



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:44 PM UTC

PDB ID : 2WBY / pdb_00002wby
Title : Crystal structure of human insulin-degrading enzyme in complex with insulin
Authors : Manolopoulou, M.; Guo, Q.; Malito, E.; Schilling, A.B.; Tang, W.J.
Deposited on : 2009-03-06
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 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

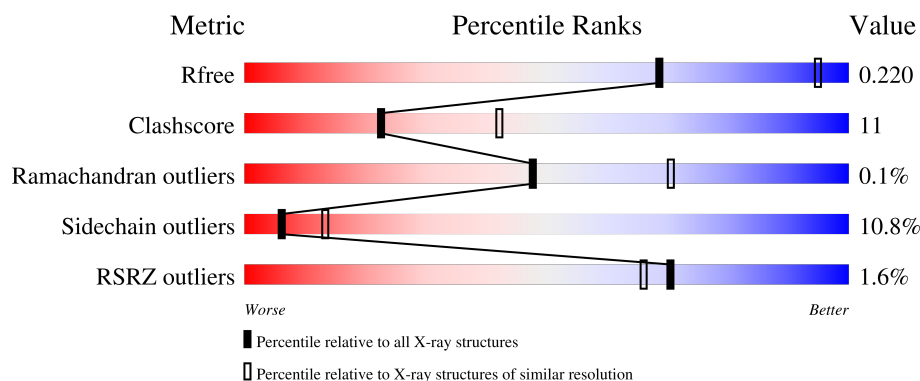
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 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	990	10% 72% 21% . . .
1	B	990	69% 23% . . .
2	C	20	10% 75% 25%
2	E	20	5% 60% 30% 10%
3	D	19	26% 63% 21% 11% 5%

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Mol	Chain	Length	Quality of chain
3	F	19	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ZN	A	3012	-	-	X	-
4	ZN	B	3012	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16926 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 INSULIN-DEGRADING ENZYME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	958	Total	C	N	O	S	0	0	1
			7813	5032	1313	1445	23			
1	B	955	Total	C	N	O	S	0	0	1
			7787	5018	1307	1440	22			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	110	LEU	CYS	engineered mutation	UNP P14735
A	111	GLN	GLU	engineered mutation	UNP P14735
A	171	SER	CYS	engineered mutation	UNP P14735
A	178	ALA	CYS	engineered mutation	UNP P14735
A	257	VAL	CYS	engineered mutation	UNP P14735
A	414	LEU	CYS	engineered mutation	UNP P14735
A	573	ASN	CYS	engineered mutation	UNP P14735
A	590	SER	CYS	engineered mutation	UNP P14735
A	789	SER	CYS	engineered mutation	UNP P14735
A	812	ALA	CYS	engineered mutation	UNP P14735
A	819	ALA	CYS	engineered mutation	UNP P14735
A	904	SER	CYS	engineered mutation	UNP P14735
A	966	ASN	CYS	engineered mutation	UNP P14735
A	974	ALA	CYS	engineered mutation	UNP P14735
B	110	LEU	CYS	engineered mutation	UNP P14735
B	111	GLN	GLU	engineered mutation	UNP P14735
B	171	SER	CYS	engineered mutation	UNP P14735
B	178	ALA	CYS	engineered mutation	UNP P14735
B	257	VAL	CYS	engineered mutation	UNP P14735
B	414	LEU	CYS	engineered mutation	UNP P14735
B	573	ASN	CYS	engineered mutation	UNP P14735
B	590	SER	CYS	engineered mutation	UNP P14735
B	789	SER	CYS	engineered mutation	UNP P14735
B	812	ALA	CYS	engineered mutation	UNP P14735
B	819	ALA	CYS	engineered mutation	UNP P14735

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Chain	Residue	Modelled	Actual	Comment	Reference
B	904	SER	CYS	engineered mutation	UNP P14735
B	966	ASN	CYS	engineered mutation	UNP P14735
B	974	ALA	CYS	engineered mutation	UNP P14735

- Molecule 2 is a protein called INSULIN A CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	20	Total	C	N	O	S	0	0	0
			155	95	23	33	4			
2	E	20	Total	C	N	O	S	0	0	0
			155	95	23	33	4			

- Molecule 3 is a protein called INSULIN B CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	18	Total	C	N	O	S	0	0	0
			143	94	24	24	1			
3	F	19	Total	C	N	O	S	0	0	0
			149	97	25	25	2			

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	408	Total	O	0	0
			408	408		
5	B	295	Total	O	0	0
			295	295		
5	C	6	Total	O	0	0
			6	6		
5	D	4	Total	O	0	0
			4	4		
5	E	5	Total	O	0	0
			5	5		

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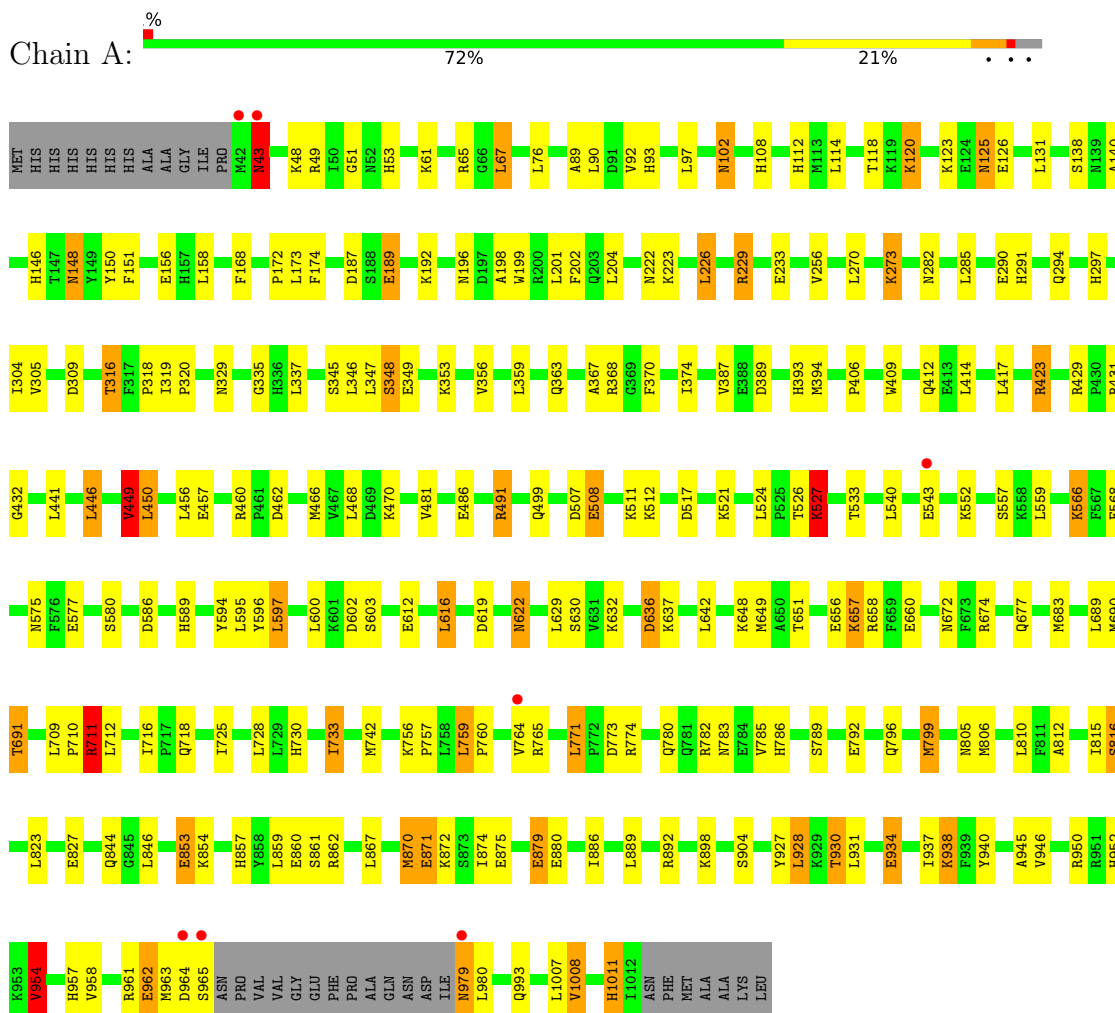
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	F	4	Total	O	0	0
			4	4		

