



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:23 AM UTC

PDB ID : 1EKM / pdb_00001ekm
Title : CRYSTAL STRUCTURE AT 2.5 Å RESOLUTION OF ZINC-SUBSTITUTED COPPER AMINE OXIDASE OF HANSENULA POLYMORPHA EXPRESSED IN ESCHERICHIA COLI
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Deposited on : 2000-03-09
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

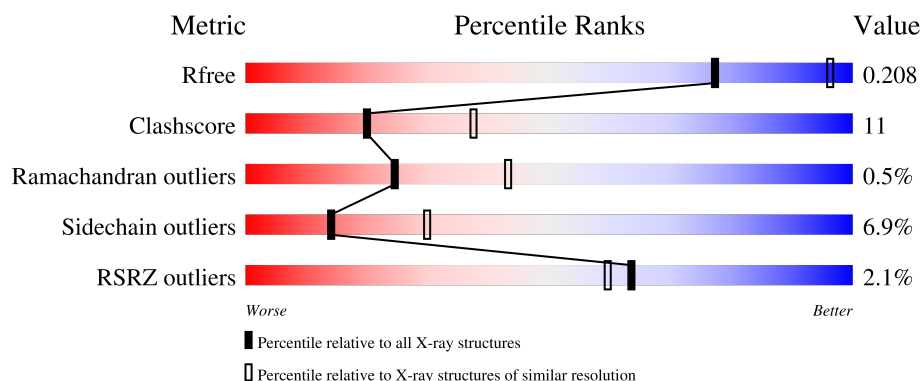
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	656	3% 72% 24% .
1	B	656	2% 72% 24% .
1	C	656	% 73% 22% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17070 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 COPPER AMINE OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	656	Total	C	N	O	S	0	0	0
			5197	3308	893	973	23			
1	B	656	Total	C	N	O	S	0	0	0
			5197	3308	893	973	23			
1	C	656	Total	C	N	O	S	0	0	0
			5197	3308	893	973	23			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		

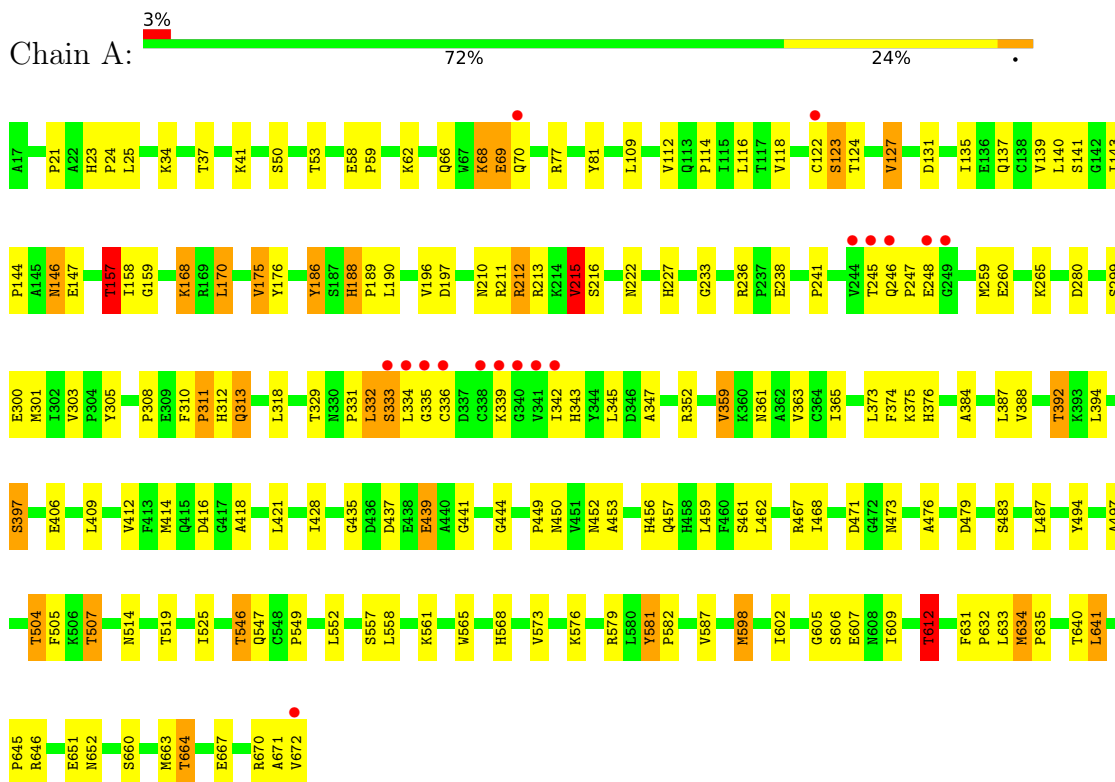
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	492	Total	O	0	0
			492	492		
3	B	491	Total	O	0	0
			491	491		
3	C	493	Total	O	0	0
			493	493		

