



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 2, 2026 – 02:21 AM UTC

PDB ID : 5HPT / pdb_00005hpt
Title : System-wide modulation of HECT E3 ligases with selective ubiquitin variant probes: WWP1, Ubv P2.3 and UBCH7
Authors : Wu, K.-P.; Schulman, B.A.
Deposited on : 2016-01-20
Resolution : 2.84 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

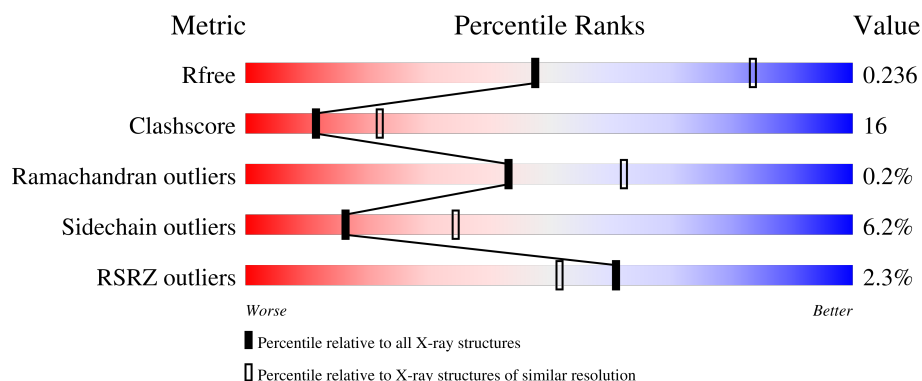
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.84 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	1520 (2.86-2.82)
Clashscore	190562	1559 (2.86-2.82)
Ramachandran outliers	187476	1517 (2.86-2.82)
Sidechain outliers	187428	1518 (2.86-2.82)
RSRZ outliers	180081	1521 (2.86-2.82)

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	383	
1	D	383	
1	G	383	
2	B	83	
2	E	83	

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Mol	Chain	Length	Quality of chain
2	H	83	64%22%5%10%
3	C	161	2% 55%32%7%6%
3	F	161	2% 55%34%7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13529 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 WWP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	373	Total	C	N	O	S	0	0	0
			3111	2013	520	558	20			
1	D	371	Total	C	N	O	S	0	0	0
			3082	1994	516	552	20			
1	G	367	Total	C	N	O	S	0	0	0
			3058	1980	509	549	20			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	535	GLY	-	expression tag	UNP Q9H0M0
A	536	SER	-	expression tag	UNP Q9H0M0
D	535	GLY	-	expression tag	UNP Q9H0M0
D	536	SER	-	expression tag	UNP Q9H0M0
G	535	GLY	-	expression tag	UNP Q9H0M0
G	536	SER	-	expression tag	UNP Q9H0M0

- Molecule 2 is a protein called Ubiquitin variant P2.3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	76	Total	C	N	O	Se	0	0	0
			607	388	101	116	2			
2	E	76	Total	C	N	O	Se	0	0	0
			607	388	101	116	2			
2	H	75	Total	C	N	O	Se	0	0	0
			598	383	99	114	2			

- Molecule 3 is a protein called Ubiquitin-conjugating enzyme E2 L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	151	Total	C	N	O	S	0	0	0
			1234	790	214	225	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	150	Total	C	N	O	S	0	0	0
			1227	785	213	224	5			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	155	GLY	-	expression tag	UNP P68036
C	156	GLY	-	expression tag	UNP P68036
C	157	HIS	-	expression tag	UNP P68036
C	158	HIS	-	expression tag	UNP P68036
C	159	HIS	-	expression tag	UNP P68036
C	160	HIS	-	expression tag	UNP P68036
C	161	HIS	-	expression tag	UNP P68036
C	162	HIS	-	expression tag	UNP P68036
F	155	GLY	-	expression tag	UNP P68036
F	156	GLY	-	expression tag	UNP P68036
F	157	HIS	-	expression tag	UNP P68036
F	158	HIS	-	expression tag	UNP P68036
F	159	HIS	-	expression tag	UNP P68036
F	160	HIS	-	expression tag	UNP P68036
F	161	HIS	-	expression tag	UNP P68036
F	162	HIS	-	expression tag	UNP P68036

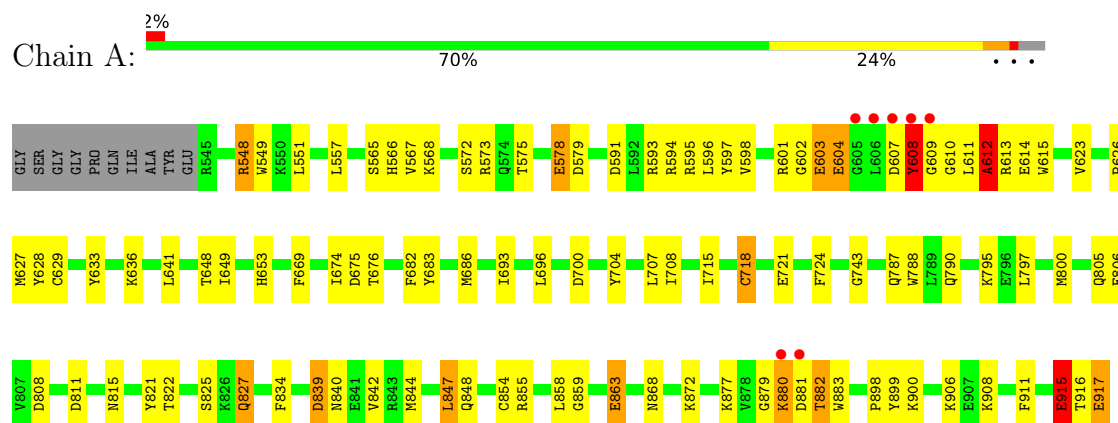
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	O	0	0
			3	3		
4	C	1	Total	O	0	0
			1	1		
4	D	1	Total	O	0	0
			1	1		

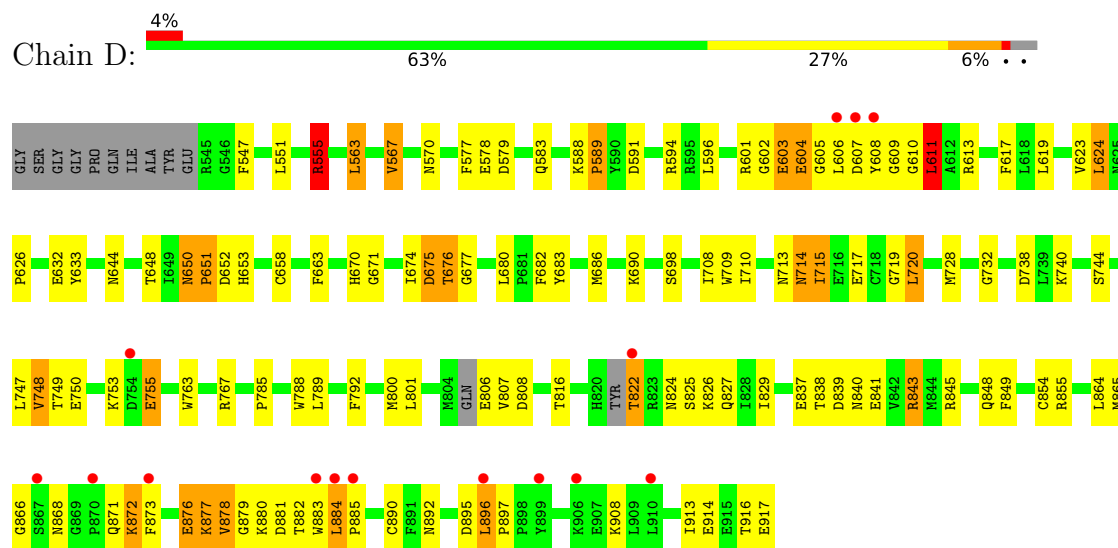
3 Residue-property plots

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.

