.46
1:C:124:GLU:HB3	1:C:189:MET:SD	2.56	0.46
1:C:729:TRP:CZ3	1:C:754:ALA:HB2	2.51	0.46
1:B:646:GLY:N	1:B:731:TYR:CD1	2.84	0.46
1:C:643:VAL:HG12	1:C:644:TYR:N	2.31	0.46
1:D:371:ARG:CB	1:D:372:PRO:HD3	2.46	0.46
1:A:211:VAL:HG11	1:A:322:PHE:CZ	2.51	0.46
1:A:540:ARG:NH1	1:A:542:THR:O	2.47	0.46
1:B:263:SER:O	1:B:272:THR:HG22	2.16	0.46
1:B:494:TRP:CB	1:B:519:LYS:HA	2.45	0.46
1:B:227:GLN:N	1:B:235:ASP:OD2	2.45	0.46
1:D:131:ARG:NE	1:D:248:GLU:OE1	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:ASN:HD22	1:A:395:GLN:CD	2.24	0.45
1:B:209:LEU:H	1:B:223:THR:HG22	1.82	0.45
1:B:804:HIS:CD2	1:B:816:THR:OG1	2.70	0.45
1:C:548:HIS:CD2	1:C:563:TYR:HB3	2.51	0.45
1:C:651:LEU:HD23	1:C:651:LEU:HA	1.83	0.45
1:D:741:ILE:HG22	1:D:742:HIS:CD2	2.52	0.45
1:D:807:LEU:HB2	1:D:839:ARG:HG2	1.97	0.45
1:D:814:PHE:O	1:D:818:PHE:N	2.46	0.45
1:A:797:PRO:O	1:A:798:ASN:HB2	2.17	0.45
1:C:376:LEU:C	1:C:376:LEU:HD23	2.41	0.45
1:D:545:GLY:O	1:D:654:ASN:ND2	2.47	0.45
1:B:42:ARG:NH1	1:B:852:GLU:OE2	2.41	0.45
1:B:432:GLN:HE21	1:B:432:GLN:HB2	1.63	0.45
1:D:350:GLU:CD	1:D:371:ARG:HG2	2.41	0.45
1:D:687:LEU:O	1:D:691:GLY:N	2.44	0.45
1:A:238:SER:O	1:A:280:VAL:N	2.41	0.45
1:B:629:HIS:NE2	1:B:665:ASN:ND2	2.65	0.45
1:A:631:LEU:O	1:A:633:PRO:HD3	2.17	0.45
1:A:645:GLY:HA3	1:A:735:LEU:HD11	1.97	0.45
1:D:702:ILE:O	1:D:706:VAL:HG23	2.17	0.45
1:A:299:LYS:HE3	1:B:287:VAL:HB	1.99	0.45
1:B:376:LEU:C	1:B:376:LEU:CD1	2.90	0.45
1:B:766:TYR:CE1	2:F:233:PRO:HD3	2.51	0.45
1:C:641:LEU:HD21	1:C:705:GLN:HE21	1.82	0.45
1:D:200:PHE:CZ	1:D:324:THR:HG21	2.52	0.45
1:D:307:ARG:O	1:D:310:SER:CB	2.61	0.45
1:D:363:TYR:CB	1:D:380:LEU:HD22	2.47	0.45
1:D:429:PRO:HA	1:D:441:PHE:CB	2.47	0.45
1:D:362:LYS:CD	1:D:432:GLN:HE22	2.30	0.44
1:A:773:VAL:CG1	1:A:775:GLU:CD	2.90	0.44
1:B:716:TYR:HB3	1:B:718:PHE:CE2	2.52	0.44
1:C:84:ASN:ND2	1:C:139:ILE:O	2.45	0.44
1:D:58:PHE:CZ	1:D:560:VAL:HG23	2.52	0.44
1:D:382:PRO:HA	1:D:383:PRO:HD3	1.88	0.44
1:D:444:ALA:HB1	1:D:452:CYS:SG	2.57	0.44
1:A:207:SER:HB3	1:A:238:SER:HB2	2.00	0.44
1:B:632:GLN:O	1:B:633:PRO:C	2.60	0.44
1:D:573:HIS:HE2	1:D:597:GLU:CD	2.25	0.44
1:C:757:THR:HA	1:C:786:VAL:HG22	2.00	0.44
1:D:308:THR:HG21	1:D:781:TYR:HE2	1.83	0.44
1:A:367:MET:CE	1:A:376:LEU:HD11	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:LEU:O	1:B:88:TYR:HA	2.17	0.44
1:B:118:HIS:HB3	1:B:120:VAL:HG23	1.99	0.44
1:B:370:ASP:CG	1:B:375:TRP:HB3	2.42	0.44
1:C:773:VAL:CG1	1:C:775:GLU:HG2	2.48	0.44
1:C:834:ILE:HD12	1:D:832:LEU:HD21	2.00	0.44
1:B:740:LEU:HD23	1:B:793:LEU:HD22	2.00	0.44
1:C:540:ARG:NH1	1:C:544:PRO:HD3	2.32	0.44
