



# Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 10:56 pm BST

PDB ID : 3I3T  
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](mailto: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.

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

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

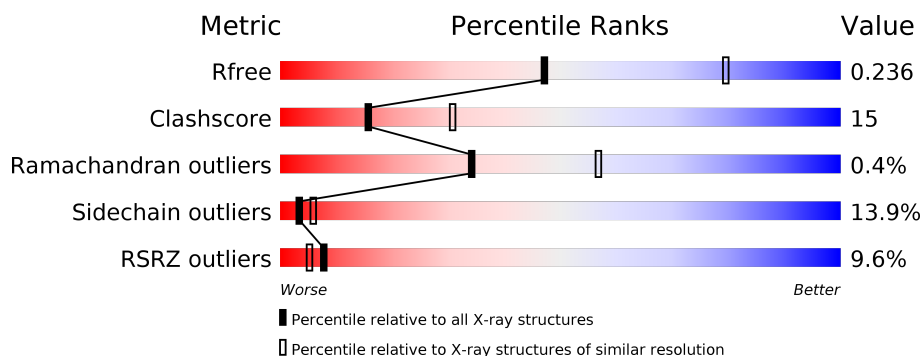
# 1 Overall quality at a glance i

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))
$R_{free}$	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	<div> <div>11%</div> <div> <div>54%</div> <div>26%</div> <div>5% •</div> <div>15%</div> </div> </div>
1	C	355	<div> <div>6%</div> <div> <div>58%</div> <div>23%</div> <div>6%</div> <div>13%</div> </div> </div>
1	E	355	<div> <div>5%</div> <div> <div>58%</div> <div>23%</div> <div>6% •</div> <div>13%</div> </div> </div>
1	G	355	<div> <div>9%</div> <div> <div>55%</div> <div>25%</div> <div>6%</div> <div>14%</div> </div> </div>
2	B	75	<div> <div>16%</div> <div> <div>80%</div> <div>19%</div> <div>•</div> </div> </div>
2	D	75	<div> <div>11%</div> <div> <div>64%</div> <div>35%</div> <div>•</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	F	75	<div><div></div><div>4%</div><div>69%</div><div>28%</div><div></div></div>
2	H	75	<div><div></div><div>16%</div><div>83%</div><div>16%</div><div></div></div>

## 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			

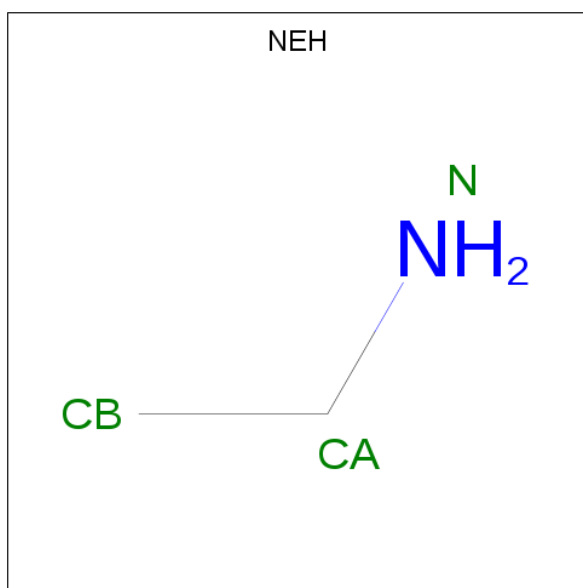
- Molecule 2 is a protein called Ubiquitin.

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 (three-letter code: ZN) (formula: Zn).

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

- Molecule 4 is ETHANAMINE (three-letter code: NEH) (formula: C<sub>2</sub>H<sub>7</sub>N).