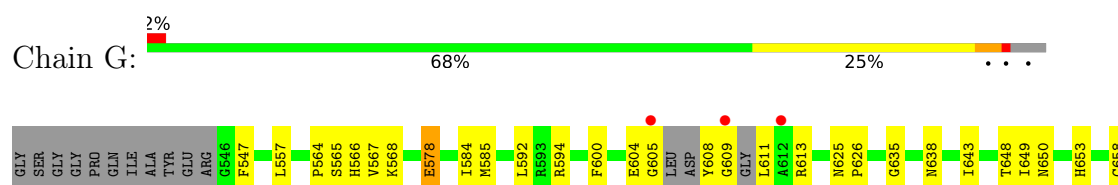
- Molecule 1: NEDD4-like E3 ubiquitin-protein ligase WWP1

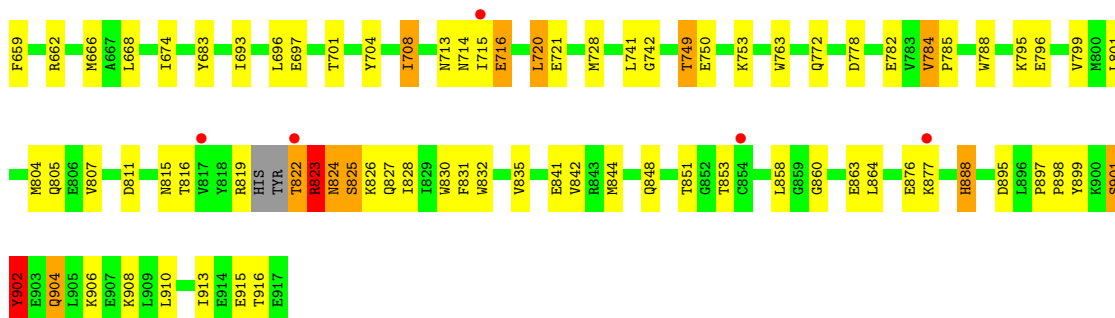


- Molecule 1: NEDD4-like E3 ubiquitin-protein ligase WWP1

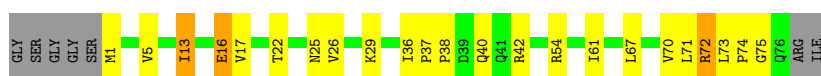


- Molecule 1: NEDD4-like E3 ubiquitin-protein ligase WWP1





- Molecule 2: Ubiquitin variant P2.3



- Molecule 2: Ubiquitin variant P2.3



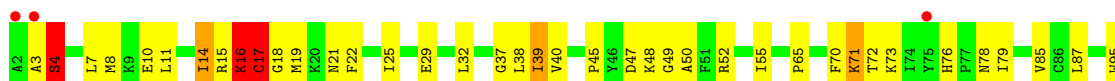
- Molecule 2: Ubiquitin variant P2.3

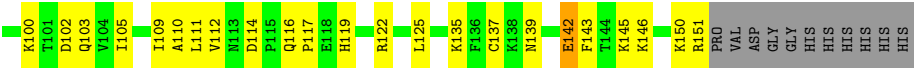


- Molecule 3: Ubiquitin-conjugating enzyme E2 L3



- Molecule 3: Ubiquitin-conjugating enzyme E2 L3





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	114.00Å 118.90Å 158.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	95.15 – 2.84 95.15 – 2.84	Depositor EDS
% Data completeness (in resolution range)	99.5 (95.15-2.84) 91.3 (95.15-2.84)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.95 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.218 , 0.237 0.218 , 0.236	Depositor DCC
R_{free} test set	2008 reflections (3.89%)	wwPDB-VP
Wilson B-factor (Å ²)	67.1	Xtriage
Anisotropy	0.367	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 49.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.023 for k,h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13529	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.66% 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	0.74	2/3193 (0.1%)	1.12	12/4309 (0.3%)
1	D	0.73	1/3161 (0.0%)	1.08	19/4264 (0.4%)
1	G	0.63	0/3135	1.05	12/4226 (0.3%)
2	B	0.68	0/615	1.09	3/828 (0.4%)
2	E	0.64	0/615	1.12	5/828 (0.6%)
2	H	0.70	0/606	1.05	0/816
3	C	0.65	0/1265	1.12	8/1709 (0.5%)
3	F	0.61	1/1257 (0.1%)	1.21	7/1697 (0.4%)
All	All	0.69	4/13847 (0.0%)	1.10	66/18677 (0.4%)

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	2
1	D	0	2
1	G	0	1
2	H	0	1
3	C	0	1
3	F	0	2
All	All	0	9

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	612	ALA	CA-CB	-7.44	1.42	1.52
3	F	16	LYS	C-N	6.58	1.41	1.33
1	D	748	VAL	CA-CB	6.12	1.62	1.54
1	A	915	GLU	CA-C	-5.13	1.47	1.53

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	17	CYS	O-C-N	19.46	145.61	123.42
3	F	17	CYS	CA-C-N	-13.31	95.32	121.41
3	F	17	CYS	C-N-CA	-13.31	95.32	121.41
1	A	613	ARG	N-CA-C	-11.15	99.67	113.38
1	A	675	ASP	N-CA-C	10.98	122.82	111.07
3	C	124	ASP	N-CA-C	-10.97	87.43	110.80
2	E	64	GLY	N-CA-C	-9.55	90.56	113.18
1	A	604	GLU	N-CA-C	9.47	121.69	111.36
1	G	915	GLU	N-CA-C	8.76	123.82	111.30
1	A	858	LEU	N-CA-C	-8.46	97.49	110.10
1	G	721	GLU	N-CA-C	8.32	123.94	109.96
1	A	610	GLY	N-CA-C	8.24	125.99	111.73
1	D	613	ARG	N-CA-C	-7.96	103.59	113.38
2	E	63	MSE	N-CA-C	7.89	127.61	110.80
3	C	124	ASP	CB-CA-C	-7.53	95.43	110.42
1	G	902	TYR	N-CA-C	7.32	120.31	111.82
2	B	73	LEU	CA-C-N	7.12	128.75	119.84
2	B	73	LEU	C-N-CA	7.12	128.75	119.84
1	D	650	ASN	CA-C-N	6.99	128.58	119.84
1	D	650	ASN	C-N-CA	6.99	128.58	119.84
1	D	876	GLU	N-CA-C	6.94	125.57	110.80
1	G	720	LEU	N-CA-C	6.87	125.44	110.80
1	G	716	GLU	N-CA-C	-6.71	105.07	112.72
3	F	49	GLY	N-CA-C	-6.47	99.49	111.14
3	F	87	LEU	CA-C-N	6.47	125.97	119.24
3	F	87	LEU	C-N-CA	6.47	125.97	119.24
1	A	675	ASP	CB-CA-C	-6.42	100.81	110.88
1	A	858	LEU	CB-CA-C	6.38	119.85	109.90
1	D	717	GLU	N-CA-C	-6.33	105.84	112.93
1	A	608	TYR	CA-CB-CG	6.22	125.09	113.90
1	D	896	LEU	CA-C-N	6.15	124.09	119.66
1	D	896	LEU	C-N-CA	6.15	124.09	119.66
3	C	14	ILE	N-CA-C	-6.12	106.95	111.90
2	E	61	ILE	O-C-N	-6.11	114.01	122.31
1	D	884	LEU	CA-C-N	-6.07	113.52	119.78
1	D	884	LEU	C-N-CA	-6.07	113.52	119.78
1	A	700	ASP	N-CA-C	6.04	119.88	107.37
1	D	675	ASP	N-CA-C	5.90	118.37	108.23
1	G	823	ARG	CA-C-N	5.86	132.25	121.70
1	G	823	ARG	C-N-CA	5.86	132.25	121.70
1	D	877	LYS	N-CA-C	5.72	119.15	109.76
1	G	749	THR	CB-CA-C	-5.71	107.27	114.40
1	D	719	GLY	N-CA-C	-5.62	106.43	115.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	114	ASP	CA-C-N	5.52	126.29	120.11
3	C	114	ASP	C-N-CA	5.52	126.29	120.11
1	D	567	VAL	CA-C-N	-5.49	115.36	123.05
1	D	567	VAL	C-N-CA	-5.49	115.36	123.05
1	D	555	ARG	N-CA-C	-5.44	106.14	112.89
1	A	879	GLY	N-CA-C	5.44	121.67	113.02
3	C	64	LYS	CA-C-N	-5.37	114.85	120.38
3	C	64	LYS	C-N-CA	-5.37	114.85	120.38
2	B	61	ILE	CB-CA-C	5.35	117.01	111.23
3	C	20	LYS	N-CA-C	5.34	117.80	111.33
2	E	61	ILE	N-CA-C	-5.33	106.06	113.00
1	D	644	ASN	CA-C-N	-5.31	114.35	119.87
1	D	644	ASN	C-N-CA	-5.31	114.35	119.87
1	G	824	ASN	N-CA-C	5.19	125.54	111.00
2	E	60	ASN	CB-CA-C	-5.15	104.28	111.80
1	D	611	LEU	N-CA-C	5.11	116.50	107.61
3	F	4	SER	N-CA-C	-5.07	105.88	111.71
1	A	847	LEU	N-CA-C	-5.07	105.84	112.23
1	D	658	CYS	CB-CA-C	-5.06	101.27	110.63
1	G	825	SER	N-CA-C	5.05	116.35	109.18
1	A	882	THR	N-CA-C	-5.05	106.96	113.02
1	G	784	VAL	CA-C-N	5.00	126.09	119.84
1	G	784	VAL	C-N-CA	5.00	126.09	119.84