1:C:697:MET:HE3	1:C:770:TYR:HB3	2.00	0.44
1:D:56:PHE:HA	1:D:73:TYR:O	2.18	0.44
1:D:226:HIS:HA	1:D:235:ASP:OD1	2.18	0.44
1:D:371:ARG:NH1	1:D:768:GLU:OE2	2.49	0.44
1:A:158:SER:HB2	1:A:188:ARG:HH21	1.82	0.44
1:B:236:PRO:HD2	1:B:237:LYS:H	1.83	0.44
1:B:808:ASP:CG	1:B:811:VAL:O	2.61	0.44
1:C:308:THR:HG21	1:C:781:TYR:HE2	1.81	0.44
1:C:420:TRP:HZ3	1:C:694:LYS:CB	2.29	0.44
1:B:57:GLN:HB2	1:B:73:TYR:HB2	2.00	0.43
1:B:192:LYS:NZ	1:B:256:TYR:O	2.50	0.43
1:C:444:ALA:HB1	1:C:452:CYS:SG	2.57	0.43
1:D:698:GLY:O	1:D:738:MET:HE2	2.19	0.43
1:A:400:ALA:O	1:A:403:VAL:HG23	2.18	0.43
1:A:807:LEU:HB2	1:A:839:ARG:HG2	1.99	0.43
1:B:29:HIS:CE1	1:B:37:ILE:HD11	2.53	0.43
1:B:308:THR:HG21	1:B:781:TYR:HE2	1.83	0.43
1:A:412:VAL:CG1	1:A:441:PHE:CZ	3.02	0.43
1:A:426:ILE:HD12	1:A:498:ALA:HB2	2.01	0.43
1:D:375:TRP:O	1:D:375:TRP:CD1	2.71	0.43
1:D:413:TYR:CE1	1:D:457:VAL:HG21	2.54	0.43
1:A:380:LEU:HD11	1:A:439:LEU:HD22	2.00	0.43
1:B:773:VAL:CG1	1:B:775:GLU:CD	2.91	0.43
1:B:806:PHE:HB2	1:B:834:ILE:HG23	2.00	0.43
1:C:307:ARG:HA	1:C:763:ASP:HA	2.00	0.43
1:C:442:LEU:HD23	1:C:456:LYS:HA	1.99	0.43
1:C:773:VAL:CG1	1:C:775:GLU:CD	2.92	0.43
1:D:696:GLN:HB2	1:D:699:GLN:CD	2.43	0.43
1:A:339:VAL:CG2	1:A:385:LEU:O	2.67	0.43
1:C:432:GLN:O	1:C:433:SER:CB	2.66	0.43
1:D:432:GLN:CG	1:D:439:LEU:HD13	2.49	0.43
1:A:741:ILE:HD13	1:A:789:HIS:HB2	2.00	0.43
1:C:709:LEU:HD21	1:C:724:VAL:HG21	2.01	0.43
1:D:77:MET:HB3	1:D:78:PRO:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:518:THR:O	1:B:519:LYS:C	2.61	0.43
1:C:272:THR:HG22	1:C:323:GLN:HE21	1.82	0.43
1:D:790:VAL:HG11	1:D:823:LEU:HA	2.00	0.43
1:A:814:PHE:O	1:A:818:PHE:N	2.45	0.43
1:C:319:LEU:HD12	1:C:386:PHE:CG	2.54	0.43
1:D:337:GLU:CD	1:D:389:SER:HB3	2.44	0.43
1:D:764:THR:HA	1:D:768:GLU:HG3	2.01	0.43
1:B:373:GLN:NE2	1:B:765:GLY:O	2.48	0.43
1:B:738:MET:SD	1:B:786:VAL:HG12	2.58	0.43
1:C:445:ASN:HB3	1:C:455:TYR:CE1	2.54	0.43
1:C:783:ALA:HA	1:C:789:HIS:HE2	1.84	0.43
1:D:188:ARG:HG2	1:D:203:PHE:CE1	2.54	0.43
1:B:209:LEU:HD11	1:B:275:ILE:HG21	2.01	0.42
1:B:528:TYR:CE1	1:B:540:ARG:HB2	2.54	0.42
1:C:439:LEU:HD23	1:C:441:PHE:CD2	2.54	0.42
1:C:757:THR:HB	1:C:787:ALA:HB2	2.01	0.42
1:D:355:ALA:HA	1:D:366:ALA:HA	2.01	0.42
1:B:354:ARG:NH2	1:B:425:ASP:OD1	2.53	0.42
1:C:397:LEU:HA	1:C:400:ALA:HB3	2.00	0.42
1:C:417:THR:HG22	1:C:421:ILE:HG12	2.00	0.42
1:C:483:ILE:HG22	1:C:485:GLU:O	2.19	0.42
1:C:807:LEU:O	1:C:839:ARG:NH1	2.52	0.42
1:C:814:PHE:CD1	1:C:814:PHE:C	2.96	0.42
1:D:165:GLY:HA2	1:D:170:PHE:CE1	2.54	0.42
1:A:445:ASN:HB3	1:A:455:TYR:CE1	2.54	0.42
1:C:419:VAL:HB	1:C:420:TRP:H	1.66	0.42