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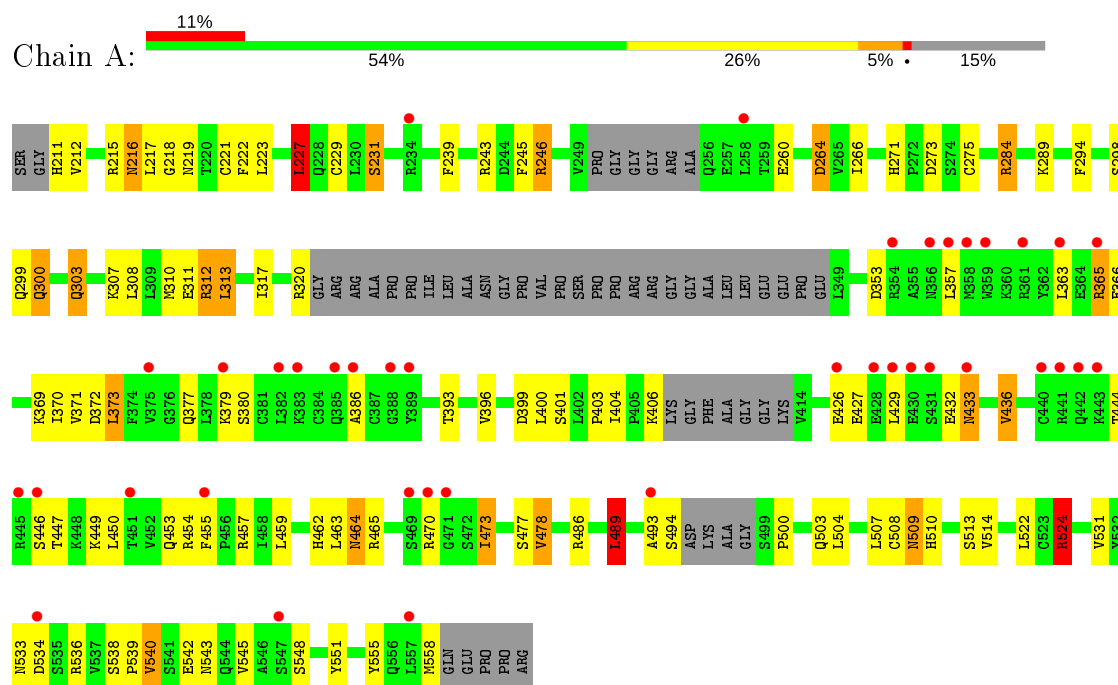
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	3	Total	O	0	0
			3	3		

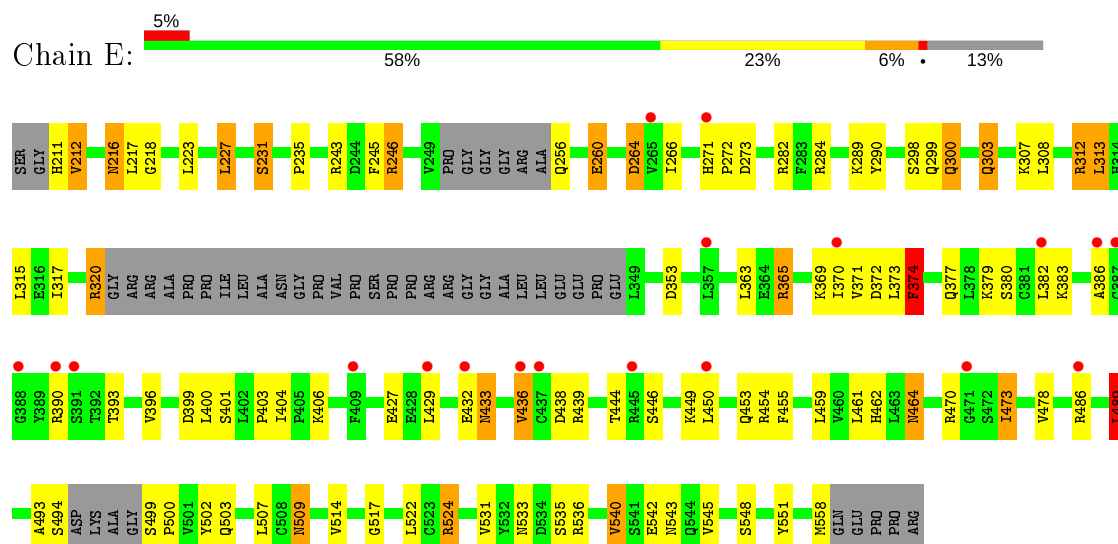
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