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	603	GLU	Peptide
1	A	612	ALA	Peptide
3	C	151	ARG	Peptide
1	D	714	ASN	Peptide
1	D	876	GLU	Peptide
3	F	16	LYS	Mainchain
3	F	17	CYS	Mainchain
1	G	901	SER	Peptide
2	H	62	LYS	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	3111	0	3044	85	0
1	D	3082	0	3008	117	1
1	G	3058	0	2994	95	2
2	B	607	0	633	16	0
2	E	607	0	633	29	0
2	H	598	0	625	16	0
3	C	1234	0	1245	46	1
3	F	1227	0	1236	44	0
4	A	3	0	0	1	0
4	C	1	0	0	0	0
4	D	1	0	0	1	0
All	All	13529	0	13418	431	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 16.

All (431) 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:D:878:VAL:HB	1:D:879:GLY:CA	1.62	1.29
1:G:822:THR:O	1:G:825:SER:HB3	1.18	1.27
1:A:881:ASP:OD2	1:A:900:LYS:HE2	1.31	1.22
3:C:13:GLU:O	3:C:17:CYS:SG	2.02	1.17
1:D:806:GLU:HG3	1:D:807:VAL:HB	1.17	1.16
1:D:916:THR:O	1:D:917:GLU:HG2	1.49	1.12
1:D:878:VAL:CB	1:D:879:GLY:HA2	1.78	1.11
1:D:877:LYS:O	1:D:878:VAL:CG2	2.01	1.07
1:G:822:THR:O	1:G:825:SER:CB	2.02	1.06
1:G:720:LEU:O	1:G:720:LEU:HD23	1.56	1.05
1:D:877:LYS:O	1:D:878:VAL:HG23	1.58	1.03
1:D:878:VAL:HG21	1:D:883:TRP:HE1	1.22	1.02
3:F:17:CYS:SG	3:F:19:MET:HE3	1.99	1.02
1:D:715:ILE:HG22	1:D:750:GLU:OE2	1.60	1.01
1:D:877:LYS:HG3	1:D:878:VAL:HG22	1.39	1.01
1:D:806:GLU:HB2	1:D:807:VAL:HA	1.42	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:591:ASP:OD1	1:D:594:ARG:NH1	1.97	0.97
1:D:877:LYS:C	1:D:878:VAL:HG22	1.87	0.96
1:D:806:GLU:HG3	1:D:807:VAL:CB	1.95	0.96
1:D:807:VAL:HG22	1:D:808:ASP:N	1.81	0.95
1:D:807:VAL:HG22	1:D:808:ASP:H	1.28	0.94
1:A:548:ARG:HG3	1:A:549:TRP:N	1.85	0.91
1:A:548:ARG:HD3	1:D:606:LEU:HD23	1.54	0.88
1:A:573:ARG:NE	1:A:603:GLU:OE2	2.05	0.88
1:G:720:LEU:HD23	1:G:720:LEU:C	1.99	0.85
1:D:567:VAL:HG11	1:D:591:ASP:O	1.76	0.85
1:D:878:VAL:HB	1:D:879:GLY:HA2	0.87	0.85
3:C:123:ALA:C	3:C:124:ASP:O	2.05	0.84
1:G:822:THR:C	1:G:825:SER:CB	2.51	0.83
1:A:607:ASP:HB3	1:A:608:TYR:HA	1.60	0.82
2:H:59:TYR:HB2	2:H:61:ILE:HD12	1.61	0.82
1:D:807:VAL:CG2	1:D:808:ASP:H	1.92	0.82
1:G:720:LEU:O	1:G:720:LEU:CD2	2.27	0.82
1:D:877:LYS:C	1:D:878:VAL:CG2	2.45	0.81
1:D:806:GLU:CB	1:D:807:VAL:HA	2.10	0.81
3:C:78:ASN:HD22	3:C:111:LEU:HD11	1.44	0.81
1:A:915:GLU:O	1:A:915:GLU:HG3	1.79	0.80
2:E:61:ILE:O	2:E:62:LYS:C	2.18	0.79
1:D:623:VAL:HG23	1:D:624:LEU:HD13	1.62	0.79
1:D:877:LYS:O	1:D:878:VAL:HG22	1.79	0.79
1:A:881:ASP:OD2	1:A:900:LYS:CE	2.23	0.78
1:A:915:GLU:O	1:A:915:GLU:CG	2.29	0.78
1:D:865:MET:O	1:D:892:ASN:ND2	2.17	0.77
1:G:804:MET:HE1	1:G:841:GLU:HA	1.65	0.76
2:H:23:ILE:HD13	2:H:50:LEU:HB3	1.65	0.76
3:F:17:CYS:SG	3:F:19:MET:CE	2.74	0.76
1:G:585:MET:HE1	1:G:662:ARG:HD2	1.66	0.76
1:G:823:ARG:N	1:G:825:SER:HB2	2.01	0.75
1:D:877:LYS:HG3	1:D:878:VAL:CG2	2.15	0.74
2:H:42:ARG:HG2	2:H:72:ARG:HD3	1.70	0.74
1:G:822:THR:C	1:G:825:SER:HB2	2.13	0.73
1:G:611:LEU:HD21	1:G:613:ARG:HH11	1.53	0.73
2:E:23:ILE:HB	2:E:52:ASP:HA	1.70	0.72
1:G:811:ASP:O	1:G:815:ASN:ND2	2.22	0.72
3:F:79:ILE:HG12	3:F:85:VAL:HG22	1.70	0.72
2:E:24:GLU:HG2	2:E:52:ASP:HB2	1.71	0.71
3:C:122:ARG:O	3:C:124:ASP:O	2.09	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:806:GLU:OE2	1:D:807:VAL:HG23	1.90	0.71
2:B:42:ARG:HG3	2:B:72:ARG:HD2	1.73	0.71
1:A:608:TYR:HB2	1:A:609:GLY:C	2.16	0.70
3:C:78:ASN:ND2	3:C:111:LEU:HD11	2.07	0.69
1:A:548:ARG:HG3	1:A:549:TRP:H	1.56	0.69
3:F:76:HIS:HE2	3:F:112:VAL:HA	1.56	0.69
1:D:602:GLY:N	1:D:603:GLU:HA	2.07	0.69
2:E:63:MSE:HG3	2:E:64:GLY:N	2.05	0.69
1:D:715:ILE:CG2	1:D:750:GLU:OE2	2.39	0.69
1:D:715:ILE:HG12	1:D:715:ILE:O	1.91	0.69
3:F:47:ASP:O	3:F:48:LYS:HD2	1.94	0.68
2:B:5:VAL:HG12	2:B:67:LEU:HB2	1.75	0.68
1:D:878:VAL:CB	1:D:879:GLY:CA	2.49	0.68
3:F:22:PHE:CE1	3:F:37:GLY:HA3	2.29	0.67
1:D:579:ASP:O	1:D:583:GLN:HG2	1.93	0.67
1:G:650:ASN:ND2	2:H:73:LEU:HD13	2.09	0.67
3:F:10:GLU:OE2	3:F:100:LYS:HD2	1.95	0.67
2:B:1:MSE:HG2	2:B:17:VAL:O	1.95	0.66
1:D:877:LYS:CG	1:D:878:VAL:HG22	2.21	0.66
1:D:806:GLU:N	1:D:840:ASN:OD1	2.29	0.66
2:E:59:TYR:HB2	2:E:61:ILE:CD1	2.26	0.66
1:A:787:GLN:HG2	1:A:787:GLN:O	1.96	0.65
1:A:806:GLU:OE2	1:D:617:PHE:HE2	1.80	0.65
2:B:16:GLU:O	2:B:29:LYS:NZ	2.28	0.65
1:D:740:LYS:NZ	1:D:755:GLU:OE2	2.30	0.64
1:D:879:GLY:O	1:D:882:THR:OG1	2.08	0.64
2:H:59:TYR:CB	2:H:61:ILE:HD12	2.27	0.64
1:D:570:ASN:OD1	1:D:601:ARG:HD3	1.98	0.64
2:E:58:ASP:OD1	2:E:58:ASP:N	2.30	0.64
1:D:596:LEU:HD12	1:D:670:HIS:ND1	2.13	0.63
3:C:81:GLU:OE2	3:C:122:ARG:NH2	2.31	0.63
1:G:611:LEU:HD21	1:G:613:ARG:NH1	2.15	0.62
1:A:899:TYR:CE1	1:A:908:LYS:HD2	2.34	0.62
1:G:650:ASN:HB3	2:H:73:LEU:HD22	1.81	0.62
3:F:142:GLU:O	3:F:145:LYS:HB3	1.99	0.62
1:G:823:ARG:H	1:G:825:SER:HB2	1.65	0.62
1:G:823:ARG:H	1:G:825:SER:N	1.98	0.62
1:A:648:THR:HG22	1:A:653:HIS:CE1	2.34	0.61
1:G:795:LYS:HZ1	1:G:916:THR:HG21	1.66	0.61
1:D:839:ASP:O	1:D:843:ARG:CZ	2.48	0.61