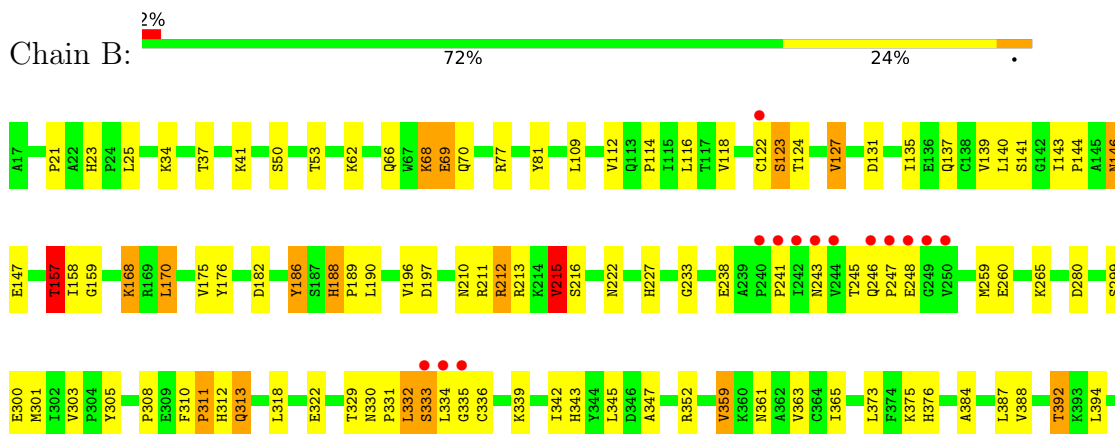
3 Residue-property plots

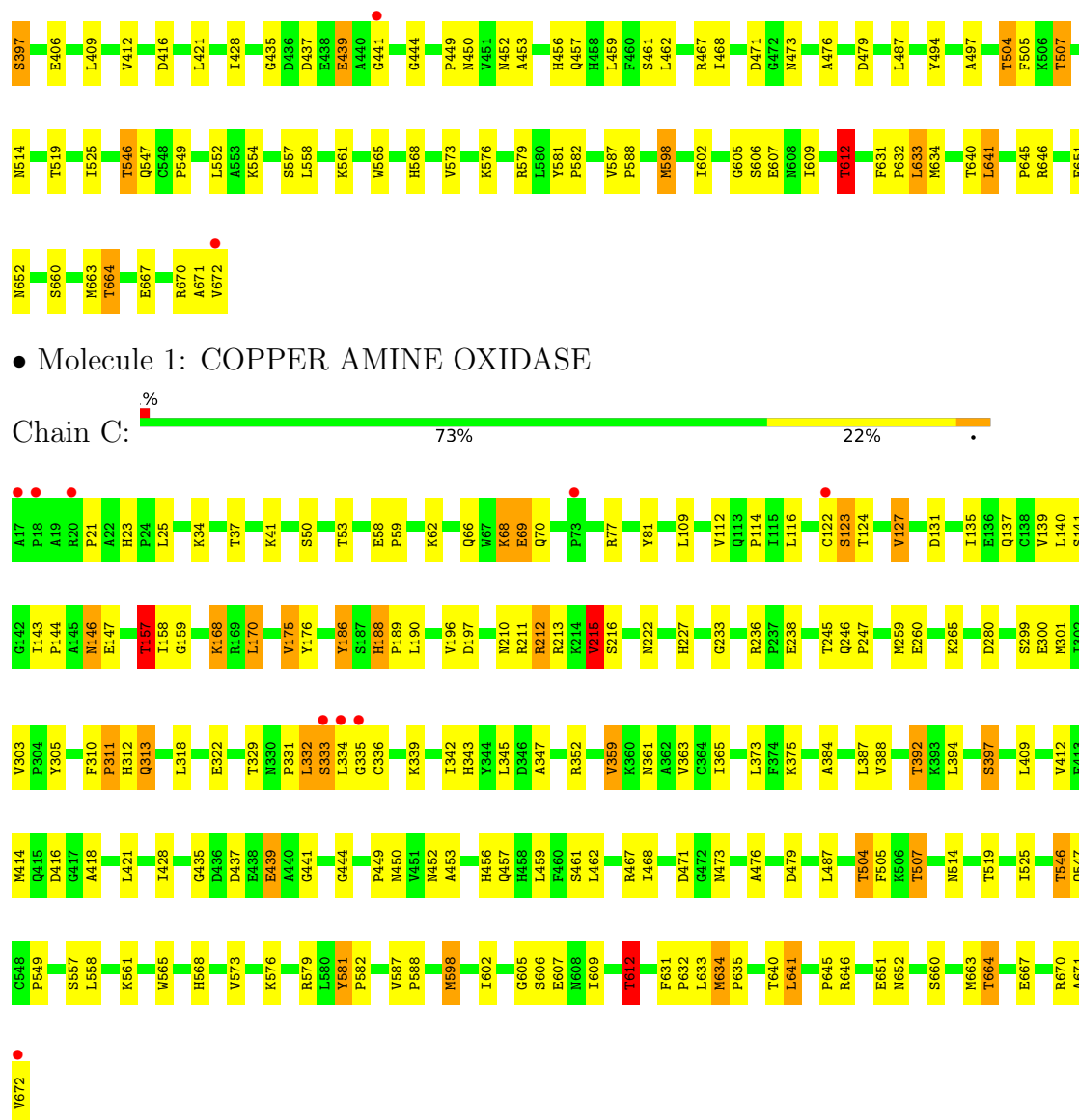
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: COPPER AMINE OXIDASE





• Molecule 1: COPPER AMINE OXIDASE

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	139.23Å 153.51Å 223.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	500.00 – 2.50 111.70 – 2.50	Depositor EDS
% Data completeness (in resolution range)	77.9 (500.00-2.50) 77.9 (111.70-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 2.39Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.183 , 0.208 0.183 , 0.208	Depositor DCC
R_{free} test set	6852 reflections (10.12%)	wwPDB-VP
Wilson B-factor (Å ²)	24.0	Xtriage
Anisotropy	0.392	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 44.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	17070	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.52	1/5348 (0.0%)	1.09	30/7280 (0.4%)
1	B	0.52	1/5348 (0.0%)	1.09	28/7280 (0.4%)
1	C	0.52	1/5348 (0.0%)	1.09	30/7280 (0.4%)
All	All	0.52	3/16044 (0.0%)	1.09	88/21840 (0.4%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	598	MET	SD-CE	-5.35	1.66	1.79
1	A	598	MET	SD-CE	-5.34	1.66	1.79
1	C	598	MET	SD-CE	-5.32	1.66	1.79

