



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 06:55 PM UTC

PDB ID : 3I3T / pdb_00003i3t
Title : Crystal structure of covalent ubiquitin-USP21 complex
Authors : Neculai, D.; Avvakumov, G.V.; Walker, J.R.; Xue, S.; Butler-Cole, C.; Weigelt, J.; Bountra, C.; Edwards, A.M.; Arrowsmith, C.H.; Bochkarev, A.; Dhe-Paganon, S.; Structural Genomics Consortium (SGC)
Deposited on : 2009-06-30
Resolution : 2.59 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

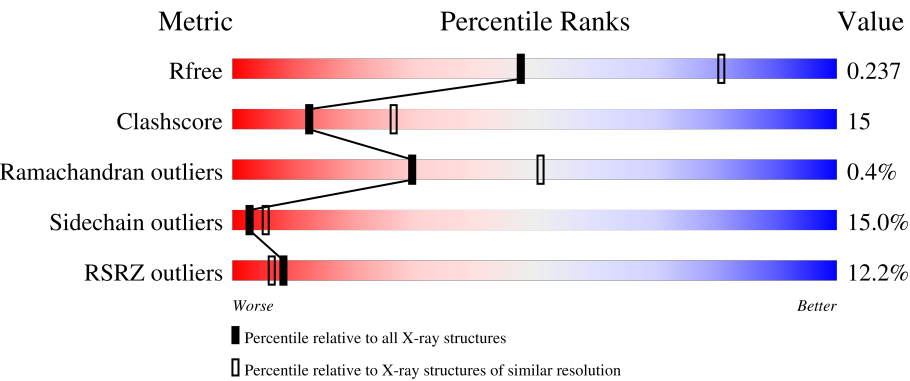
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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	355	9% 51% 27% 6% 15%
1	C	355	12% 52% 29% 5% 13%
1	E	355	12% 54% 27% 6% 13%
1	G	355	8% 53% 25% 6% 14%
2	B	75	9% 81% 15%

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Mol	Chain	Length	Quality of chain
2	D	75	 16% 64% 33% •
2	F	75	 20% 68% 25% 7%
2	H	75	 9% 81% 16% •

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 12456 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 Ubiquitin carboxyl-terminal hydrolase 21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	303	Total	C	N	O	S	0	1	0
			2460	1549	442	452	17			
1	C	310	Total	C	N	O	S	0	1	0
			2506	1579	452	458	17			
1	E	310	Total	C	N	O	S	0	0	0
			2497	1574	450	456	17			
1	G	304	Total	C	N	O	S	0	1	0
			2468	1555	446	450	17			

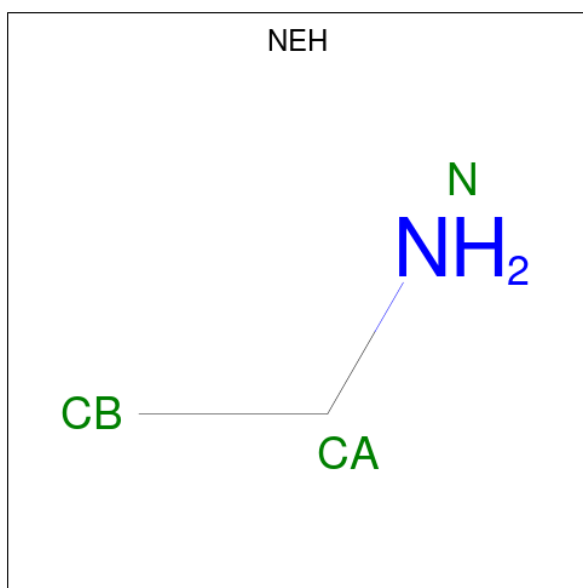
- Molecule 2 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	75	Total	C	N	O	S	0	0	0
			597	376	104	116	1			
2	D	75	Total	C	N	O	S	0	0	0
			597	376	104	116	1			
2	F	75	Total	C	N	O	S	0	0	0
			597	376	104	116	1			
2	H	75	Total	C	N	O	S	0	0	0
			597	376	104	116	1			

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		
3	E	1	Total	Zn	0	0
			1	1		
3	G	1	Total	Zn	0	0
			1	1		

- Molecule 4 is ETHANAMINE (CCD ID: NEH) (formula: C_2H_7N).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	N	0	0
			3	2	1		
4	D	1	Total	C	N	0	0
			3	2	1		
4	F	1	Total	C	N	0	0
			3	2	1		
4	H	1	Total	C	N	0	0
			3	2	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	20	Total	O	0	0
			20	20		
5	C	19	Total	O	0	0
			19	19		
5	E	31	Total	O	0	0
			31	31		
5	G	33	Total	O	0	0
			33	33		
5	B	2	Total	O	0	0
			2	2		
5	D	7	Total	O	0	0
			7	7		
5	F	6	Total	O	0	0
			6	6		

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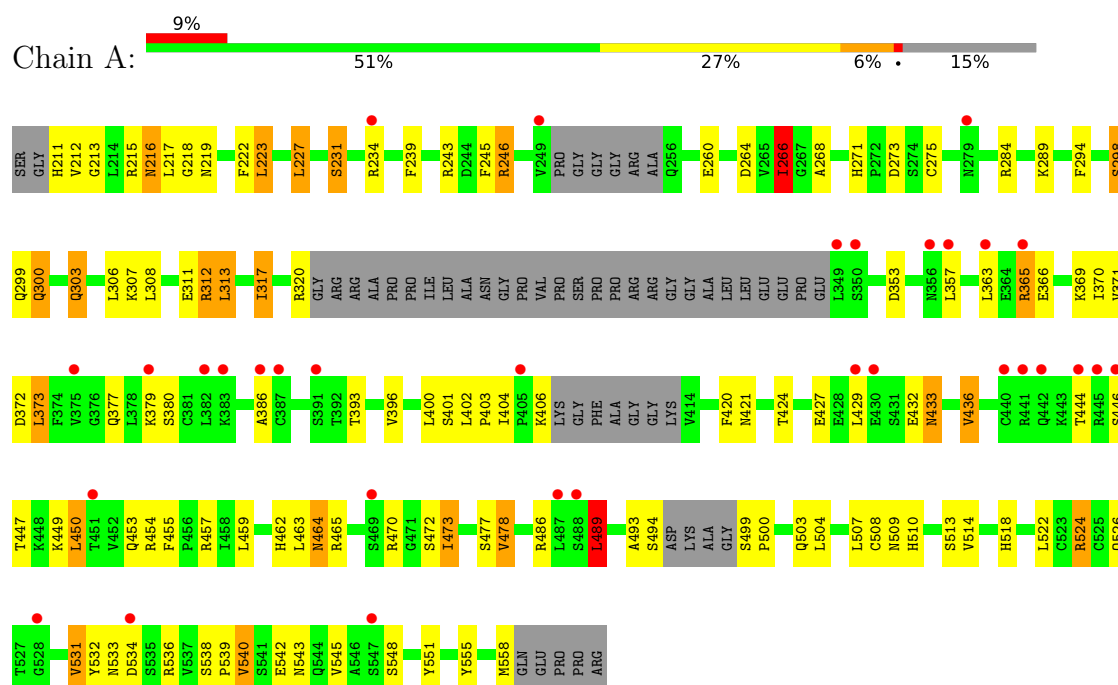
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	3	Total	O	0	0
			3	3		

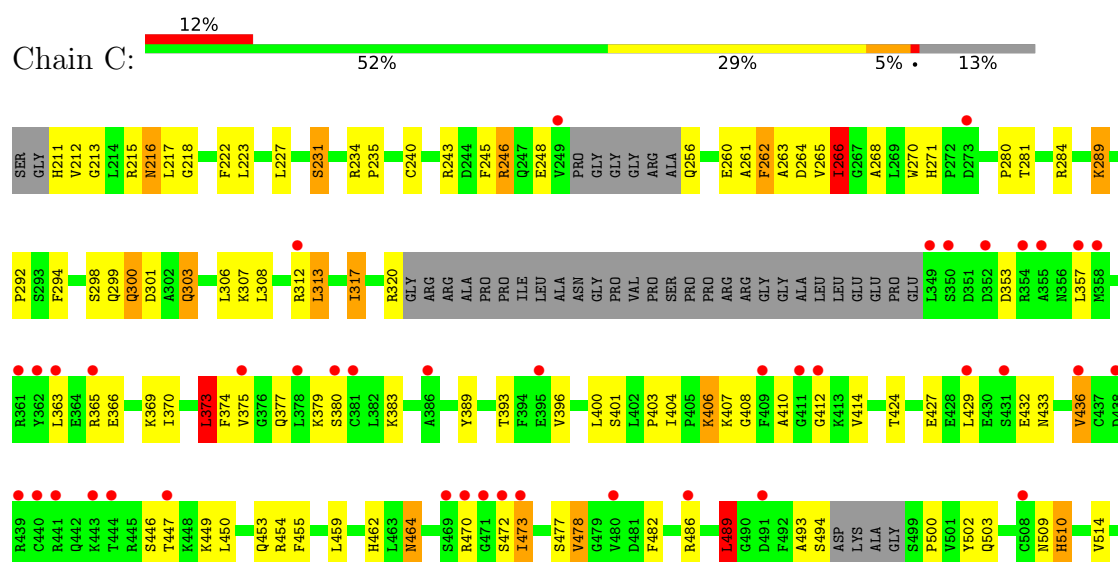
3 Residue-property plots

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: Ubiquitin carboxyl-terminal hydrolase 21