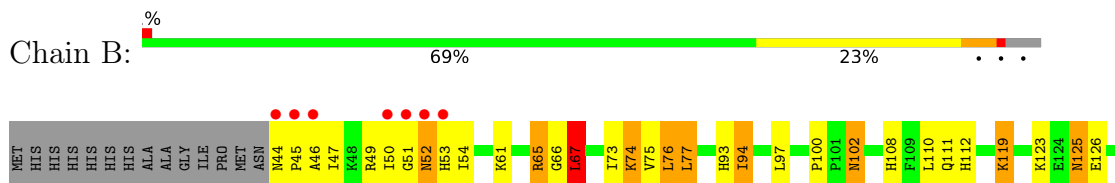
3 Residue-property plots

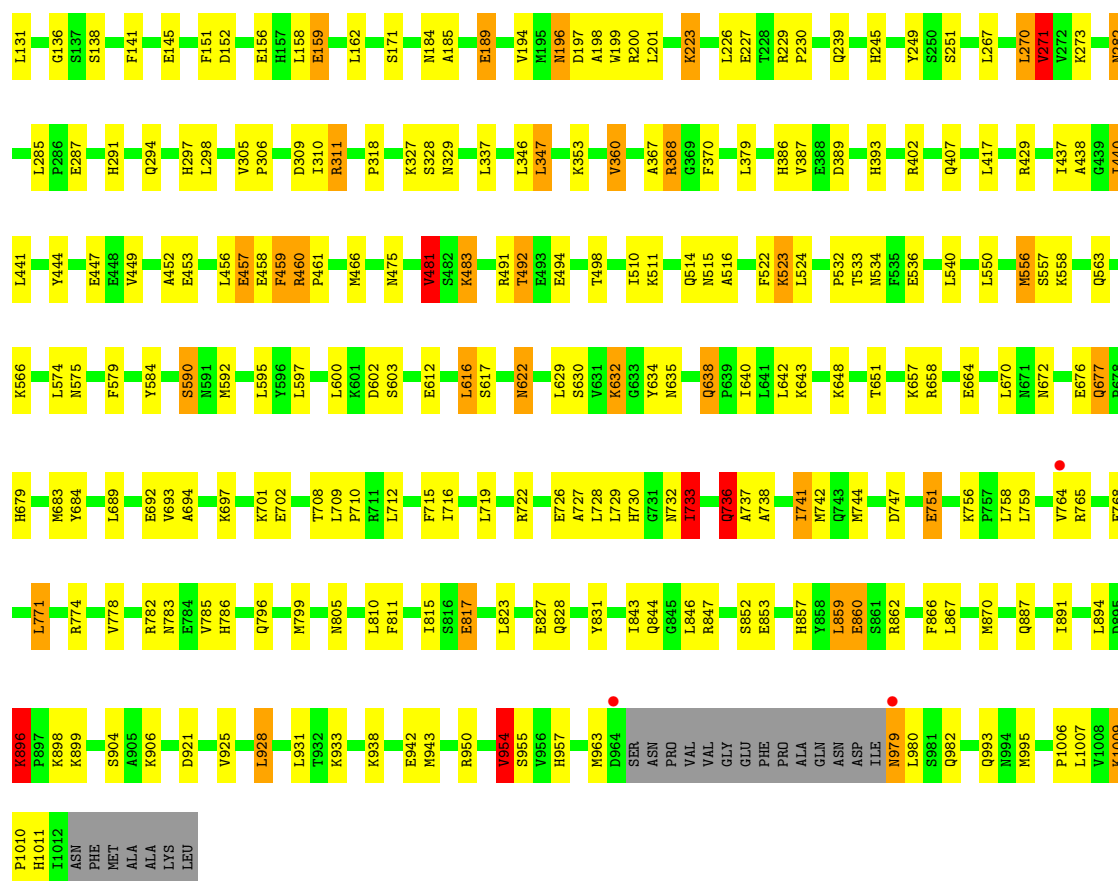
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

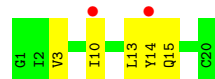
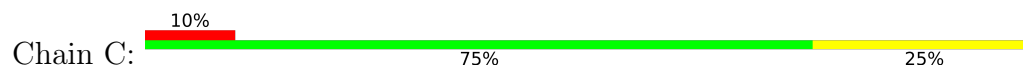


• Molecule 1: INSULIN-DEGRADING ENZYME

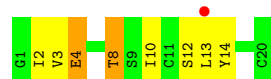




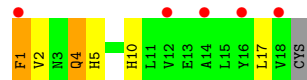
● Molecule 2: INSULIN A CHAIN



● Molecule 2: INSULIN A CHAIN



● Molecule 3: INSULIN B CHAIN



● Molecule 3: INSULIN B CHAIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	262.32Å 262.32Å 90.61Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	32.08 – 2.60 32.08 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (32.08-2.60) 99.8 (32.08-2.60)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.39 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.164 , 0.218 0.168 , 0.220	Depositor DCC
R_{free} test set	5438 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	31.3	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 45.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.019 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16926	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.82% 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	1.35	22/8007 (0.3%)	1.30	40/10833 (0.4%)
1	B	1.34	24/7982 (0.3%)	1.29	45/10801 (0.4%)
2	C	1.53	0/156	1.52	0/209
2	E	1.48	1/156 (0.6%)	1.34	0/209
3	D	1.74	1/146 (0.7%)	1.50	0/198
3	F	1.67	3/152 (2.0%)	1.48	1/206 (0.5%)
All	All	1.36	51/16599 (0.3%)	1.30	86/22456 (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	1

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	189	GLU	CD-OE2	10.00	1.44	1.25
1	B	764	VAL	CA-CB	9.84	1.65	1.53
1	A	189	GLU	CD-OE1	9.27	1.43	1.25
1	B	716	ILE	CA-CB	8.22	1.58	1.54
1	B	741	ILE	CA-CB	7.47	1.63	1.54
1	B	305	VAL	CA-CB	6.88	1.61	1.53
1	B	329	ASN	C-O	-6.83	1.20	1.23
1	A	527	LYS	CG-CD	6.70	1.72	1.52
1	A	566	LYS	C-O	-6.61	1.15	1.24
1	A	1011	HIS	C-N	-6.55	1.24	1.33
1	A	1008	VAL	CA-CB	6.53	1.62	1.54
1	B	670	LEU	C-O	-6.43	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	271	VAL	CA-CB	6.31	1.62	1.54
1	A	305	VAL	CA-CB	6.29	1.60	1.53
1	A	367	ALA	CA-CB	-6.22	1.45	1.53
1	A	619	ASP	N-CA	-6.20	1.38	1.46
1	B	492	THR	C-O	-6.19	1.16	1.23
1	B	1011	HIS	C-N	-6.14	1.24	1.33
2	E	8	THR	CA-CB	6.07	1.62	1.53
3	D	1	PHE	N-CA	5.83	1.57	1.46
1	B	736	GLN	N-CA	-5.79	1.39	1.46
1	B	74	LYS	CE-NZ	5.70	1.66	1.49
1	A	409	TRP	CA-C	5.68	1.60	1.52
1	B	47	ILE	C-O	-5.67	1.18	1.24
1	B	239	GLN	CG-CD	5.64	1.66	1.52
1	B	1009	LYS	CA-C	5.62	1.59	1.52
1	A	387	VAL	CA-CB	-5.48	1.48	1.54
3	F	1	PHE	N-CA	5.44	1.56	1.46
1	A	857	HIS	CA-CB	5.44	1.62	1.53
1	A	273	LYS	N-CA	-5.43	1.40	1.46
1	B	67	LEU	CA-C	-5.43	1.46	1.52
1	A	146	HIS	CA-C	-5.41	1.46	1.52
3	F	18	VAL	CA-CB	5.41	1.61	1.54
1	A	120	LYS	CA-C	5.39	1.60	1.52
1	A	189	GLU	CG-CD	5.35	1.65	1.52
1	B	311	ARG	N-CA	-5.29	1.40	1.46
1	B	481	VAL	C-O	5.29	1.29	1.24
1	B	94	ILE	C-O	5.27	1.29	1.24
1	A	657	LYS	CA-C	5.25	1.59	1.52
1	B	481	VAL	CA-CB	5.23	1.60	1.54
1	B	632	LYS	CD-CE	5.21	1.68	1.52
1	A	89	ALA	C-O	5.19	1.30	1.23
1	A	946	VAL	CA-C	5.13	1.59	1.52
1	B	407	GLN	C-O	5.11	1.29	1.24
1	B	438	ALA	CA-C	5.11	1.59	1.52
1	B	811	PHE	N-CA	-5.09	1.40	1.46
1	A	543	GLU	CA-C	5.05	1.61	1.52
1	A	202	PHE	CA-C	5.04	1.59	1.52
1	A	406	PRO	C-O	-5.04	1.17	1.23
1	A	577	GLU	CG-CD	5.04	1.64	1.52
3	F	12	VAL	CA-CB	5.01	1.59	1.54