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	581	TYR	CA-C-N	8.93	129.83	119.47
1	B	581	TYR	C-N-CA	8.93	129.83	119.47
1	A	581	TYR	CA-C-N	8.93	129.82	119.47
1	A	581	TYR	C-N-CA	8.93	129.82	119.47
1	C	581	TYR	CA-C-N	8.92	129.82	119.47
1	C	581	TYR	C-N-CA	8.92	129.82	119.47
1	B	157	THR	N-CA-C	-8.31	98.78	110.50
1	A	157	THR	N-CA-C	-8.28	98.83	110.50
1	C	157	THR	N-CA-C	-8.27	98.84	110.50
1	A	634	MET	N-CA-C	8.22	120.00	109.72
1	C	634	MET	N-CA-C	8.22	119.99	109.72
1	B	634	MET	N-CA-C	8.21	119.98	109.72
1	C	334	LEU	N-CA-C	8.13	120.94	111.02
1	A	334	LEU	N-CA-C	8.11	120.92	111.02
1	B	334	LEU	N-CA-C	8.11	120.91	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	246	GLN	CA-C-N	7.81	128.53	119.47
1	A	246	GLN	C-N-CA	7.81	128.53	119.47
1	B	246	GLN	CA-C-N	7.81	128.53	119.47
1	B	246	GLN	C-N-CA	7.81	128.53	119.47
1	C	246	GLN	CA-C-N	7.78	128.50	119.47
1	C	246	GLN	C-N-CA	7.78	128.50	119.47
1	A	332	LEU	N-CA-C	7.56	121.76	112.54
1	C	332	LEU	N-CA-C	7.55	121.75	112.54
1	B	332	LEU	N-CA-C	7.53	121.73	112.54
1	A	397	SER	N-CA-C	7.17	119.82	109.14
1	B	397	SER	N-CA-C	7.16	119.81	109.14
1	C	397	SER	N-CA-C	7.15	119.79	109.14
1	A	158	ILE	N-CA-C	-6.57	104.46	113.00
1	B	158	ILE	N-CA-C	-6.54	104.50	113.00
1	B	188	HIS	N-CA-C	6.45	120.11	109.79
1	C	188	HIS	N-CA-C	6.45	120.11	109.79
1	A	188	HIS	N-CA-C	6.45	120.11	109.79
1	C	331	PRO	N-CA-C	-6.45	100.04	110.74
1	B	331	PRO	N-CA-C	-6.43	100.06	110.74
1	C	170	LEU	N-CA-C	6.38	119.94	109.85
1	B	170	LEU	N-CA-C	6.38	119.93	109.85
1	A	170	LEU	N-CA-C	6.37	119.91	109.85
1	C	158	ILE	N-CA-C	-6.32	104.47	113.07
1	B	336	CYS	N-CA-C	-6.28	102.58	111.56
1	A	336	CYS	N-CA-C	-6.27	102.59	111.56
1	C	336	CYS	N-CA-C	-6.27	102.60	111.56
1	B	416	ASP	N-CA-C	-6.18	105.38	113.17
1	A	416	ASP	N-CA-C	-6.18	105.38	113.17
1	C	416	ASP	N-CA-C	-6.14	105.44	113.17
1	A	373	LEU	N-CA-C	-6.06	104.03	112.45
1	B	373	LEU	N-CA-C	-6.04	104.05	112.45
1	C	373	LEU	N-CA-C	-6.04	104.05	112.45
1	A	331	PRO	N-CA-C	-6.02	100.07	112.47
1	A	196	VAL	N-CA-C	5.78	116.91	108.53
1	B	186	TYR	N-CA-C	5.77	119.79	112.87
1	C	196	VAL	N-CA-C	5.77	116.89	108.53
1	B	196	VAL	N-CA-C	5.76	116.89	108.53
1	A	186	TYR	N-CA-C	5.75	119.77	112.87
1	A	233	GLY	N-CA-C	5.74	119.44	112.49
1	C	233	GLY	N-CA-C	5.72	119.41	112.49
1	B	233	GLY	N-CA-C	5.70	119.39	112.49
1	C	186	TYR	N-CA-C	5.70	119.71	112.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	157	THR	CB-CA-C	-5.53	99.37	109.54
1	B	157	THR	CB-CA-C	-5.53	99.37	109.54
1	C	157	THR	CB-CA-C	-5.52	99.39	109.54
1	A	612	THR	CB-CA-C	-5.51	102.48	114.10
1	C	612	THR	CB-CA-C	-5.50	102.49	114.10
1	B	384	ALA	N-CA-C	-5.50	105.44	111.82
1	B	612	THR	CB-CA-C	-5.50	102.49	114.10
1	A	384	ALA	N-CA-C	-5.48	105.46	111.82
1	C	384	ALA	N-CA-C	-5.47	105.47	111.82
1	C	525	ILE	N-CA-C	-5.35	98.78	107.28
1	A	525	ILE	N-CA-C	-5.32	98.81	107.28
1	A	606	SER	N-CA-C	5.31	119.76	113.28
1	C	606	SER	N-CA-C	5.31	119.76	113.28
1	B	525	ILE	N-CA-C	-5.30	98.85	107.28
1	B	606	SER	N-CA-C	5.29	119.74	113.28
1	B	587	VAL	N-CA-C	5.25	120.21	108.88
1	B	215	VAL	CB-CA-C	-5.24	102.70	111.29
1	A	587	VAL	N-CA-C	5.24	120.19	108.88
1	A	215	VAL	CB-CA-C	-5.22	102.73	111.29
1	C	587	VAL	N-CA-C	5.22	120.15	108.88
1	C	215	VAL	CB-CA-C	-5.21	102.74	111.29
1	C	412	VAL	N-CA-C	5.19	115.44	108.17
1	C	660	SER	N-CA-C	-5.19	106.80	113.23
1	A	660	SER	N-CA-C	-5.17	106.82	113.23
1	A	412	VAL	N-CA-C	5.17	115.41	108.17
1	B	412	VAL	N-CA-C	5.16	115.40	108.17
1	B	660	SER	N-CA-C	-5.16	106.83	113.23
1	C	175	VAL	N-CA-C	5.03	116.04	109.21
1	C	236	ARG	N-CA-C	-5.03	102.85	110.39
1	A	175	VAL	N-CA-C	5.02	116.04	109.21
1	A	236	ARG	N-CA-C	-5.02	102.86	110.39

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	5197	0	5037	139	0
1	B	5197	0	5037	133	0
1	C	5197	0	5037	107	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	492	0	0	10	1
3	B	491	0	0	9	0
3	C	493	0	0	6	0
All	All	17070	0	15111	350	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 11.