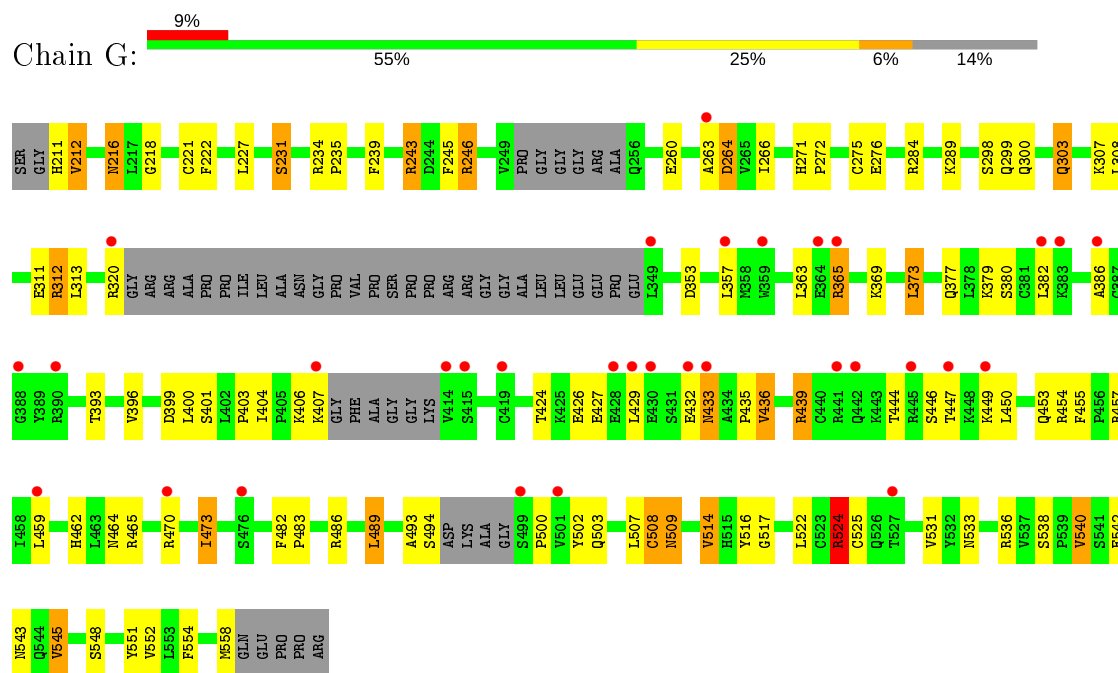
- Molecule 1: Ubiquitin carboxyl-terminal hydrolase 21



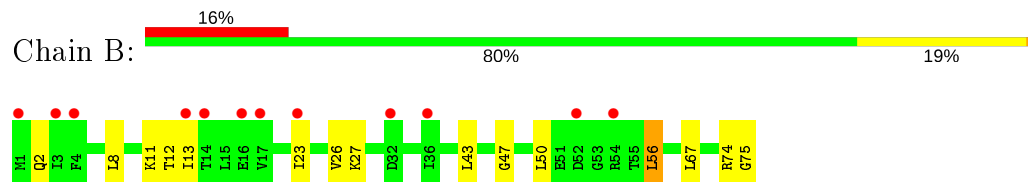
Chain E:



Chain G:



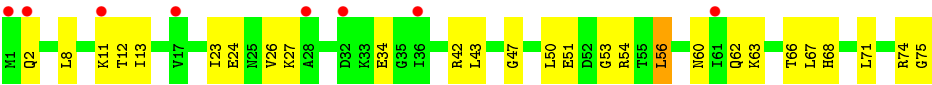
Chain B:



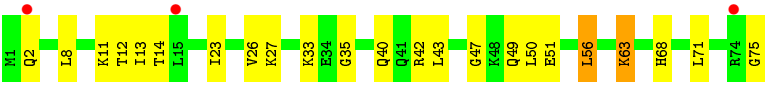
Chain D:



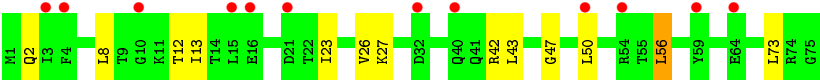
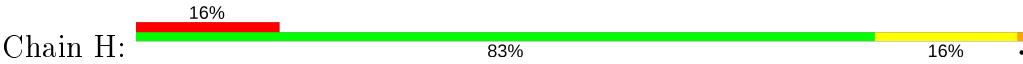




● Molecule 2: Ubiquitin



● Molecule 2: Ubiquitin



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.43 Å   83.66 Å   118.79 Å 88.71°   75.73°   85.11°	Depositor
Resolution (Å)	83.37 – 2.59 83.36 – 2.59	Depositor EDS
% Data completeness (in resolution range)	95.8 (83.37-2.59) 99.3 (83.36-2.59)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.14 (at 2.58 Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, $R_{free}$	0.186 , 0.218 0.209 , 0.236	Depositor DCC
$R_{free}$ test set	3400 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	46.9	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 64.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	1.09	5/2509 (0.2%)	1.17	17/3382 (0.5%)
1	C	1.01	3/2557 (0.1%)	1.02	8/3445 (0.2%)
1	E	1.07	5/2548 (0.2%)	1.05	10/3433 (0.3%)
1	G	1.01	4/2520 (0.2%)	1.05	8/3395 (0.2%)
2	B	0.79	0/603	0.84	0/811
2	D	0.85	0/603	0.89	1/811 (0.1%)
2	F	0.79	0/603	0.87	0/811
2	H	0.81	0/603	0.89	1/811 (0.1%)
All	All	1.00	17/12546 (0.1%)	1.04	45/16899 (0.3%)

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	545	VAL	CB-CG2	-13.44	1.24	1.52
1	A	545	VAL	CB-CG1	-13.13	1.25	1.52
1	E	374	PHE	CE1-CZ	-10.01	1.18	1.37
1	E	374	PHE	CG-CD1	-9.85	1.24	1.38
1	E	374	PHE	CE2-CZ	-9.35	1.19	1.37
1	E	374	PHE	CG-CD2	-8.53	1.25	1.38
1	A	229	CYS	CB-SG	6.63	1.93	1.82
1	G	525	CYS	CB-SG	-6.40	1.71	1.82
1	C	523	CYS	CB-SG	6.15	1.92	1.82
1	G	545	VAL	CB-CG1	-5.92	1.40	1.52
1	C	545	VAL	CB-CG2	-5.76	1.40	1.52
1	E	260	GLU	CG-CD	5.72	1.60	1.51
1	C	545	VAL	CB-CG1	-5.54	1.41	1.52
1	G	508	CYS	CB-SG	-5.54	1.72	1.81
1	A	508	CYS	CB-SG	-5.50	1.72	1.81
1	A	221	CYS	CB-SG	-5.41	1.73	1.81
1	G	554	PHE	CE2-CZ	5.26	1.47	1.37