1:C:563:TYR:CZ	1:C:571:CYS:HB2	2.54	0.42
1:C:758:VAL:HG12	1:C:761:ALA:H	1.85	0.42
1:D:527:LEU:HB3	1:D:542:THR:HG23	2.02	0.42
1:B:376:LEU:O	1:B:414:GLU:HA	2.19	0.42
1:D:155:ALA:HB3	1:D:160:PHE:CD1	2.53	0.42
1:A:811:VAL:HG13	1:A:815:HIS:ND1	2.34	0.42
1:C:724:VAL:CG1	1:C:746:VAL:O	2.68	0.42
1:C:737:LEU:HD12	1:C:786:VAL:HG21	2.00	0.42
1:C:319:LEU:HD12	1:C:386:PHE:CD1	2.55	0.42
1:C:520:ASP:HB2	1:C:528:TYR:OH	2.20	0.42
1:B:54:HIS:CE1	1:B:75:LEU:HB2	2.55	0.42
1:D:82:ARG:HD2	1:D:83:GLU:HB3	2.02	0.42
1:D:243:THR:HG21	1:D:280:VAL:HG11	2.00	0.42
1:D:730:SER:N	1:D:753:GLY:O	2.53	0.42
1:C:208:ASP:OD1	1:C:223:THR:CG2	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:319:LEU:HD21	1:C:357:TRP:HH2	1.85	0.42
1:C:520:ASP:OD2	1:C:540:ARG:NE	2.47	0.42
1:A:625:ILE:HD12	1:A:675:VAL:HG22	2.02	0.41
1:A:766:TYR:O	1:A:770:TYR:CD2	2.73	0.41
1:B:88:TYR:OH	1:B:172:VAL:O	2.38	0.41
1:B:805:GLY:HA2	1:B:835:TYR:HB2	2.01	0.41
1:C:318:LYS:HD2	1:C:337:GLU:HA	2.02	0.41
1:C:812:HIS:O	1:C:813:PHE:C	2.62	0.41
1:D:405:ARG:O	1:D:465:GLY:HA2	2.20	0.41
1:B:58:PHE:CE2	1:B:72:LEU:HD11	2.55	0.41
1:C:243:THR:HG21	1:C:280:VAL:HG11	2.02	0.41
1:C:448:LYS:HD3	1:C:455:TYR:CE2	2.54	0.41
1:C:527:LEU:HB3	1:C:542:THR:HG23	2.01	0.41
1:C:528:TYR:CD1	1:C:540:ARG:HB2	2.56	0.41
1:D:359:ARG:NE	1:D:431:PRO:HD3	2.35	0.41
1:A:145:HIS:O	1:A:149:GLY:N	2.53	0.41
1:A:337:GLU:HG2	1:A:389:SER:OG	2.20	0.41
1:A:357:TRP:CE3	1:A:364:ALA:HB2	2.55	0.41
1:A:639:THR:HA	1:A:673:ALA:O	2.20	0.41
1:B:154:GLN:HE22	1:B:189:MET:HE3	1.86	0.41
1:C:641:LEU:HD22	1:C:747:PHE:CE1	2.56	0.41
1:D:212:ALA:HA	1:D:218:GLU:O	2.21	0.41
1:D:236:PRO:HB2	1:D:283:SER:OG	2.19	0.41
1:A:457:VAL:HG22	1:A:486:GLU:HG3	2.02	0.41
1:B:697:MET:HE3	1:B:770:TYR:HB2	2.02	0.41
1:D:725:ALA:HB2	1:D:863:LEU:HD22	2.03	0.41
1:D:771:MET:O	1:D:772:ASP:CB	2.69	0.41
1:B:60:GLN:HG3	1:B:70:HIS:CE1	2.56	0.41
1:B:645:GLY:HA3	1:B:735:LEU:CD1	2.49	0.41
1:B:751:ILE:HG23	1:B:801:LEU:HD23	2.02	0.41
1:B:243:THR:HG21	1:B:280:VAL:HG11	2.02	0.41
1:B:797:PRO:O	1:B:798:ASN:HB2	2.19	0.41
1:C:764:THR:HB	1:C:768:GLU:OE1	2.20	0.41
1:D:350:GLU:HG2	1:D:371:ARG:HG2	2.02	0.41
1:D:644:TYR:O	1:D:735:LEU:HD12	2.21	0.41
1:A:131:ARG:NE	1:A:248:GLU:HG2	2.35	0.41
1:A:231:ASN:OD1	1:A:231:ASN:N	2.52	0.41
1:A:239:ALA:HB1	1:A:277:TYR:CE1	2.55	0.41
1:B:426:ILE:HD12	1:B:498:ALA:HB2	2.01	0.41
1:C:623:GLY:HA2	1:C:652:VAL:HG21	2.02	0.41
1:C:801:LEU:HD12	1:C:831:GLN:CB	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:609:GLU:HB3	1:A:625:ILE:CG2	2.50	0.41
1:B:371:ARG:HB3	1:B:372:PRO:HD3	2.01	0.41
1:C:58:PHE:CZ	1:C:560:VAL:HG23	2.56	0.41