All (350) 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:546:THR:HG21	1:B:546:THR:CG2	1.22	1.60
1:A:546:THR:CG2	1:B:546:THR:HG21	1.24	1.57
1:A:546:THR:CG2	1:B:546:THR:CG2	1.96	1.18
1:A:664:THR:HG22	1:A:667:GLU:H	1.26	0.99
1:C:664:THR:HG22	1:C:667:GLU:H	1.26	0.98
1:A:546:THR:HG21	1:B:546:THR:HG23	1.48	0.96
1:B:664:THR:HG22	1:B:667:GLU:H	1.26	0.95
1:A:313:GLN:HG2	1:B:494:TYR:CD1	2.00	0.95
1:C:23:HIS:HD2	1:C:25:LEU:H	1.08	0.95
1:B:23:HIS:HD2	1:B:25:LEU:H	1.08	0.95
1:B:311:PRO:HA	1:B:313:GLN:HE22	1.35	0.92
1:A:546:THR:CG2	1:B:546:THR:HG23	2.00	0.91
1:A:23:HIS:HD2	1:A:25:LEU:H	1.08	0.90
1:A:311:PRO:HA	1:A:313:GLN:HE22	1.35	0.90
1:A:546:THR:HG23	1:B:546:THR:CG2	2.03	0.89
1:C:311:PRO:HA	1:C:313:GLN:HE22	1.35	0.88
1:A:494:TYR:CD1	1:B:313:GLN:HG2	2.09	0.88
1:B:598:MET:HE2	1:B:602:ILE:HG13	1.63	0.81
1:C:598:MET:HE2	1:C:602:ILE:HG13	1.63	0.81
1:C:311:PRO:HA	1:C:313:GLN:NE2	1.96	0.81
1:A:311:PRO:HA	1:A:313:GLN:NE2	1.97	0.80
1:B:311:PRO:HA	1:B:313:GLN:NE2	1.96	0.79
1:A:546:THR:HG23	1:B:546:THR:HG21	1.54	0.79
1:A:598:MET:HE2	1:A:602:ILE:HG13	1.63	0.79
1:A:546:THR:HG21	1:B:546:THR:HG22	1.58	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:PRO:HG2	1:A:147:GLU:HG3	1.67	0.76
1:B:144:PRO:HG2	1:B:147:GLU:HG3	1.67	0.76
1:A:546:THR:HG22	1:B:546:THR:HG21	1.57	0.76
1:B:23:HIS:CD2	1:B:25:LEU:H	2.00	0.75
1:C:144:PRO:HG2	1:C:147:GLU:HG3	1.67	0.75
1:B:157:THR:HB	1:B:159:GLY:H	1.53	0.74
1:A:157:THR:HB	1:A:159:GLY:H	1.53	0.73
1:C:157:THR:HB	1:C:159:GLY:H	1.53	0.73
1:C:23:HIS:CD2	1:C:25:LEU:H	2.01	0.73
1:B:507:THR:HG23	1:B:605:GLY:O	1.89	0.73
1:C:507:THR:HG23	1:C:605:GLY:O	1.89	0.73
1:A:23:HIS:CD2	1:A:25:LEU:H	2.00	0.73
1:C:392:THR:HG22	3:C:804:HOH:O	1.89	0.72
1:B:392:THR:HG22	3:B:873:HOH:O	1.89	0.72
1:A:392:THR:HG22	3:A:767:HOH:O	1.89	0.71
1:A:546:THR:HG21	1:B:546:THR:HG21	0.77	0.71
1:A:507:THR:HG23	1:A:605:GLY:O	1.89	0.71
1:B:50:SER:HB2	1:B:352:ARG:HG2	1.73	0.71
1:A:50:SER:HB2	1:A:352:ARG:HG2	1.73	0.70
1:B:137:GLN:OE1	1:B:212:ARG:NH2	2.25	0.70
1:C:137:GLN:OE1	1:C:212:ARG:NH2	2.25	0.69
1:B:664:THR:HG21	3:B:715:HOH:O	1.92	0.69
1:C:50:SER:HB2	1:C:352:ARG:HG2	1.73	0.69
1:A:137:GLN:OE1	1:A:212:ARG:NH2	2.25	0.68
1:A:664:THR:HG22	1:A:667:GLU:N	2.07	0.68
1:C:664:THR:HG22	1:C:667:GLU:N	2.07	0.68
1:A:68:LYS:HE2	1:A:280:ASP:OD2	1.95	0.67
1:C:68:LYS:HE2	1:C:280:ASP:OD2	1.95	0.67
1:B:664:THR:HG22	1:B:667:GLU:N	2.07	0.66
1:B:670:ARG:NH2	3:B:786:HOH:O	2.28	0.66
1:B:68:LYS:HE2	1:B:280:ASP:OD2	1.95	0.66
1:A:146:ASN:N	1:A:146:ASN:HD22	1.94	0.65
1:A:631:PHE:CG	1:A:632:PRO:HA	2.32	0.65
1:B:631:PHE:CG	1:B:632:PRO:HA	2.32	0.65
1:C:631:PHE:CG	1:C:632:PRO:HA	2.32	0.65
1:B:146:ASN:HD22	1:B:146:ASN:N	1.94	0.64
1:C:146:ASN:N	1:C:146:ASN:HD22	1.94	0.64
1:C:211:ARG:NH2	1:C:435:GLY:HA3	2.13	0.63
1:A:211:ARG:NH2	1:A:435:GLY:HA3	2.13	0.63
1:B:211:ARG:NH2	1:B:435:GLY:HA3	2.13	0.63
1:A:452:ASN:C	1:A:452:ASN:HD22	2.08	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:GLU:HB2	1:B:241:PRO:HD2	1.82	0.61
1:B:452:ASN:C	1:B:452:ASN:HD22	2.07	0.61
1:A:123:SER:O	1:A:127:VAL:HG12	2.01	0.61
1:B:123:SER:O	1:B:127:VAL:HG12	2.01	0.61
1:B:439:GLU:C	1:B:441:GLY:H	2.09	0.60
1:C:123:SER:O	1:C:127:VAL:HG12	2.01	0.60
1:B:573:VAL:HG11	1:B:598:MET:HE1	1.84	0.60
1:A:573:VAL:HG11	1:A:598:MET:HE1	1.84	0.60
1:A:376:HIS:ND1	1:B:406:GLU:OE2	2.35	0.60
1:C:598:MET:HE2	1:C:602:ILE:CG1	2.32	0.59
1:A:439:GLU:C	1:A:441:GLY:H	2.09	0.59
1:B:452:ASN:HD22	1:B:453:ALA:N	2.01	0.59
1:C:573:VAL:HG11	1:C:598:MET:HE1	1.84	0.59
1:A:598:MET:HE2	1:A:602:ILE:CG1	2.32	0.59
1:C:452:ASN:C	1:C:452:ASN:HD22	2.07	0.59
1:C:598:MET:CE	1:C:602:ILE:HG13	2.33	0.59
1:B:146:ASN:HD22	1:B:146:ASN:H	1.51	0.58
1:A:598:MET:CE	1:A:602:ILE:HG13	2.33	0.58
1:C:573:VAL:CG1	1:C:598:MET:HE1	2.34	0.58
1:B:190:LEU:CD2	1:B:215:VAL:HG13	2.34	0.58
1:B:573:VAL:CG1	1:B:598:MET:HE1	2.34	0.58