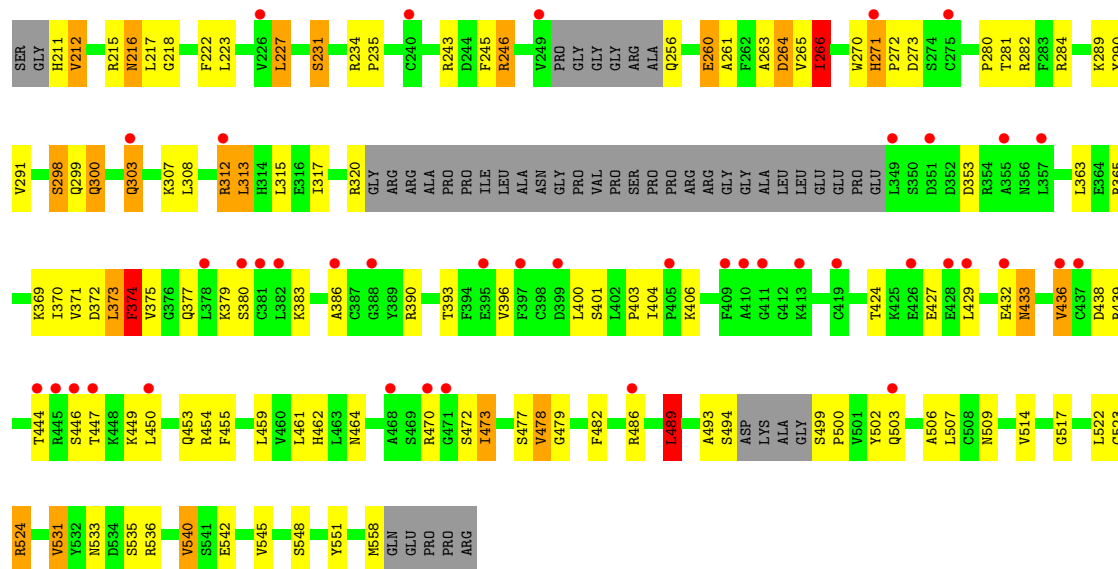


• Molecule 1: Ubiquitin carboxyl-terminal hydrolase 21

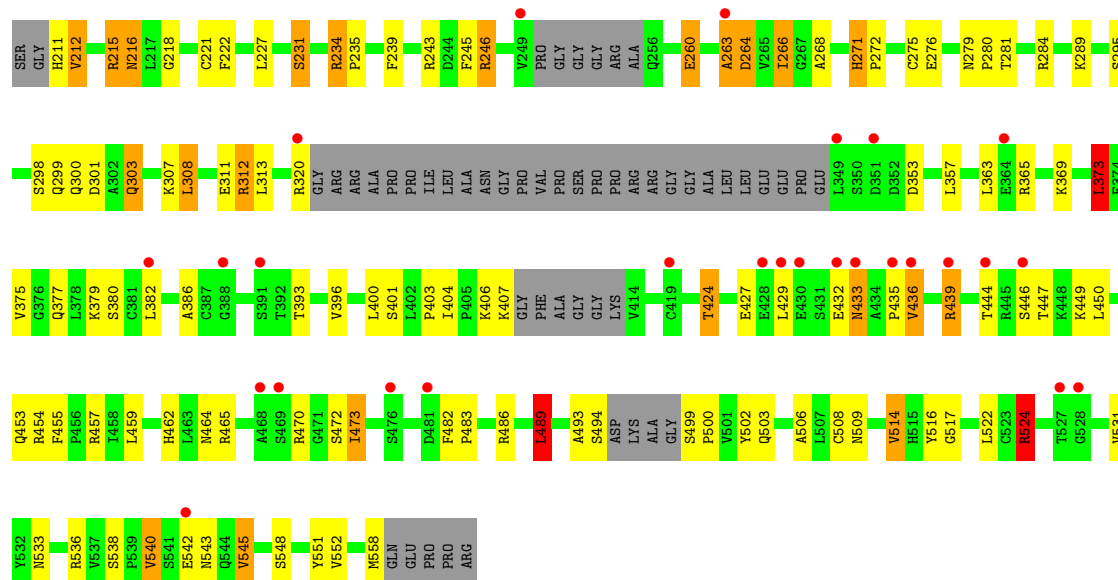




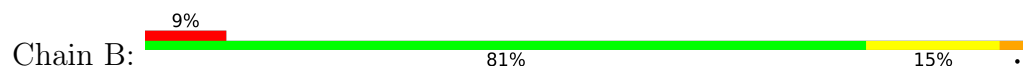
• Molecule 1: Ubiquitin carboxyl-terminal hydrolase 21

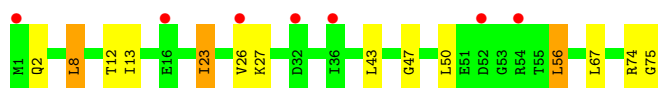


• Molecule 1: Ubiquitin carboxyl-terminal hydrolase 21

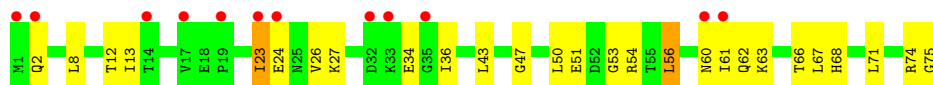


• Molecule 2: Ubiquitin





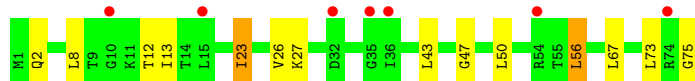
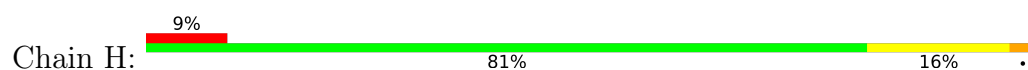
● Molecule 2: Ubiquitin



● Molecule 2: Ubiquitin



● Molecule 2: Ubiquitin



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	58.43Å 83.66Å 118.79Å 88.71° 75.73° 85.11°	Depositor
Resolution (Å)	83.37 – 2.59 83.37 – 2.59	Depositor EDS
% Data completeness (in resolution range)	95.8 (83.37-2.59) 99.6 (83.37-2.59)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.186 , 0.218 0.207 , 0.237	Depositor DCC
R_{free} test set	3400 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	46.9	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 51.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.059 for -h,-k,-h+l	Xtriage
Reported twinning fraction	0.540 for H, K, L 0.460 for -H, -K, -H+L	Depositor
Outliers	0 of 67375 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	12456	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.91% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	1.25	10/2509 (0.4%)	1.35	19/3382 (0.6%)
1	C	1.25	12/2557 (0.5%)	1.31	19/3445 (0.6%)
1	E	1.27	11/2548 (0.4%)	1.30	21/3433 (0.6%)
1	G	1.22	6/2520 (0.2%)	1.29	18/3395 (0.5%)
2	B	1.03	0/603	1.10	1/811 (0.1%)
2	D	1.09	1/603 (0.2%)	1.12	1/811 (0.1%)
2	F	1.03	0/603	1.10	5/811 (0.6%)
2	H	1.02	0/603	1.09	0/811
All	All	1.21	40/12546 (0.3%)	1.27	84/16899 (0.5%)

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	270	TRP	C-O	8.98	1.31	1.23
1	A	545	VAL	CB-CG2	-8.46	1.24	1.52
1	A	545	VAL	CB-CG1	-8.27	1.25	1.52
1	G	545	VAL	CA-CB	7.55	1.63	1.54
1	E	374	PHE	CG-CD1	-7.08	1.24	1.38
1	E	298	SER	C-O	-6.98	1.15	1.23
1	A	266	ILE	CA-CB	6.91	1.62	1.54
1	E	374	PHE	CE1-CZ	-6.77	1.18	1.38
1	C	532	TYR	CA-C	-6.69	1.44	1.52
1	C	266	ILE	CA-CB	6.56	1.64	1.54
1	C	545	VAL	CA-CB	6.38	1.62	1.54
1	E	374	PHE	CE2-CZ	-6.36	1.19	1.38
1	A	532	TYR	CA-C	-6.35	1.45	1.52
1	E	374	PHE	CG-CD2	-6.14	1.25	1.38
2	D	61	ILE	CA-CB	6.05	1.60	1.53
1	C	268	ALA	CA-CB	-5.99	1.43	1.53
1	C	510	HIS	N-CA	5.99	1.53	1.46
1	E	261	ALA	CA-CB	-5.98	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	291	VAL	CA-CB	5.98	1.61	1.54
1	A	246	ARG	CA-C	5.85	1.60	1.52
1	C	552	VAL	CA-CB	5.83	1.61	1.54
1	C	414	VAL	CA-CB	5.81	1.60	1.54
1	G	301	ASP	CA-C	5.72	1.59	1.52
1	A	532	TYR	N-CA	5.67	1.53	1.46
1	A	213	GLY	C-O	5.64	1.29	1.23
1	C	262	PHE	CA-C	5.43	1.59	1.52
1	E	375	VAL	CA-CB	5.43	1.61	1.54
1	G	279	ASN	N-CA	5.37	1.52	1.46
1	C	261	ALA	N-CA	-5.37	1.39	1.46
1	C	213	GLY	N-CA	5.32	1.48	1.44
1	C	261	ALA	CA-C	5.26	1.59	1.52
1	G	215	ARG	CA-C	-5.22	1.46	1.52
1	E	261	ALA	CA-C	5.15	1.59	1.52
1	A	298	SER	C-O	-5.13	1.17	1.23
1	E	266	ILE	CA-CB	5.09	1.61	1.54
1	C	375	VAL	CA-C	-5.08	1.46	1.52
1	G	506	ALA	CA-CB	5.07	1.62	1.53
1	A	518	HIS	CA-C	5.06	1.58	1.52
1	A	508	CYS	CA-C	-5.05	1.46	1.52
1	G	375	VAL	CA-C	-5.03	1.46	1.52