1:C:191:PRO:HA	1:C:202:SER:O	2.21	0.41
1:C:464:GLN:HG3	1:C:464:GLN:O	2.20	0.41
1:C:740:LEU:HD23	1:C:793:LEU:HD22	2.03	0.41
1:D:670:LEU:HD12	1:D:856:LEU:HD22	2.03	0.41
1:D:705:GLN:O	1:D:709:LEU:HB2	2.21	0.41
1:A:158:SER:HB2	1:A:188:ARG:NH2	2.35	0.41
1:A:527:LEU:HB3	1:A:542:THR:HG23	2.03	0.41
1:B:644:TYR:CZ	1:B:649:VAL:HG21	2.56	0.41
1:C:735:LEU:HD23	1:C:735:LEU:HA	1.81	0.41
1:D:60:GLN:NE2	1:D:557:ASP:OD2	2.52	0.41
1:B:512:LEU:HD23	1:B:531:SER:HA	2.04	0.40
1:D:693:LEU:O	1:D:694:LYS:C	2.64	0.40
1:A:368:PHE:CE2	1:A:379:VAL:HG21	2.57	0.40
1:A:371:ARG:CG	1:A:371:ARG:NH1	2.77	0.40
1:B:131:ARG:HG3	1:B:247:GLN:NE2	2.35	0.40
1:B:372:PRO:O	1:B:373:GLN:C	2.64	0.40
1:B:405:ARG:O	1:B:465:GLY:HA2	2.22	0.40
1:C:801:LEU:HD12	1:C:831:GLN:HB2	2.02	0.40
1:D:151:PHE:O	1:D:161:HIS:HA	2.21	0.40
1:A:339:VAL:HG13	1:A:387:ILE:HG23	2.03	0.40
1:A:369:LEU:HG	1:A:376:LEU:HD12	2.03	0.40
1:A:825:ARG:NH2	1:B:837:ASN:HD22	2.17	0.40
1:B:519:LYS:HB3	1:B:528:TYR:CZ	2.56	0.40
1:B:680:ARG:NH2	1:B:704:ASP:OD1	2.55	0.40
1:C:319:LEU:O	1:C:336:LYS:N	2.54	0.40
1:C:342:PHE:CD1	1:C:342:PHE:C	2.99	0.40
1:D:160:PHE:CE2	1:D:179:GLU:HG2	2.55	0.40
1:D:412:VAL:HG13	1:D:441:PHE:CE2	2.56	0.40
1:B:412:VAL:HG21	1:B:439:LEU:HD22	2.04	0.40
1:B:494:TRP:CD1	1:B:494:TRP:H	2.40	0.40
1:B:785:SER:HB2	1:B:788:LEU:HD12	2.03	0.40
1:C:308:THR:HB	1:C:763:ASP:O	2.21	0.40
1:C:751:ILE:HG23	1:C:801:LEU:HD23	2.02	0.40
1:D:369:LEU:HD21	1:D:376:LEU:HB2	2.03	0.40
1:D:521:THR:CG2	1:D:524:GLU:HB2	2.51	0.40
1:D:651:LEU:HA	1:D:651:LEU:HD23	1.85	0.40
1:B:376:LEU:HB2	1:B:421:ILE:HG21	2.03	0.40
1:B:595:MET:HE3	1:B:595:MET:HB3	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:806:PHE:HB3	1:B:836:PRO:HA	2.03	0.40
1:C:192:LYS:NZ	1:C:256:TYR:O	2.49	0.40
1:C:494:TRP:CE3	1:C:519:LYS:HB2	2.57	0.40
1:C:693:LEU:O	1:C:694:LYS:C	2.65	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	790/898 (88%)	735 (93%)	52 (7%)	3 (0%)	30	65
1	B	785/898 (87%)	729 (93%)	55 (7%)	1 (0%)	48	80
1	C	790/898 (88%)	735 (93%)	50 (6%)	5 (1%)	21	56
1	D	794/898 (88%)	730 (92%)	61 (8%)	3 (0%)	30	65
All	All	3159/3592 (88%)	2929 (93%)	218 (7%)	12 (0%)	30	65

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	232	VAL
1	A	465	GLY
1	D	772	ASP
1	C	207	SER
1	C	348	LYS
1	C	814	PHE
1	A	772	ASP
1	B	236	PRO
1	C	419	VAL
1	C	839	ARG
1	D	419	VAL

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Mol	Chain	Res	Type
1	D	339	VAL

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	712/785 (91%)	664 (93%)	48 (7%)	15	46
1	B	712/785 (91%)	666 (94%)	46 (6%)	15	47
