



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 09:09 am BST

PDB ID : 5TJ7
Title : Structure of WWP2 WW2-2,3-linker-HECT aa 334-398 linked to 485-865
Authors : Chen, Z.; Gabelli, S.B.
Deposited on : 2016-10-03
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

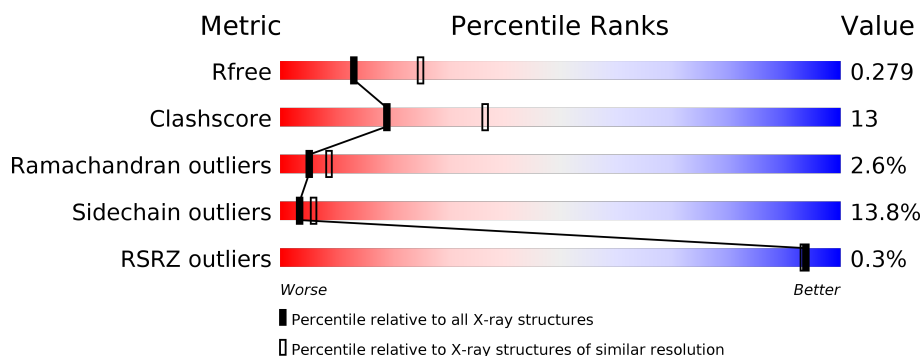
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 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	447	 64% 28% 6% •
1	B	447	 62% 30% 7% •
1	C	447	 66% 27% • •
1	D	447	 60% 30% 8% •

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15912 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 NEDD4-like E3 ubiquitin-protein ligase WWP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	436	Total	C	N	O	S	0	0	0
			3705	2379	635	670	21			
1	B	445	Total	C	N	O	S	0	0	0
			3756	2408	645	682	21			
1	C	435	Total	C	N	O	S	0	0	0
			3692	2370	634	667	21			
1	D	445	Total	C	N	O	S	0	0	0
			3756	2408	645	682	21			

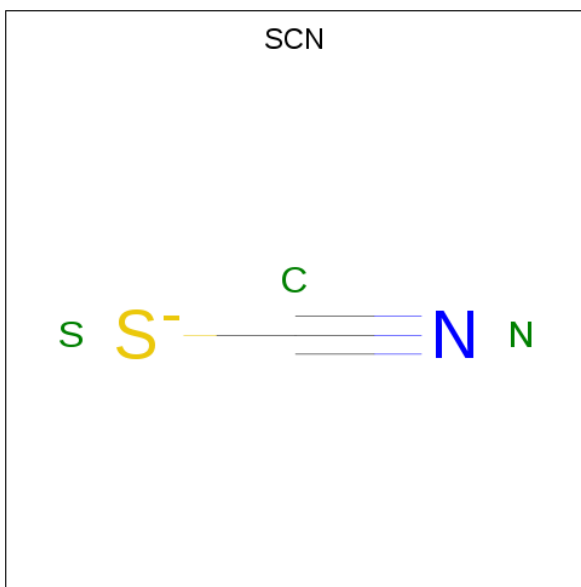
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	333	GLY	-	expression tag	UNP O00308
B	333	GLY	-	expression tag	UNP O00308
C	333	GLY	-	expression tag	UNP O00308
D	333	GLY	-	expression tag	UNP O00308

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Na	0	0
			1	1		
2	A	1	Total	Na	0	0
			1	1		
2	D	1	Total	Na	0	0
			1	1		

- Molecule 3 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	N	S	0	0
			3	1	1	1		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total	Cl	0	0
			1	1		

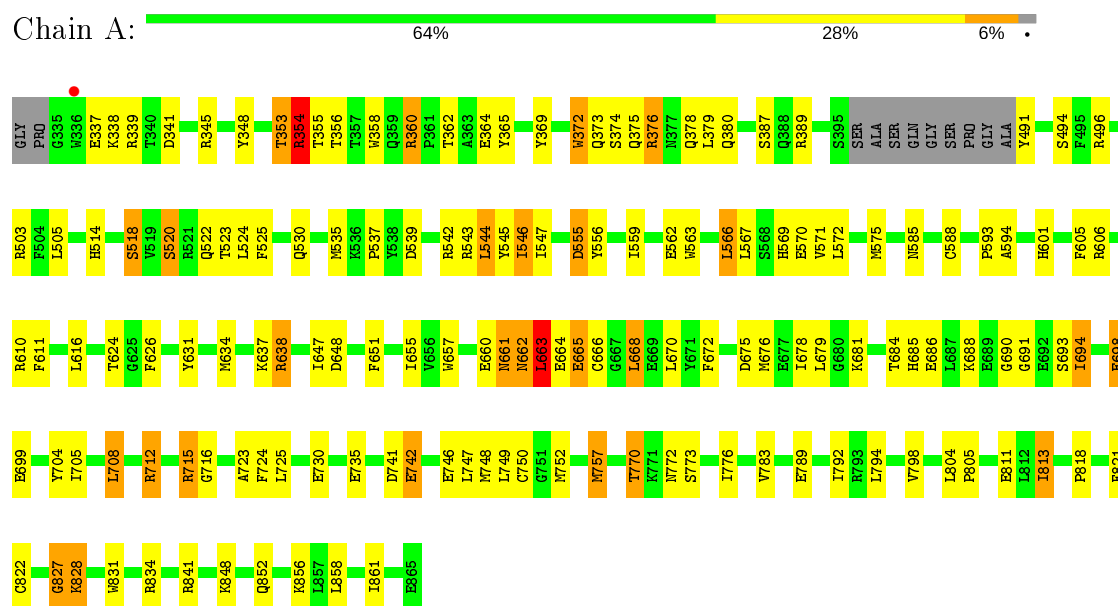
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	273	Total	O	0	0
			273	273		
5	B	229	Total	O	0	0
			229	229		
5	C	235	Total	O	0	0
			235	235		
5	D	259	Total	O	0	0
			259	259		

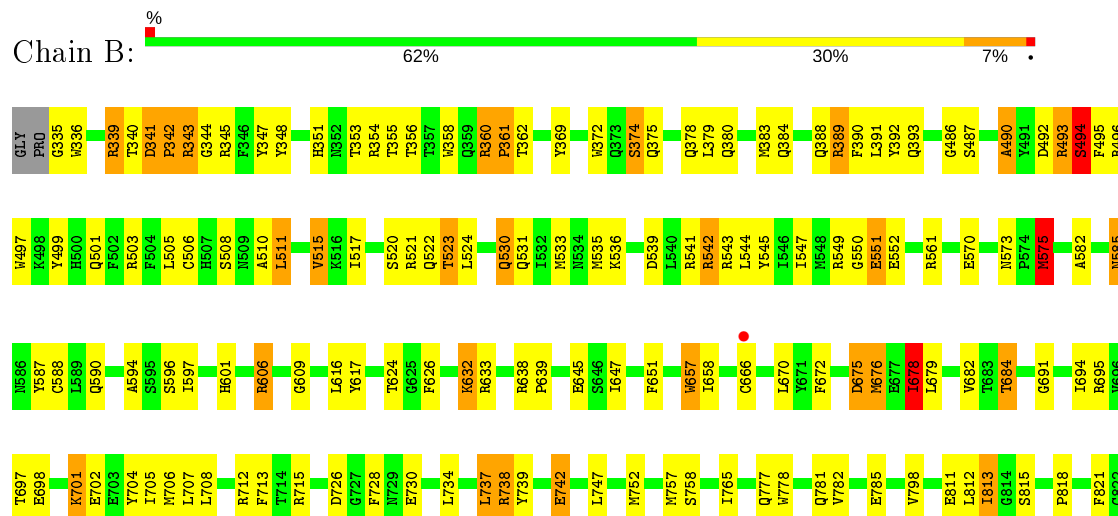
3 Residue-property plots

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: NEDD4-like E3 ubiquitin-protein ligase WWP2