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	234	ARG	CA-C-N	-11.08	107.44	119.19
1	C	234	ARG	C-N-CA	-11.08	107.44	119.19
1	A	545	VAL	CG1-CB-CG2	-11.06	86.48	110.80
1	G	234	ARG	CA-C-N	-10.06	108.21	119.28
1	G	234	ARG	C-N-CA	-10.06	108.21	119.28
1	A	365	ARG	NE-CZ-NH2	9.98	128.18	119.20
1	A	234	ARG	CA-C-N	-9.62	108.70	119.28
1	A	234	ARG	C-N-CA	-9.62	108.70	119.28
1	A	365	ARG	NE-CZ-NH1	-9.19	112.31	121.50
1	E	472	SER	N-CA-C	8.60	120.60	108.74
1	G	472	SER	N-CA-C	8.05	119.85	108.74
1	G	489	LEU	N-CA-C	7.82	122.89	111.87
1	A	271	HIS	CA-C-N	-7.80	111.56	119.99
1	A	271	HIS	C-N-CA	-7.80	111.56	119.99
1	C	472	SER	N-CA-C	7.62	119.26	108.74
1	A	472	SER	N-CA-C	7.55	119.16	108.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	271	HIS	CA-C-N	-7.32	112.44	119.76
1	G	271	HIS	C-N-CA	-7.32	112.44	119.76
1	A	365	ARG	CD-NE-CZ	7.25	134.55	124.40
1	C	489	LEU	N-CA-C	6.96	121.69	111.87
1	E	234	ARG	CA-C-N	-6.94	111.65	119.28
1	E	234	ARG	C-N-CA	-6.94	111.65	119.28
1	A	489	LEU	N-CA-C	6.85	121.32	112.41
1	C	223	LEU	N-CA-C	-6.83	104.58	113.12
1	C	374	PHE	N-CA-C	6.71	121.64	113.38
1	E	270	TRP	CA-C-N	-6.67	114.46	123.46
1	E	270	TRP	C-N-CA	-6.67	114.46	123.46
1	G	545	VAL	N-CA-CB	6.54	118.94	110.57
1	E	482	PHE	CA-C-N	6.48	126.24	119.76
1	E	482	PHE	C-N-CA	6.48	126.24	119.76
1	E	222	PHE	N-CA-C	-6.47	104.65	112.54
1	E	271	HIS	CA-C-N	-6.38	113.38	119.76
1	E	271	HIS	C-N-CA	-6.38	113.38	119.76
1	G	373	LEU	N-CA-C	6.38	118.11	111.03
1	C	410	ALA	N-CA-C	-6.37	103.59	112.25
1	C	373	LEU	N-CA-C	6.33	117.86	110.97
1	E	489	LEU	N-CA-C	6.27	120.71	111.87
1	E	479	GLY	N-CA-C	-6.22	104.08	111.36
1	G	499	SER	CA-C-N	6.14	125.90	119.76
1	G	499	SER	C-N-CA	6.14	125.90	119.76
1	C	482	PHE	CA-C-N	6.01	125.95	119.76
1	C	482	PHE	C-N-CA	6.01	125.95	119.76
1	E	531	VAL	CB-CA-C	-6.00	102.52	110.98
2	D	36	ILE	N-CA-C	5.94	114.43	107.77
1	C	523	CYS	N-CA-C	5.87	119.05	109.24
1	A	499	SER	CA-C-N	5.87	125.63	119.76
1	A	499	SER	C-N-CA	5.87	125.63	119.76
1	C	270	TRP	CA-C-N	-5.85	115.57	123.46
1	C	270	TRP	C-N-CA	-5.85	115.57	123.46
1	A	402	LEU	N-CA-C	5.84	117.03	109.72
1	G	260	GLU	N-CA-C	-5.81	104.64	110.97
2	B	8	LEU	N-CA-C	5.73	118.26	111.33
1	G	524	ARG	NE-CZ-NH1	-5.69	115.81	121.50
1	E	265	VAL	N-CA-C	-5.58	105.41	110.82
1	E	523	CYS	N-CA-C	5.54	118.43	109.40
1	A	507	LEU	CB-CA-C	-5.50	97.36	109.56
1	E	264	ASP	N-CA-C	5.42	119.89	113.16
1	C	545	VAL	N-CA-CB	5.39	117.46	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	263	ALA	CA-C-N	-5.38	112.65	122.38
1	E	263	ALA	C-N-CA	-5.38	112.65	122.38
1	E	507	LEU	CB-CA-C	-5.38	98.14	109.38
1	A	317	ILE	N-CA-C	5.24	117.14	112.17
1	A	223	LEU	N-CA-C	-5.21	105.20	112.45
1	G	295	SER	N-CA-C	-5.21	103.51	110.55
1	G	264	ASP	N-CA-C	5.20	119.72	113.17
1	G	263	ALA	CA-C-N	-5.19	113.97	122.54
1	G	263	ALA	C-N-CA	-5.19	113.97	122.54
1	A	526	GLN	N-CA-C	5.19	117.67	111.71
1	A	531	VAL	CB-CA-C	-5.17	103.97	111.68
2	F	36	ILE	CA-C-N	-5.17	115.94	119.66
2	F	36	ILE	C-N-CA	-5.17	115.94	119.66
2	F	7	THR	CA-C-N	5.16	127.45	120.38
2	F	7	THR	C-N-CA	5.16	127.45	120.38
1	C	265	VAL	N-CA-C	-5.14	105.70	110.53
2	F	8	LEU	N-CA-C	5.14	117.54	111.33
1	A	268	ALA	N-CA-C	5.11	117.52	111.33
1	C	260	GLU	CA-C-N	-5.11	112.11	121.52
1	C	260	GLU	C-N-CA	-5.11	112.11	121.52
1	E	506	ALA	N-CA-C	5.09	116.80	108.55
1	C	265	VAL	N-CA-CB	5.06	117.05	110.57
1	G	308	LEU	N-CA-C	-5.06	106.62	112.89
1	G	268	ALA	N-CA-C	5.05	118.21	111.75
1	E	260	GLU	CA-CB-CG	5.03	124.16	114.10
1	C	317	ILE	N-CA-C	5.03	116.95	112.17

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	2460	0	2412	79	0
1	C	2506	0	2464	100	0
1	E	2497	0	2457	106	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	2468	0	2433	69	0
2	B	597	0	626	13	0
2	D	597	0	626	26	0
2	F	597	0	626	23	0
2	H	597	0	626	14	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
4	B	3	0	5	1	0
4	D	3	0	4	0	0
4	F	3	0	4	0	0
4	H	3	0	5	1	0
5	A	20	0	0	3	0
5	B	2	0	0	0	0
5	C	19	0	0	3	0
5	D	7	0	0	4	0
5	E	31	0	0	3	0
5	F	6	0	0	1	0
5	G	33	0	0	0	0
5	H	3	0	0	1	0
All	All	12456	0	12288	374	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 15.