1	C	714/785 (91%)	676 (95%)	38 (5%)	20	54
1	D	715/785 (91%)	673 (94%)	42 (6%)	18	50
2	E	2/2 (100%)	2 (100%)	0	100	100
2	F	2/2 (100%)	2 (100%)	0	100	100
2	G	2/2 (100%)	2 (100%)	0	100	100
2	H	2/2 (100%)	2 (100%)	0	100	100
All	All	2861/3148 (91%)	2687 (94%)	174 (6%)	17	49

All (174) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	ASP
1	A	60	GLN
1	A	125	GLU
1	A	130	GLU
1	A	141	SER
1	A	147	GLU
1	A	150	LEU
1	A	172	VAL
1	A	183	GLN
1	A	209	LEU
1	A	214	ILE
1	A	223	THR
1	A	226	HIS
1	A	231	ASN

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Mol	Chain	Res	Type
1	A	274	ARG
1	A	287	VAL
1	A	288	ILE
1	A	296	GLU
1	A	319	LEU
1	A	326	SER
1	A	339	VAL
1	A	371	ARG
1	A	389	SER
1	A	403	VAL
1	A	419	VAL
1	A	447	CYS
1	A	469	SER
1	A	520	ASP
1	A	551	SER
1	A	595	MET
1	A	624	MET
1	A	625	ILE
1	A	632	GLN
1	A	682	SER
1	A	683	CYS
1	A	688	ARG
1	A	697	MET
1	A	700	VAL
1	A	701	GLU
1	A	719	ILE
1	A	749	VAL
1	A	764	THR
1	A	778	GLN
1	A	821	SER
1	A	843	ARG
1	A	846	GLU
1	A	847	SER
1	A	860	GLN
1	B	104	SER
1	B	123	ARG
1	B	128	LEU
1	B	130	GLU
1	B	136	VAL
1	B	147	GLU
1	B	150	LEU
1	B	189	MET

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Mol	Chain	Res	Type
1	B	209	LEU
1	B	211	VAL
1	B	214	ILE
1	B	226	HIS
1	B	232	VAL
1	B	233	LEU
1	B	238	SER
1	B	251	ASP
1	B	287	VAL
1	B	300	THR
1	B	307	ARG
1	B	351	TYR
1	B	376	LEU
1	B	389	SER
1	B	390	THR
1	B	408	GLN
1	B	412	VAL
1	B	419	VAL
1	B	432	GLN
1	B	447	CYS
1	B	469	SER
1	B	473	SER
1	B	503	LYS
1	B	516	GLN
1	B	539	VAL
1	B	549	SER
1	B	567	SER
1	B	696	GLN
1	B	700	VAL
1	B	712	VAL
1	B	714	GLU
1	B	719	ILE
1	B	773	VAL
1	B	778	GLN
1	B	790	VAL
1	B	809	GLU
1	B	810	ASN
1	B	847	SER
1	C	102	LEU
1	C	104	SER
1	C	115	THR
1	C	128	LEU

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Mol	Chain	Res	Type
1	C	130	GLU
1	C	136	VAL
1	C	171	MET
1	C	172	VAL
1	C	189	MET
1	C	209	LEU
1	C	221	ARG
1	C	223	THR
1	C	226	HIS
1	C	248	GLU
1	C	272	THR
1	C	342	PHE
1	C	343	SER
1	C	345	LEU
1	C	351	TYR
1	C	362	LYS
1	C	392	ASN
1	C	411	VAL
1	C	419	VAL
1	C	433	SER
1	C	447	CYS
1	C	464	GLN
1	C	491	SER
1	C	506	VAL
1	C	557	ASP
1	C	558	MET
1	C	597	GLU
1	C	604	ASP
1	C	609	GLU
1	C	631	LEU
1	C	662	LEU
1	C	703	GLU
1	C	712	VAL
1	C	773	VAL
1	D	20	PRO
1	D	25	GLN
1	D	101	LEU
1	D	125	GLU
1	D	128	LEU
1	D	130	GLU
1	D	136	VAL
1	D	158	SER

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Mol	Chain	Res	Type
1	D	168	ASN
1	D	172	VAL
1	D	184	CYS
1	D	189	MET
1	D	209	LEU
1	D	220	ARG
1	D	223	THR
1	D	233	LEU
1	D	238	SER
1	D	259	CYS
1	D	263	SER
1	D	319	LEU
1	D	324	THR
1	D	334	GLN
1	D	343	SER
1	D	345	LEU
1	D	371	ARG
1	D	379	VAL
1	D	390	THR