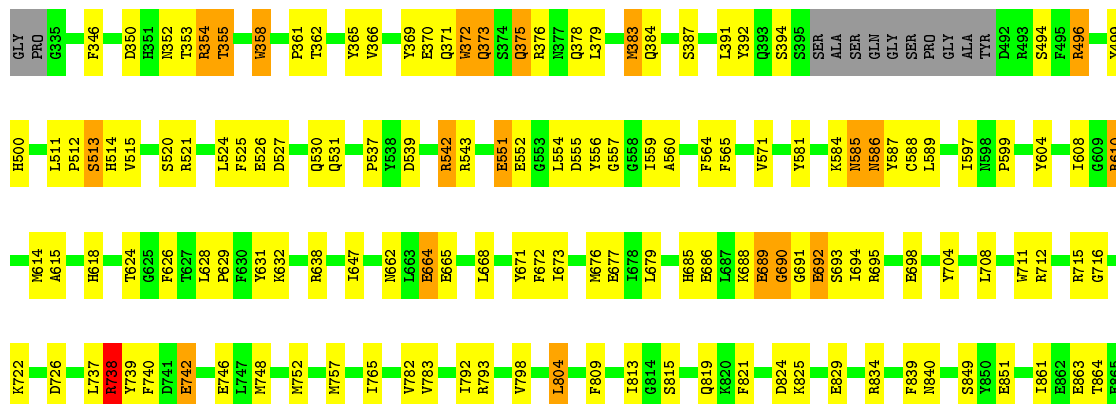
- Molecule 1: NEDD4-like E3 ubiquitin-protein ligase WWP2





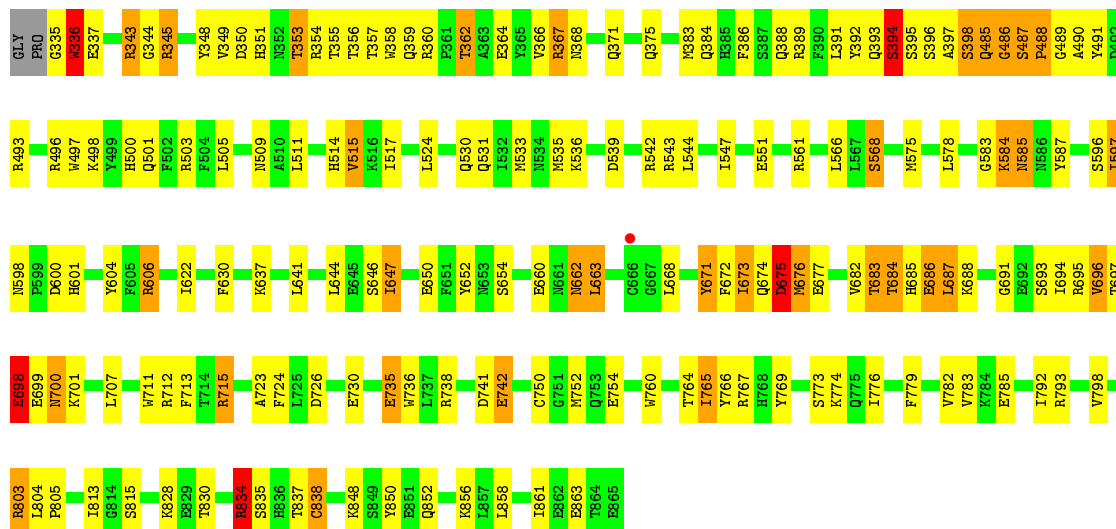
- Molecule 1: NEDD4-like E3 ubiquitin-protein ligase WWP2

Chain C: 66% 27%



- Molecule 1: NEDD4-like E3 ubiquitin-protein ligase WWP2

Chain D: 60% 30% 8%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	72.00Å 73.91Å 82.38Å 89.99° 89.66° 90.01°	Depositor
Resolution (Å)	50.00 – 2.60 43.80 – 2.60	Depositor EDS
% Data completeness (in resolution range)	90.1 (50.00-2.60) 90.0 (43.80-2.60)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.15 (at 2.61Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.207 , 0.284 0.206 , 0.279	Depositor DCC
R_{free} test set	2310 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	27.1	Xtriage
Anisotropy	0.212	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 22.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.040 for k,-h,l 0.040 for -k,h,l 0.163 for h,-k,-l 0.477 for -h,k,-l 0.160 for -h,-k,l 0.039 for k,h,-l 0.044 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	15912	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.49% 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

Bond lengths and bond angles in the following residue types are not validated in this section: NA, SCN, CL

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	0.65	0/3807	1.00	8/5135 (0.2%)
1	B	0.67	0/3860	1.06	18/5210 (0.3%)
1	C	0.63	0/3793	1.01	11/5116 (0.2%)
1	D	0.66	0/3860	1.04	11/5210 (0.2%)
All	All	0.65	0/15320	1.03	48/20671 (0.2%)

There are no bond length outliers.

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	561	ARG	NE-CZ-NH1	8.96	124.78	120.30
1	C	690	GLY	N-CA-C	-8.75	91.22	113.10
1	B	561	ARG	NE-CZ-NH1	8.01	124.31	120.30
1	B	354	ARG	NE-CZ-NH2	7.54	124.07	120.30
1	B	493	ARG	NE-CZ-NH2	7.50	124.05	120.30
1	D	367	ARG	NE-CZ-NH2	7.34	123.97	120.30
1	B	493	ARG	NE-CZ-NH1	-7.27	116.67	120.30
1	D	561	ARG	NE-CZ-NH2	-6.94	116.83	120.30
1	A	354	ARG	NE-CZ-NH1	6.80	123.70	120.30
1	D	606	ARG	NE-CZ-NH1	6.75	123.67	120.30
1	D	486	GLY	N-CA-C	-6.53	96.77	113.10
1	B	606	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	A	353	THR	N-CA-C	-6.32	93.94	111.00
1	D	360	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	C	610	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	C	738	ARG	NE-CZ-NH1	-6.09	117.25	120.30
1	B	542	ARG	NE-CZ-NH1	5.97	123.29	120.30
1	B	515	VAL	CB-CA-C	-5.94	100.12	111.40
1	C	511	LEU	CA-CB-CG	5.91	128.90	115.30
1	B	561	ARG	NE-CZ-NH2	-5.91	117.34	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	841	ARG	NE-CZ-NH1	-5.87	117.37	120.30
1	D	803	ARG	NE-CZ-NH2	5.83	123.22	120.30
1	D	834	ARG	NE-CZ-NH2	5.70	123.15	120.30
1	A	638	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	B	541	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	C	834	ARG	NE-CZ-NH2	-5.57	117.51	120.30
1	B	341	ASP	CB-CG-OD1	5.54	123.28	118.30
1	B	834	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	C	542	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	C	542	ARG	NE-CZ-NH2	-5.51	117.55	120.30
1	B	339	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	A	610	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	C	824	ASP	CB-CG-OD2	-5.28	113.55	118.30
1	D	394	SER	C-N-CA	5.27	134.87	121.70
1	B	499	TYR	CB-CG-CD1	-5.24	117.86	121.00
1	B	606	ARG	NE-CZ-NH1	5.23	122.91	120.30
1	D	606	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	B	354	ARG	NE-CZ-NH1	-5.15	117.72	120.30
1	B	575	MET	CA-CB-CG	5.14	122.03	113.30
1	B	389	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	C	610	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	C	694	ILE	N-CA-C	-5.10	97.24	111.00
1	A	638	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	C	354	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	A	715	ARG	NE-CZ-NH1	-5.06	117.77	120.30
1	D	712	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	A	376	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	A	827	GLY	CA-C-N	-5.01	106.17	117.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3705	0	3580	98	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3756	0	3628	98	0
1	C	3692	0	3572	84	0
1	D	3756	0	3628	113	2
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	D	1	0	0	0	0
3	C	3	0	0	0	0
4	D	1	0	0	0	0
5	A	273	0	0	2	0
5	B	229	0	0	1	0
5	C	235	0	0	2	0
5	D	259	0	0	3	0
All	All	15912	0	14408	381	2