1:D:609:GLY:N	1:D:610:GLY:HA2	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:704:TYR:CZ	1:A:708:ILE:HD12	2.36	0.61
1:D:916:THR:O	1:D:917:GLU:CG	2.38	0.61
3:F:17:CYS:O	3:F:18:GLY:C	2.41	0.61
1:A:627:MET:HE3	2:B:71:LEU:HD13	1.82	0.61
2:E:56:LEU:HA	2:E:61:ILE:HD13	1.82	0.61
1:G:795:LYS:NZ	1:G:916:THR:HG21	2.16	0.60
1:G:823:ARG:N	1:G:825:SER:CB	2.63	0.60
1:A:578:GLU:HB3	2:B:75:GLY:HA2	1.84	0.60
1:A:806:GLU:OE2	1:D:617:PHE:CE2	2.54	0.60
3:F:22:PHE:HE1	3:F:37:GLY:HA3	1.66	0.60
1:A:827:GLN:NE2	1:A:899:TYR:O	2.33	0.60
1:D:567:VAL:CG1	1:D:591:ASP:O	2.49	0.60
1:A:715:ILE:O	1:A:718:CYS:HB2	2.01	0.60
1:G:825:SER:O	1:G:828:ILE:N	2.35	0.60
1:G:547:PHE:HB3	1:G:841:GLU:OE2	2.02	0.60
3:C:46:TYR:OH	3:C:75:TYR:O	2.10	0.59
3:F:47:ASP:OD1	3:F:48:LYS:N	2.34	0.59
1:G:819:ARG:HB3	1:G:876:GLU:HA	1.84	0.59
1:G:902:TYR:C	1:G:904:GLN:H	2.09	0.59
2:H:22:THR:HG22	2:H:25:ASN:ND2	2.17	0.59
3:F:55:ILE:HD11	3:F:105:ILE:HD11	1.84	0.59
3:C:31:ASN:O	3:C:33:LEU:N	2.34	0.59
1:D:878:VAL:HG21	1:D:883:TRP:NE1	2.06	0.59
1:G:827:GLN:HG3	1:G:877:LYS:HZ3	1.67	0.59
1:A:593:ARG:HG2	1:A:669:PHE:CE2	2.38	0.59
2:E:73:LEU:O	2:E:76:GLN:HB2	2.03	0.59
2:H:22:THR:HG22	2:H:25:ASN:HD21	1.68	0.58
1:A:629:CYS:HA	4:A:1002:HOH:O	2.03	0.58
3:C:122:ARG:HB3	3:C:125:LEU:HD12	1.85	0.58
1:G:830:TRP:HB3	1:G:902:TYR:HD2	1.68	0.58
3:F:142:GLU:O	3:F:145:LYS:N	2.35	0.58
3:C:114:ASP:OD1	3:C:114:ASP:N	2.36	0.58
3:C:124:ASP:O	3:C:125:LEU:HB2	2.03	0.58
3:C:135:LYS:O	3:C:139:ASN:ND2	2.32	0.57
1:D:603:GLU:HB3	1:D:604:GLU:O	2.04	0.57
1:D:806:GLU:HG3	1:D:807:VAL:CA	2.34	0.57
1:G:830:TRP:CD2	1:G:902:TYR:HB2	2.39	0.57
1:A:607:ASP:CB	1:A:608:TYR:HA	2.30	0.57
1:A:859:GLY:HA3	1:A:863:GLU:OE2	2.04	0.57
2:B:22:THR:HG22	2:B:25:ASN:CG	2.30	0.57
1:D:710:ILE:O	1:D:753:LYS:HD3	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:607:ASP:N	1:A:607:ASP:OD1	2.37	0.57
3:C:27:VAL:HG11	3:C:32:LEU:HD22	1.87	0.56
3:C:140:ALA:O	3:C:144:THR:HG23	2.05	0.56
3:C:2:ALA:HA	3:C:3:ALA:C	2.30	0.56
2:E:23:ILE:HD13	2:E:50:LEU:HB3	1.87	0.56
1:G:713:ASN:O	1:G:753:LYS:NZ	2.38	0.56
1:G:578:GLU:CD	1:G:578:GLU:H	2.13	0.56
1:A:601:ARG:HA	1:A:604:GLU:HG3	1.86	0.56
1:A:593:ARG:HG2	1:A:669:PHE:CZ	2.40	0.56
2:H:45:PHE:CE1	2:H:65:SER:HB3	2.42	0.55
3:F:76:HIS:NE2	3:F:112:VAL:HA	2.20	0.55
1:G:714:ASN:HB3	1:G:716:GLU:HG2	1.88	0.55
3:F:102:ASP:OD1	3:F:103:GLN:N	2.40	0.55
3:F:17:CYS:O	3:F:19:MET:N	2.40	0.55
3:C:20:LYS:O	3:C:23:ARG:NH1	2.33	0.55
1:D:555:ARG:NH1	1:D:671:GLY:HA2	2.22	0.55
1:G:609:GLY:O	1:G:611:LEU:N	2.40	0.55
3:C:151:ARG:HB2	3:C:152:PRO:C	2.31	0.54
1:D:749:THR:O	1:D:753:LYS:HB2	2.07	0.54
1:D:806:GLU:CB	1:D:807:VAL:CA	2.84	0.54
1:D:807:VAL:CG2	1:D:808:ASP:N	2.49	0.54
1:G:565:SER:OG	1:G:566:HIS:N	2.41	0.54
1:A:682:PHE:CE2	1:A:686:MET:HE2	2.42	0.54
1:D:896:LEU:HD12	1:D:897:PRO:HD2	1.90	0.54
1:A:868:ASN:OD1	3:C:93:GLU:HG2	2.08	0.54
3:C:7:LEU:HD13	3:C:32:LEU:O	2.08	0.54
2:H:18:GLU:N	2:H:21:ASP:OD2	2.41	0.54
1:A:787:GLN:O	1:A:790:GLN:HG2	2.08	0.53
3:C:44:PRO:HG3	3:C:47:ASP:OD2	2.08	0.53
1:G:831:PHE:O	1:G:835:VAL:HG13	2.08	0.53
1:G:827:GLN:HG3	1:G:877:LYS:NZ	2.23	0.53
1:G:643:ILE:HD13	1:G:772:GLN:HB3	1.89	0.53
1:D:884:LEU:HB3	1:D:885:PRO:HD2	1.89	0.53
1:G:600:PHE:O	1:G:604:GLU:HG3	2.09	0.53
3:C:123:ALA:O	3:C:124:ASP:C	2.40	0.53
1:G:827:GLN:HB2	1:G:877:LYS:HZ1	1.74	0.53
2:E:59:TYR:HB2	2:E:61:ILE:HD11	1.91	0.52
1:D:877:LYS:HG2	1:D:895:ASP:CB	2.39	0.52
1:G:592:LEU:HB3	1:G:666:MET:HG3	1.89	0.52
3:C:26:GLN:HG2	3:C:27:VAL:H	1.74	0.52
3:F:10:GLU:HG2	3:F:100:LYS:HE3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:135:LYS:O	3:F:139:ASN:ND2	2.37	0.52
1:A:612:ALA:HB1	1:A:615:TRP:CB	2.40	0.52
2:B:22:THR:HG22	2:B:25:ASN:OD1	2.10	0.52
1:G:906:LYS:O	1:G:910:LEU:HB2	2.10	0.52
2:E:26:VAL:HA	2:E:29:LYS:HG3	1.91	0.52
1:G:804:MET:HG3	1:G:844:MET:SD	2.50	0.52
2:H:42:ARG:NE	2:H:49:GLN:OE1	2.41	0.52
1:A:840:ASN:O	1:A:844:MET:HG3	2.10	0.52
2:E:3:ILE:HG22	2:E:63:MSE:O	2.10	0.52
3:C:122:ARG:C	3:C:124:ASP:O	2.52	0.52
3:F:76:HIS:H	3:F:122:ARG:NH2	2.07	0.52
1:D:601:ARG:C	1:D:603:GLU:HA	2.34	0.51
1:A:548:ARG:HH11	1:D:606:LEU:CD2	2.23	0.51
3:C:27:VAL:CG1	3:C:32:LEU:HD22	2.40	0.51
1:D:547:PHE:HB3	1:D:841:GLU:OE1	2.11	0.51
3:F:3:ALA:O	3:F:7:LEU:HB2	2.10	0.51
1:G:827:GLN:NE2	1:G:898:PRO:HA	2.25	0.51
1:D:785:PRO:HD2	1:D:788:TRP:CD2	2.46	0.51
1:G:795:LYS:HB3	1:G:848:GLN:OE1	2.10	0.51
3:C:12:GLU:O	3:C:16:LYS:HG2	2.11	0.51
1:D:849:PHE:CG	1:D:913:ILE:HG22	2.45	0.51
1:D:792:PHE:CD2	1:D:800:MET:HE1	2.46	0.51
1:G:778:ASP:O	1:G:782:GLU:HG3	2.11	0.51
2:B:22:THR:O	2:B:26:VAL:HG23	2.11	0.51
3:F:72:THR:HG22	3:F:73:LYS:O	2.11	0.51
1:G:823:ARG:N	1:G:825:SER:N	2.58	0.50
1:A:565:SER:OG	1:A:566:HIS:N	2.44	0.50
1:A:721:GLU:HB2	3:C:6:ARG:HB2	1.93	0.50
1:A:880:LYS:HG3	1:A:883:TRP:CE2	2.47	0.50
1:G:816:THR:HG21	1:G:832:TRP:HZ2	1.77	0.50