1	D	407	VAL
1	D	423	VAL
1	D	447	CYS
1	D	483	ILE
1	D	551	SER
1	D	582	ASP
1	D	662	LEU
1	D	688	ARG
1	D	700	VAL
1	D	712	VAL
1	D	722	SER
1	D	748	LYS
1	D	764	THR
1	D	790	VAL
1	D	810	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (93) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	HIS
1	A	60	GLN
1	A	70	HIS
1	A	84	ASN

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Mol	Chain	Res	Type
1	A	107	GLN
1	A	113	GLN
1	A	183	GLN
1	A	205	ASN
1	A	206	ASN
1	A	231	ASN
1	A	247	GLN
1	A	323	GLN
1	A	340	GLN
1	A	374	GLN
1	A	377	GLN
1	A	392	ASN
1	A	395	GLN
1	A	408	GLN
1	A	525	HIS
1	A	548	HIS
1	A	650	GLN
1	A	665	ASN
1	A	778	GLN
1	A	804	HIS
1	A	817	ASN
1	A	831	GLN
1	A	833	GLN
1	B	29	HIS
1	B	54	HIS
1	B	84	ASN
1	B	118	HIS
1	B	247	GLN
1	B	323	GLN
1	B	334	GLN
1	B	340	GLN
1	B	424	HIS
1	B	432	GLN
1	B	507	ASN
1	B	525	HIS
1	B	548	HIS
1	B	562	HIS
1	B	650	GLN
1	B	665	ASN
1	B	695	ASN
1	B	778	GLN
1	B	804	HIS

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Mol	Chain	Res	Type
1	B	810	ASN
1	B	815	HIS
1	B	822	GLN
1	B	837	ASN
1	C	39	HIS
1	C	117	HIS
1	C	118	HIS
1	C	161	HIS
1	C	206	ASN
1	C	247	GLN
1	C	323	GLN
1	C	340	GLN
1	C	406	ASN
1	C	432	GLN
1	C	445	ASN
1	C	464	GLN
1	C	507	ASN
1	C	548	HIS
1	C	554	GLN
1	C	562	HIS
1	C	648	GLN
1	C	665	ASN
1	C	684	GLN
1	C	695	ASN
1	C	705	GLN
1	C	710	GLN
1	C	804	HIS
1	C	860	GLN
1	D	29	HIS
1	D	183	GLN
1	D	205	ASN
1	D	247	GLN
1	D	334	GLN
1	D	408	GLN
1	D	432	GLN
1	D	516	GLN
1	D	562	HIS
1	D	684	GLN
1	D	705	GLN
1	D	742	HIS
1	D	804	HIS
1	D	810	ASN

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Mol	Chain	Res	Type
1	D	817	ASN
1	D	822	GLN
1	D	831	GLN
1	D	837	ASN
1	D	860	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	808/898 (89%)	0.88	80 (9%) 13 7	10, 25, 60, 83	0
1	B	805/898 (89%)	0.83	58 (7%) 21 11	8, 24, 53, 81	0
1	C	808/898 (89%)	0.91	80 (9%) 13 7	9, 23, 54, 80	0
1	D	812/898 (90%)	0.93	87 (10%) 11 6	9, 23, 55, 77	0
2	E	2/2 (100%)	3.14	2 (100%) 0 0	43, 43, 43, 44	0
2	F	2/2 (100%)	2.66	2 (100%) 0 0	30, 30, 30, 31	0
2	G	2/2 (100%)	4.32	2 (100%) 0 0	38, 38, 38, 38	0
2	H	2/2 (100%)	4.01	2 (100%) 0 0	42, 42, 42, 45	0
All	All	3241/3600 (90%)	0.89	313 (9%) 13 7	8, 24, 56, 83	0

All (313) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	233	PRO	5.9
1	D	232	VAL	5.6
2	H	233	PRO	5.4
1	A	394	GLU	5.3
1	A	118	HIS	5.2
1	A	233	LEU	5.2
1	C	232	VAL	5.0
1	A	864	HIS	4.9
1	B	124	GLU	4.7
1	A	397	LEU	4.7
1	A	266	GLY	4.6
1	D	701	GLU	4.6
1	D	20	PRO	4.4
1	C	168	ASN	4.4
1	B	297	GLU	4.4
1	B	20	PRO	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	396	ARG	4.3
1	D	645	GLY	4.3