1:B:598:MET:HE2	1:B:602:ILE:CG1	2.32	0.58
1:C:439:GLU:C	1:C:441:GLY:H	2.09	0.58
1:A:452:ASN:HD22	1:A:453:ALA:N	2.01	0.58
1:A:573:VAL:CG1	1:A:598:MET:HE1	2.34	0.58
1:A:565:TRP:CD1	1:A:582:PRO:HB2	2.39	0.58
1:C:565:TRP:CD1	1:C:582:PRO:HB2	2.39	0.58
1:B:565:TRP:CD1	1:B:582:PRO:HB2	2.39	0.58
1:B:468:ILE:H	1:B:473:ASN:HD21	1.52	0.57
1:C:190:LEU:CD2	1:C:215:VAL:HG13	2.34	0.57
1:C:468:ILE:H	1:C:473:ASN:HD21	1.52	0.57
1:A:190:LEU:CD2	1:A:215:VAL:HG13	2.34	0.57
1:B:598:MET:CE	1:B:602:ILE:HG13	2.33	0.57
1:C:452:ASN:HD22	1:C:453:ALA:N	2.01	0.57
1:A:146:ASN:HD22	1:A:146:ASN:H	1.51	0.56
1:A:557:SER:O	1:A:561:LYS:HG3	2.05	0.56
1:A:313:GLN:HG2	1:B:494:TYR:CE1	2.39	0.56
1:B:347:ALA:HB3	1:B:359:VAL:HG13	1.88	0.56
1:C:557:SER:O	1:C:561:LYS:HG3	2.05	0.56
1:C:146:ASN:HD22	1:C:146:ASN:H	1.51	0.56
1:C:439:GLU:C	1:C:441:GLY:N	2.63	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:ILE:H	1:A:473:ASN:HD21	1.52	0.56
1:B:557:SER:O	1:B:561:LYS:HG3	2.05	0.56
1:C:671:ALA:O	1:C:672:VAL:HB	2.06	0.56
1:A:347:ALA:HB3	1:A:359:VAL:HG13	1.88	0.55
1:A:439:GLU:C	1:A:441:GLY:N	2.63	0.55
1:B:124:THR:O	1:B:127:VAL:HG13	2.07	0.55
1:B:146:ASN:H	1:B:146:ASN:ND2	2.05	0.55
1:C:312:HIS:HD2	3:C:1064:HOH:O	1.89	0.55
1:A:146:ASN:H	1:A:146:ASN:ND2	2.05	0.55
1:B:671:ALA:O	1:B:672:VAL:HB	2.06	0.55
1:B:439:GLU:C	1:B:441:GLY:N	2.63	0.55
1:A:671:ALA:O	1:A:672:VAL:HB	2.06	0.54
1:C:347:ALA:HB3	1:C:359:VAL:HG13	1.88	0.54
1:A:312:HIS:HD2	3:A:977:HOH:O	1.90	0.54
1:B:479:ASP:HB3	1:B:519:THR:HB	1.90	0.54
1:A:124:THR:O	1:A:127:VAL:HG13	2.07	0.54
1:C:504:THR:HG21	3:C:1099:HOH:O	2.08	0.54
1:C:124:THR:O	1:C:127:VAL:HG13	2.07	0.54
1:A:479:ASP:HB3	1:A:519:THR:HB	1.89	0.54
1:A:514:ASN:OD1	1:A:568:HIS:HA	2.07	0.54
1:C:375:LYS:HG3	1:C:388:VAL:HG22	1.90	0.54
1:C:546:THR:HB	3:C:1060:HOH:O	2.08	0.54
1:B:312:HIS:HD2	3:B:1085:HOH:O	1.90	0.53
1:B:514:ASN:OD1	1:B:568:HIS:HA	2.07	0.53
1:C:146:ASN:H	1:C:146:ASN:ND2	2.05	0.53
1:A:375:LYS:HG3	1:A:388:VAL:HG22	1.90	0.53
1:B:375:LYS:HG3	1:B:388:VAL:HG22	1.90	0.53
1:C:514:ASN:OD1	1:C:568:HIS:HA	2.07	0.53
1:A:504:THR:HG21	3:A:994:HOH:O	2.08	0.53
1:C:479:ASP:HB3	1:C:519:THR:HB	1.90	0.53
1:C:664:THR:CG2	1:C:667:GLU:H	2.12	0.53
1:A:376:HIS:HA	1:B:406:GLU:CD	2.34	0.52
1:B:452:ASN:C	1:B:452:ASN:ND2	2.67	0.52
1:B:504:THR:HG21	3:B:1102:HOH:O	2.08	0.52
1:B:576:LYS:HB2	1:B:579:ARG:HD2	1.92	0.52
1:A:631:PHE:CD1	1:A:632:PRO:HA	2.45	0.52
1:B:144:PRO:HG2	1:B:147:GLU:CG	2.40	0.52
1:C:631:PHE:CD1	1:C:632:PRO:HA	2.45	0.52
1:A:459:LEU:HD21	1:A:549:PRO:HG2	1.92	0.52
1:A:641:LEU:C	1:A:641:LEU:HD23	2.35	0.52
1:B:168:LYS:HD3	1:B:197:ASP:OD2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:168:LYS:HD3	1:C:197:ASP:OD2	2.10	0.52
1:B:459:LEU:HD21	1:B:549:PRO:HG2	1.92	0.52
1:C:459:LEU:HD21	1:C:549:PRO:HG2	1.92	0.51
1:C:576:LYS:HB2	1:C:579:ARG:HD2	1.92	0.51
1:C:452:ASN:C	1:C:452:ASN:ND2	2.67	0.51
1:B:476:ALA:HB2	1:B:504:THR:HA	1.92	0.51
1:B:664:THR:CG2	1:B:667:GLU:H	2.12	0.51
1:A:483:SER:O	1:B:554:LYS:NZ	2.44	0.51
1:B:641:LEU:C	1:B:641:LEU:HD23	2.35	0.51
1:C:146:ASN:N	1:C:146:ASN:ND2	2.59	0.51
1:A:241:PRO:HD2	1:B:248:GLU:HB2	1.92	0.51
1:A:452:ASN:C	1:A:452:ASN:ND2	2.67	0.51
1:A:168:LYS:HD3	1:A:197:ASP:OD2	2.10	0.51
1:A:547:GLN:NE2	1:A:640:THR:H	2.09	0.51
1:A:576:LYS:HB2	1:A:579:ARG:HD2	1.92	0.51
1:B:68:LYS:HE2	1:B:280:ASP:CG	2.36	0.51
1:B:631:PHE:CD1	1:B:632:PRO:HA	2.45	0.51
1:C:641:LEU:HD23	1:C:641:LEU:C	2.35	0.51
1:A:245:THR:C	1:A:247:PRO:HD3	2.36	0.51
1:C:476:ALA:HB2	1:C:504:THR:HA	1.92	0.51
1:A:476:ALA:HB2	1:A:504:THR:HA	1.92	0.50
1:A:497:ALA:HB2	1:B:308:PRO:HB3	1.94	0.50
1:C:68:LYS:HE2	1:C:280:ASP:CG	2.35	0.50
1:B:245:THR:C	1:B:247:PRO:HD3	2.36	0.50
1:B:547:GLN:NE2	1:B:640:THR:H	2.09	0.50
1:A:494:TYR:CE1	1:B:313:GLN:HG2	2.47	0.50
1:B:387:LEU:C	1:B:387:LEU:HD23	2.37	0.50
1:A:68:LYS:HE2	1:A:280:ASP:CG	2.35	0.49