All (374) 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:E:503:GLN:NE2	1:E:524:ARG:HH12	1.12	1.42
1:G:503:GLN:NE2	1:G:524:ARG:HH12	1.07	1.42
1:G:503:GLN:HE21	1:G:524:ARG:NH1	1.15	1.41
1:C:289:LYS:HE2	1:E:315:LEU:CD2	1.48	1.40
1:C:503:GLN:NE2	1:C:524:ARG:HH12	1.26	1.29
1:A:503:GLN:HE21	1:A:524:ARG:NH1	1.29	1.28
1:C:289:LYS:CE	1:E:315:LEU:HD21	1.69	1.21
1:E:282:ARG:HH12	2:D:54:ARG:CD	1.53	1.19
1:E:503:GLN:HE21	1:E:524:ARG:NH1	1.41	1.19
1:A:503:GLN:NE2	1:A:524:ARG:HH12	1.40	1.19
1:C:503:GLN:HE21	1:C:524:ARG:NH1	1.39	1.18
1:E:503:GLN:NE2	1:E:524:ARG:NH1	1.92	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:509:ASN:HD21	1:G:548:SER:HB3	1.03	1.16
1:E:509:ASN:HD21	1:E:548:SER:HB3	1.06	1.14
1:C:407:LYS:HB3	1:C:412:GLY:HA2	1.30	1.13
1:C:503:GLN:NE2	1:C:524:ARG:NH1	1.96	1.10
1:E:282:ARG:NH1	2:D:54:ARG:NE	2.00	1.10
1:C:509:ASN:HD21	1:C:548:SER:HB3	1.05	1.10
1:G:439[A]:ARG:HH11	1:G:439[A]:ARG:CG	1.63	1.10
1:E:282:ARG:HH12	2:D:54:ARG:NE	1.50	1.09
1:C:292:PRO:HG3	1:E:290:TYR:CD1	1.87	1.08
1:A:509:ASN:HD21	1:A:548:SER:HB3	1.10	1.06
1:A:509:ASN:ND2	1:A:548:SER:HB3	1.71	1.04
1:G:439[A]:ARG:NH1	1:G:439[A]:ARG:HG2	1.65	1.03
1:E:282:ARG:HH12	2:D:54:ARG:HD3	1.18	1.01
1:C:509:ASN:ND2	1:C:548:SER:HB3	1.75	1.01
1:E:509:ASN:ND2	1:E:548:SER:HB3	1.77	0.99
1:G:439[A]:ARG:HH11	1:G:439[A]:ARG:HG2	0.84	0.99
1:G:503:GLN:NE2	1:G:524:ARG:NH1	1.84	0.99
1:E:282:ARG:NH1	2:D:54:ARG:HE	1.56	0.98
1:G:509:ASN:ND2	1:G:548:SER:HB3	1.79	0.97
1:C:289:LYS:HE2	1:E:315:LEU:HD21	0.93	0.93
1:C:289:LYS:HE2	1:E:315:LEU:HD23	1.52	0.92
1:E:401:SER:HB2	1:E:462:HIS:HD2	1.39	0.88
1:C:401:SER:HB2	1:C:462:HIS:HD2	1.40	0.86
1:G:231:SER:HB2	1:G:266:ILE:HD12	1.57	0.86
1:C:294:PHE:CE2	1:C:300[B]:GLN:HG2	2.10	0.86
1:E:436:VAL:H	2:F:2:GLN:HE22	1.20	0.86
1:E:282:ARG:NH1	2:D:54:ARG:CD	2.36	0.85
1:E:282:ARG:NH1	2:D:54:ARG:HD3	1.93	0.83
1:C:256:GLN:OE1	5:C:86:HOH:O	1.97	0.82
1:E:231:SER:HB2	1:E:266:ILE:HD12	1.61	0.81
1:A:246:ARG:HD2	1:A:260[B]:GLU:OE2	1.81	0.80
1:E:307:LYS:HE3	2:F:47:GLY:O	1.83	0.79
1:E:320:ARG:HD2	1:E:363:LEU:O	1.82	0.79
1:C:289:LYS:CE	1:E:315:LEU:CD2	2.41	0.79
1:A:433:ASN:OD1	2:B:13:ILE:HA	1.83	0.78
1:G:433:ASN:OD1	2:H:13:ILE:HA	1.83	0.78
1:A:503:GLN:NE2	1:A:524:ARG:NH1	2.08	0.78
1:C:216:ASN:HD22	1:C:218:GLY:H	1.30	0.78
1:C:407:LYS:CB	1:C:412:GLY:HA2	2.12	0.77
2:D:68:HIS:NE2	5:D:81:HOH:O	2.16	0.76
1:C:216:ASN:ND2	1:C:218:GLY:H	1.83	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:292:PRO:HG3	1:E:290:TYR:CE1	2.21	0.75
1:G:489:LEU:H	1:G:489:LEU:HD22	1.50	0.74
1:E:216:ASN:ND2	1:E:218:GLY:H	1.85	0.74
1:E:216:ASN:HD22	1:E:218:GLY:H	1.34	0.74
1:E:503:GLN:HE21	1:E:524:ARG:HH12	0.74	0.74
1:A:436:VAL:HG13	2:B:2:GLN:HE22	1.53	0.73
1:G:401:SER:HB2	1:G:462:HIS:HD2	1.53	0.73
1:G:489:LEU:HD22	1:G:489:LEU:N	2.05	0.72
1:C:231:SER:HB2	1:C:266:ILE:HD12	1.70	0.72
1:C:320:ARG:HD2	1:C:363:LEU:O	1.90	0.71
1:A:509:ASN:HD21	1:A:548:SER:CB	1.97	0.71
1:G:320:ARG:HD2	1:G:363:LEU:O	1.91	0.71
1:C:307:LYS:HE3	2:D:47:GLY:O	1.90	0.70
1:C:380:SER:HB3	1:C:450:LEU:HD12	1.72	0.70
1:C:503:GLN:HE21	1:C:524:ARG:HH12	0.72	0.70
1:E:433:ASN:OD1	2:F:13:ILE:HA	1.93	0.69
1:E:243:ARG:HD2	1:E:246:ARG:NH1	2.08	0.69
1:E:401:SER:HB2	1:E:462:HIS:CD2	2.26	0.69
1:A:489:LEU:HD22	1:A:489:LEU:H	1.57	0.69
1:C:401:SER:HB2	1:C:462:HIS:CD2	2.27	0.68
2:H:27:LYS:HE2	2:H:43:LEU:HD23	1.76	0.67
1:A:462:HIS:HE1	1:A:551:TYR:CZ	2.12	0.67
1:A:320:ARG:HD2	1:A:363:LEU:O	1.95	0.67
1:G:436:VAL:HG13	2:H:2:GLN:HE22	1.59	0.66
1:E:380:SER:HB3	1:E:450:LEU:HD12	1.78	0.66
1:G:221:CYS:H	4:H:76:NEH:HB1	1.60	0.65
1:C:433:ASN:OD1	2:D:13:ILE:HA	1.96	0.65
1:A:534:ASP:OD1	5:A:73:HOH:O	2.15	0.65
1:C:289:LYS:NZ	1:E:315:LEU:HD21	2.11	0.65
1:G:303:GLN:HG2	1:G:462:HIS:CE1	2.32	0.65
2:F:27:LYS:HE2	2:F:43:LEU:HD23	1.78	0.65
1:C:216:ASN:HD22	1:C:217:LEU:N	1.94	0.64
1:A:380:SER:HB3	1:A:450:LEU:HD12	1.79	0.64
1:G:307:LYS:HE3	2:H:47:GLY:O	1.98	0.64
1:E:433:ASN:HD21	2:F:33:LYS:HE2	1.63	0.63
1:A:243:ARG:HD2	1:A:246:ARG:NH1	2.13	0.63
1:G:243:ARG:HD2	1:G:246:ARG:NH1	2.14	0.63
1:A:294:PHE:CE2	1:A:300:GLN:HG2	2.33	0.63
1:A:243:ARG:HH22	1:A:264:ASP:HB3	1.64	0.63
1:A:489:LEU:HD22	1:A:489:LEU:N	2.13	0.62
1:C:455:PHE:HE1	1:C:493:ALA:HB2	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:509:ASN:HD21	1:C:548:SER:CB	1.96	0.62
2:D:27:LYS:HE2	2:D:43:LEU:HD23	1.81	0.62
1:C:243:ARG:HD2	1:C:246:ARG:NH1	2.14	0.62
1:G:473:ILE:H	1:G:473:ILE:HD12	1.64	0.62
1:G:522:LEU:HD23	1:G:531:VAL:HG22	1.81	0.62
1:A:231:SER:HB2	1:A:266:ILE:HD12	1.81	0.62
1:A:473:ILE:HD12	1:A:473:ILE:H	1.65	0.62
1:E:439:ARG:HD2	5:E:38:HOH:O	2.00	0.61
1:C:473:ILE:HD12	1:C:473:ILE:N	2.15	0.61
1:G:401:SER:HB2	1:G:462:HIS:CD2	2.34	0.61
1:C:243:ARG:HH22	1:C:264:ASP:HB3	1.65	0.61
1:C:300[B]:GLN:HG3	1:C:301:ASP:N	2.16	0.61
1:G:216:ASN:HD22	1:G:218:GLY:H	1.47	0.61
1:A:455:PHE:HE1	1:A:493:ALA:HB2	1.66	0.60
1:C:455:PHE:CE1	1:C:493:ALA:HB2	2.36	0.60
1:G:216:ASN:ND2	1:G:218:GLY:H	1.99	0.60
1:E:473:ILE:HD12	1:E:473:ILE:H	1.66	0.60
1:C:303:GLN:HG2	1:C:462:HIS:CE1	2.36	0.60
1:E:374:PHE:N	1:E:374:PHE:HD1	2.00	0.60
1:A:455:PHE:CE1	1:A:493:ALA:HB2	2.37	0.59
1:C:245:PHE:HB2	1:C:317:ILE:HG22	1.83	0.59
1:C:462:HIS:HE1	1:C:551:TYR:CZ	2.21	0.59
1:G:455:PHE:CE1	1:G:493:ALA:HB2	2.38	0.59
1:C:522:LEU:HD23	1:C:531:VAL:HG22	1.85	0.59
2:B:26:VAL:HG21	2:B:56:LEU:HD11	1.84	0.59
2:B:27:LYS:HE2	2:B:43:LEU:HD23	1.85	0.59
1:A:522:LEU:HD23	1:A:531:VAL:HG22	1.84	0.59
1:G:380:SER:HB3	1:G:450:LEU:HD12	1.85	0.59
1:A:380:SER:HA	1:A:449:LYS:O	2.02	0.59
1:E:374:PHE:N	1:E:374:PHE:CD1	2.69	0.59