1	D	437	ASP	4.2
1	C	135	GLY	4.2
1	D	118	HIS	4.1
1	A	234	ASP	4.1
1	B	425	ASP	4.1
1	C	264	TRP	4.1
1	A	472	PHE	4.0
1	C	645	GLY	4.0
1	D	85	SER	3.9
1	A	392	ASN	3.9
1	C	683	CYS	3.9
1	C	52	ALA	3.9
1	B	327	GLN	3.8
1	B	251	ASP	3.8
1	D	396	ARG	3.8
2	E	233	PRO	3.8
1	C	20	PRO	3.7
1	C	396	ARG	3.7
1	A	65	SER	3.7
1	A	79	TYR	3.6
1	D	185	SER	3.6
1	A	390	THR	3.6
1	A	471	PRO	3.6
1	A	101	LEU	3.6
1	A	231	ASN	3.6
1	B	535	ALA	3.5
1	A	683	CYS	3.5
1	C	114	ALA	3.5
1	C	702	ILE	3.5
1	C	117	HIS	3.5
1	C	22	ALA	3.5
1	B	111	HIS	3.4
1	C	437	ASP	3.4
1	C	116	PRO	3.4
1	A	391	GLU	3.4
1	C	111	HIS	3.4
1	C	475	GLY	3.3
1	D	168	ASN	3.3
1	C	398	ALA	3.3
1	D	21	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	393	GLU	3.3
1	D	438	GLU	3.2
1	D	436	GLU	3.2
1	C	570	PRO	3.2
1	D	394	GLU	3.2
1	B	683	CYS	3.2
1	A	40	GLY	3.2
1	C	112	PHE	3.2
1	D	43	LYS	3.1
1	A	841	SER	3.1
1	D	55	ASP	3.1
1	A	395	GLN	3.1
1	B	437	ASP	3.1
1	A	393	GLU	3.1
1	C	55	ASP	3.1
1	D	163	ARG	3.1
1	D	395	GLN	3.1
1	A	158	SER	3.0
1	A	469	SER	3.0
1	C	478	GLU	3.0
1	D	110	ASP	3.0
1	C	121	TYR	3.0
1	B	841	SER	3.0
1	C	101	LEU	3.0
1	D	183	GLN	3.0
1	C	444	ALA	3.0
1	A	111	HIS	3.0
1	A	810	ASN	3.0
1	B	394	GLU	3.0
1	B	407	VAL	3.0
1	D	472	PHE	3.0
2	F	233	PRO	2.9
1	D	604	ASP	2.9
1	C	386	PHE	2.9
1	D	464	GLN	2.9
1	D	297	GLU	2.9
1	A	135	GLY	2.9
1	C	477	ASP	2.9
1	D	33	GLY	2.9
1	C	82	ARG	2.9
1	B	644	TYR	2.9
1	C	470	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	399	SER	2.8
1	A	535	ALA	2.8
1	A	701	GLU	2.8
1	D	137	PHE	2.8
1	A	865	HIS	2.8
1	D	535	ALA	2.8
1	D	598	ALA	2.8
1	D	52	ALA	2.8
1	A	604	ASP	2.8
1	C	83	GLU	2.8
1	D	392	ASN	2.8
1	B	491	SER	2.8
1	C	344	SER	2.8
1	B	126	GLU	2.8
1	C	395	GLN	2.8
1	C	301	ASP	2.7
1	B	121	TYR	2.7
1	B	598	ALA	2.7
1	A	844	CYS	2.7
1	C	469	SER	2.7
1	D	56	PHE	2.7
1	D	175	MET	2.7
1	D	391	GLU	2.7
1	D	476	GLU	2.7
1	B	43	LYS	2.7
2	G	232	MET	2.7
1	C	297	GLU	2.7
1	D	775	GLU	2.7
1	A	166	GLY	2.7
1	C	185	SER	2.7
1	B	264	TRP	2.7
1	D	359	ARG	2.7
1	B	118	HIS	2.7
1	D	312	ASN	2.7
1	A	284	GLU	2.7
1	B	470	GLU	2.7
1	D	63	ASP	2.7
1	D	397	LEU	2.7
1	B	347	PRO	2.7
1	B	21	ALA	2.7
2	H	232	MET	2.6
1	D	266	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	301	ASP	2.6
1	C	223	THR	2.6
1	A	557	ASP	2.6
1	C	763	ASP	2.6
1	A	248	GLU	2.6
1	B	424	HIS	2.6
1	B	464	GLN	2.6
1	A	439	LEU	2.6
1	D	101	LEU	2.6
1	C	402	ALA	2.6
1	B	348	LYS	2.6
1	A	842	ILE	2.6
1	A	558	MET	2.6
1	D	411	VAL	2.6
1	D	463	SER	2.5
1	B	360	ASP	2.5
1	C	476	GLU	2.5
2	E	232	MET	2.5
1	B	429	PRO	2.5
1	C	657	LYS	2.5
1	B	391	GLU	2.5
1	D	599	ALA	2.5
1	D	412	VAL	2.5
1	C	126	GLU	2.5
1	C	394	GLU	2.5
1	A	93	LYS	2.5