2:E:18:GLU:N	2:E:21:ASP:OD2	2.30	0.50
1:G:897:PRO:HB2	1:G:899:TYR:CE1	2.46	0.50
1:A:844:MET:HE2	1:A:854:CYS:HB2	1.94	0.50
1:A:548:ARG:NH1	1:D:606:LEU:CD2	2.75	0.50
3:F:29:GLU:HA	3:F:32:LEU:HD23	1.93	0.50
3:F:39:ILE:HD11	3:F:70:PHE:HE2	1.77	0.50
3:F:45:PRO:HG3	3:F:137:CYS:SG	2.52	0.50
3:F:78:ASN:HB2	3:F:111:LEU:HD21	1.94	0.50
1:G:823:ARG:H	1:G:824:ASN:C	2.19	0.50
2:B:40:GLN:HA	2:B:72:ARG:HG3	1.93	0.50
1:G:830:TRP:CE2	1:G:902:TYR:HB2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:608:TYR:CD2	1:A:611:LEU:HB2	2.47	0.49
1:A:911:PHE:O	1:A:915:GLU:HB3	2.11	0.49
1:D:619:LEU:HD23	1:D:663:PHE:CE1	2.47	0.49
3:C:13:GLU:C	3:C:17:CYS:SG	2.89	0.49
3:F:122:ARG:HE	3:F:125:LEU:HD13	1.75	0.49
3:C:3:ALA:O	3:C:4:SER:OG	2.25	0.49
3:C:102:ASP:OD1	3:C:103:GLN:N	2.46	0.49
1:A:612:ALA:HA	1:A:614:GLU:H	1.78	0.49
1:G:605:GLY:O	1:G:608:TYR:HA	2.13	0.49
1:G:715:ILE:HG12	1:G:750:GLU:OE2	2.11	0.49
1:D:845:ARG:HE	1:D:914:GLU:HA	1.77	0.49
1:G:888:HIS:HE1	1:G:895:ASP:OD2	1.95	0.49
1:D:877:LYS:HG2	1:D:895:ASP:HB2	1.94	0.48
1:G:611:LEU:CD2	1:G:613:ARG:HH11	2.23	0.48
2:H:14:THR:O	2:H:33:LYS:NZ	2.46	0.48
2:H:61:ILE:HG12	2:H:67:LEU:HD21	1.95	0.48
1:G:826:LYS:O	1:G:830:TRP:CE3	2.66	0.48
1:D:878:VAL:CG2	1:D:883:TRP:HE1	2.11	0.48
1:G:604:GLU:O	1:G:605:GLY:C	2.56	0.48
1:D:555:ARG:NH1	4:D:1001:HOH:O	2.22	0.48
1:G:785:PRO:HG2	1:G:788:TRP:CE2	2.49	0.48
1:A:916:THR:O	1:A:917:GLU:C	2.56	0.48
1:A:805:GLN:H	1:A:844:MET:CE	2.26	0.48
1:G:864:LEU:HD23	1:G:864:LEU:HA	1.69	0.48
1:A:815:ASN:O	1:A:872:LYS:HB3	2.14	0.48
2:E:2:GLN:HA	2:E:15:LEU:O	2.14	0.48
1:A:636:LYS:H	1:A:636:LYS:HD2	1.78	0.47
1:G:823:ARG:H	1:G:825:SER:CB	2.23	0.47
2:H:1:MSE:O	2:H:16:GLU:HA	2.14	0.47
1:A:683:TYR:CD1	1:A:797:LEU:HD23	2.49	0.47
1:A:806:GLU:CD	1:D:617:PHE:HE2	2.21	0.47
2:E:38:PRO:HA	2:E:41:GLN:NE2	2.30	0.47
3:C:22:PHE:HA	3:C:38:LEU:O	2.14	0.47
1:D:868:ASN:OD1	1:D:871:GLN:NE2	2.48	0.47
2:E:23:ILE:HA	2:E:26:VAL:HG12	1.97	0.47
3:F:4:SER:O	3:F:8:MET:HB2	2.15	0.47
1:G:592:LEU:HD13	1:G:666:MET:HE2	1.97	0.47
2:B:22:THR:HG23	2:B:25:ASN:H	1.78	0.47
3:C:20:LYS:HA	3:C:23:ARG:HH22	1.80	0.47
3:C:60:GLU:OE1	3:C:60:GLU:N	2.48	0.47
1:G:825:SER:H	1:G:828:ILE:HB	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:763:TRP:O	1:D:767:ARG:HB3	2.15	0.47
1:D:849:PHE:CD2	1:D:913:ILE:HG22	2.49	0.47
2:E:61:ILE:O	2:E:65:SER:OG	2.26	0.47
3:F:14:ILE:O	3:F:17:CYS:SG	2.67	0.47
1:A:899:TYR:C	1:A:900:LYS:HD3	2.40	0.47
1:A:683:TYR:HD1	1:A:686:MET:HE3	1.81	0.47
1:G:826:LYS:O	1:G:830:TRP:CD2	2.68	0.47
3:C:11:LEU:O	3:C:14:ILE:HG22	2.14	0.46
3:C:105:ILE:HG22	3:C:109:ILE:HD12	1.97	0.46
2:E:23:ILE:HD12	2:E:51:GLU:O	2.14	0.46
1:A:839:ASP:HB2	1:A:842:VAL:HG23	1.97	0.46
1:G:844:MET:HE3	1:G:844:MET:HB2	1.68	0.46
1:A:608:TYR:HB2	1:A:609:GLY:O	2.14	0.46
1:D:605:GLY:C	1:D:607:ASP:H	2.23	0.46
1:D:674:ILE:HG12	1:D:801:LEU:HD22	1.98	0.46
1:D:848:GLN:HG3	1:D:854:CYS:HB3	1.97	0.46
1:G:804:MET:CE	1:G:841:GLU:HA	2.43	0.46
1:A:626:PRO:HG2	1:A:633:TYR:CE2	2.50	0.46
1:G:693:ILE:HG13	1:G:696:LEU:HD12	1.96	0.46
1:G:823:ARG:HB2	1:G:824:ASN:C	2.41	0.46
1:A:567:VAL:N	1:A:595:ARG:O	2.47	0.46
1:D:738:ASP:HB3	1:D:740:LYS:O	2.16	0.46
1:D:840:ASN:ND2	1:D:840:ASN:O	2.48	0.46
3:F:109:ILE:HG13	3:F:110:ALA:N	2.31	0.46
1:G:851:THR:HG22	1:G:853:THR:HG22	1.97	0.46
1:D:880:LYS:O	1:D:881:ASP:C	2.56	0.46
1:D:826:LYS:HB2	1:D:827:GLN:NE2	2.30	0.46
3:F:11:LEU:O	3:F:15:ARG:HB2	2.16	0.46
3:C:73:LYS:HA	3:C:73:LYS:HD3	1.79	0.45
1:G:683:TYR:CE1	1:G:801:LEU:HD12	2.50	0.45
1:G:811:ASP:OD2	1:G:860:GLY:HA3	2.16	0.45
1:G:830:TRP:CH2	1:G:901:SER:HA	2.52	0.45
1:A:683:TYR:CD1	1:A:686:MET:HE3	2.52	0.45
1:A:821:TYR:CE2	1:A:877:LYS:HB2	2.51	0.45
3:F:38:LEU:HD21	3:F:50:ALA:HB1	1.98	0.45
1:A:612:ALA:HB1	1:A:615:TRP:HB3	1.98	0.45
1:G:858:LEU:C	1:G:863:GLU:OE2	2.60	0.45
3:F:16:LYS:HG3	3:F:16:LYS:O	2.17	0.45
1:G:858:LEU:O	1:G:863:GLU:OE2	2.34	0.45
3:F:151:ARG:HA	3:F:151:ARG:HD2	1.72	0.45
1:D:824:ASN:HB3	1:D:829:ILE:HG13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:5:VAL:HB	2:E:13:ILE:HB	1.97	0.45
3:F:21:ASN:O	3:F:39:ILE:HA	2.17	0.45
3:C:22:PHE:CE1	3:C:53:ILE:HD11	2.52	0.45
1:D:732:GLY:O	2:E:46:ALA:HA	2.17	0.45
2:E:41:GLN:O	2:E:72:ARG:NH2	2.50	0.45
1:A:676:THR:HG22	1:A:855:ARG:NH1	2.32	0.44
1:D:675:ASP:O	1:D:676:THR:HG22	2.18	0.44
1:D:709:TRP:CD1	1:D:713:ASN:ND2	2.85	0.44
2:E:63:MSE:C	2:E:65:SER:H	2.24	0.44
3:F:139:ASN:HB3	3:F:143:PHE:CE2	2.51	0.44
1:G:635:GLY:H	1:G:638:ASN:HB3	1.80	0.44
2:H:45:PHE:HE1	2:H:65:SER:HB3	1.81	0.44
1:D:632:GLU:HG3	1:D:633:TYR:O	2.17	0.44
3:F:65:PRO:HB3	3:F:95:TRP:CD2	2.52	0.44
1:G:741:LEU:HB3	1:G:742:GLY:H	1.43	0.44
2:B:25:ASN:O	2:B:29:LYS:HG3	2.17	0.44
1:D:551:LEU:O	1:D:555:ARG:HB2	2.18	0.44
1:D:567:VAL:HG11	1:D:591:ASP:HB3	2.00	0.44
1:D:839:ASP:O	1:D:843:ARG:NH1	2.51	0.44
3:F:71:LYS:HE2	3:F:71:LYS:HA	1.99	0.44