1:G:473:ILE:HD12	1:G:473:ILE:N	2.18	0.59
1:E:489:LEU:H	1:E:489:LEU:HD22	1.68	0.58
1:E:473:ILE:HD12	1:E:473:ILE:N	2.19	0.58
1:E:439:ARG:HG2	1:E:439:ARG:HH11	1.69	0.58
1:E:243:ARG:HH22	1:E:264:ASP:HB3	1.68	0.58
1:G:455:PHE:HE1	1:G:493:ALA:HB2	1.68	0.58
1:E:489:LEU:HD23	1:E:500:PRO:HG2	1.84	0.58
1:A:522:LEU:CD2	1:A:531:VAL:HG22	2.33	0.58
1:A:436:VAL:HG13	2:B:2:GLN:NE2	2.19	0.58
1:E:299:GLN:HB3	2:F:75:GLY:C	2.28	0.58
1:C:453:GLN:NE2	1:C:494:SER:OG	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:489:LEU:HD23	1:C:500:PRO:HG2	1.86	0.57
1:E:462:HIS:HE1	1:E:551:TYR:CZ	2.23	0.57
1:C:489:LEU:HD22	1:C:489:LEU:N	2.19	0.57
1:G:436:VAL:H	2:H:2:GLN:HE22	1.50	0.57
1:A:216:ASN:HD22	1:A:218:GLY:H	1.53	0.57
1:C:312:ARG:HE	1:C:312:ARG:HA	1.70	0.57
1:E:489:LEU:HD22	1:E:489:LEU:N	2.20	0.57
1:G:439[A]:ARG:CG	1:G:439[A]:ARG:NH1	2.34	0.57
1:A:473:ILE:HD12	1:A:473:ILE:N	2.20	0.56
2:D:66:THR:HB	5:D:81:HOH:O	2.06	0.56
1:A:216:ASN:HD22	1:A:217:LEU:N	2.03	0.56
1:E:380:SER:HA	1:E:449:LYS:O	2.05	0.56
1:A:429:LEU:HD21	2:B:12:THR:HB	1.86	0.56
1:G:369:LYS:HE3	1:G:373:LEU:HD21	1.86	0.56
1:A:216:ASN:ND2	1:A:218:GLY:H	2.04	0.56
1:E:522:LEU:CD2	1:E:531:VAL:HG22	2.36	0.55
1:A:303:GLN:HG2	1:A:462:HIS:CE1	2.40	0.55
1:A:371:VAL:O	1:A:372:ASP:C	2.47	0.55
1:G:243:ARG:HH22	1:G:264:ASP:HB3	1.71	0.55
2:H:26:VAL:HG21	2:H:56:LEU:HD11	1.87	0.55
1:C:522:LEU:CD2	1:C:531:VAL:HG22	2.36	0.55
1:C:489:LEU:HD22	1:C:489:LEU:H	1.72	0.55
1:E:245:PHE:HB2	1:E:317:ILE:HG22	1.89	0.55
1:A:436:VAL:H	2:B:2:GLN:HE22	1.52	0.55
1:A:307:LYS:HE3	2:B:47:GLY:O	2.06	0.55
2:D:26:VAL:HG21	2:D:56:LEU:HD11	1.89	0.55
1:G:436:VAL:HG13	2:H:2:GLN:NE2	2.23	0.55
1:C:473:ILE:HD12	1:C:473:ILE:H	1.71	0.54
1:E:436:VAL:H	2:F:2:GLN:NE2	1.98	0.54
2:H:27:LYS:HG2	2:H:43:LEU:HD21	1.90	0.54
1:A:477:SER:O	1:A:478:VAL:C	2.51	0.54
1:G:311:GLU:HG3	5:H:77:HOH:O	2.07	0.54
1:G:403:PRO:C	1:G:404:ILE:HD13	2.33	0.54
1:E:303:GLN:HG2	1:E:462:HIS:CE1	2.42	0.54
1:A:453:GLN:NE2	1:A:494:SER:OG	2.40	0.54
1:C:245:PHE:HB2	1:C:317:ILE:CG2	2.37	0.54
1:A:510:HIS:NE2	2:B:74:ARG:O	2.37	0.54
1:E:379:LYS:O	1:E:450:LEU:HA	2.08	0.54
1:G:221:CYS:SG	1:G:222:PHE:N	2.82	0.53
1:C:436:VAL:HG13	2:D:2:GLN:HE22	1.72	0.53
1:E:453:GLN:NE2	1:E:494:SER:OG	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:489:LEU:HD23	1:G:500:PRO:HG2	1.91	0.53
1:E:256:GLN:O	1:E:260:GLU:HG3	2.09	0.53
1:G:453:GLN:NE2	1:G:494:SER:OG	2.41	0.53
1:G:522:LEU:CD2	1:G:531:VAL:HG22	2.39	0.53
1:A:223:LEU:HD23	1:A:227:LEU:HD22	1.90	0.53
1:A:401:SER:HB2	1:A:462:HIS:HD2	1.74	0.53
1:A:509:ASN:ND2	1:A:548:SER:CB	2.61	0.53
1:C:294:PHE:CZ	1:C:300[B]:GLN:HG2	2.42	0.52
1:C:406:LYS:O	1:C:407:LYS:HG3	2.09	0.52
1:E:373:LEU:HB2	1:E:374:PHE:CD1	2.43	0.52
1:C:377:GLN:HB3	1:C:454:ARG:HB2	1.91	0.52
1:E:522:LEU:HD23	1:E:531:VAL:HG22	1.92	0.52
1:G:380:SER:HA	1:G:449:LYS:O	2.10	0.52
1:C:403:PRO:C	1:C:404:ILE:HD13	2.35	0.52
1:C:300[B]:GLN:CG	1:C:301:ASP:N	2.72	0.52
1:E:373:LEU:CB	1:E:374:PHE:CD1	2.93	0.52
1:E:377:GLN:HB3	1:E:454:ARG:HB2	1.92	0.52
1:A:377:GLN:HB3	1:A:454:ARG:HB2	1.92	0.52
1:E:312:ARG:HE	1:E:312:ARG:HA	1.74	0.52
1:G:429:LEU:HD21	2:H:12:THR:HB	1.91	0.52
1:E:531:VAL:CG2	1:E:540:VAL:HG21	2.40	0.52
1:E:401:SER:HA	1:E:462:HIS:HB3	1.92	0.51
1:E:429:LEU:HD21	2:F:12:THR:HB	1.92	0.51
1:A:222:PHE:CD1	1:A:222:PHE:C	2.88	0.51
1:C:526:GLN:NE2	5:C:101:HOH:O	2.44	0.51
1:A:531:VAL:CG2	1:A:540:VAL:HG21	2.41	0.51
1:G:531:VAL:CG2	1:G:540:VAL:HG21	2.41	0.51
1:E:320:ARG:CD	1:E:363:LEU:O	2.57	0.51
1:E:403:PRO:C	1:E:404:ILE:HD13	2.36	0.51
1:G:379:LYS:O	1:G:450:LEU:HA	2.11	0.50
1:A:436:VAL:O	1:A:436:VAL:CG2	2.60	0.50
1:E:436:VAL:HG13	2:F:2:GLN:HE22	1.76	0.50
2:F:35:GLY:CA	5:F:78:HOH:O	2.59	0.50
1:G:514:VAL:HA	2:H:73:LEU:HD12	1.93	0.50
1:E:433:ASN:OD1	2:F:14:THR:N	2.43	0.49
1:C:380:SER:HA	1:C:449:LYS:O	2.13	0.49
2:B:23:ILE:HG22	2:B:27:LYS:HE3	1.93	0.49
1:E:438:ASP:OD2	2:F:63:LYS:CE	2.61	0.49
1:G:462:HIS:HE1	1:G:551:TYR:CZ	2.31	0.49
1:E:369:LYS:HE3	1:E:373:LEU:HD21	1.94	0.49
2:D:24:GLU:OE1	2:D:53:GLY:N	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:GLN:HB3	2:B:75:GLY:C	2.37	0.49
1:E:313:LEU:O	1:E:317:ILE:HG12	2.14	0.48
1:C:436:VAL:H	2:D:2:GLN:HE22	1.61	0.48
1:G:234:ARG:O	1:G:235:PRO:C	2.54	0.48
1:A:245:PHE:HB2	1:A:317:ILE:CG2	2.43	0.48
1:G:533:ASN:HD22	1:G:536:ARG:HH11	1.60	0.48
1:E:216:ASN:HD22	1:E:217:LEU:N	2.12	0.48
1:C:379:LYS:O	1:C:450:LEU:HA	2.14	0.48
1:C:531:VAL:CG2	1:C:540:VAL:HG21	2.43	0.48
1:C:216:ASN:HD22	1:C:216:ASN:C	2.22	0.48
1:A:312:ARG:HE	1:A:312:ARG:HA	1.78	0.47
1:A:457:ARG:N	5:A:58:HOH:O	2.04	0.47
1:A:219:ASN:O	4:B:76:NEH:HA3	2.13	0.47
1:G:275:CYS:O	1:G:276:GLU:C	2.56	0.47
1:C:262:PHE:O	1:C:263:ALA:C	2.55	0.47
1:C:473:ILE:HG21	2:D:71:LEU:CD1	2.44	0.47
1:C:303:GLN:HE21	1:C:462:HIS:CG	2.33	0.47
1:E:312:ARG:HE	1:E:312:ARG:CA	2.26	0.47
1:E:535:SER:HG	1:G:516:TYR:HD1	1.61	0.47
1:C:320:ARG:CD	1:C:363:LEU:O	2.61	0.47
1:E:436:VAL:HG13	2:F:2:GLN:NE2	2.30	0.47
1:A:379:LYS:O	1:A:450:LEU:HA	2.13	0.47
1:A:503:GLN:HE21	1:A:524:ARG:HH12	0.57	0.47
1:E:243:ARG:CD	1:E:246:ARG:NH1	2.77	0.47
5:E:103:HOH:O	2:F:68:HIS:HE1	1.97	0.47
1:G:386:ALA:HB2	1:G:444:THR:HG21	1.95	0.47
1:A:462:HIS:HE1	1:A:551:TYR:OH	1.96	0.47
2:F:26:VAL:HG21	2:F:56:LEU:HD11	1.97	0.47
1:G:377:GLN:HB3	1:G:454:ARG:HB2	1.97	0.47
1:C:401:SER:HA	1:C:462:HIS:HB3	1.97	0.46
1:E:373:LEU:HB2	1:E:374:PHE:HD1	1.79	0.46
1:C:477:SER:O	1:C:478:VAL:C	2.59	0.46
1:E:313:LEU:HB3	1:E:370:ILE:CD1	2.45	0.46
1:E:371:VAL:O	1:E:372:ASP:C	2.57	0.46
2:D:27:LYS:HE2	2:D:43:LEU:CD2	2.46	0.46