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 13.

All (381) 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:668:LEU:HD11	1:A:670:LEU:HD21	1.32	1.09
1:C:673:ILE:HG23	1:C:692:GLU:HA	1.34	1.08
1:A:668:LEU:CD1	1:A:670:LEU:CD2	2.32	1.08
1:A:668:LEU:CD1	1:A:670:LEU:HD22	1.87	1.03
1:B:335:GLY:HA3	1:B:351:HIS:HB2	1.40	1.02
1:A:668:LEU:HD11	1:A:670:LEU:CD2	1.91	0.99
1:D:675:ASP:OD2	1:D:682:VAL:O	1.86	0.93
1:D:485:GLN:HE22	1:D:489:GLY:CA	1.82	0.90
1:D:697:THR:HA	1:D:700:ASN:HD21	1.35	0.89
1:B:340:THR:HG23	1:C:556:TYR:HB2	1.56	0.86
1:D:487:SER:O	1:D:489:GLY:N	2.09	0.85
1:B:393:GLN:HE21	1:B:486:GLY:HA2	1.43	0.83
1:C:673:ILE:CG2	1:C:692:GLU:HA	2.08	0.82
1:D:487:SER:C	1:D:489:GLY:H	1.83	0.82
1:D:485:GLN:HE22	1:D:489:GLY:N	1.81	0.79
1:C:686:GLU:OE1	1:C:690:GLY:O	2.02	0.78
1:D:485:GLN:HE22	1:D:489:GLY:HA2	1.46	0.78
1:A:798:VAL:HG11	1:A:821:PHE:CE1	2.19	0.77
1:C:671:TYR:HB3	1:C:692:GLU:O	1.84	0.76
1:A:668:LEU:HD12	1:A:670:LEU:HD22	1.68	0.75
1:A:828:LYS:HD2	1:A:831:TRP:CD1	2.22	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:546:ILE:CD1	1:A:563:TRP:HB2	2.17	0.74
1:A:668:LEU:HD12	1:A:670:LEU:CD2	2.18	0.73
1:B:523:THR:HG21	1:C:392:TYR:CD2	2.24	0.73
1:D:343:ARG:HD3	1:D:345:ARG:HG3	1.69	0.72
1:A:662:ASN:O	1:A:663:LEU:HD22	1.89	0.72
1:A:663:LEU:HD22	1:A:698:GLU:OE2	1.91	0.71
1:B:515:VAL:HG23	1:B:542:ARG:HB2	1.72	0.70
1:C:588:CYS:SG	1:C:647:ILE:HA	2.33	0.68
1:A:588:CYS:SG	1:A:647:ILE:HG22	2.34	0.68
1:C:391:LEU:HD13	1:C:499:TYR:CE1	2.29	0.67
1:D:485:GLN:NE2	1:D:489:GLY:N	2.42	0.67
1:B:335:GLY:CA	1:B:351:HIS:HB2	2.22	0.67
1:A:341:ASP:HB2	1:A:345:ARG:O	1.95	0.67
1:A:827:GLY:HA2	1:A:828:LYS:HE2	1.75	0.67
1:B:340:THR:HG23	1:C:556:TYR:CB	2.25	0.67
1:B:638:ARG:HG3	1:B:639:PRO:HD2	1.77	0.67
1:A:546:ILE:HD13	1:A:563:TRP:HB2	1.77	0.67
1:D:583:GLY:HA3	1:D:587:TYR:HB3	1.77	0.66
1:A:841:ARG:NH1	1:C:689:GLU:OE1	2.28	0.66
1:D:536:LYS:O	1:D:539:ASP:HB2	1.94	0.66
1:A:747:LEU:HD11	1:A:752:MET:HG2	1.75	0.66
1:D:487:SER:C	1:D:489:GLY:N	2.47	0.66
1:D:726:ASP:O	1:D:730:GLU:HG3	1.95	0.66
1:D:675:ASP:OD1	1:D:676:MET:N	2.28	0.66
1:D:804:LEU:HD22	1:D:805:PRO:CD	2.26	0.66
1:D:343:ARG:O	1:D:345:ARG:N	2.29	0.65
1:A:353:THR:HG23	1:A:369:TYR:CE2	2.32	0.65
1:C:798:VAL:HG11	1:C:821:PHE:CD1	2.32	0.65
1:D:487:SER:O	1:D:490:ALA:N	2.22	0.65
1:A:353:THR:HG23	1:A:369:TYR:CD2	2.32	0.64
1:C:691:GLY:O	1:C:693:SER:N	2.29	0.64
1:D:662:ASN:N	1:D:662:ASN:HD22	1.94	0.64
1:B:651:PHE:HZ	1:B:708:LEU:HD22	1.64	0.63
1:D:662:ASN:HD21	1:D:701:LYS:NZ	1.96	0.63
1:D:644:LEU:HB2	1:D:652:TYR:HD1	1.62	0.63
1:D:852:GLN:O	1:D:856:LYS:HG3	1.99	0.63
1:B:633:ARG:HD3	1:B:713:PHE:CE2	2.35	0.62
1:D:696:VAL:HG13	1:D:697:THR:H	1.64	0.62
1:C:496:ARG:NH2	1:C:496:ARG:HB3	2.14	0.62
1:D:486:GLY:H	1:D:488:PRO:HD2	1.64	0.62
1:A:353:THR:CG2	1:A:369:TYR:CE2	2.83	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:660:GLU:O	1:A:662:ASN:N	2.33	0.62
1:B:501:GLN:HA	1:B:501:GLN:HE21	1.65	0.61
1:D:684:THR:O	1:D:684:THR:HG23	2.01	0.61
1:A:522:GLN:NE2	5:A:1001:HOH:O	2.33	0.61
1:A:794:LEU:HD13	1:A:861:ILE:HD11	1.83	0.61
1:B:678:ILE:C	1:B:678:ILE:HD12	2.21	0.60
1:C:624:THR:HG21	1:C:626:PHE:CZ	2.35	0.60
1:A:546:ILE:HD12	1:A:563:TRP:CG	2.36	0.60
1:D:343:ARG:HD3	1:D:345:ARG:CG	2.31	0.60
1:D:696:VAL:HG22	1:D:697:THR:HG22	1.82	0.60
1:B:501:GLN:HG3	1:B:739:TYR:CE2	2.36	0.60
1:A:676:MET:HB3	1:A:685:HIS:HE1	1.66	0.60
1:B:633:ARG:HD3	1:B:713:PHE:CZ	2.37	0.60
1:B:501:GLN:HA	1:B:501:GLN:NE2	2.16	0.59
1:A:535:MET:HG3	5:A:1003:HOH:O	2.03	0.59
1:D:362:THR:O	1:D:366:VAL:HG23	2.03	0.58
1:A:672:PHE:CZ	1:A:704:TYR:HB2	2.39	0.58
1:B:339:ARG:NH1	1:C:557:GLY:HA3	2.19	0.58
1:B:573:ASN:OD1	1:B:575:MET:HG2	2.02	0.58
1:C:350:ASP:HB3	1:C:355:THR:HG22	1.85	0.58
1:D:485:GLN:NE2	1:D:488:PRO:C	2.57	0.58
1:D:677:GLU:HG3	5:D:1062:HOH:O	2.03	0.58
1:B:632:LYS:HE2	1:B:742:GLU:OE2	2.03	0.58
1:C:672:PHE:CZ	1:C:704:TYR:HB2	2.39	0.58
1:C:711:TRP:CH2	1:C:715:ARG:HD2	2.39	0.58
1:D:578:LEU:HD11	1:D:604:TYR:HB3	1.86	0.58
1:A:375:GLN:O	1:A:379:LEU:HG	2.02	0.57
1:A:588:CYS:SG	1:A:647:ILE:HA	2.44	0.57
1:D:386:PHE:O	1:D:389:ARG:HG3	2.04	0.57
1:A:712:ARG:HD3	1:A:712:ARG:O	2.04	0.57
1:D:487:SER:HB2	1:D:488:PRO:HD3	1.84	0.57
1:A:663:LEU:CD2	1:A:698:GLU:OE2	2.52	0.57