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	52	ASN	N-CA-C	18.75	133.90	111.02
1	A	189	GLU	CG-CD-OE2	-12.84	88.88	118.40
1	A	636	ASP	N-CA-C	12.59	127.87	111.75
1	A	189	GLU	CG-CD-OE1	11.78	145.50	118.40
1	B	52	ASN	CB-CA-C	-10.74	93.84	110.92
1	B	189	GLU	CG-CD-OE1	-10.34	94.62	118.40
1	B	452	ALA	CA-C-N	-9.43	107.30	122.66
1	B	452	ALA	C-N-CA	-9.43	107.30	122.66
1	B	360	VAL	CB-CA-C	-8.30	98.25	110.62
1	B	46	ALA	N-CA-C	-8.04	103.47	113.20
1	A	954	VAL	CB-CA-C	-8.04	98.11	110.50
1	B	189	GLU	CG-CD-OE2	7.99	136.78	118.40
1	B	733	ILE	CB-CA-C	-7.77	100.44	111.40
1	A	637	LYS	N-CA-C	-7.66	101.09	113.19
1	A	816	SER	N-CA-C	7.56	119.21	110.97
1	B	954	VAL	CB-CA-C	-7.52	98.92	110.50
1	A	656	GLU	N-CA-C	7.51	119.11	111.07
1	B	311	ARG	CB-CA-C	7.40	121.97	110.14
1	A	282	ASN	N-CA-C	6.97	121.02	111.54
1	B	100	PRO	CA-C-N	6.88	127.16	119.32
1	B	100	PRO	C-N-CA	6.88	127.16	119.32
1	B	189	GLU	N-CA-C	-6.79	102.96	111.11
1	B	694	ALA	CB-CA-C	6.71	121.22	109.89
1	B	817	GLU	CA-C-N	-6.67	111.72	119.32
1	B	817	GLU	C-N-CA	-6.67	111.72	119.32
1	A	189	GLU	CB-CG-CD	6.56	123.75	112.60
1	A	636	ASP	CB-CA-C	-6.44	97.96	110.46
1	B	282	ASN	CB-CA-C	-6.44	102.74	111.89
1	B	638	GLN	CA-C-N	-6.32	112.03	119.05
1	B	638	GLN	C-N-CA	-6.32	112.03	119.05
1	B	677	GLN	N-CA-C	6.31	118.62	109.84
1	B	305	VAL	N-CA-C	6.27	114.09	107.76
1	A	651	THR	N-CA-C	-6.16	103.07	112.99
1	B	896	LYS	N-CA-C	6.15	116.67	109.60
1	B	453	GLU	CB-CA-C	6.08	120.48	111.17
1	A	189	GLU	N-CA-C	-6.08	103.81	111.11
1	A	616	LEU	CA-C-N	-6.08	112.60	122.82
1	A	616	LEU	C-N-CA	-6.08	112.60	122.82
1	A	853	GLU	N-CA-C	-5.98	105.81	113.23
1	B	239	GLN	N-CA-C	-5.97	104.78	111.28
1	B	533	THR	N-CA-C	-5.96	106.99	114.56
1	B	460	ARG	CG-CD-NE	-5.93	98.96	112.00
1	A	892	ARG	NE-CZ-NH2	5.92	124.53	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	459	PHE	CA-C-N	-5.91	114.88	122.98
1	B	459	PHE	C-N-CA	-5.91	114.88	122.98
1	A	449	VAL	CB-CA-C	-5.89	103.03	112.16
1	A	870	MET	N-CA-C	5.85	117.66	111.28
1	B	387	VAL	N-CA-C	5.76	116.40	110.36
1	B	159	GLU	N-CA-C	5.75	117.55	111.28
1	A	527	LYS	CB-CG-CD	5.65	124.29	111.30
1	B	928	LEU	CB-CA-C	-5.62	99.23	110.42
1	A	508	GLU	N-CA-CB	-5.62	101.86	110.12
1	A	677	GLN	N-CA-C	5.53	117.72	110.08
1	B	368	ARG	CA-C-N	-5.53	116.86	123.44
1	B	368	ARG	C-N-CA	-5.53	116.86	123.44
1	B	694	ALA	N-CA-C	-5.50	99.30	108.32
1	A	871	GLU	N-CA-C	-5.49	105.22	111.14
1	A	962	GLU	N-CA-C	5.47	119.12	112.23
1	A	691	THR	CB-CA-C	-5.43	100.35	109.48
1	B	239	GLN	CA-CB-CG	5.43	124.96	114.10
1	B	456	LEU	N-CA-C	-5.41	100.21	109.24
1	A	92	VAL	CB-CA-C	-5.39	103.51	110.84
1	A	65	ARG	NE-CZ-NH1	-5.35	116.15	121.50
1	B	310	ILE	CA-C-N	-5.34	115.24	122.77
1	B	310	ILE	C-N-CA	-5.34	115.24	122.77
1	A	335	GLY	N-CA-C	-5.32	105.97	112.77
1	A	733	ILE	N-CA-C	5.31	116.01	108.42
1	A	566	LYS	N-CA-C	-5.29	99.54	110.80
1	A	716	ILE	O-C-N	5.21	123.76	120.42
1	A	533	THR	CA-C-N	-5.20	115.86	122.77
1	A	533	THR	C-N-CA	-5.20	115.86	122.77
1	B	511	LYS	N-CA-CB	5.20	117.76	110.12
1	A	43	ASN	N-CA-C	5.19	117.76	110.23
3	F	15	LEU	N-CA-C	5.17	117.81	111.82
1	B	197	ASP	N-CA-C	5.15	116.90	111.28
1	A	349	GLU	N-CA-C	5.12	116.54	111.07
1	B	651	THR	N-CA-C	-5.12	105.11	113.19
1	A	711	ARG	NE-CZ-NH2	5.11	123.80	119.20
1	B	557	SER	N-CA-C	5.10	116.82	108.55
1	A	980	LEU	N-CA-C	5.08	117.89	109.46
1	B	189	GLU	CB-CG-CD	5.05	121.19	112.60
1	B	612	GLU	CA-CB-CG	-5.03	104.05	114.10
1	A	51	GLY	N-CA-C	-5.02	104.95	112.89
1	A	533	THR	CB-CA-C	-5.02	101.71	109.29
1	A	580	SER	CA-C-N	5.00	124.79	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	580	SER	C-N-CA	5.00	124.79	119.28