1:B:259:MET:CE	1:B:365:ILE:HG21	2.43	0.49
1:C:547:GLN:NE2	1:C:640:THR:H	2.09	0.49
1:A:259:MET:CE	1:A:365:ILE:HG21	2.43	0.49
1:C:245:THR:C	1:C:247:PRO:HD3	2.36	0.49
1:B:645:PRO:O	1:B:646:ARG:HD2	2.13	0.49
1:A:645:PRO:O	1:A:646:ARG:HD2	2.13	0.49
1:C:259:MET:CE	1:C:365:ILE:HG21	2.43	0.49
1:B:546:THR:HB	3:B:771:HOH:O	2.12	0.49
1:C:387:LEU:C	1:C:387:LEU:HD23	2.37	0.49
1:C:645:PRO:O	1:C:646:ARG:HD2	2.12	0.49
1:A:387:LEU:C	1:A:387:LEU:HD23	2.37	0.48
1:A:670:ARG:C	1:A:672:VAL:H	2.22	0.48
1:C:670:ARG:C	1:C:672:VAL:H	2.21	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:670:ARG:NH2	3:A:1164:HOH:O	2.45	0.48
1:B:397:SER:HB2	1:B:409:LEU:O	2.14	0.48
1:A:69:GLU:OE2	1:A:467:ARG:NH2	2.47	0.48
1:B:641:LEU:C	1:B:641:LEU:CD2	2.87	0.48
1:B:670:ARG:C	1:B:672:VAL:H	2.21	0.48
1:C:444:GLY:HA3	1:C:452:ASN:HD21	1.78	0.48
1:C:69:GLU:OE2	1:C:467:ARG:NH2	2.47	0.47
1:B:116:LEU:HD12	1:B:157:THR:HG23	1.97	0.47
1:A:144:PRO:HG2	1:A:147:GLU:CG	2.40	0.47
1:B:444:GLY:HA3	1:B:452:ASN:HD21	1.78	0.47
1:C:310:PHE:HA	1:C:313:GLN:HE21	1.79	0.47
1:A:247:PRO:HG2	1:B:243:ASN:ND2	2.30	0.47
1:A:310:PHE:HA	1:A:313:GLN:HE21	1.79	0.47
1:B:69:GLU:OE2	1:B:467:ARG:NH2	2.47	0.47
1:C:260:GLU:HG2	1:C:265:LYS:HG3	1.97	0.47
1:C:397:SER:HB2	1:C:409:LEU:O	2.14	0.47
1:C:437:ASP:HB2	3:C:988:HOH:O	2.15	0.47
1:A:116:LEU:HD12	1:A:157:THR:HG23	1.97	0.47
1:A:345:LEU:HB2	1:A:363:VAL:HB	1.97	0.47
1:A:641:LEU:C	1:A:641:LEU:CD2	2.87	0.47
1:B:260:GLU:HG2	1:B:265:LYS:HG3	1.97	0.47
1:B:310:PHE:HA	1:B:313:GLN:HE21	1.79	0.47
1:B:461:SER:HB2	1:B:565:TRP:CE3	2.50	0.47
1:A:397:SER:HB2	1:A:409:LEU:O	2.14	0.47
1:A:124:THR:HA	1:A:127:VAL:CG1	2.45	0.47
1:C:124:THR:HA	1:C:127:VAL:CG1	2.45	0.47
1:C:461:SER:HB2	1:C:565:TRP:CE3	2.50	0.46
1:A:461:SER:HB2	1:A:565:TRP:CE3	2.50	0.46
1:B:124:THR:HA	1:B:127:VAL:CG1	2.46	0.46
1:A:375:LYS:O	1:B:406:GLU:HG3	2.16	0.46
1:B:467:ARG:HH11	1:B:471:ASP:CG	2.23	0.46
1:C:301:MET:O	1:C:318:LEU:HA	2.15	0.46
1:C:467:ARG:HH11	1:C:471:ASP:CG	2.23	0.46
1:A:664:THR:HG21	3:A:1089:HOH:O	2.16	0.46
1:B:437:ASP:HB2	3:B:1025:HOH:O	2.15	0.46
1:C:131:ASP:O	1:C:135:ILE:HG13	2.16	0.46
1:C:186:TYR:CD2	1:C:428:ILE:HG21	2.51	0.46
1:C:345:LEU:HB2	1:C:363:VAL:HB	1.97	0.46
1:A:186:TYR:CD2	1:A:428:ILE:HG21	2.51	0.46
1:B:131:ASP:O	1:B:135:ILE:HG13	2.16	0.46
1:A:444:GLY:HA3	1:A:452:ASN:HD21	1.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:641:LEU:C	1:C:641:LEU:CD2	2.87	0.46
1:A:313:GLN:HG2	1:B:494:TYR:CG	2.47	0.46
1:B:301:MET:O	1:B:318:LEU:HA	2.15	0.46
1:C:144:PRO:HG2	1:C:147:GLU:CG	2.39	0.46
1:C:671:ALA:O	1:C:672:VAL:CB	2.64	0.46
1:C:116:LEU:HD12	1:C:157:THR:HG23	1.97	0.46
1:C:190:LEU:HD21	1:C:215:VAL:HG13	1.98	0.46
1:A:301:MET:O	1:A:318:LEU:HA	2.15	0.46
1:B:66:GLN:HG2	1:B:70:GLN:NE2	2.31	0.46
1:B:671:ALA:O	1:B:672:VAL:CB	2.64	0.46
1:A:247:PRO:HG2	1:B:243:ASN:HD22	1.81	0.46
1:A:62:LYS:HB3	1:A:62:LYS:HE2	1.70	0.45
1:A:131:ASP:O	1:A:135:ILE:HG13	2.16	0.45
1:A:260:GLU:HG2	1:A:265:LYS:HG3	1.97	0.45
1:A:437:ASP:HB2	3:A:916:HOH:O	2.15	0.45
1:A:467:ARG:HH11	1:A:471:ASP:CG	2.23	0.45
1:C:141:SER:O	1:C:215:VAL:HG22	2.16	0.45
1:A:299:SER:O	1:A:300:GLU:HB2	2.16	0.45
1:A:671:ALA:O	1:A:672:VAL:CB	2.64	0.45
1:B:141:SER:O	1:B:215:VAL:HG22	2.16	0.45
1:A:21:PRO:HG3	1:A:77:ARG:CZ	2.46	0.45
1:C:21:PRO:HG3	1:C:77:ARG:CZ	2.46	0.45
1:A:66:GLN:HG2	1:A:70:GLN:NE2	2.31	0.45
1:B:186:TYR:CD2	1:B:428:ILE:HG21	2.51	0.45
1:B:299:SER:O	1:B:300:GLU:HB2	2.16	0.45
1:B:651:GLU:O	1:B:652:ASN:C	2.60	0.45
1:B:175:VAL:HG11	1:B:190:LEU:HD12	1.99	0.45
1:B:345:LEU:HB2	1:B:363:VAL:HB	1.97	0.45
1:A:546:THR:HB	3:A:1147:HOH:O	2.16	0.45
1:B:21:PRO:HG3	1:B:77:ARG:CZ	2.47	0.45
1:B:310:PHE:HA	1:B:313:GLN:NE2	2.32	0.45
1:A:141:SER:O	1:A:215:VAL:HG22	2.16	0.45
1:B:190:LEU:HD21	1:B:215:VAL:HG13	1.98	0.45
1:C:299:SER:O	1:C:300:GLU:HB2	2.16	0.45