1:C:798:VAL:HG11	1:C:821:PHE:CE1	2.39	0.57
1:D:671:TYR:HA	1:D:695:ARG:O	2.05	0.57
1:A:624:THR:HG21	1:A:626:PHE:CZ	2.40	0.57
1:A:798:VAL:HG11	1:A:821:PHE:HE1	1.66	0.56
1:B:675:ASP:HA	1:B:684:THR:HA	1.87	0.56
1:C:376:ARG:O	1:C:379:LEU:HB2	2.05	0.56
1:B:701:LYS:O	1:B:704:TYR:HB3	2.05	0.56
1:A:594:ALA:HB1	1:A:679:LEU:HD21	1.86	0.56
1:B:353:THR:CG2	1:B:369:TYR:CD2	2.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:644:LEU:HD23	1:D:713:PHE:CZ	2.41	0.56
1:A:537:PRO:HB3	1:A:730:GLU:HB3	1.87	0.56
1:D:683:THR:OG1	1:D:684:THR:N	2.37	0.56
1:B:651:PHE:CZ	1:B:708:LEU:HD22	2.42	0.55
1:C:673:ILE:HG22	1:C:685:HIS:O	2.07	0.55
1:B:543:ARG:NH2	1:B:545:TYR:OH	2.40	0.55
1:A:555:ASP:OD1	1:A:559:ILE:HB	2.06	0.55
1:C:689:GLU:HG2	1:C:690:GLY:N	2.22	0.55
1:A:798:VAL:HG11	1:A:821:PHE:CD1	2.41	0.55
1:A:668:LEU:HD13	1:A:670:LEU:HD22	1.83	0.55
1:B:588:CYS:SG	1:B:647:ILE:HA	2.47	0.55
1:D:804:LEU:HD22	1:D:805:PRO:HD2	1.88	0.54
1:D:697:THR:OG1	1:D:698:GLU:N	2.40	0.54
1:C:496:ARG:HH12	1:C:500:HIS:CE1	2.24	0.54
1:B:492:ASP:N	1:B:492:ASP:OD1	2.40	0.54
1:A:555:ASP:O	1:A:556:TYR:HB2	2.07	0.54
1:C:793:ARG:HG2	1:C:861:ILE:HG22	1.90	0.54
1:A:634:MET:HA	1:A:725:LEU:HD21	1.89	0.54
1:D:676:MET:HG2	1:D:715:ARG:HD2	1.88	0.54
1:B:353:THR:HG21	1:B:369:TYR:CD2	2.43	0.54
1:C:537:PRO:HD3	1:C:610:ARG:NH2	2.23	0.53
1:B:530:GLN:HG3	1:B:531:GLN:N	2.24	0.53
1:C:632:LYS:HE3	1:C:742:GLU:HG2	1.91	0.53
1:A:665:GLU:OE1	1:A:665:GLU:N	2.42	0.53
1:C:689:GLU:O	1:C:691:GLY:N	2.42	0.53
1:D:793:ARG:HG2	1:D:861:ILE:HG23	1.90	0.53
1:B:590:GLN:HE22	1:B:712:ARG:HH22	1.57	0.53
1:C:496:ARG:HH21	1:C:496:ARG:HB3	1.73	0.53
1:C:793:ARG:HG2	1:C:861:ILE:CG2	2.39	0.53
1:B:495:PHE:CE2	1:B:747:LEU:HD23	2.43	0.53
1:D:358:TRP:O	1:D:597:ILE:CD1	2.57	0.53
1:A:813:ILE:HA	1:A:818:PRO:HA	1.91	0.53
1:B:378:GLN:HA	1:D:509:ASN:OD1	2.09	0.53
1:A:789:GLU:HA	1:A:792:ILE:HD12	1.91	0.53
1:D:336:TRP:CH2	1:D:348:TYR:CE2	2.97	0.52
1:D:515:VAL:HG22	1:D:542:ARG:HB2	1.91	0.52
1:C:515:VAL:HG11	1:C:539:ASP:O	2.09	0.52
1:D:662:ASN:ND2	1:D:662:ASN:N	2.57	0.52
1:D:671:TYR:O	1:D:672:PHE:CD1	2.62	0.52
1:A:547:ILE:O	1:A:547:ILE:HG13	2.10	0.52
1:B:734:LEU:O	1:B:738:ARG:NH1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:779:PHE:O	1:D:783:VAL:HG23	2.09	0.52
1:C:525:PHE:HE2	1:C:571:VAL:HG12	1.74	0.52
1:A:686:GLU:HB3	1:A:688:LYS:O	2.11	0.51
1:A:678:ILE:O	1:A:678:ILE:CG2	2.59	0.51
1:D:644:LEU:HB2	1:D:652:TYR:CD1	2.43	0.51
1:B:616:LEU:HD13	1:B:737:LEU:HD21	1.92	0.51
1:B:633:ARG:CD	1:B:713:PHE:CZ	2.93	0.51
1:D:673:ILE:O	1:D:685:HIS:O	2.28	0.51
1:D:697:THR:HA	1:D:700:ASN:ND2	2.15	0.51
1:B:521:ARG:NH1	1:B:551:GLU:OE2	2.40	0.50
1:D:685:HIS:O	1:D:686:GLU:HB2	2.11	0.50
1:A:631:TYR:CE2	1:A:746:GLU:HG3	2.47	0.50
1:C:631:TYR:CE2	1:C:746:GLU:HG3	2.47	0.50
1:D:393:GLN:O	1:D:394:SER:OG	2.26	0.50
1:A:678:ILE:O	1:A:678:ILE:HG23	2.11	0.50
1:D:343:ARG:NH2	1:D:600:ASP:OD1	2.42	0.50
1:A:616:LEU:HD13	1:A:749:LEU:HG	1.93	0.50
1:B:342:PRO:O	1:B:344:GLY:N	2.43	0.50
1:B:390:PHE:O	1:B:752:MET:HB2	2.11	0.50
1:D:675:ASP:N	1:D:685:HIS:O	2.40	0.50
1:A:555:ASP:O	1:A:556:TYR:CB	2.60	0.50
1:A:661:ASN:O	1:A:662:ASN:C	2.48	0.50
1:C:581:TYR:CE1	1:C:589:LEU:HB2	2.47	0.50
1:B:520:SER:HB2	1:B:549:ARG:HH12	1.76	0.49
1:D:337:GLU:HB3	1:D:349:VAL:HB	1.94	0.49
1:D:587:TYR:CD2	1:D:815:SER:HA	2.47	0.49
1:B:490:ALA:O	1:B:497:TRP:NE1	2.46	0.49
1:A:828:LYS:CD	1:A:831:TRP:CD1	2.94	0.49
1:C:530:GLN:HB2	5:C:1028:HOH:O	2.10	0.49
1:B:672:PHE:CD1	1:B:694:ILE:HG22	2.46	0.49
1:B:501:GLN:HG2	1:B:739:TYR:CZ	2.46	0.49
1:C:587:TYR:CD2	1:C:815:SER:HA	2.48	0.49
1:B:594:ALA:HA	1:B:678:ILE:HD13	1.95	0.49
1:B:645:GLU:HG2	1:B:838:CYS:SG	2.52	0.49
1:C:355:THR:HG21	1:C:365:TYR:OH	2.12	0.49
1:C:689:GLU:C	1:C:691:GLY:N	2.65	0.49
1:D:355:THR:HG23	1:D:575:MET:HG2	1.95	0.49
1:C:353:THR:HG23	1:C:366:VAL:HG22	1.94	0.49
1:D:486:GLY:N	1:D:488:PRO:HD2	2.26	0.49
1:D:769:TYR:CD2	1:D:776:ILE:HD11	2.47	0.49
1:A:544:LEU:O	1:A:545:TYR:CD1	2.66	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:353:THR:O	1:C:354:ARG:HB3	2.13	0.49
1:C:371:GLN:O	1:C:375:GLN:HB2	2.13	0.49
1:D:336:TRP:CZ3	1:D:348:TYR:CD2	3.01	0.49
1:D:497:TRP:CH2	1:D:501:GLN:HG3	2.48	0.48
1:D:675:ASP:OD2	1:D:682:VAL:C	2.51	0.48