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	979	ASN	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7813	0	7744	156	0
1	B	7787	0	7715	172	0
2	C	155	0	144	5	0
2	E	155	0	143	8	0
3	D	143	0	142	14	0
3	F	149	0	146	12	0
4	A	1	0	0	2	0
4	B	1	0	0	3	0
5	A	408	0	0	24	0
5	B	295	0	0	14	0
5	C	6	0	0	0	0
5	D	4	0	0	1	0
5	E	5	0	0	0	0
5	F	4	0	0	0	0
All	All	16926	0	16034	339	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (339) 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:491:ARG:HG3	1:A:491:ARG:HH11	1.02	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:3012:ZN:ZN	3:F:1:PHE:N	1.11	1.14
4:A:3012:ZN:ZN	3:D:1:PHE:N	1.17	1.06
1:B:189:GLU:OE2	3:F:1:PHE:N	1.90	1.03
1:B:119:LYS:HE3	1:B:171:SER:HB2	1.44	0.98
1:B:189:GLU:OE2	4:B:3012:ZN:ZN	1.11	0.97
1:A:491:ARG:HH11	1:A:491:ARG:CG	1.75	0.97
1:A:431:ARG:HD3	5:A:2206:HOH:O	1.64	0.96
1:A:764:VAL:HA	5:A:2305:HOH:O	1.67	0.92
1:A:674:ARG:HD3	5:A:2321:HOH:O	1.68	0.91
1:A:423:ARG:HH11	1:A:423:ARG:CG	1.84	0.90
1:A:189:GLU:OE1	3:D:1:PHE:N	1.98	0.90
1:A:102:ASN:H	1:A:102:ASN:HD22	1.20	0.89
4:B:3012:ZN:ZN	3:F:1:PHE:H2	0.60	0.89
2:E:4:GLU:HG3	3:F:11:LEU:HD22	1.55	0.89
1:A:491:ARG:HG3	1:A:491:ARG:NH1	1.80	0.89
1:B:93:HIS:HE1	1:B:368:ARG:HH21	1.27	0.83
1:B:125:ASN:HD22	1:B:125:ASN:H	1.26	0.83
1:B:77:LEU:HD21	1:B:271:VAL:HG11	1.61	0.82
1:A:316:THR:HG23	5:A:2131:HOH:O	1.80	0.81
1:B:622:ASN:HD22	1:B:622:ASN:H	1.28	0.81
1:A:711:ARG:HG2	1:A:711:ARG:HH21	1.46	0.80
1:B:440:ILE:HD11	1:B:449:VAL:HB	1.64	0.80
1:B:102:ASN:HD22	1:B:102:ASN:H	1.30	0.79
1:A:199:TRP:HA	3:D:4:GLN:HE22	1.48	0.78
1:B:294:GLN:H	1:B:297:HIS:HD2	1.29	0.78
1:A:294:GLN:H	1:A:297:HIS:HD2	1.27	0.78
1:A:423:ARG:HH11	1:A:423:ARG:HG3	1.48	0.78
1:A:196:ASN:HD22	1:A:199:TRP:H	1.29	0.78
1:B:783:ASN:HD22	1:B:785:VAL:H	1.32	0.77
1:B:108:HIS:NE2	1:B:189:GLU:OE2	2.18	0.77
1:B:771:LEU:HD21	1:B:954:VAL:HG22	1.65	0.77
1:A:815:ILE:HG22	1:A:870:MET:HG3	1.65	0.77
1:A:771:LEU:HD21	1:A:954:VAL:HG22	1.65	0.76
2:E:10:ILE:HG23	3:F:3:ASN:HB3	1.67	0.76
1:A:125:ASN:H	1:A:125:ASN:HD22	1.32	0.76
1:A:521:LYS:NZ	5:A:2231:HOH:O	2.17	0.75
1:B:368:ARG:HD2	5:B:2125:HOH:O	1.85	0.75
1:B:494:GLU:HG2	5:B:2170:HOH:O	1.86	0.75
1:A:934:GLU:HG2	1:B:53:HIS:CE1	2.22	0.74
1:A:53:HIS:HE1	5:A:2012:HOH:O	1.71	0.74
1:A:429:ARG:HB2	2:C:14:TYR:OH	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:LYS:HE3	5:A:2215:HOH:O	1.86	0.74
1:B:49:ARG:NH2	1:B:447:GLU:OE1	2.21	0.73
1:A:309:ASP:H	1:A:672:ASN:HD21	1.35	0.73
1:B:309:ASP:H	1:B:672:ASN:HD21	1.36	0.73
1:B:51:GLY:N	1:B:66:GLY:O	2.20	0.73
1:B:184:ASN:HD21	1:B:223:LYS:NZ	1.87	0.73
1:A:636:ASP:O	1:A:636:ASP:OD2	2.07	0.73
1:A:316:THR:CG2	5:A:2131:HOH:O	2.34	0.72
1:A:927:TYR:O	1:A:930:THR:HB	1.90	0.72
1:B:579:PHE:HE2	1:B:765:ARG:NH1	1.87	0.72
1:A:389:ASP:O	1:A:393:HIS:HD2	1.72	0.72
1:B:386:HIS:HE1	5:B:2132:HOH:O	1.72	0.72
1:B:782:ARG:NH2	1:B:963:MET:O	2.23	0.71
1:A:309:ASP:H	1:A:672:ASN:ND2	1.89	0.70
1:A:799:MET:HE3	1:A:1008:VAL:HG22	1.72	0.70
1:B:441:LEU:HD23	1:B:449:VAL:HG11	1.73	0.70
1:A:730:HIS:HD2	1:A:904:SER:OG	1.75	0.70
1:A:879:GLU:HG3	5:A:2362:HOH:O	1.92	0.69
1:B:309:ASP:H	1:B:672:ASN:ND2	1.91	0.69
1:A:880:GLU:HG3	1:B:457:GLU:HG2	1.75	0.69
1:B:556:MET:HE3	1:B:556:MET:HA	1.73	0.68
2:C:10:ILE:HG12	3:D:4:GLN:O	1.93	0.68
1:B:108:HIS:NE2	3:F:1:PHE:N	2.41	0.68
1:A:950:ARG:HD2	5:A:2312:HOH:O	1.94	0.68
1:B:632:LYS:NZ	5:B:2213:HOH:O	2.11	0.68
1:B:676:GLU:OE2	1:B:676:GLU:HA	1.93	0.67
1:A:783:ASN:HD22	1:A:785:VAL:H	1.42	0.66
1:A:329:ASN:HD21	1:A:363:GLN:HE22	1.43	0.66
1:B:579:PHE:CE2	1:B:765:ARG:NH1	2.63	0.66
1:B:267:LEU:O	1:B:271:VAL:HG12	1.95	0.66
1:A:783:ASN:ND2	1:A:785:VAL:H	1.93	0.66
1:A:93:HIS:HE1	1:A:368:ARG:HH21	1.42	0.65
1:B:112:HIS:NE2	3:F:1:PHE:N	2.44	0.65
1:A:229:ARG:HD2	1:A:233:GLU:OE2	1.97	0.65
1:A:491:ARG:CD	5:A:2219:HOH:O	2.45	0.65
1:A:622:ASN:HD22	1:A:622:ASN:H	1.44	0.64
1:A:189:GLU:OE2	3:D:1:PHE:HA	1.98	0.64
1:A:423:ARG:CG	1:A:423:ARG:NH1	2.56	0.64
1:B:783:ASN:ND2	1:B:785:VAL:H	1.96	0.64
1:A:491:ARG:HD2	5:A:2219:HOH:O	1.98	0.63
1:B:906:LYS:HE2	1:B:921:ASP:OD2	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:979:ASN:N	1:B:979:ASN:HD22	1.95	0.63
1:A:782:ARG:NH1	1:A:963:MET:O	2.30	0.63
3:D:4:GLN:HG3	3:D:5:HIS:N	2.14	0.63
1:B:771:LEU:HD21	1:B:954:VAL:CG2	2.27	0.62
1:A:316:THR:HB	1:A:374:ILE:HG22	1.80	0.62
1:A:102:ASN:H	1:A:102:ASN:ND2	1.97	0.62
1:B:112:HIS:NE2	1:B:189:GLU:OE2	2.33	0.62
1:A:112:HIS:NE2	3:D:1:PHE:N	2.49	0.61
1:A:827:GLU:OE1	1:A:862:ARG:HD3	2.01	0.61
4:A:3012:ZN:ZN	3:D:1:PHE:H2	1.07	0.61
1:B:125:ASN:HD22	1:B:125:ASN:N	1.96	0.61
1:B:93:HIS:CE1	1:B:368:ARG:HH21	2.13	0.60
1:B:110:LEU:HD23	1:B:110:LEU:C	2.25	0.60
1:B:847:ARG:NH1	5:B:2257:HOH:O	2.09	0.60
1:B:306:PRO:O	1:B:483:LYS:HE3	2.01	0.60
1:B:827:GLU:OE1	1:B:862:ARG:HD3	2.00	0.60
1:B:616:LEU:HD21	1:B:638:GLN:HG2	1.84	0.60
1:B:860:GLU:OE2	1:B:957:HIS:HE1	1.84	0.60
1:A:771:LEU:HD21	1:A:954:VAL:CG2	2.31	0.60
1:B:491:ARG:HD2	5:B:2167:HOH:O	2.02	0.59
1:B:294:GLN:H	1:B:297:HIS:CD2	2.14	0.59
1:A:783:ASN:ND2	1:A:786:HIS:H	2.00	0.59
1:B:783:ASN:ND2	1:B:786:HIS:H	2.01	0.59
1:A:725:ILE:HG21	1:A:742:MET:HE1	1.84	0.59
1:B:108:HIS:CE1	1:B:189:GLU:OE2	2.56	0.59