1:A:548:ARG:NH1	1:D:606:LEU:HD21	2.32	0.44
1:D:648:THR:HG22	1:D:653:HIS:NE2	2.33	0.44
1:G:697:GLU:O	1:G:701:THR:HG22	2.17	0.44
1:G:902:TYR:C	1:G:904:GLN:N	2.73	0.44
1:A:834:PHE:CD1	1:A:906:LYS:HG3	2.52	0.44
1:D:806:GLU:CG	1:D:807:VAL:HA	2.48	0.44
1:D:896:LEU:HA	1:D:897:PRO:HD3	1.84	0.44
3:C:89:VAL:HG13	3:C:90:ILE:HG23	1.99	0.44
1:D:610:GLY:O	1:D:611:LEU:HG	2.17	0.44
1:D:626:PRO:HG2	1:D:633:TYR:CZ	2.53	0.44
1:D:816:THR:HG23	1:D:873:PHE:HD1	1.83	0.44
1:A:821:TYR:CZ	1:A:877:LYS:HB2	2.53	0.44
1:D:588:LYS:O	1:D:589:PRO:C	2.60	0.44
1:A:682:PHE:HE2	1:A:686:MET:HE2	1.83	0.43
3:F:142:GLU:O	3:F:146:LYS:N	2.45	0.43
1:A:548:ARG:HH11	1:D:606:LEU:HD21	1.83	0.43
1:D:822:THR:O	1:D:825:SER:OG	2.36	0.43
1:A:575:THR:OG1	1:A:579:ASP:OD2	2.23	0.43
1:A:628:TYR:CE1	2:B:74:PRO:HD3	2.52	0.43
1:A:707:LEU:HD23	1:A:707:LEU:HA	1.86	0.43
3:C:41:PRO:HG3	3:C:112:VAL:HG11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:714:ASN:ND2	1:D:715:ILE:H	2.16	0.43
1:G:557:LEU:HD23	1:G:557:LEU:HA	1.91	0.43
1:A:808:ASP:OD2	1:A:811:ASP:HB2	2.18	0.43
2:E:23:ILE:HG22	2:E:27:LYS:HE3	2.01	0.43
2:E:56:LEU:CD2	2:E:61:ILE:HD13	2.48	0.43
1:D:682:PHE:CE2	1:D:686:MET:HE2	2.53	0.43
2:E:59:TYR:HB2	2:E:61:ILE:HD12	2.01	0.43
1:A:839:ASP:OD1	1:A:839:ASP:N	2.52	0.43
3:C:19:MET:HB3	3:C:22:PHE:O	2.17	0.43
3:C:125:LEU:O	3:C:126:ALA:C	2.61	0.43
3:F:117:PRO:C	3:F:119:HIS:H	2.27	0.43
1:G:910:LEU:HD12	1:G:910:LEU:HA	1.77	0.43
2:H:1:MSE:H2	2:H:63:MSE:HB2	1.84	0.43
1:A:573:ARG:CD	1:D:806:GLU:HA	2.49	0.42
1:A:724:PHE:O	1:A:743:GLY:C	2.62	0.42
1:A:800:MET:HE2	1:A:800:MET:HB3	1.76	0.42
3:C:47:ASP:OD1	3:C:47:ASP:N	2.52	0.42
1:A:598:VAL:HB	1:A:612:ALA:HB3	2.00	0.42
1:D:650:ASN:HA	1:D:651:PRO:HD2	1.83	0.42
1:G:648:THR:HG22	1:G:653:HIS:CE1	2.54	0.42
1:A:612:ALA:HB1	1:A:615:TRP:HB2	2.00	0.42
1:G:749:THR:OG1	1:G:750:GLU:N	2.47	0.42
3:F:3:ALA:O	3:F:4:SER:C	2.62	0.42
1:G:625:ASN:HA	1:G:626:PRO:HD3	1.91	0.42
1:G:819:ARG:HD3	1:G:819:ARG:C	2.44	0.42
1:A:795:LYS:HD3	1:A:848:GLN:HB3	2.01	0.42
1:A:693:ILE:O	1:A:696:LEU:HB2	2.20	0.42
2:E:56:LEU:HD22	2:E:61:ILE:HD13	2.01	0.42
1:D:605:GLY:O	1:D:608:TYR:HD1	2.02	0.42
1:D:872:LYS:O	1:D:873:PHE:C	2.62	0.42
1:D:884:LEU:HD22	1:D:908:LYS:HG2	2.01	0.42
3:F:21:ASN:O	3:F:40:VAL:N	2.39	0.42
1:G:830:TRP:CG	1:G:902:TYR:HB2	2.54	0.42
3:F:116:GLN:HA	3:F:117:PRO:HD3	1.72	0.42
1:D:677:GLY:H	1:D:855:ARG:NH1	2.18	0.42
1:D:866:GLY:HA3	1:D:871:GLN:HG2	2.01	0.42
1:A:859:GLY:HA3	1:A:863:GLU:CD	2.45	0.41
1:D:864:LEU:HD12	1:D:864:LEU:HA	1.96	0.41
2:E:37:PRO:HA	2:E:38:PRO:HD3	1.91	0.41
1:A:557:LEU:HD13	1:A:788:TRP:CG	2.56	0.41
1:D:806:GLU:CG	1:D:807:VAL:CA	2.97	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:837:GLU:HG3	1:D:838:THR:N	2.35	0.41
3:F:16:LYS:HA	3:F:16:LYS:HD3	1.71	0.41
1:G:877:LYS:HA	1:G:877:LYS:HD3	1.92	0.41
2:B:37:PRO:HA	2:B:38:PRO:HD3	1.92	0.41
1:D:604:GLU:CD	1:D:604:GLU:H	2.28	0.41
2:E:23:ILE:O	2:E:26:VAL:HG12	2.21	0.41
1:G:547:PHE:CE1	1:G:796:GLU:HB3	2.56	0.41
1:A:572:SER:HB3	1:A:601:ARG:HG3	2.02	0.41
1:A:602:GLY:H	1:A:604:GLU:CD	2.28	0.41
2:B:36:ILE:HA	2:B:37:PRO:HD2	1.89	0.41
2:E:38:PRO:HA	2:E:41:GLN:HE21	1.85	0.41
1:D:577:PHE:C	1:D:577:PHE:CD1	2.99	0.41
1:G:842:VAL:HG13	1:G:913:ILE:HD11	2.02	0.41
1:A:595:ARG:NH1	1:A:597:TYR:HE1	2.19	0.41
1:A:674:ILE:O	1:A:674:ILE:HG13	2.17	0.41
1:A:822:THR:HG23	1:A:825:SER:H	1.86	0.41
1:D:682:PHE:CD2	1:D:686:MET:HE2	2.56	0.41
1:D:709:TRP:CD1	1:D:713:ASN:HD22	2.39	0.41
1:D:880:LYS:C	1:D:882:THR:N	2.77	0.41
1:G:564:PRO:O	1:G:594:ARG:NH1	2.53	0.41
1:G:832:TRP:HE3	1:G:835:VAL:HG21	1.84	0.41
1:A:900:LYS:HD3	1:A:900:LYS:N	2.35	0.41
1:A:591:ASP:HA	1:A:594:ARG:HD2	2.03	0.41
3:C:67:LYS:HE3	3:C:67:LYS:HB3	1.77	0.41
3:C:78:ASN:OD1	3:C:78:ASN:N	2.53	0.41
3:C:129:TYR:O	3:C:133:ARG:HG3	2.21	0.41
1:D:714:ASN:HD22	1:D:750:GLU:CD	2.29	0.41
1:G:584:ILE:HG22	1:G:585:MET:HE2	2.02	0.41
1:G:784:VAL:HA	1:G:785:PRO:HD3	1.89	0.41
2:B:5:VAL:CG2	2:B:13:ILE:HB	2.51	0.41
1:D:563:LEU:HA	1:D:563:LEU:HD12	1.81	0.41
1:G:825:SER:OG	1:G:826:LYS:N	2.52	0.41
1:A:847:LEU:HD12	1:A:847:LEU:HA	1.90	0.40
1:A:877:LYS:NZ	1:A:898:PRO:HG3	2.37	0.40
1:D:720:LEU:HD23	1:D:720:LEU:HA	1.73	0.40
3:F:7:LEU:HD23	3:F:7:LEU:HA	1.86	0.40
1:G:658:CYS:O	1:G:662:ARG:HG3	2.21	0.40
3:C:40:VAL:HG13	3:C:152:PRO:HB2	2.03	0.40
1:G:585:MET:HE3	1:G:659:PHE:HD1	1.86	0.40
3:C:150:LYS:HB2	3:C:151:ARG:HA	2.04	0.40
1:D:683:TYR:CD1	1:D:686:MET:HE3	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:704:TYR:CZ	1:G:708:ILE:HD12	2.56	0.40
1:G:728:MET:HB2	1:G:763:TRP:HZ2	1.85	0.40
1:G:902:TYR:O	1:G:904:GLN:N	2.55	0.40
1:D:677:GLY:N	1:D:855:ARG:NH1	2.69	0.40
1:G:611:LEU:CD2	1:G:613:ARG:NH1	2.82	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)
3:C:146:LYS:O	1:G:568:LYS:NZ[4_445]	1.99	0.21
1:D:608:TYR:OH	1:G:908:LYS:NZ[4_455]	2.00	0.20