1:C:597:ILE:HB	1:C:679:LEU:HD11	1.94	0.48
1:B:828:LYS:HD2	1:B:828:LYS:N	2.28	0.48
1:D:741:ASP:HB2	1:D:742:GLU:OE2	2.14	0.48
1:A:353:THR:HG22	1:A:354:ARG:H	1.78	0.48
1:C:375:GLN:NE2	1:C:375:GLN:O	2.45	0.48
1:D:765:ILE:HD12	1:D:766:TYR:N	2.29	0.48
1:B:833:PRO:HD2	1:B:860:ALA:HB2	1.95	0.48
1:C:525:PHE:CE2	1:C:571:VAL:HG12	2.48	0.48
1:A:372:TRP:HZ3	1:A:569:HIS:O	1.97	0.47
1:A:691:GLY:HA2	1:A:694:ILE:HG23	1.96	0.47
1:A:822:CYS:HB3	1:A:841:ARG:HG3	1.96	0.47
1:C:614:MET:O	1:C:618:HIS:CD2	2.67	0.47
1:D:531:GLN:O	1:D:535:MET:HG2	2.13	0.47
1:A:520:SER:HB2	1:A:523:THR:OG1	2.15	0.47
1:B:852:GLN:O	1:B:856:LYS:HG3	2.14	0.47
1:D:760:TRP:O	1:D:764:THR:OG1	2.27	0.47
1:D:834:ARG:HG3	1:D:834:ARG:HH21	1.79	0.47
1:A:605:PHE:O	1:A:724:PHE:HA	2.14	0.47
1:D:392:TYR:CE2	1:D:496:ARG:HG3	2.50	0.47
1:B:340:THR:O	1:B:345:ARG:O	2.33	0.47
1:B:638:ARG:HA	1:B:638:ARG:HE	1.79	0.47
1:B:678:ILE:O	1:B:678:ILE:HD12	2.15	0.47
1:B:798:VAL:HG11	1:B:821:PHE:CD1	2.49	0.47
1:D:533:MET:CE	1:D:606:ARG:HD2	2.45	0.47
1:B:657:TRP:C	1:B:657:TRP:CD1	2.88	0.47
1:A:353:THR:CG2	1:A:369:TYR:CD2	2.96	0.47
1:B:523:THR:OG1	1:C:496:ARG:CD	2.63	0.47
1:D:364:GLU:HG3	1:D:368:ASN:OD1	2.15	0.47
1:A:757:MET:SD	1:A:783:VAL:HG12	2.55	0.46
1:C:819:GLN:NE2	1:C:839:PHE:HB3	2.31	0.46
1:D:630:PHE:CZ	1:D:724:PHE:CE2	3.03	0.46
1:B:798:VAL:HG11	1:B:821:PHE:CE1	2.51	0.46
1:A:567:LEU:HD23	1:A:611:PHE:CE1	2.50	0.46
1:B:676:MET:HG3	1:B:678:ILE:HG22	1.96	0.46
1:D:335:GLY:CA	1:D:351:HIS:HB2	2.45	0.46
1:A:770:THR:O	1:A:776:ILE:HG13	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:393:GLN:NE2	1:B:486:GLY:HA2	2.22	0.46
1:B:501:GLN:CG	1:B:739:TYR:CZ	2.98	0.46
1:C:358:TRP:CD2	1:C:599:PRO:HD2	2.51	0.46
1:C:369:TYR:O	1:C:372:TRP:HD1	1.99	0.46
1:B:594:ALA:O	1:B:597:ILE:HG22	2.15	0.46
1:B:392:TYR:CE2	1:B:496:ARG:HG3	2.50	0.46
1:B:523:THR:OG1	1:C:496:ARG:HD2	2.16	0.46
1:C:521:ARG:NH1	1:C:551:GLU:OE1	2.37	0.46
1:B:778:TRP:HB3	1:B:853:LEU:HD22	1.98	0.46
1:C:515:VAL:HG13	1:C:542:ARG:HB2	1.97	0.46
1:D:754:GLU:HG2	5:D:1116:HOH:O	2.15	0.46
1:A:348:TYR:CE2	1:A:360:ARG:HG3	2.51	0.46
1:B:702:GLU:O	1:B:705:ILE:HG12	2.16	0.46
1:D:335:GLY:HA2	1:D:351:HIS:HB2	1.98	0.46
1:D:357:THR:HG23	1:D:359:GLN:O	2.16	0.46
1:B:347:TYR:CD2	1:B:356:THR:HG23	2.51	0.45
1:A:524:LEU:HD22	1:A:566:LEU:HB3	1.98	0.45
1:A:852:GLN:O	1:A:856:LYS:HG2	2.16	0.45
1:B:506:CYS:HG	1:B:617:TYR:HD1	1.63	0.45
1:B:515:VAL:CG2	1:B:539:ASP:O	2.65	0.45
1:D:350:ASP:O	1:D:353:THR:O	2.33	0.45
1:B:380:GLN:NE2	1:D:735:GLU:HG2	2.31	0.45
1:D:815:SER:HB3	1:D:838:CYS:HB3	1.98	0.45
1:D:357:THR:OG1	1:D:359:GLN:HG2	2.16	0.45
1:B:374:SER:O	1:B:378:GLN:NE2	2.49	0.45
1:C:584:LYS:O	1:C:586:ASN:N	2.48	0.45
1:C:624:THR:HG21	1:C:626:PHE:CE2	2.52	0.45
1:A:676:MET:HB3	1:A:685:HIS:CE1	2.50	0.45
1:B:524:LEU:HD23	1:B:570:GLU:HG3	1.98	0.45
1:C:664:GLU:HG3	1:C:665:GLU:H	1.82	0.45
1:D:584:LYS:O	1:D:585:ASN:HB2	2.17	0.45
1:D:673:ILE:HD11	1:D:711:TRP:CZ3	2.52	0.45
1:A:741:ASP:HB2	1:A:742:GLU:OE2	2.16	0.45
1:C:632:LYS:HG3	1:C:742:GLU:CG	2.46	0.45
1:D:391:LEU:HA	1:D:391:LEU:HD23	1.92	0.45
1:A:524:LEU:CD2	1:A:566:LEU:HB3	2.47	0.45
1:C:739:TYR:CE1	1:D:493:ARG:HD2	2.51	0.45
1:B:624:THR:HG21	1:B:626:PHE:CZ	2.51	0.45
1:B:823:ILE:HG12	1:B:842:LEU:HD23	1.98	0.45
1:A:546:ILE:CD1	1:A:563:TRP:CG	3.00	0.44
1:A:616:LEU:HD11	1:A:748:MET:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:511:LEU:HB2	1:B:542:ARG:HG2	2.00	0.44
1:A:355:THR:HG23	1:A:575:MET:HG3	2.00	0.44
1:B:582:ALA:HB3	1:B:647:ILE:O	2.17	0.44
1:D:485:GLN:NE2	1:D:489:GLY:HA2	2.25	0.44
1:A:567:LEU:HA	1:A:570:GLU:HB2	1.99	0.44
1:C:672:PHE:CD2	1:C:688:LYS:HE2	2.53	0.44
1:A:372:TRP:HH2	1:A:570:GLU:HA	1.82	0.44
1:B:348:TYR:N	1:B:348:TYR:CD1	2.85	0.44
1:B:340:THR:CG2	1:C:556:TYR:HB2	2.37	0.44
1:C:383:MET:CE	1:C:565:PHE:HB3	2.47	0.44
1:A:546:ILE:HD12	1:A:563:TRP:CD1	2.53	0.44
1:B:353:THR:HG22	1:B:355:THR:HG23	1.99	0.44
1:C:839:PHE:O	1:C:840:ASN:HB2	2.16	0.44
1:D:568:SER:OG	1:D:622:ILE:HB	2.17	0.44
1:B:336:TRP:CD1	1:B:361:PRO:HD2	2.53	0.43
1:C:757:MET:SD	1:C:783:VAL:HG12	2.58	0.43
1:D:335:GLY:O	1:D:336:TRP:CB	2.66	0.43
1:D:672:PHE:HB3	1:D:688:LYS:CG	2.48	0.43
1:C:512:PRO:O	1:C:513:SER:HB3	2.17	0.43
1:D:514:HIS:HA	1:D:542:ARG:HB3	1.99	0.43