1:B:602:ASP:OD1	1:B:658:ARG:HD3	2.03	0.58
1:B:162:LEU:HD23	1:B:270:LEU:CD1	2.32	0.58
1:B:771:LEU:HB2	1:B:796:GLN:OE1	2.04	0.58
1:B:692:GLU:HG2	1:B:693:VAL:HG23	1.86	0.58
1:B:184:ASN:HD21	1:B:223:LYS:HZ3	1.50	0.58
1:A:964:ASP:O	1:A:965:SER:CB	2.51	0.57
1:A:432:GLY:HA3	2:C:14:TYR:CE1	2.40	0.57
1:A:49:ARG:NH1	5:A:2005:HOH:O	2.38	0.57
2:E:4:GLU:HG3	3:F:11:LEU:CD2	2.33	0.57
1:A:441:LEU:HD23	1:A:449:VAL:HG11	1.86	0.57
1:A:566:LYS:O	1:A:568:PHE:CD1	2.56	0.57
1:A:789:SER:HB2	1:A:958:VAL:O	2.03	0.56
1:A:622:ASN:H	1:A:622:ASN:ND2	2.03	0.56
1:B:52:ASN:C	1:B:53:HIS:ND1	2.64	0.56
1:B:298:LEU:HD13	1:B:475:ASN:CB	2.36	0.56
1:A:898:LYS:HE3	5:A:2026:HOH:O	2.04	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:ARG:HG2	1:B:50:ILE:N	2.21	0.55
1:B:196:ASN:HD22	1:B:199:TRP:H	1.52	0.55
1:A:67:LEU:HD23	1:A:67:LEU:N	2.21	0.55
1:A:934:GLU:OE1	1:B:53:HIS:HE1	1.90	0.55
1:A:125:ASN:HD22	1:A:125:ASN:N	2.03	0.55
1:B:67:LEU:HB2	1:B:75:VAL:HB	1.89	0.55
1:B:189:GLU:CD	3:F:1:PHE:H2	2.11	0.54
1:B:622:ASN:H	1:B:622:ASN:ND2	2.01	0.54
1:A:431:ARG:CD	5:A:2206:HOH:O	2.36	0.54
1:B:602:ASP:OD1	1:B:658:ARG:CD	2.55	0.54
1:A:815:ILE:CG2	1:A:870:MET:HG3	2.36	0.54
1:A:806:MET:HE3	1:A:928:LEU:HG	1.90	0.54
1:A:711:ARG:HH21	1:A:711:ARG:CG	2.18	0.54
1:A:112:HIS:CE1	1:A:189:GLU:OE1	2.57	0.53
1:A:229:ARG:HG2	5:A:2101:HOH:O	2.08	0.53
1:A:359:LEU:C	1:A:359:LEU:HD23	2.33	0.53
1:A:291:HIS:CD2	1:A:370:PHE:HB2	2.44	0.53
1:B:386:HIS:CE1	5:B:2132:HOH:O	2.53	0.53
1:A:423:ARG:HH11	1:A:423:ARG:HG2	1.69	0.53
1:B:815:ILE:HG22	1:B:870:MET:HG3	1.90	0.53
1:B:575:ASN:OD1	1:B:630:SER:HB3	2.08	0.53
1:A:799:MET:CE	1:A:1008:VAL:HG22	2.39	0.53
1:B:906:LYS:CE	1:B:921:ASP:OD2	2.57	0.53
1:B:708:THR:HB	1:B:710:PRO:HD2	1.90	0.53
2:E:10:ILE:CG2	3:F:3:ASN:HB3	2.37	0.53
1:A:393:HIS:HE1	5:A:2155:HOH:O	1.91	0.52
1:B:196:ASN:ND2	1:B:198:ALA:H	2.06	0.52
1:A:874:ILE:HG22	1:A:937:ILE:HD11	1.91	0.52
1:B:185:ALA:HB2	1:B:828:GLN:HE22	1.74	0.52
1:A:491:ARG:CG	1:A:491:ARG:NH1	2.48	0.52
1:A:709:LEU:HB3	1:A:710:PRO:CD	2.40	0.52
1:B:558:LYS:HB3	1:B:726:GLU:HG3	1.91	0.52
1:A:771:LEU:HB2	1:A:796:GLN:OE1	2.10	0.52
1:B:679:HIS:O	1:B:683:MET:HG3	2.09	0.52
1:A:187:ASP:OD1	1:A:222:ASN:HB2	2.10	0.52
1:A:222:ASN:O	1:A:226:LEU:HB2	2.10	0.52
1:A:316:THR:HG22	5:A:2169:HOH:O	2.10	0.52
1:B:76:LEU:HD12	1:B:437:ILE:HG21	1.91	0.52
1:B:49:ARG:CG	1:B:50:ILE:N	2.71	0.51
1:A:827:GLU:OE1	1:A:862:ARG:CD	2.58	0.51
1:B:768:GLU:HB3	1:B:843:ILE:HG13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:GLU:HG3	1:B:831:TYR:CE1	2.46	0.51
1:B:563:GLN:HG3	1:B:733:ILE:O	2.10	0.51
1:A:90:LEU:HD12	1:A:256:VAL:HG22	1.93	0.51
1:A:460:ARG:HD2	1:A:462:ASP:OD2	2.10	0.51
1:B:162:LEU:HD23	1:B:270:LEU:HD11	1.91	0.51
1:B:440:ILE:HD11	1:B:449:VAL:CB	2.39	0.51
1:B:979:ASN:N	1:B:979:ASN:ND2	2.58	0.51
1:A:880:GLU:CG	1:B:457:GLU:HG2	2.39	0.51
1:B:429:ARG:HG2	1:B:429:ARG:HH11	1.74	0.51
1:B:805:ASN:HD22	1:B:844:GLN:HE22	1.58	0.51
1:B:386:HIS:HD2	1:B:389:ASP:OD2	1.93	0.50
2:E:3:VAL:HG23	2:E:3:VAL:O	2.11	0.50
1:A:102:ASN:HD22	1:A:102:ASN:N	1.95	0.50
1:B:441:LEU:CD2	1:B:449:VAL:HG11	2.40	0.50
1:A:294:GLN:H	1:A:297:HIS:CD2	2.19	0.50
1:B:196:ASN:ND2	1:B:199:TRP:H	2.09	0.50
1:B:440:ILE:HG12	1:B:444:TYR:HD2	1.76	0.50
1:A:196:ASN:ND2	1:A:199:TRP:H	2.06	0.50
1:A:771:LEU:HB3	1:A:952:HIS:HB3	1.93	0.50
1:B:402:ARG:NH2	5:B:2140:HOH:O	2.42	0.50
1:A:596:TYR:CD2	1:A:597:LEU:HD13	2.47	0.49
1:B:664:GLU:HB3	5:B:2219:HOH:O	2.10	0.49
1:B:510:ILE:O	1:B:514:GLN:HG3	2.12	0.49
1:B:534:ASN:ND2	1:B:536:GLU:H	2.10	0.49
1:B:742:MET:HA	1:B:742:MET:HE3	1.95	0.49
1:A:805:ASN:HD22	1:A:844:GLN:HE22	1.61	0.49
1:B:346:LEU:HA	1:B:522:PHE:CE2	2.47	0.49
1:A:131:LEU:CD1	1:A:138:SER:HB2	2.43	0.49
1:A:961:ARG:HD2	1:A:962:GLU:OE1	2.12	0.49
1:A:812:ALA:O	1:A:816:SER:HB2	2.13	0.48
1:B:684:TYR:OH	1:B:697:LYS:HG2	2.13	0.48
1:B:689:LEU:CD2	1:B:995:MET:HG2	2.43	0.48
1:B:860:GLU:OE2	1:B:957:HIS:CE1	2.67	0.48
1:A:389:ASP:O	1:A:393:HIS:CD2	2.61	0.48
1:B:575:ASN:O	1:B:727:ALA:HA	2.14	0.48
1:B:603:SER:OG	1:B:648:LYS:HE3	2.13	0.48
1:B:852:SER:HB3	1:B:859:LEU:HD21	1.94	0.48
1:B:184:ASN:HD21	1:B:223:LYS:HZ2	1.57	0.48
1:B:729:LEU:HD12	1:B:738:ALA:HB1	1.95	0.48
1:A:799:MET:HE3	1:A:1008:VAL:CG2	2.43	0.48
1:B:73:ILE:HG13	1:B:251:SER:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:526:THR:O	1:A:527:LYS:C	2.56	0.47
1:B:151:PHE:CD1	1:B:151:PHE:C	2.92	0.47
1:B:189:GLU:OE1	3:F:1:PHE:HA	2.13	0.47
1:A:575:ASN:ND2	1:A:630:SER:OG	2.48	0.47
1:A:940:TYR:CE1	1:A:945:ALA:HB2	2.48	0.47
1:A:636:ASP:OD2	1:A:636:ASP:C	2.57	0.47
1:B:189:GLU:CD	3:F:1:PHE:HA	2.40	0.47
1:B:622:ASN:HD22	1:B:622:ASN:N	2.07	0.47
1:B:747:ASP:O	1:B:751:GLU:HB2	2.15	0.47
1:B:866:PHE:CZ	1:B:870:MET:HG2	2.50	0.47
1:B:311:ARG:HG3	1:B:379:LEU:HB2	1.96	0.47
1:B:93:HIS:HD2	1:B:145:GLU:O	1.98	0.46
1:A:566:LYS:O	1:A:568:PHE:CE1	2.68	0.46
1:B:145:GLU:CD	1:B:367:ALA:HB1	2.40	0.46
1:B:592:MET:HE3	1:B:715:PHE:CD1	2.51	0.46
1:A:450:LEU:HB2	5:A:2209:HOH:O	2.15	0.46
1:B:774:ARG:HG2	1:B:774:ARG:HH11	1.81	0.46
1:A:140:ALA:HA	1:A:148:ASN:O	2.16	0.46
1:B:550:LEU:HD11	1:B:558:LYS:HG2	1.96	0.46
2:C:3:VAL:HG23	2:C:3:VAL:O	2.15	0.46
1:A:319:ILE:HB	1:A:320:PRO:HD2	1.97	0.46
1:A:689:LEU:C	1:A:690:MET:HE2	2.40	0.46