2:D:2:GLN:N	5:D:104:HOH:O	2.48	0.46
1:A:239:PHE:CE2	1:A:245:PHE:HB3	2.50	0.46
1:C:312:ARG:HA	1:C:312:ARG:NE	2.30	0.46
1:C:407:LYS:HB3	1:C:412:GLY:CA	2.22	0.46
1:C:510:HIS:NE2	2:D:74:ARG:O	2.42	0.46
1:A:455:PHE:CG	1:A:500:PRO:HG3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:489:LEU:HD21	1:E:502:TYR:CD2	2.51	0.46
1:G:403:PRO:O	1:G:404:ILE:HD13	2.16	0.46
2:B:43:LEU:N	2:B:43:LEU:HD22	2.30	0.46
1:E:212:VAL:HB	1:E:272:PRO:HG3	1.98	0.45
1:C:429:LEU:HD21	2:D:12:THR:HB	1.99	0.45
1:E:369:LYS:HG3	1:E:373:LEU:CD2	2.46	0.45
1:E:312:ARG:HA	1:E:312:ARG:NE	2.31	0.45
1:G:320:ARG:CD	1:G:363:LEU:O	2.63	0.45
2:B:27:LYS:HG2	2:B:43:LEU:HD21	1.98	0.45
1:A:401:SER:HA	1:A:462:HIS:HB3	1.97	0.45
1:C:289:LYS:HZ1	1:E:315:LEU:HD21	1.81	0.45
1:E:373:LEU:CB	1:E:374:PHE:HD1	2.30	0.45
1:C:243:ARG:HB3	1:C:246:ARG:HD3	1.99	0.45
1:C:533:ASN:HD22	1:C:536:ARG:HH11	1.65	0.45
1:G:212:VAL:HB	1:G:272:PRO:HG3	1.99	0.45
2:H:23:ILE:O	2:H:27:LYS:HG3	2.17	0.45
1:C:299:GLN:HB3	2:D:75:GLY:C	2.41	0.45
1:E:473:ILE:HG21	2:F:71:LEU:CD1	2.47	0.45
1:E:235:PRO:HB2	1:E:373:LEU:HD11	1.99	0.45
1:C:216:ASN:ND2	1:C:217:LEU:N	2.61	0.44
1:E:245:PHE:HB2	1:E:317:ILE:CG2	2.47	0.44
1:G:489:LEU:N	1:G:489:LEU:CD2	2.75	0.44
1:C:462:HIS:HE1	1:C:551:TYR:OH	2.00	0.44
1:E:436:VAL:O	1:E:436:VAL:CG2	2.65	0.44
1:A:222:PHE:CD1	1:A:223:LEU:N	2.86	0.44
1:A:401:SER:HB2	1:A:462:HIS:CD2	2.51	0.44
1:E:533:ASN:HD22	1:E:536:ARG:HH11	1.66	0.44
1:E:386:ALA:HB2	1:E:444:THR:HG21	2.00	0.44
1:G:312:ARG:HE	1:G:312:ARG:HA	1.82	0.44
2:F:23:ILE:O	2:F:27:LYS:HG3	2.17	0.44
2:H:27:LYS:HE2	2:H:43:LEU:CD2	2.45	0.44
1:E:280:PRO:O	1:E:281:THR:C	2.61	0.44
1:E:299:GLN:HE22	1:E:517:GLY:H	1.65	0.44
1:A:307:LYS:O	1:A:311:GLU:HG3	2.18	0.43
1:E:223:LEU:HD23	1:E:227:LEU:HD22	1.99	0.43
1:A:386:ALA:HB2	1:A:444:THR:HG21	1.99	0.43
1:A:363:LEU:HA	1:A:366:GLU:O	2.18	0.43
1:C:363:LEU:HA	1:C:366:GLU:O	2.17	0.43
1:E:489:LEU:HD21	1:E:502:TYR:CE2	2.53	0.43
1:G:299:GLN:HE22	1:G:517:GLY:H	1.65	0.43
1:G:436:VAL:O	1:G:436:VAL:CG2	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:455:PHE:CG	1:G:500:PRO:HG3	2.53	0.43
2:H:23:ILE:HG22	2:H:27:LYS:HE3	2.00	0.43
1:A:455:PHE:CD1	1:A:500:PRO:HG3	2.53	0.43
1:A:513:SER:HB2	5:A:17:HOH:O	2.17	0.43
1:E:455:PHE:CE1	1:E:493:ALA:HB2	2.54	0.43
1:E:473:ILE:HD13	2:F:40:GLN:HE22	1.84	0.43
1:E:477:SER:O	1:E:478:VAL:C	2.62	0.43
1:C:464:ASN:HD22	1:C:464:ASN:HA	1.60	0.43
1:A:245:PHE:HB2	1:A:317:ILE:HG22	2.00	0.43
1:A:313:LEU:HB3	1:A:370:ILE:CD1	2.49	0.43
1:A:403:PRO:C	1:A:404:ILE:HD13	2.43	0.43
1:C:280:PRO:O	1:C:281:THR:C	2.57	0.43
1:E:303:GLN:HE21	1:E:462:HIS:CG	2.37	0.43
1:A:369:LYS:HE3	1:A:373:LEU:HD21	2.01	0.43
1:E:464:ASN:HD22	1:E:464:ASN:HA	1.58	0.43
1:A:223:LEU:HD23	1:A:227:LEU:CD2	2.49	0.42
1:E:216:ASN:HD22	1:E:216:ASN:C	2.27	0.42
1:G:299:GLN:HB3	2:H:75:GLY:C	2.43	0.42
2:D:60:ASN:OD1	2:D:62:GLN:NE2	2.48	0.42
1:A:504:LEU:HD13	1:A:555:TYR:CZ	2.55	0.42
1:E:455:PHE:CG	1:E:500:PRO:HG3	2.55	0.42
1:C:243:ARG:CD	1:C:246:ARG:NH1	2.81	0.42
1:C:299:GLN:HE22	1:C:517:GLY:H	1.67	0.42
1:E:433:ASN:ND2	2:F:33:LYS:HE2	2.30	0.42
1:E:455:PHE:HE1	1:E:493:ALA:HB2	1.85	0.42
2:F:42:ARG:NE	2:F:49:GLN:OE1	2.39	0.42
1:A:312:ARG:HE	1:A:312:ARG:CA	2.31	0.42
1:C:455:PHE:CG	1:C:500:PRO:HG3	2.54	0.42
1:E:383:LYS:HG2	1:E:390:ARG:HG2	2.01	0.42
2:F:43:LEU:N	2:F:43:LEU:HD22	2.35	0.42
1:C:455:PHE:HE1	1:C:493:ALA:CB	2.32	0.42
1:A:533:ASN:HD22	1:A:536:ARG:HH11	1.67	0.42
1:G:239:PHE:CE2	1:G:245:PHE:HB3	2.55	0.42
2:F:23:ILE:HD13	2:F:51:GLU:O	2.19	0.42
1:C:313:LEU:HB3	1:C:370:ILE:CD1	2.50	0.42
1:G:508:CYS:HB2	1:G:552:VAL:HB	2.01	0.42
1:A:403:PRO:O	1:A:404:ILE:HD13	2.19	0.41
1:E:499:SER:HA	1:E:500:PRO:HD2	1.93	0.41
1:G:482:PHE:HA	1:G:483:PRO:HD3	1.83	0.41
2:D:2:GLN:HG2	5:D:104:HOH:O	2.19	0.41
2:D:23:ILE:HD13	2:D:51:GLU:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:231:SER:CB	1:G:266:ILE:HD12	2.39	0.41
1:A:462:HIS:CE1	1:A:551:TYR:CZ	3.02	0.41
1:C:235:PRO:HB2	1:C:373:LEU:HD11	2.02	0.41
1:G:280:PRO:O	1:G:281:THR:C	2.62	0.41
2:D:27:LYS:CE	2:D:43:LEU:HD23	2.50	0.41
1:C:292:PRO:CB	1:E:290:TYR:HA	2.51	0.41
1:C:455:PHE:HB3	1:C:502:TYR:OH	2.20	0.41
1:C:489:LEU:HD21	1:C:502:TYR:CD2	2.56	0.41
1:C:222:PHE:CD1	1:C:222:PHE:C	2.99	0.41
1:A:313:LEU:HB3	1:A:370:ILE:HD11	2.03	0.41
1:C:240:CYS:HG	1:C:262:PHE:HE2	1.64	0.41
1:C:248:GLU:HG3	5:C:53:HOH:O	2.20	0.41
1:C:383:LYS:HA	1:C:389:TYR:O	2.21	0.41
1:G:489:LEU:HD21	1:G:502:TYR:CD2	2.56	0.41
2:F:23:ILE:HG22	2:F:27:LYS:HE3	2.03	0.41
1:A:463:LEU:O	1:A:465:ARG:N	2.53	0.41
1:A:538:SER:HA	1:A:539:PRO:HD3	1.98	0.41
1:E:461:LEU:HD23	1:E:461:LEU:HA	1.84	0.41
1:G:312:ARG:HE	1:G:312:ARG:CA	2.32	0.41
1:A:489:LEU:HD23	1:A:500:PRO:HG2	2.03	0.40
1:C:369:LYS:HE3	1:C:373:LEU:HD21	2.04	0.40
1:E:300:GLN:HG2	5:E:1:HOH:O	2.20	0.40
1:A:464:ASN:HD22	1:A:464:ASN:HA	1.54	0.40
1:C:294:PHE:CE2	1:C:300[B]:GLN:CG	2.93	0.40
1:A:420:PHE:O	1:A:421:ASN:C	2.64	0.40
1:G:382:LEU:HD11	1:G:435:PRO:HG3	2.04	0.40
1:G:424:THR:O	1:G:449:LYS:HG3	2.21	0.40
1:C:408:GLY:H	1:C:412:GLY:C	2.30	0.40
1:C:489:LEU:HD21	1:C:502:TYR:CE2	2.56	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	294/355 (83%)	272 (92%)	21 (7%)	1 (0%)	36	58
1	C	303/355 (85%)	287 (95%)	14 (5%)	2 (1%)	18	38
1	E	302/355 (85%)	279 (92%)	22 (7%)	1 (0%)	36	58
1	G	295/355 (83%)	272 (92%)	21 (7%)	2 (1%)	18	38
2	B	73/75 (97%)	68 (93%)	5 (7%)	0	100	100
2	D	73/75 (97%)	71 (97%)	2 (3%)	0	100	100
2	F	73/75 (97%)	69 (94%)	4 (6%)	0	100	100
2	H	73/75 (97%)	69 (94%)	4 (6%)	0	100	100
All	All	1486/1720 (86%)	1387 (93%)	93 (6%)	6 (0%)	30	51