1:B:633:ARG:HG2	1:B:713:PHE:CZ	2.52	0.43
1:C:690:GLY:O	1:C:691:GLY:O	2.37	0.43
1:D:687:LEU:O	1:D:688:LYS:HB2	2.18	0.43
1:A:655:ILE:HG23	1:A:705:ILE:HG12	2.00	0.43
1:C:527:ASP:O	1:C:531:GLN:HG3	2.18	0.43
1:D:644:LEU:HD23	1:D:713:PHE:CE2	2.53	0.43
1:D:691:GLY:HA2	1:D:694:ILE:HD12	1.98	0.43
1:B:676:MET:O	1:B:682:VAL:HA	2.18	0.43
1:C:804:LEU:HD21	1:C:809:PHE:CZ	2.54	0.43
1:D:353:THR:O	1:D:355:THR:N	2.51	0.43
1:A:339:ARG:HD3	1:A:339:ARG:HA	1.83	0.43
1:B:632:LYS:HE2	1:B:742:GLU:HG2	1.99	0.43
1:D:662:ASN:HD21	1:D:701:LYS:HZ3	1.64	0.43
1:D:498:LYS:NZ	5:D:1003:HOH:O	2.48	0.43
1:D:646:SER:O	1:D:647:ILE:HG23	2.18	0.43
1:B:672:PHE:CE1	1:B:694:ILE:HG22	2.53	0.43
1:D:700:ASN:HD22	1:D:700:ASN:C	2.22	0.43
1:D:752:MET:HE3	1:D:792:ILE:HD12	2.01	0.43
1:D:393:GLN:O	1:D:394:SER:CB	2.67	0.43
1:D:491:TYR:CE1	1:D:493:ARG:HA	2.54	0.43
1:A:657:TRP:O	1:A:661:ASN:HB2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:546:ILE:CD1	1:A:563:TRP:CB	2.92	0.42
1:D:345:ARG:HA	1:D:345:ARG:NH2	2.33	0.42
1:A:518:SER:HB3	1:A:547:ILE:HD11	2.01	0.42
1:A:588:CYS:SG	1:A:647:ILE:CB	3.08	0.42
1:C:722:LYS:HD3	1:C:726:ASP:OD2	2.19	0.42
1:A:811:GLU:OE2	1:C:695:ARG:NH1	2.52	0.42
1:B:587:TYR:CD2	1:B:815:SER:HA	2.54	0.42
1:D:598:ASN:C	1:D:598:ASN:OD1	2.57	0.42
1:B:347:TYR:CE2	1:B:356:THR:HG23	2.54	0.42
1:B:811:GLU:O	1:B:812:LEU:C	2.56	0.42
1:C:664:GLU:HG3	1:C:665:GLU:N	2.35	0.42
1:C:752:MET:HG2	1:C:792:ILE:HD13	2.02	0.42
1:B:492:ASP:C	1:B:494:SER:H	2.21	0.42
1:B:506:CYS:SG	1:B:617:TYR:CD1	3.13	0.42
1:C:370:GLU:HA	1:C:373:GLN:HB2	2.01	0.42
1:B:726:ASP:O	1:B:730:GLU:HG3	2.20	0.42
1:C:628:LEU:N	1:C:629:PRO:CD	2.82	0.42
1:C:662:ASN:O	1:C:665:GLU:HG2	2.19	0.42
1:C:740:PHE:CE2	1:C:748:MET:HE1	2.55	0.42
1:C:494:SER:OG	1:C:496:ARG:HB2	2.20	0.42
1:A:372:TRP:CZ3	1:A:569:HIS:O	2.73	0.41
1:A:572:LEU:HD21	1:A:624:THR:HG23	2.02	0.41
1:B:343:ARG:NH2	5:B:1003:HOH:O	2.53	0.41
1:B:813:ILE:HA	1:B:818:PRO:HA	2.02	0.41
1:A:690:GLY:O	1:A:693:SER:HB2	2.20	0.41
1:B:360:ARG:O	1:B:362:THR:HG23	2.19	0.41
1:D:351:HIS:H	1:D:351:HIS:CD2	2.38	0.41
1:D:785:GLU:OE2	1:D:850:TYR:OH	2.38	0.41
1:A:525:PHE:CE2	1:A:571:VAL:HG12	2.55	0.41
1:A:648:ASP:HB3	1:A:651:PHE:HB3	2.02	0.41
1:D:336:TRP:CZ3	1:D:348:TYR:CE2	3.09	0.41
1:A:593:PRO:HB3	1:A:716:GLY:HA3	2.03	0.41
1:D:834:ARG:HG3	1:D:834:ARG:NH2	2.34	0.41
1:A:804:LEU:HD12	1:A:805:PRO:HD2	2.03	0.41
1:B:742:GLU:HG3	1:B:742:GLU:H	1.50	0.41
1:D:335:GLY:HA3	1:D:351:HIS:N	2.35	0.41
1:A:539:ASP:HA	1:A:542:ARG:HE	1.84	0.41
1:D:355:THR:HG23	1:D:575:MET:HE3	2.01	0.41
1:A:679:LEU:HD23	1:A:679:LEU:HA	1.92	0.41
1:A:606:ARG:HA	1:A:723:ALA:O	2.21	0.41
1:B:549:ARG:O	1:B:551:GLU:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:750:CYS:SG	1:D:803:ARG:HD2	2.61	0.41
1:A:355:THR:HG23	1:A:575:MET:CE	2.51	0.41
1:B:511:LEU:CB	1:B:542:ARG:HG2	2.50	0.41
1:B:675:ASP:N	1:B:675:ASP:OD1	2.54	0.41
1:C:581:TYR:HB2	1:C:585:ASN:HA	2.03	0.41
1:D:485:GLN:HG2	1:D:500:HIS:CE1	2.56	0.41
1:D:511:LEU:HD23	1:D:511:LEU:HA	1.91	0.41
1:B:510:ALA:HA	1:B:617:TYR:OH	2.21	0.41
1:B:679:LEU:H	1:B:679:LEU:HD12	1.85	0.41
1:A:588:CYS:SG	1:A:647:ILE:CG2	3.06	0.41
1:C:531:GLN:NE2	5:C:1004:HOH:O	2.54	0.41
1:C:604:TYR:O	1:C:608:ILE:HG13	2.21	0.41
1:C:564:PHE:CE2	1:C:615:ALA:HA	2.55	0.41
1:C:632:LYS:HG3	1:C:742:GLU:HG2	2.03	0.41
1:D:335:GLY:HA2	1:D:351:HIS:CD2	2.56	0.41
1:B:697:THR:O	1:B:701:LYS:HG3	2.21	0.41
1:B:609:GLY:O	1:B:728:PHE:HA	2.21	0.41
1:D:505:LEU:HD21	1:D:736:TRP:CD1	2.56	0.41
1:D:798:VAL:HA	1:D:835:SER:HB2	2.03	0.41
1:A:355:THR:HG21	1:A:365:TYR:OH	2.21	0.40
1:A:655:ILE:HD11	1:A:708:LEU:HD13	2.03	0.40
1:B:505:LEU:HD12	1:B:505:LEU:HA	1.89	0.40
1:C:383:MET:HE2	1:C:565:PHE:CD2	2.57	0.40
1:A:518:SER:HA	1:A:547:ILE:HG12	2.03	0.40
1:B:355:THR:HG21	1:B:369:TYR:CZ	2.56	0.40
1:B:777:GLN:O	1:B:781:GLN:HG3	2.21	0.40
1:C:555:ASP:HB2	1:C:559:ILE:HD12	2.03	0.40
1:D:606:ARG:HA	1:D:723:ALA:O	2.21	0.40
1:C:560:ALA:O	1:C:564:PHE:HD1	2.04	0.40
1:C:737:LEU:O	1:C:740:PHE:HD2	2.04	0.40
1:A:389:ARG:HD2	1:A:750:CYS:O	2.21	0.40
1:C:665:GLU:O	1:C:665:GLU:HG3	2.22	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:770:THR:OG1	1:D:674:GLN:NE2[1_554]	1.54	0.66
1:A:356:THR:N	1:D:398:SER:OG[1_455]	1.92	0.28