1:B:522:PHE:C	1:B:523:LYS:HD3	2.41	0.46
1:A:67:LEU:N	1:A:67:LEU:CD2	2.79	0.46
1:A:730:HIS:CD2	1:A:904:SER:OG	2.62	0.46
1:A:783:ASN:HD22	1:A:786:HIS:H	1.62	0.46
1:A:586:ASP:OD1	1:A:589:HIS:HD2	1.99	0.46
1:B:778:VAL:HG22	1:B:955:SER:HB2	1.98	0.46
1:B:328:SER:HB2	1:B:458:GLU:O	2.16	0.46
1:A:552:LYS:HB3	1:A:559:LEU:HB3	1.97	0.45
1:B:245:HIS:O	1:B:249:TYR:HB2	2.16	0.45
1:B:709:LEU:HB3	1:B:710:PRO:HD3	1.98	0.45
1:B:131:LEU:CD1	1:B:138:SER:HB2	2.47	0.45
1:A:860:GLU:OE2	1:A:957:HIS:HE1	2.00	0.45
1:B:347:LEU:HD23	1:B:347:LEU:HA	1.67	0.45
1:A:938:LYS:HB3	1:A:938:LYS:HE2	1.24	0.45
3:D:4:GLN:HG3	3:D:5:HIS:H	1.81	0.45
3:D:4:GLN:HE21	3:D:4:GLN:HB2	1.53	0.45
1:A:291:HIS:CE1	1:A:318:PRO:HB3	2.52	0.45
1:A:345:SER:OG	1:A:348:SER:HB3	2.17	0.45
1:A:799:MET:HE1	1:A:1008:VAL:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:886:ILE:HG23	1:A:928:LEU:HD13	1.98	0.45
1:B:123:LYS:HB3	1:B:126:GLU:HB2	1.99	0.44
1:B:52:ASN:O	1:B:53:HIS:ND1	2.50	0.44
1:A:48:LYS:O	1:A:49:ARG:HB3	2.17	0.44
1:B:102:ASN:H	1:B:102:ASN:ND2	2.07	0.44
1:B:635:ASN:OD1	1:B:732:ASN:ND2	2.47	0.44
1:A:172:PRO:HG2	1:A:174:PHE:CE1	2.52	0.44
1:A:507:ASP:O	1:A:511:LYS:HD3	2.18	0.44
1:B:389:ASP:O	1:B:393:HIS:HD2	2.00	0.44
1:B:730:HIS:HD2	1:B:904:SER:OG	2.00	0.44
1:B:196:ASN:ND2	1:B:198:ALA:N	2.65	0.44
1:A:880:GLU:OE1	1:B:327:LYS:HE3	2.18	0.43
1:B:44:ASN:HB3	1:B:45:PRO:HB3	2.00	0.43
1:B:162:LEU:HD23	1:B:270:LEU:HD13	1.99	0.43
1:B:894:LEU:HG	1:B:925:VAL:HG21	2.00	0.43
1:A:649:MET:HE3	1:A:649:MET:HB2	1.85	0.43
1:A:196:ASN:HD21	1:A:198:ALA:HB3	1.82	0.43
1:A:540:LEU:HD12	1:A:540:LEU:HA	1.80	0.43
1:B:429:ARG:HD3	2:E:14:TYR:OH	2.18	0.43
1:A:806:MET:CE	1:A:928:LEU:HG	2.49	0.43
1:B:736:GLN:HE21	1:B:736:GLN:C	2.26	0.43
1:B:774:ARG:HG2	1:B:774:ARG:NH1	2.34	0.43
1:A:199:TRP:CH2	3:D:2:VAL:HG23	2.54	0.43
1:A:709:LEU:O	1:A:710:PRO:C	2.61	0.43
1:B:136:GLY:HA3	1:B:152:ASP:O	2.18	0.43
1:B:291:HIS:CE1	1:B:318:PRO:HB3	2.54	0.43
1:A:759:LEU:O	1:A:760:PRO:C	2.61	0.43
1:B:515:ASN:O	1:B:516:ALA:C	2.62	0.43
1:B:584:TYR:CD2	1:B:590:SER:HB2	2.54	0.43
1:B:896:LYS:HB2	1:B:896:LYS:HE2	1.83	0.43
1:B:532:PRO:HG3	1:B:634:TYR:CD2	2.53	0.43
1:A:329:ASN:ND2	5:A:2142:HOH:O	2.52	0.43
1:A:43:ASN:ND2	5:A:2001:HOH:O	2.52	0.42
1:A:151:PHE:CD1	1:A:151:PHE:C	2.96	0.42
1:A:456:LEU:HD23	1:A:456:LEU:HA	1.81	0.42
1:A:552:LYS:HE2	1:A:557:SER:OG	2.19	0.42
1:A:934:GLU:HG3	1:B:52:ASN:HB3	2.01	0.42
1:B:534:ASN:ND2	1:B:534:ASN:C	2.77	0.42
1:A:346:LEU:HD21	1:A:394:MET:HG2	2.01	0.42
1:A:48:LYS:HB2	1:A:48:LYS:HE3	1.83	0.42
1:A:108:HIS:NE2	3:D:1:PHE:N	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:491:ARG:NE	5:A:2219:HOH:O	2.51	0.42
1:A:602:ASP:OD1	1:A:658:ARG:HD3	2.19	0.42
1:B:622:ASN:ND2	1:B:622:ASN:N	2.67	0.42
1:B:353:LYS:NZ	5:B:2120:HOH:O	2.52	0.42
1:B:737:ALA:O	1:B:741:ILE:HG12	2.20	0.42
1:A:198:ALA:HB1	3:D:4:GLN:OE1	2.20	0.42
1:A:457:GLU:HG2	5:A:2083:HOH:O	2.19	0.42
1:B:125:ASN:N	1:B:125:ASN:ND2	2.67	0.42
1:B:574:LEU:O	1:B:630:SER:HA	2.20	0.42
1:B:950:ARG:HH11	1:B:950:ARG:HD2	1.72	0.42
1:A:304:ILE:HB	1:A:481:VAL:HG22	2.01	0.42
1:B:291:HIS:CD2	1:B:370:PHE:HB2	2.55	0.42
1:B:311:ARG:HA	1:B:481:VAL:O	2.19	0.42
1:B:799:MET:HE1	1:B:1006:PRO:HG2	2.02	0.42
1:A:204:LEU:CD2	1:A:304:ILE:HD12	2.50	0.42
1:B:298:LEU:HD13	1:B:475:ASN:HB3	2.02	0.42
1:B:556:MET:HA	1:B:556:MET:CE	2.46	0.42
1:B:943:MET:HE3	1:B:943:MET:HB3	1.91	0.42
1:B:141:PHE:CD1	2:E:12:SER:HB3	2.55	0.42
1:B:843:ILE:HG22	1:B:844:GLN:H	1.85	0.42
1:A:423:ARG:NH1	1:A:423:ARG:HG2	2.29	0.41
1:A:711:ARG:HG2	1:A:711:ARG:NH2	2.22	0.41
1:A:756:LYS:HB3	1:A:757:PRO:HD2	2.02	0.41
1:B:982:GLN:HA	5:B:2290:HOH:O	2.20	0.41
3:D:10:HIS:CD2	5:D:2002:HOH:O	2.72	0.41
1:A:114:LEU:HD13	1:A:168:PHE:HB3	2.01	0.41
1:A:446:LEU:O	1:A:449:VAL:HG22	2.20	0.41
1:A:683:MET:HA	1:A:792:GLU:OE2	2.19	0.41
2:E:2:ILE:O	2:E:3:VAL:C	2.63	0.41
1:A:123:LYS:HB3	1:A:126:GLU:HB2	2.03	0.41
1:B:459:PHE:CE2	1:B:461:PRO:HG3	2.55	0.41
1:B:887:GLN:HE21	1:B:891:ILE:HD11	1.85	0.41
1:A:594:TYR:HD1	1:A:622:ASN:HD21	1.68	0.41
1:A:773:ASP:O	1:A:774:ARG:HB2	2.20	0.41
1:B:768:GLU:OE1	5:B:2231:HOH:O	2.22	0.41
1:A:961:ARG:NH2	5:A:2396:HOH:O	2.52	0.41
1:B:159:GLU:OE2	1:B:273:LYS:NZ	2.51	0.41
1:B:200:ARG:NH2	1:B:498:THR:HA	2.34	0.41
1:B:227:GLU:C	1:B:230:PRO:HD2	2.46	0.41
1:B:65:ARG:HD3	5:B:2011:HOH:O	2.21	0.41
2:C:14:TYR:CD1	2:C:14:TYR:C	2.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:ARG:HH11	1:A:368:ARG:HD3	1.74	0.41
1:A:150:TYR:HD1	1:A:431:ARG:HG2	1.86	0.40
1:B:689:LEU:HD23	1:B:995:MET:HG2	2.02	0.40
1:B:828:GLN:NE2	5:B:2246:HOH:O	2.54	0.40
1:A:173:LEU:O	1:A:174:PHE:C	2.65	0.40
1:B:53:HIS:ND1	1:B:53:HIS:N	2.69	0.40
1:B:196:ASN:ND2	1:B:196:ASN:C	2.80	0.40
1:B:429:ARG:NH1	1:B:429:ARG:CG	2.83	0.40
1:A:118:THR:HG22	1:A:172:PRO:HA	2.04	0.40
1:B:429:ARG:HG2	1:B:429:ARG:NH1	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	954/990 (96%)	918 (96%)	36 (4%)	0	100	100
1	B	951/990 (96%)	921 (97%)	29 (3%)	1 (0%)	48	70
2	C	18/20 (90%)	16 (89%)	2 (11%)	0	100	100
2	E	18/20 (90%)	17 (94%)	1 (6%)	0	100	100
3	D	16/19 (84%)	12 (75%)	4 (25%)	0	100	100
3	F	17/19 (90%)	17 (100%)	0	0	100	100
All	All	1974/2058 (96%)	1901 (96%)	72 (4%)	1 (0%)	48	70