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	371/383 (97%)	360 (97%)	11 (3%)	0	100	100
1	D	365/383 (95%)	343 (94%)	21 (6%)	1 (0%)	36	55
1	G	359/383 (94%)	335 (93%)	24 (7%)	0	100	100
2	B	74/83 (89%)	73 (99%)	1 (1%)	0	100	100
2	E	74/83 (89%)	71 (96%)	3 (4%)	0	100	100
2	H	73/83 (88%)	70 (96%)	3 (4%)	0	100	100
3	C	149/161 (92%)	138 (93%)	9 (6%)	2 (1%)	9	20
3	F	148/161 (92%)	140 (95%)	8 (5%)	0	100	100
All	All	1613/1720 (94%)	1530 (95%)	80 (5%)	3 (0%)	43	62

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	120	PRO
1	D	878	VAL
3	C	125	LEU

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	338/344 (98%)	321 (95%)	17 (5%)	22	44
1	D	334/344 (97%)	307 (92%)	27 (8%)	11	24
1	G	333/344 (97%)	319 (96%)	14 (4%)	26	51
2	B	69/71 (97%)	64 (93%)	5 (7%)	13	28
2	E	69/71 (97%)	65 (94%)	4 (6%)	18	38
2	H	68/71 (96%)	63 (93%)	5 (7%)	13	27
3	C	135/143 (94%)	125 (93%)	10 (7%)	13	27
3	F	134/143 (94%)	124 (92%)	10 (8%)	12	27
All	All	1480/1531 (97%)	1388 (94%)	92 (6%)	16	34