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	432/447 (97%)	391 (90%)	34 (8%)	7 (2%)	9	19
1	B	443/447 (99%)	394 (89%)	37 (8%)	12 (3%)	5	8
1	C	431/447 (96%)	396 (92%)	25 (6%)	10 (2%)	6	11
1	D	443/447 (99%)	387 (87%)	39 (9%)	17 (4%)	3	4
All	All	1749/1788 (98%)	1568 (90%)	135 (8%)	46 (3%)	5	9

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	663	LEU
1	A	666	CYS
1	B	360	ARG
1	B	494	SER
1	C	585	ASN
1	C	829	GLU
1	D	344	GLY
1	D	394	SER
1	D	397	ALA
1	D	487	SER
1	D	675	ASP
1	D	698	GLU
1	A	354	ARG
1	A	555	ASP
1	A	661	ASN
1	B	585	ASN
1	B	678	ILE
1	B	691	GLY
1	C	513	SER
1	C	716	GLY
1	C	738	ARG
1	D	395	SER

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Mol	Chain	Res	Type
1	D	488	PRO
1	D	585	ASN
1	D	668	LEU
1	D	686	GLU
1	D	696	VAL
1	A	338	LYS
1	B	487	SER
1	B	550	GLY
1	C	692	GLU
1	C	863	GLU
1	D	354	ARG
1	D	362	THR
1	D	663	LEU
1	A	585	ASN
1	B	342	PRO
1	B	361	PRO
1	B	490	ALA
1	C	346	PHE
1	C	352	ASN
1	B	666	CYS
1	B	737	LEU
1	D	336	TRP
1	C	361	PRO
1	D	647	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	400/406 (98%)	345 (86%)	55 (14%)	3	6
1	B	405/406 (100%)	344 (85%)	61 (15%)	3	4
1	C	399/406 (98%)	359 (90%)	40 (10%)	7	14
1	D	405/406 (100%)	339 (84%)	66 (16%)	2	3
All	All	1609/1624 (99%)	1387 (86%)	222 (14%)	3	6