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1010	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	848/879 (96%)	758 (89%)	90 (11%)	6	14
1	B	845/879 (96%)	753 (89%)	92 (11%)	6	13
2	C	19/19 (100%)	17 (90%)	2 (10%)	6	14
2	E	19/19 (100%)	16 (84%)	3 (16%)	2	4
3	D	16/17 (94%)	14 (88%)	2 (12%)	4	9
3	F	17/17 (100%)	15 (88%)	2 (12%)	5	10
All	All	1764/1830 (96%)	1573 (89%)	191 (11%)	6	13

All (191) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	ASN
1	A	61	LYS
1	A	67	LEU
1	A	76	LEU
1	A	97	LEU
1	A	102	ASN
1	A	120	LYS
1	A	125	ASN
1	A	148	ASN
1	A	156	GLU
1	A	158	LEU
1	A	192	LYS
1	A	201	LEU
1	A	223	LYS
1	A	226	LEU
1	A	229	ARG
1	A	270	LEU
1	A	273	LYS
1	A	285	LEU
1	A	290	GLU
1	A	316	THR
1	A	337	LEU

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Mol	Chain	Res	Type
1	A	347	LEU
1	A	348	SER
1	A	353	LYS
1	A	356	VAL
1	A	412	GLN
1	A	414	LEU
1	A	417	LEU
1	A	423	ARG
1	A	446	LEU
1	A	449	VAL
1	A	450	LEU
1	A	466	MET
1	A	468	LEU
1	A	486	GLU
1	A	491	ARG
1	A	499	GLN
1	A	508	GLU
1	A	512	LYS
1	A	517	ASP
1	A	524	LEU
1	A	527	LYS
1	A	595	LEU
1	A	597	LEU
1	A	600	LEU
1	A	603	SER
1	A	612	GLU
1	A	616	LEU
1	A	622	ASN
1	A	629	LEU
1	A	632	LYS
1	A	642	LEU
1	A	648	LYS
1	A	657	LYS
1	A	660	GLU
1	A	691	THR
1	A	711	ARG
1	A	712	LEU
1	A	718	GLN
1	A	728	LEU
1	A	733	ILE
1	A	759	LEU
1	A	765	ARG