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	548	ARG
1	A	551	LEU
1	A	568	LYS
1	A	578	GLU
1	A	596	LEU
1	A	608	TYR
1	A	623	VAL
1	A	641	LEU
1	A	649	ILE
1	A	718	CYS
1	A	827	GLN
1	A	839	ASP
1	A	863	GLU

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Mol	Chain	Res	Type
1	A	880	LYS
1	A	882	THR
1	A	915	GLU
1	A	917	GLU
2	B	13	ILE
2	B	16	GLU
2	B	54	ARG
2	B	70	VAL
2	B	72	ARG
3	C	27	VAL
3	C	67	LYS
3	C	78	ASN
3	C	85	VAL
3	C	93	GLU
3	C	109	ILE
3	C	116	GLN
3	C	124	ASP
3	C	149	GLU
3	C	150	LYS
1	D	555	ARG
1	D	563	LEU
1	D	578	GLU
1	D	589	PRO
1	D	603	GLU
1	D	604	GLU
1	D	611	LEU
1	D	624	LEU
1	D	651	PRO
1	D	652	ASP
1	D	676	THR
1	D	680	LEU
1	D	690	LYS
1	D	698	SER
1	D	708	ILE
1	D	715	ILE
1	D	720	LEU
1	D	728	MET
1	D	744	SER
1	D	747	LEU
1	D	748	VAL
1	D	755	GLU
1	D	789	LEU

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Mol	Chain	Res	Type
1	D	822	THR
1	D	843	ARG
1	D	872	LYS
1	D	890	CYS
2	E	24	GLU
2	E	58	ASP
2	E	65	SER
2	E	73	LEU
3	F	4	SER
3	F	14	ILE
3	F	16	LYS
3	F	25	ILE
3	F	39	ILE
3	F	52	ARG
3	F	71	LYS
3	F	114	ASP
3	F	142	GLU
3	F	150	LYS
1	G	567	VAL
1	G	578	GLU
1	G	649	ILE
1	G	668	LEU
1	G	674	ILE
1	G	708	ILE
1	G	799	VAL
1	G	805	GLN
1	G	807	VAL
1	G	822	THR
1	G	823	ARG
1	G	888	HIS
1	G	902	TYR
1	G	904	GLN
2	H	25	ASN
2	H	34	GLU
2	H	61	ILE
2	H	62	LYS
2	H	72	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	553	HIS

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Mol	Chain	Res	Type
1	A	566	HIS
1	A	737	HIS
1	A	833	GLN
2	B	60	ASN
3	C	94	ASN
1	D	650	ASN
1	D	714	ASN
1	D	737	HIS
1	D	745	ASN
1	D	827	GLN
1	D	840	ASN
1	D	871	GLN
1	G	566	HIS
1	G	827	GLN
1	G	888	HIS
2	H	25	ASN

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 ⓘ

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	373/383 (97%)	-0.04	7 (1%) 66 59	42, 64, 104, 134	0
1	D	371/383 (96%)	0.30	15 (4%) 42 33	39, 69, 162, 199	0
1	G	367/383 (95%)	0.24	8 (2%) 62 53	49, 83, 124, 151	0
2	B	74/83 (89%)	-0.10	0 100 100	54, 78, 94, 104	0
2	E	74/83 (89%)	0.35	1 (1%) 73 67	64, 103, 130, 138	0
2	H	73/83 (87%)	0.31	0 100 100	76, 95, 119, 133	0
3	C	151/161 (93%)	0.31	3 (1%) 65 57	56, 92, 144, 159	0
3	F	150/161 (93%)	0.52	3 (2%) 65 57	68, 121, 153, 167	0
All	All	1633/1720 (94%)	0.21	37 (2%) 61 52	39, 82, 141, 199	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	605	GLY	4.9
1	G	822	THR	4.7
1	D	822	THR	4.1
3	F	2	ALA	4.0
1	D	607	ASP	3.5
1	A	606	LEU	3.4
3	F	3	ALA	3.2
1	D	606	LEU	3.1
1	D	910	LEU	3.1
1	A	605	GLY	3.0
1	D	754	ASP	2.9
1	A	608	TYR	2.8
1	D	906	LYS	2.7
1	D	899	TYR	2.7
3	C	151	ARG	2.5
1	D	608	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	607	ASP	2.5
2	E	4	LEU	2.5
1	A	609	GLY	2.5
1	G	612	ALA	2.4
1	D	873	PHE	2.4
3	F	75	TYR	2.4
1	D	870	PRO	2.4
1	G	877	LYS	2.3
1	A	881	ASP	2.3
1	D	896	LEU	2.3
1	D	885	PRO	2.3
1	D	883	TRP	2.2
3	C	3	ALA	2.2
1	D	884	LEU	2.2
1	G	609	GLY	2.2
3	C	130	SER	2.2
1	A	880	LYS	2.1
1	G	715	ILE	2.1
1	D	867	SER	2.0
1	G	854	CYS	2.0
1	G	817	VAL	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.