All (222) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	337	GLU
1	A	354	ARG
1	A	358	TRP
1	A	360	ARG
1	A	362	THR
1	A	364	GLU
1	A	372	TRP
1	A	373	GLN
1	A	374	SER
1	A	376	ARG
1	A	378	GLN
1	A	380	GLN
1	A	387	SER
1	A	491	TYR
1	A	494	SER
1	A	496	ARG
1	A	503	ARG
1	A	505	LEU
1	A	514	HIS
1	A	518	SER
1	A	520	SER
1	A	530	GLN
1	A	543	ARG
1	A	544	LEU
1	A	546	ILE
1	A	562	GLU
1	A	566	LEU
1	A	601	HIS
1	A	637	LYS
1	A	638	ARG
1	A	662	ASN
1	A	663	LEU
1	A	664	GLU
1	A	665	GLU
1	A	668	LEU
1	A	675	ASP
1	A	681	LYS
1	A	684	THR
1	A	694	ILE
1	A	698	GLU
1	A	699	GLU
1	A	708	LEU

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Mol	Chain	Res	Type
1	A	712	ARG
1	A	715	ARG
1	A	735	GLU
1	A	742	GLU
1	A	757	MET
1	A	770	THR
1	A	772	ASN
1	A	773	SER
1	A	813	ILE
1	A	828	LYS
1	A	834	ARG
1	A	848	LYS
1	A	858	LEU
1	B	341	ASP
1	B	343	ARG
1	B	358	TRP
1	B	372	TRP
1	B	374	SER
1	B	375	GLN
1	B	379	LEU
1	B	383	MET
1	B	384	GLN
1	B	388	GLN
1	B	389	ARG
1	B	391	LEU
1	B	493	ARG
1	B	494	SER
1	B	503	ARG
1	B	508	SER
1	B	511	LEU
1	B	517	ILE
1	B	522	GLN
1	B	523	THR
1	B	530	GLN
1	B	533	MET
1	B	535	MET
1	B	536	LYS
1	B	544	LEU
1	B	547	ILE
1	B	551	GLU
1	B	552	GLU
1	B	575	MET

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Mol	Chain	Res	Type
1	B	585	ASN
1	B	596	SER
1	B	601	HIS
1	B	606	ARG
1	B	632	LYS
1	B	657	TRP
1	B	658	ILE
1	B	670	LEU
1	B	675	ASP
1	B	676	MET
1	B	678	ILE
1	B	684	THR
1	B	695	ARG
1	B	698	GLU
1	B	701	LYS
1	B	706	MET
1	B	707	LEU
1	B	715	ARG
1	B	738	ARG
1	B	742	GLU
1	B	757	MET
1	B	758	SER
1	B	765	ILE
1	B	782	VAL
1	B	785	GLU
1	B	813	ILE
1	B	828	LYS
1	B	829	GLU
1	B	830	THR
1	B	838	CYS
1	B	848	LYS
1	B	856	LYS
1	C	355	THR
1	C	358	TRP
1	C	362	THR
1	C	372	TRP
1	C	373	GLN
1	C	375	GLN
1	C	378	GLN
1	C	383	MET
1	C	384	GLN
1	C	387	SER

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Mol	Chain	Res	Type
1	C	394	SER
1	C	496	ARG
1	C	514	HIS
1	C	520	SER
1	C	524	LEU
1	C	526	GLU
1	C	543	ARG
1	C	551	GLU
1	C	552	GLU
1	C	554	LEU
1	C	586	ASN
1	C	638	ARG
1	C	664	GLU
1	C	668	LEU
1	C	676	MET
1	C	677	GLU
1	C	689	GLU
1	C	698	GLU
1	C	708	LEU
1	C	712	ARG
1	C	738	ARG
1	C	742	GLU
1	C	765	ILE
1	C	782	VAL
1	C	804	LEU
1	C	813	ILE
1	C	825	LYS
1	C	849	SER
1	C	851	GLU
1	C	864	THR
1	D	336	TRP
1	D	343	ARG
1	D	345	ARG
1	D	353	THR
1	D	356	THR
1	D	367	ARG
1	D	371	GLN
1	D	375	GLN
1	D	383	MET
1	D	384	GLN
1	D	388	GLN
1	D	396	SER

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Mol	Chain	Res	Type
1	D	398	SER
1	D	485	GLN
1	D	503	ARG
1	D	515	VAL
1	D	517	ILE
1	D	524	LEU
1	D	530	GLN
1	D	543	ARG
1	D	544	LEU
1	D	547	ILE
1	D	551	GLU
1	D	566	LEU
1	D	568	SER
1	D	584	LYS
1	D	596	SER
1	D	597	ILE
1	D	601	HIS
1	D	637	LYS
1	D	641	LEU
1	D	650	GLU
1	D	654	SER
1	D	660	GLU
1	D	662	ASN
1	D	663	LEU
1	D	671	TYR
1	D	673	ILE
1	D	675	ASP
1	D	676	MET
1	D	683	THR
1	D	684	THR
1	D	687	LEU
1	D	693	SER
1	D	698	GLU
1	D	699	GLU
1	D	700	ASN
1	D	707	LEU
1	D	715	ARG
1	D	735	GLU
1	D	738	ARG
1	D	742	GLU
1	D	765	ILE
1	D	767	ARG

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Mol	Chain	Res	Type
1	D	773	SER
1	D	774	LYS
1	D	782	VAL
1	D	813	ILE
1	D	828	LYS
1	D	830	THR
1	D	834	ARG
1	D	837	THR
1	D	838	CYS
1	D	848	LYS
1	D	858	LEU
1	D	863	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	368	ASN
1	A	393	GLN
1	A	514	HIS
1	A	534	ASN
1	A	569	HIS
1	A	685	HIS
1	B	371	GLN
1	B	378	GLN
1	B	384	GLN
1	B	388	GLN
1	B	393	GLN
1	B	485	GLN
1	B	501	GLN
1	B	530	GLN
1	B	531	GLN
1	B	569	HIS
1	B	685	HIS
1	C	368	ASN
1	C	384	GLN
1	C	500	HIS
1	C	534	ASN
1	C	618	HIS
1	C	653	ASN
1	C	729	ASN
1	D	351	HIS
1	D	359	GLN

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Mol	Chain	Res	Type
1	D	380	GLN
1	D	384	GLN
1	D	388	GLN
1	D	485	GLN
1	D	530	GLN
1	D	531	GLN
1	D	661	ASN
1	D	662	ASN
1	D	700	ASN
1	D	729	ASN
1	D	761	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SCN	C	900	-	1,2,2	0.04	0	0,1,1	0.00	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	436/447 (97%)	-0.47	1 (0%) 95 95	11, 23, 36, 43	0
1	B	445/447 (99%)	-0.46	3 (0%) 87 86	10, 23, 36, 41	0
1	C	435/447 (97%)	-0.47	0 100 100	11, 23, 35, 42	0
1	D	445/447 (99%)	-0.46	1 (0%) 95 95	10, 23, 38, 46	0
All	All	1761/1788 (98%)	-0.47	5 (0%) 94 93	10, 23, 36, 46	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	864	THR	2.7
1	B	666	CYS	2.4
1	D	666	CYS	2.2
1	B	865	GLU	2.1
1	A	336	TRP	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 carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NA	A	901	1/1	0.82	0.12	24,24,24,24	0
4	CL	D	900	1/1	0.86	0.12	45,45,45,45	0
2	NA	D	901	1/1	0.87	0.11	21,21,21,21	0
3	SCN	C	900	3/3	0.95	0.11	37,37,37,41	0
2	NA	B	901	1/1	0.97	0.09	11,11,11,11	0

6.5 Other polymers [i](#)

There are no such residues in this entry.