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	478	VAL
1	E	478	VAL
1	G	263	ALA
1	G	465	ARG
1	C	478	VAL
1	C	550	GLY

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	276/309 (89%)	230 (83%)	46 (17%)	2	4
1	C	279/309 (90%)	234 (84%)	45 (16%)	2	4
1	E	278/309 (90%)	234 (84%)	44 (16%)	2	4
1	G	277/309 (90%)	226 (82%)	51 (18%)	1	3
2	B	68/68 (100%)	63 (93%)	5 (7%)	13	29
2	D	68/68 (100%)	61 (90%)	7 (10%)	7	15
2	F	68/68 (100%)	62 (91%)	6 (9%)	9	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	68/68 (100%)	63 (93%)	5 (7%)	13	29
All	All	1382/1508 (92%)	1173 (85%)	209 (15%)	3	5

All (209) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	211	HIS
1	A	212	VAL
1	A	215	ARG
1	A	216	ASN
1	A	227	LEU
1	A	231	SER
1	A	266	ILE
1	A	273	ASP
1	A	275	CYS
1	A	284	ARG
1	A	289	LYS
1	A	298	SER
1	A	300	GLN
1	A	303	GLN
1	A	306	LEU
1	A	308	LEU
1	A	312	ARG
1	A	313	LEU
1	A	353	ASP
1	A	357	LEU
1	A	365	ARG
1	A	373	LEU
1	A	393	THR
1	A	396	VAL
1	A	400	LEU
1	A	406	LYS
1	A	424	THR
1	A	427	GLU
1	A	432	GLU
1	A	433	ASN
1	A	436	VAL
1	A	446	SER
1	A	447	THR
1	A	450	LEU
1	A	459	LEU
1	A	464	ASN

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Mol	Chain	Res	Type
1	A	470	ARG
1	A	473	ILE
1	A	486	ARG
1	A	489	LEU
1	A	514	VAL
1	A	524	ARG
1	A	540	VAL
1	A	542	GLU
1	A	543	ASN
1	A	558	MET
1	C	211	HIS
1	C	212	VAL
1	C	215	ARG
1	C	216	ASN
1	C	227	LEU
1	C	231	SER
1	C	246	ARG
1	C	266	ILE
1	C	271	HIS
1	C	284	ARG
1	C	289	LYS
1	C	298	SER
1	C	300[A]	GLN
1	C	300[B]	GLN
1	C	303	GLN
1	C	306	LEU
1	C	308	LEU
1	C	313	LEU
1	C	353	ASP
1	C	357	LEU
1	C	365	ARG
1	C	373	LEU
1	C	393	THR
1	C	396	VAL
1	C	400	LEU
1	C	406	LYS
1	C	424	THR
1	C	427	GLU
1	C	432	GLU
1	C	436	VAL
1	C	446	SER
1	C	447	THR

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Mol	Chain	Res	Type
1	C	459	LEU
1	C	464	ASN
1	C	470	ARG
1	C	473	ILE
1	C	486	ARG
1	C	489	LEU
1	C	514	VAL
1	C	524	ARG
1	C	540	VAL
1	C	542	GLU
1	C	543	ASN
1	C	545	VAL
1	C	558	MET
1	E	211	HIS
1	E	212	VAL
1	E	215	ARG
1	E	216	ASN
1	E	227	LEU
1	E	231	SER
1	E	246	ARG
1	E	266	ILE
1	E	271	HIS
1	E	273	ASP
1	E	284	ARG
1	E	289	LYS
1	E	298	SER
1	E	300	GLN
1	E	303	GLN
1	E	308	LEU
1	E	312	ARG
1	E	313	LEU
1	E	353	ASP
1	E	365	ARG
1	E	373	LEU
1	E	374	PHE
1	E	393	THR
1	E	396	VAL
1	E	400	LEU
1	E	406	LYS
1	E	424	THR
1	E	427	GLU
1	E	432	GLU

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Mol	Chain	Res	Type
1	E	433	ASN
1	E	436	VAL
1	E	446	SER
1	E	447	THR
1	E	459	LEU
1	E	470	ARG
1	E	473	ILE
1	E	486	ARG
1	E	489	LEU
1	E	514	VAL
1	E	524	ARG
1	E	540	VAL
1	E	542	GLU
1	E	545	VAL
1	E	558	MET
1	G	211	HIS
1	G	212	VAL
1	G	215	ARG
1	G	216	ASN
1	G	227	LEU
1	G	231	SER
1	G	246	ARG
1	G	260	GLU
1	G	266	ILE
1	G	271	HIS
1	G	284	ARG
1	G	289	LYS
1	G	298	SER
1	G	300	GLN
1	G	303	GLN
1	G	308	LEU
1	G	312	ARG
1	G	313	LEU
1	G	353	ASP
1	G	357	LEU
1	G	365	ARG
1	G	373	LEU
1	G	393	THR
1	G	396	VAL
1	G	400	LEU
1	G	406	LYS
1	G	407	LYS

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Mol	Chain	Res	Type
1	G	424	THR
1	G	427	GLU
1	G	432	GLU
1	G	433	ASN
1	G	436	VAL
1	G	439[A]	ARG
1	G	439[B]	ARG
1	G	446	SER
1	G	447	THR
1	G	457	ARG
1	G	459	LEU
1	G	464	ASN
1	G	470	ARG
1	G	473	ILE
1	G	486	ARG
1	G	489	LEU
1	G	514	VAL
1	G	524	ARG
1	G	538	SER
1	G	540	VAL
1	G	542	GLU
1	G	543	ASN
1	G	545	VAL
1	G	558	MET
2	B	8	LEU
2	B	23	ILE
2	B	50	LEU
2	B	56	LEU
2	B	67	LEU
2	D	8	LEU
2	D	23	ILE
2	D	34	GLU
2	D	50	LEU
2	D	56	LEU
2	D	63	LYS
2	D	67	LEU
2	F	8	LEU
2	F	23	ILE
2	F	43	LEU
2	F	50	LEU
2	F	56	LEU
2	F	63	LYS

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Mol	Chain	Res	Type
2	H	8	LEU
2	H	23	ILE
2	H	50	LEU
2	H	56	LEU
2	H	67	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	211	HIS
1	A	216	ASN
1	A	219	ASN
1	A	256	GLN
1	A	288	GLN
1	A	299	GLN
1	A	453	GLN
1	A	462	HIS
1	A	464	ASN
1	A	503	GLN
1	A	509	ASN
1	C	216	ASN
1	C	219	ASN
1	C	299	GLN
1	C	453	GLN
1	C	462	HIS
1	C	464	ASN
1	C	503	GLN
1	C	509	ASN
1	C	526	GLN
1	C	556	GLN
1	E	216	ASN
1	E	219	ASN
1	E	288	GLN
1	E	299	GLN
1	E	453	GLN
1	E	462	HIS
1	E	464	ASN
1	E	503	GLN
1	E	509	ASN
1	G	216	ASN
1	G	219	ASN
1	G	299	GLN