1:A:190:LEU:HD21	1:A:215:VAL:HG13	1.98	0.44
1:C:634:MET:HA	1:C:635:PRO:HD3	1.93	0.44
1:A:333:SER:HB2	1:A:361:ASN:OD1	2.18	0.44
1:A:375:LYS:HE2	3:A:1074:HOH:O	2.16	0.44
1:B:62:LYS:HB3	1:B:62:LYS:HE2	1.70	0.44
1:C:333:SER:HB2	1:C:361:ASN:OD1	2.18	0.44
1:C:66:GLN:HG2	1:C:70:GLN:NE2	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:VAL:HG11	1:A:190:LEU:HD12	1.99	0.44
1:A:449:PRO:O	1:A:450:ASN:HB2	2.18	0.44
1:C:175:VAL:HG11	1:C:190:LEU:HD12	1.99	0.44
1:A:308:PRO:HB3	1:B:497:ALA:HB2	2.00	0.44
1:A:310:PHE:HA	1:A:313:GLN:NE2	2.32	0.44
1:B:333:SER:HB2	1:B:361:ASN:OD1	2.18	0.44
1:B:449:PRO:O	1:B:450:ASN:HB2	2.18	0.44
1:B:139:VAL:HA	1:B:143:ILE:O	2.18	0.43
1:B:476:ALA:CB	1:B:504:THR:HA	2.48	0.43
1:C:310:PHE:HA	1:C:313:GLN:NE2	2.32	0.43
1:C:651:GLU:O	1:C:652:ASN:C	2.60	0.43
1:A:53:THR:O	1:A:81:TYR:HA	2.18	0.43
1:A:176:TYR:CE1	1:A:189:PRO:HB3	2.53	0.43
1:A:664:THR:HG23	1:B:182:ASP:OD1	2.18	0.43
1:B:53:THR:O	1:B:81:TYR:HA	2.18	0.43
1:A:342:ILE:HG22	1:A:343:HIS:N	2.34	0.43
1:B:176:TYR:CE1	1:B:189:PRO:HB3	2.53	0.43
1:A:581:TYR:HA	1:A:582:PRO:HD3	1.59	0.43
1:C:53:THR:O	1:C:81:TYR:HA	2.18	0.43
1:C:176:TYR:CE1	1:C:189:PRO:HB3	2.53	0.43
1:C:449:PRO:O	1:C:450:ASN:HB2	2.18	0.43
1:A:476:ALA:CB	1:A:504:THR:HA	2.48	0.43
1:A:651:GLU:O	1:A:652:ASN:C	2.60	0.43
1:C:476:ALA:CB	1:C:504:THR:HA	2.48	0.43
1:A:23:HIS:HA	1:A:24:PRO:HD3	1.95	0.42
1:A:573:VAL:HG11	1:A:598:MET:CE	2.48	0.42
1:B:573:VAL:HG11	1:B:598:MET:CE	2.48	0.42
1:C:139:VAL:HA	1:C:143:ILE:O	2.18	0.42
1:C:573:VAL:HG11	1:C:598:MET:CE	2.48	0.42
1:B:342:ILE:HG22	1:B:343:HIS:N	2.34	0.42
1:A:139:VAL:HA	1:A:143:ILE:O	2.18	0.42
1:C:62:LYS:HE2	1:C:62:LYS:HB3	1.70	0.42
1:C:37:THR:O	1:C:41:LYS:HG3	2.20	0.42
1:C:342:ILE:HG22	1:C:343:HIS:N	2.34	0.42
1:A:210:ASN:N	1:A:210:ASN:HD22	2.18	0.42
1:C:58:GLU:HA	1:C:59:PRO:HD3	1.90	0.42
1:A:37:THR:O	1:A:41:LYS:HG3	2.20	0.42
1:A:305:TYR:CD2	1:A:456:HIS:HB3	2.55	0.42
1:B:188:HIS:CD2	1:B:216:SER:HB3	2.55	0.42
1:B:305:TYR:CD2	1:B:456:HIS:HB3	2.55	0.42
1:A:58:GLU:HA	1:A:59:PRO:HD3	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:THR:O	1:B:41:LYS:HG3	2.20	0.42
1:B:505:PHE:HB3	1:B:609:ILE:HD11	2.02	0.42
1:C:414:MET:HE3	1:C:418:ALA:HB3	2.02	0.42
1:A:68:LYS:HE2	1:A:280:ASP:OD1	2.19	0.41
1:A:505:PHE:HB3	1:A:609:ILE:HD11	2.02	0.41
1:C:188:HIS:CD2	1:C:216:SER:HB3	2.55	0.41
1:A:303:VAL:HA	1:A:457:GLN:O	2.20	0.41
1:B:68:LYS:HE2	1:B:280:ASP:OD1	2.19	0.41
1:C:210:ASN:N	1:C:210:ASN:HD22	2.18	0.41
1:C:581:TYR:HA	1:C:582:PRO:HD3	1.58	0.41
1:A:188:HIS:CD2	1:A:216:SER:HB3	2.55	0.41
1:A:565:TRP:CD1	1:A:565:TRP:H	2.38	0.41
1:C:305:TYR:CD2	1:C:456:HIS:HB3	2.55	0.41
1:B:210:ASN:N	1:B:210:ASN:HD22	2.18	0.41
1:A:414:MET:HE3	1:A:418:ALA:HB3	2.02	0.41
1:A:634:MET:HA	1:A:635:PRO:HD3	1.93	0.41
1:B:303:VAL:HA	1:B:457:GLN:O	2.21	0.41
1:A:664:THR:CG2	1:A:667:GLU:H	2.12	0.41
1:B:457:GLN:HE22	1:B:552:LEU:H	1.69	0.41
1:C:222:ASN:HB3	1:C:227:HIS:ND1	2.36	0.41
1:C:303:VAL:HA	1:C:457:GLN:O	2.20	0.41
1:A:222:ASN:HB3	1:A:227:HIS:ND1	2.36	0.41
1:A:374:PHE:CD1	1:B:633:LEU:HD13	2.55	0.41
1:A:612:THR:HG21	3:A:975:HOH:O	2.21	0.41
1:B:222:ASN:HB3	1:B:227:HIS:ND1	2.36	0.41
1:C:124:THR:HA	1:C:127:VAL:HG13	2.03	0.41
1:C:505:PHE:HB3	1:C:609:ILE:HD11	2.02	0.41
1:C:565:TRP:CD1	1:C:565:TRP:H	2.38	0.41
1:A:118:VAL:HG13	3:A:905:HOH:O	2.21	0.41
1:A:457:GLN:HE22	1:A:552:LEU:H	1.69	0.41
1:B:118:VAL:HG13	3:B:1014:HOH:O	2.21	0.40
1:A:375:LYS:NZ	1:B:330:ASN:HD22	2.19	0.40
1:A:406:GLU:OE2	1:B:376:HIS:ND1	2.49	0.40
1:B:322:GLU:HG2	1:B:588:PRO:HG3	2.03	0.40
1:B:612:THR:HG21	3:B:1083:HOH:O	2.21	0.40
1:C:322:GLU:HG2	1:C:588:PRO:HG3	2.03	0.40
1:C:612:THR:HG21	3:C:1062:HOH:O	2.21	0.40
1:C:68:LYS:HE2	1:C:280:ASP:OD1	2.19	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:C:546:THR:CG2	1:C:546:THR:CG2[3_555]	1.83	0.37
3:A:1119:HOH:O	3:A:1119:HOH:O[3_555]	2.13	0.07