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Mol	Chain	Res	Type
1	A	771	LEU
1	A	780	GLN
1	A	799	MET
1	A	810	LEU
1	A	823	LEU
1	A	846	LEU
1	A	853	GLU
1	A	854	LYS
1	A	859	LEU
1	A	861	SER
1	A	867	LEU
1	A	871	GLU
1	A	872	LYS
1	A	875	GLU
1	A	879	GLU
1	A	889	LEU
1	A	928	LEU
1	A	930	THR
1	A	931	LEU
1	A	934	GLU
1	A	938	LYS
1	A	954	VAL
1	A	979	ASN
1	A	993	GLN
1	A	1007	LEU
1	A	1011	HIS
1	B	54	ILE
1	B	61	LYS
1	B	65	ARG
1	B	67	LEU
1	B	74	LYS
1	B	76	LEU
1	B	77	LEU
1	B	94	ILE
1	B	97	LEU
1	B	102	ASN
1	B	111	GLN
1	B	119	LYS
1	B	125	ASN
1	B	156	GLU
1	B	158	LEU
1	B	194	VAL

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Mol	Chain	Res	Type
1	B	196	ASN
1	B	201	LEU
1	B	223	LYS
1	B	226	LEU
1	B	229	ARG
1	B	270	LEU
1	B	271	VAL
1	B	282	ASN
1	B	285	LEU
1	B	287	GLU
1	B	337	LEU
1	B	347	LEU
1	B	360	VAL
1	B	417	LEU
1	B	440	ILE
1	B	457	GLU
1	B	460	ARG
1	B	466	MET
1	B	481	VAL
1	B	483	LYS
1	B	492	THR
1	B	523	LYS
1	B	524	LEU
1	B	540	LEU
1	B	556	MET
1	B	566	LYS
1	B	590	SER
1	B	595	LEU
1	B	597	LEU
1	B	600	LEU
1	B	616	LEU
1	B	617	SER
1	B	622	ASN
1	B	629	LEU
1	B	640	ILE
1	B	642	LEU
1	B	643	LYS
1	B	657	LYS
1	B	677	GLN
1	B	701	LYS
1	B	702	GLU
1	B	712	LEU

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Mol	Chain	Res	Type
1	B	719	LEU
1	B	722	ARG
1	B	728	LEU
1	B	733	ILE
1	B	736	GLN
1	B	744	MET
1	B	751	GLU
1	B	756	LYS
1	B	758	LEU
1	B	759	LEU
1	B	771	LEU
1	B	810	LEU
1	B	817	GLU
1	B	823	LEU
1	B	846	LEU
1	B	853	GLU
1	B	857	HIS
1	B	859	LEU
1	B	860	GLU
1	B	867	LEU
1	B	896	LYS
1	B	898	LYS
1	B	899	LYS
1	B	928	LEU
1	B	931	LEU
1	B	933	LYS
1	B	938	LYS
1	B	942	GLU
1	B	954	VAL
1	B	979	ASN
1	B	980	LEU
1	B	993	GLN
1	B	1007	LEU
1	B	1009	LYS
2	C	13	LEU
2	C	15	GLN
3	D	4	GLN
3	D	17	LEU
2	E	4	GLU
2	E	8	THR
2	E	13	LEU
3	F	4	GLN

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Mol	Chain	Res	Type
3	F	19	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	ASN
1	A	53	HIS
1	A	93	HIS
1	A	102	ASN
1	A	125	ASN
1	A	148	ASN
1	A	184	ASN
1	A	196	ASN
1	A	231	ASN
1	A	232	GLN
1	A	297	HIS
1	A	300	GLN
1	A	329	ASN
1	A	386	HIS
1	A	393	HIS
1	A	407	GLN
1	A	412	GLN
1	A	502	GLN
1	A	515	ASN
1	A	575	ASN
1	A	589	HIS
1	A	622	ASN
1	A	672	ASN
1	A	677	GLN
1	A	718	GLN
1	A	730	HIS
1	A	770	GLN
1	A	780	GLN
1	A	783	ASN
1	A	805	ASN
1	A	828	GLN
1	A	841	ASN
1	A	917	ASN
1	A	922	ASN
1	A	957	HIS
1	B	93	HIS
1	B	102	ASN

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Mol	Chain	Res	Type
1	B	125	ASN
1	B	184	ASN
1	B	196	ASN
1	B	231	ASN
1	B	294	GLN
1	B	297	HIS
1	B	376	ASN
1	B	386	HIS
1	B	393	HIS
1	B	534	ASN
1	B	589	HIS
1	B	622	ASN
1	B	672	ASN
1	B	730	HIS
1	B	736	GLN
1	B	752	HIS
1	B	780	GLN
1	B	783	ASN
1	B	805	ASN
1	B	828	GLN
1	B	887	GLN
1	B	917	ASN
1	B	922	ASN
1	B	957	HIS
3	D	4	GLN
3	F	4	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 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

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	958/990 (96%)	-0.86	7 (0%) 84 82	13, 24, 40, 71	0
1	B	955/990 (96%)	-0.73	10 (1%) 79 76	15, 28, 44, 78	0
2	C	20/20 (100%)	0.59	2 (10%) 12 9	22, 52, 60, 61	0
2	E	20/20 (100%)	0.68	1 (5%) 34 28	21, 46, 63, 67	0
3	D	18/19 (94%)	1.43	5 (27%) 1 1	26, 52, 56, 57	0
3	F	19/19 (100%)	1.47	7 (36%) 1 0	32, 49, 63, 64	0
All	All	1990/2058 (96%)	-0.73	32 (1%) 70 66	13, 26, 47, 78	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	965	SER	5.7
1	B	52	ASN	5.6
1	B	964	ASP	4.7
1	A	964	ASP	4.6
1	B	50	ILE	3.9
1	B	51	GLY	3.8
1	A	42	MET	3.5
1	B	45	PRO	3.5
1	B	44	ASN	3.4
3	D	18	VAL	3.1
3	D	16	TYR	3.0
3	F	12	VAL	2.8
3	F	1	PHE	2.8
3	F	18	VAL	2.7
3	F	16	TYR	2.7
1	A	764	VAL	2.7
2	C	10	ILE	2.6
1	B	53	HIS	2.6
1	A	43	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
3	D	1	PHE	2.6
1	B	46	ALA	2.5
3	F	19	CYS	2.4
3	D	14	ALA	2.4
1	B	764	VAL	2.4
1	B	979	ASN	2.3
3	F	14	ALA	2.3
3	F	17	LEU	2.2
2	C	14	TYR	2.2
1	A	543	GLU	2.1
2	E	13	LEU	2.0
3	D	12	VAL	2.0
1	A	979	ASN	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
4	ZN	A	3012	1/1	1.00	0.30	2,2,2,2	0
4	ZN	B	3012	1/1	1.00	0.30	2,2,2,2	0

6.5 Other polymers [i](#)

There are no such residues in this entry.