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Mol	Chain	Res	Type
1	G	453	GLN
1	G	462	HIS
1	G	464	ASN
1	G	503	GLN
1	G	509	ASN
2	B	2	GLN
2	B	25	ASN
2	B	40	GLN
2	D	2	GLN
2	D	25	ASN
2	D	31	GLN
2	F	2	GLN
2	F	31	GLN
2	F	40	GLN
2	F	68	HIS
2	H	2	GLN
2	H	25	ASN
2	H	31	GLN
2	H	40	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NEH	F	76	2	2,2,2	0.29	0	0,1,1	-	-
4	NEH	D	76	2	2,2,2	0.61	0	0,1,1	-	-
4	NEH	B	76	2	2,2,2	0.45	0	0,1,1	-	-
4	NEH	H	76	2	2,2,2	0.55	0	0,1,1	-	-

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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	76	NEH	1	0
4	H	76	NEH	1	0

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	303/355 (85%)	0.84	32 (10%) 11 9	13, 39, 70, 83	1 (0%)
1	C	310/355 (87%)	1.00	44 (14%) 6 5	10, 39, 70, 83	1 (0%)
1	E	310/355 (87%)	1.02	42 (13%) 7 5	22, 39, 70, 83	0
1	G	304/355 (85%)	0.84	27 (8%) 15 12	22, 39, 70, 83	1 (0%)
2	B	75/75 (100%)	1.13	7 (9%) 14 11	27, 49, 61, 62	0
2	D	75/75 (100%)	1.11	12 (16%) 5 4	26, 49, 61, 61	0
2	F	75/75 (100%)	1.28	15 (20%) 3 2	16, 49, 61, 62	1 (1%)
2	H	75/75 (100%)	1.12	7 (9%) 14 11	16, 49, 61, 62	1 (1%)
All	All	1527/1720 (88%)	0.97	186 (12%) 8 6	10, 42, 67, 83	5 (0%)

All (186) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	436	VAL	7.8
2	B	32	ASP	6.9
1	A	440	CYS	6.4
1	A	451	THR	5.4
2	D	32	ASP	5.3
2	H	74	ARG	5.2
2	F	74	ARG	5.1
1	E	349	LEU	5.0
1	G	263	ALA	4.9
1	C	471	GLY	4.7
1	E	429	LEU	4.6
1	A	349	LEU	4.5
1	C	350	SER	4.1
1	C	412	GLY	4.1
2	F	2	GLN	4.0
1	C	358	MET	3.9

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Mol	Chain	Res	Type	RSRZ
1	E	357	LEU	3.9
1	A	249	VAL	3.8
1	C	411	GLY	3.7
1	C	357	LEU	3.7
1	C	349	LEU	3.6
1	E	450	LEU	3.6
2	H	54	ARG	3.6
1	E	399	ASP	3.6
1	G	349	LEU	3.5
1	G	249	VAL	3.5
1	E	386	ALA	3.5
1	A	357	LEU	3.4
1	A	534	ASP	3.3
1	G	476	SER	3.3
1	A	444	THR	3.3
1	E	380	SER	3.2
1	A	430	GLU	3.2
2	F	15	LEU	3.2
1	E	381	CYS	3.2
1	E	409	PHE	3.1
1	G	428	GLU	3.1
1	E	388	GLY	3.1
2	D	14	THR	3.1
2	D	61	ILE	3.1
1	C	439	ARG	3.0
1	G	436	VAL	3.0
1	C	447	THR	3.0
2	B	1	MET	3.0
1	E	419	CYS	3.0
1	C	444	THR	3.0
2	D	24	GLU	3.0
1	C	386	ALA	3.0
1	E	486	ARG	3.0
2	B	16	GLU	2.9
1	E	447	THR	2.9
1	A	429	LEU	2.9
1	E	432	GLU	2.9
1	C	249	VAL	2.9
2	F	54	ARG	2.9
1	G	433	ASN	2.9
1	E	410	ALA	2.8
1	C	354	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
2	D	17	VAL	2.8
1	E	468	ALA	2.8
1	C	378	LEU	2.8
1	C	380	SER	2.8
1	G	527	THR	2.8
1	C	486	ARG	2.8
2	F	39	ASP	2.8
2	H	32	ASP	2.8
1	A	356	ASN	2.8
1	A	387	CYS	2.8
1	G	419	CYS	2.8
1	E	312	ARG	2.8
1	C	273	ASP	2.8
1	C	557	LEU	2.7
1	G	429	LEU	2.7
1	E	355	ALA	2.7
1	E	437	CYS	2.7
2	H	36	ILE	2.7
1	E	428	GLU	2.7
1	C	431	SER	2.7
1	C	438	ASP	2.7
1	A	383	LYS	2.7
2	D	2	GLN	2.7
1	A	405	PRO	2.6
1	C	365	ARG	2.6
1	G	542	GLU	2.6
1	C	362	TYR	2.6
1	E	503	GLN	2.6
1	E	426	GLU	2.6
1	E	446	SER	2.6
1	G	388	GLY	2.6
1	G	320	ARG	2.6
1	E	275	CYS	2.6
1	E	271	HIS	2.6
1	C	312	ARG	2.6
1	A	363	LEU	2.6
2	F	64	GLU	2.6
1	A	547	SER	2.6
1	E	405	PRO	2.5
1	E	411	GLY	2.5
1	A	442	GLN	2.5
1	C	540	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	G	469	SER	2.5
1	G	364	GLU	2.5
1	G	432	GLU	2.5
1	A	382	LEU	2.5
1	A	279	ASN	2.5
2	B	36	ILE	2.5
1	E	445	ARG	2.5
2	B	54	ARG	2.5
1	E	395	GLU	2.4
1	A	441	ARG	2.4
1	E	249	VAL	2.4
2	D	23	ILE	2.4
1	A	391	SER	2.4
1	A	528	GLY	2.4
1	E	240	CYS	2.4
1	G	382	LEU	2.4
2	H	15	LEU	2.4
1	A	350	SER	2.4
2	H	10	GLY	2.4
2	H	35	GLY	2.4
1	C	508	CYS	2.4
1	C	436	VAL	2.4
1	C	355	ALA	2.4
1	A	445	ARG	2.3
1	C	409	PHE	2.3
1	C	443	LYS	2.3
1	E	444	THR	2.3
1	G	444	THR	2.3
1	E	397	PHE	2.3
1	C	480	VAL	2.3
1	G	430	GLU	2.3
2	F	56	LEU	2.3
2	D	1	MET	2.3
2	F	37	PRO	2.3
1	A	234	ARG	2.3
1	E	382	LEU	2.3
1	C	352	ASP	2.3
2	F	11	LYS	2.3
1	C	361	ARG	2.3
1	G	439[A]	ARG	2.3
1	E	303	GLN	2.2
1	A	469	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	472	SER	2.2
1	A	386	ALA	2.2
2	D	33	LYS	2.2
1	C	469	SER	2.2
1	A	375	VAL	2.2
1	A	487	LEU	2.2
2	F	19	PRO	2.2
1	G	468	ALA	2.2
1	C	429	LEU	2.2
1	A	446	SER	2.2
1	A	488	SER	2.2
1	E	351	ASP	2.2
1	A	365	ARG	2.2
1	E	413	LYS	2.2
1	E	226	VAL	2.1
2	B	26	VAL	2.1
1	C	440	CYS	2.1
1	C	491	ASP	2.1
1	G	391	SER	2.1
2	F	33	LYS	2.1
1	E	471	GLY	2.1
2	D	35	GLY	2.1
2	D	19	PRO	2.1
2	F	23	ILE	2.1
1	G	351	ASP	2.1
1	E	470	ARG	2.1
1	G	528	GLY	2.1
2	F	16	GLU	2.1
2	B	52	ASP	2.1
1	G	446	SER	2.1
1	C	381	CYS	2.1
1	G	435	PRO	2.1
1	C	375	VAL	2.0
2	F	17	VAL	2.0
1	C	441	ARG	2.0
1	E	378	LEU	2.0
2	D	60	ASN	2.0
1	C	473	ILE	2.0
2	F	14	THR	2.0
1	G	481	ASP	2.0
1	C	470	ARG	2.0
1	C	363	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	379	LYS	2.0
1	C	395	GLU	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	NEH	H	76	3/3	0.96	0.09	29,29,30,31	0
3	ZN	E	700	1/1	0.97	0.05	68,68,68,68	0
4	NEH	D	76	3/3	0.97	0.07	22,22,22,23	0
3	ZN	A	700	1/1	0.97	0.10	74,74,74,74	0
4	NEH	F	76	3/3	0.98	0.07	21,21,22,24	0
4	NEH	B	76	3/3	0.98	0.07	23,23,24,24	0
3	ZN	C	700	1/1	0.99	0.04	71,71,71,71	0
3	ZN	G	700	1/1	0.99	0.07	74,74,74,74	0

6.5 Other polymers [i](#)

There are no such residues in this entry.