1	C	176	LYS	2.5
1	A	21	ALA	2.5
1	C	189	MET	2.5
1	D	189	MET	2.5
1	D	270	LEU	2.5
1	A	780	GLY	2.5
1	D	40	GLY	2.5
1	B	778	GLN	2.5
1	D	534	ALA	2.4
1	C	399	SER	2.4
1	D	167	LYS	2.4
1	D	557	ASP	2.4
1	D	660	LYS	2.4
1	B	384	ALA	2.4
1	C	426	ILE	2.4
1	A	534	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	82	ARG	2.4
1	A	581	ASP	2.4
1	B	169	GLY	2.4
1	D	489	LEU	2.4
1	A	168	ASN	2.4
1	C	169	GLY	2.4
1	C	312	ASN	2.4
1	B	455	TYR	2.4
1	D	499	ARG	2.4
2	F	232	MET	2.4
1	C	125	GLU	2.4
1	B	655	SER	2.4
1	A	403	VAL	2.4
1	C	241	VAL	2.4
1	B	84	ASN	2.3
1	D	648	GLN	2.3
1	C	347	PRO	2.3
1	C	348	LYS	2.3
1	D	375	TRP	2.3
1	C	397	LEU	2.3
1	C	93	LYS	2.3
1	A	474	PRO	2.3
1	D	166	GLY	2.3
1	C	639	THR	2.3
1	B	289	HIS	2.3
1	D	558	MET	2.3
1	D	554	GLN	2.3
1	A	375	TRP	2.3
1	A	665	ASN	2.3
1	B	110	ASP	2.3
1	A	172	VAL	2.3
1	C	66	GLY	2.3
1	B	101	LEU	2.3
1	D	117	HIS	2.3
1	C	85	SER	2.3
1	C	251	ASP	2.3
1	C	700	VAL	2.3
1	C	509	GLU	2.2
1	A	169	GLY	2.2
1	B	760	MET	2.2
1	B	117	HIS	2.2
1	A	232	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	745	GLN	2.2
1	B	55	ASP	2.2
1	D	156	SER	2.2
1	C	643	VAL	2.2
1	B	516	GLN	2.2
1	A	124	GLU	2.2
1	A	703	GLU	2.2
1	A	584	PRO	2.2
1	A	468	TRP	2.2
1	B	232	VAL	2.2
1	C	554	GLN	2.2
1	C	139	ILE	2.2
1	A	404	PRO	2.2
1	D	78	PRO	2.2
1	D	132	LYS	2.2
1	A	590	ARG	2.2
1	D	112	PHE	2.2
1	D	500	HIS	2.2
1	C	113	GLN	2.2
1	B	488	ALA	2.2
1	A	536	GLY	2.2
1	A	55	ASP	2.2
1	A	170	PHE	2.2
1	B	245	VAL	2.1
1	D	223	THR	2.1
1	A	327	GLN	2.1
1	C	233	LEU	2.1
1	A	185	SER	2.1
1	A	237	LYS	2.1
1	C	314	LYS	2.1
1	C	473	SER	2.1
1	D	473	SER	2.1
1	D	590	ARG	2.1
1	A	26	VAL	2.1
1	A	43	LYS	2.1
1	A	167	LYS	2.1
1	B	51	LYS	2.1
1	C	660	LYS	2.1
1	C	374	GLN	2.1
1	B	22	ALA	2.1
1	A	244	PHE	2.1
1	D	234	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	289	HIS	2.1
1	A	862	TYR	2.1
1	A	22	ALA	2.1
1	C	183	GLN	2.1
1	C	598	ALA	2.1
1	A	312	ASN	2.1
1	A	245	VAL	2.1
1	A	301	ASP	2.1
1	B	52	ALA	2.1
1	A	113	GLN	2.1
1	D	125	GLU	2.1
1	B	502	SER	2.1
1	C	120	VAL	2.1
1	D	418	ASN	2.1
1	B	371	ARG	2.1
1	C	461	LEU	2.1
1	D	840	HIS	2.1
1	B	234	ASP	2.1
1	D	582	ASP	2.1
1	A	116	PRO	2.1
1	A	286	GLU	2.1
1	C	67	PRO	2.1
1	D	187	PRO	2.1
1	B	120	VAL	2.0
1	D	127	LEU	2.0
1	D	702	ILE	2.0
1	C	226	HIS	2.0
1	D	111	HIS	2.0
1	C	410	TYR	2.0
1	C	455	TYR	2.0
1	D	114	ALA	2.0
1	D	126	GLU	2.0
1	A	163	ARG	2.0
1	B	128	LEU	2.0
1	C	693	LEU	2.0
1	A	263	SER	2.0
1	B	62	THR	2.0
1	D	444	ALA	2.0
1	D	93	LYS	2.0
1	D	184	CYS	2.0
1	D	113	GLN	2.0
1	C	405	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	619	VAL	2.0
1	D	643	VAL	2.0
1	A	127	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.