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	654/656 (100%)	620 (95%)	31 (5%)	3 (0%)	24	43
1	B	654/656 (100%)	620 (95%)	31 (5%)	3 (0%)	24	43
1	C	654/656 (100%)	620 (95%)	31 (5%)	3 (0%)	24	43
All	All	1962/1968 (100%)	1860 (95%)	93 (5%)	9 (0%)	24	43

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	SER
1	B	123	SER
1	C	123	SER
1	A	333	SER
1	A	335	GLY
1	B	333	SER
1	B	335	GLY
1	C	333	SER
1	C	335	GLY

5.3.2 Protein sidechains [i](#)

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	566/566 (100%)	527 (93%)	39 (7%)	14	30
1	B	566/566 (100%)	527 (93%)	39 (7%)	14	30
1	C	566/566 (100%)	527 (93%)	39 (7%)	14	30
All	All	1698/1698 (100%)	1581 (93%)	117 (7%)	14	30

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	LYS
1	A	68	LYS
1	A	69	GLU
1	A	109	LEU
1	A	112	VAL
1	A	114	PRO
1	A	122	CYS
1	A	127	VAL
1	A	140	LEU
1	A	146	ASN
1	A	157	THR
1	A	168	LYS
1	A	170	LEU
1	A	212	ARG
1	A	213	ARG
1	A	215	VAL
1	A	238	GLU
1	A	311	PRO
1	A	313	GLN
1	A	329	THR
1	A	332	LEU
1	A	339	LYS
1	A	359	VAL
1	A	392	THR
1	A	394	LEU
1	A	421	LEU
1	A	439	GLU
1	A	462	LEU
1	A	487	LEU
1	A	504	THR
1	A	507	THR
1	A	546	THR
1	A	558	LEU
1	A	607	GLU

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Mol	Chain	Res	Type
1	A	612	THR
1	A	633	LEU
1	A	641	LEU
1	A	663	MET
1	A	664	THR
1	B	34	LYS
1	B	68	LYS
1	B	69	GLU
1	B	109	LEU
1	B	112	VAL
1	B	114	PRO
1	B	122	CYS
1	B	127	VAL
1	B	140	LEU
1	B	146	ASN
1	B	157	THR
1	B	168	LYS
1	B	170	LEU
1	B	212	ARG
1	B	213	ARG
1	B	215	VAL
1	B	238	GLU
1	B	311	PRO
1	B	313	GLN
1	B	329	THR
1	B	332	LEU
1	B	339	LYS
1	B	359	VAL
1	B	392	THR
1	B	394	LEU
1	B	421	LEU
1	B	439	GLU
1	B	462	LEU
1	B	487	LEU
1	B	504	THR
1	B	507	THR
1	B	546	THR
1	B	558	LEU
1	B	607	GLU
1	B	612	THR
1	B	633	LEU
1	B	641	LEU

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Mol	Chain	Res	Type
1	B	663	MET
1	B	664	THR
1	C	34	LYS
1	C	68	LYS
1	C	69	GLU
1	C	109	LEU
1	C	112	VAL
1	C	114	PRO
1	C	122	CYS
1	C	127	VAL
1	C	140	LEU
1	C	146	ASN
1	C	157	THR
1	C	168	LYS
1	C	170	LEU
1	C	212	ARG
1	C	213	ARG
1	C	215	VAL
1	C	238	GLU
1	C	311	PRO
1	C	313	GLN
1	C	329	THR
1	C	332	LEU
1	C	339	LYS
1	C	359	VAL
1	C	392	THR
1	C	394	LEU
1	C	421	LEU
1	C	439	GLU
1	C	462	LEU
1	C	487	LEU
1	C	504	THR
1	C	507	THR
1	C	546	THR
1	C	558	LEU
1	C	607	GLU
1	C	612	THR
1	C	633	LEU
1	C	641	LEU
1	C	663	MET
1	C	664	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	HIS
1	A	70	GLN
1	A	146	ASN
1	A	210	ASN
1	A	218	HIS
1	A	243	ASN
1	A	288	ASN
1	A	312	HIS
1	A	313	GLN
1	A	330	ASN
1	A	348	HIS
1	A	382	ASN
1	A	450	ASN
1	A	452	ASN
1	A	457	GLN
1	A	529	ASN
1	A	547	GLN
1	A	578	ASN
1	A	611	ASN
1	B	23	HIS
1	B	70	GLN
1	B	146	ASN
1	B	210	ASN
1	B	218	HIS
1	B	243	ASN
1	B	286	HIS
1	B	288	ASN
1	B	312	HIS
1	B	313	GLN
1	B	330	ASN
1	B	450	ASN
1	B	452	ASN
1	B	457	GLN
1	B	529	ASN
1	B	547	GLN
1	B	578	ASN
1	B	611	ASN
1	C	23	HIS
1	C	70	GLN
1	C	146	ASN
1	C	210	ASN
1	C	218	HIS

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Mol	Chain	Res	Type
1	C	288	ASN
1	C	294	HIS
1	C	312	HIS
1	C	313	GLN
1	C	376	HIS
1	C	450	ASN
1	C	452	ASN
1	C	457	GLN
1	C	473	ASN
1	C	529	ASN
1	C	547	GLN
1	C	578	ASN
1	C	611	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

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 [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	656/656 (100%)	-0.28	17 (2%) 57 52	13, 21, 40, 69	0
1	B	656/656 (100%)	-0.29	16 (2%) 59 55	13, 21, 40, 69	0
1	C	656/656 (100%)	-0.31	9 (1%) 73 70	13, 21, 40, 69	0
All	All	1968/1968 (100%)	-0.29	42 (2%) 63 59	13, 21, 40, 69	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	335	GLY	4.2
1	C	17	ALA	4.0
1	A	342	ILE	4.0
1	B	335	GLY	4.0
1	A	338	CYS	3.9
1	A	249	GLY	3.7
1	B	243	ASN	3.6
1	A	335	GLY	3.5
1	A	672	VAL	3.3
1	B	122	CYS	3.3
1	B	242	ILE	3.3
1	A	244	VAL	3.2
1	C	333	SER	3.1
1	C	672	VAL	3.1
1	A	246	GLN	3.1
1	A	248	GLU	3.0
1	B	334	LEU	3.0
1	B	247	PRO	3.0
1	C	122	CYS	2.8
1	C	73	PRO	2.8
1	A	339	LYS	2.8
1	A	245	THR	2.7
1	A	340	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	672	VAL	2.6
1	B	244	VAL	2.6
1	A	334	LEU	2.5
1	C	334	LEU	2.4
1	B	246	GLN	2.3
1	B	250	VAL	2.3
1	B	240	PRO	2.3
1	A	70	GLN	2.2
1	C	18	PRO	2.2
1	A	333	SER	2.2
1	A	122	CYS	2.2
1	A	341	VAL	2.1
1	B	441	GLY	2.1
1	A	336	CYS	2.1
1	B	333	SER	2.1
1	B	241	PRO	2.1
1	C	20	ARG	2.0
1	B	248	GLU	2.0
1	B	249	GLY	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](#)

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($\text{\AA}^2$)	Q<0.9
2	ZN	B	701	1/1	0.99	0.02	21,21,21,21	0
2	ZN	A	701	1/1	1.00	0.02	21,21,21,21	0
2	ZN	C	701	1/1	1.00	0.02	21,21,21,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.