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	365	ARG	NE-CZ-NH1	-15.99	112.31	120.30
1	A	365	ARG	NE-CZ-NH2	15.76	128.18	120.30
1	A	545	VAL	CG1-CB-CG2	-15.26	86.48	110.90
1	A	246	ARG	NE-CZ-NH1	11.43	126.01	120.30
1	E	264	ASP	CB-CG-OD1	-11.36	108.08	118.30
1	G	246	ARG	NE-CZ-NH1	10.17	125.39	120.30
1	G	524	ARG	NE-CZ-NH1	-8.98	115.81	120.30
1	G	264	ASP	CB-CG-OD1	-8.00	111.10	118.30
1	A	365	ARG	CD-NE-CZ	7.82	134.55	123.60
1	C	264	ASP	CB-CG-OD1	-7.65	111.41	118.30
1	E	246	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	A	524	ARG	NE-CZ-NH1	-7.34	116.63	120.30
1	A	507	LEU	CB-CG-CD2	-7.20	98.76	111.00
1	A	246	ARG	NE-CZ-NH2	-7.13	116.74	120.30
1	A	264	ASP	CB-CG-OD1	-7.01	111.99	118.30
1	G	243	ARG	NE-CZ-NH1	-6.93	116.83	120.30
1	A	507	LEU	CB-CA-C	-6.76	97.36	110.20
2	H	42	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	E	507	LEU	CB-CA-C	-6.35	98.14	110.20
1	E	365	ARG	NE-CZ-NH1	6.29	123.45	120.30
1	A	284	ARG	NE-CZ-NH2	-6.21	117.19	120.30
1	C	399	ASP	CB-CG-OD1	6.13	123.82	118.30
1	G	365	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	E	399	ASP	CB-CG-OD1	5.98	123.68	118.30
1	C	365	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	G	399	ASP	CB-CG-OD1	5.88	123.59	118.30
1	A	310	MET	CG-SD-CE	5.88	109.60	100.20
1	E	320	ARG	NE-CZ-NH1	5.85	123.23	120.30
1	E	374	PHE	CB-CG-CD1	5.71	124.80	120.80
1	G	507	LEU	CB-CA-C	-5.63	99.50	110.20
1	C	244	ASP	CB-CG-OD1	5.59	123.33	118.30
1	A	227	LEU	CB-CG-CD2	-5.53	101.60	111.00
1	C	489	LEU	CA-CB-CG	5.47	127.88	115.30
1	A	399	ASP	CB-CG-OD1	5.39	123.15	118.30
1	A	357	LEU	CA-CB-CG	5.39	127.69	115.30
1	C	507	LEU	CB-CA-C	-5.38	99.97	110.20
1	C	246	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	E	382	LEU	CA-CB-CG	5.31	127.52	115.30
1	A	489	LEU	CA-CB-CG	5.28	127.44	115.30
2	D	42	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	C	382	LEU	CA-CB-CG	5.24	127.35	115.30
1	E	374	PHE	CD1-CG-CD2	-5.22	111.51	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	357	LEU	CA-CB-CG	5.20	127.27	115.30
1	A	507	LEU	CA-CB-CG	5.15	127.15	115.30
1	E	489	LEU	CA-CB-CG	5.08	126.98	115.30

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	77	0
1	C	2506	0	2464	96	0
1	E	2497	0	2457	103	0
1	G	2468	0	2433	67	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	13	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	363	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 (363) 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
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:CG	1:G:439[A]:ARG:HH11	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:HG2	1:G:439[A]:ARG:NH1	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:HG2	1:G:439[A]:ARG:HH11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:292:PRO:HG3	1:E:290:TYR:CE1	2.21	0.75
1:G:489:LEU:HD22	1:G:489:LEU:H	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:401:SER:HB2	1:E:462:HIS:CD2	2.26	0.69
1:E:243:ARG:HD2	1:E:246:ARG:NH1	2.08	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:H	1:E:473:ILE:HD12	1.66	0.60
1:C:303:GLN:HG2	1:C:462:HIS:CE1	2.36	0.60
1:E:374:PHE:HD1	1:E:374:PHE:N	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:522:LEU:HD23	1:C:531:VAL:HG22	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:HD22	1:E:489:LEU:H	1.68	0.58
1:E:473:ILE:N	1:E:473:ILE:HD12	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:C:489:LEU:HD23	1:C:500:PRO:HG2	1.86	0.57
1:C:453:GLN:NE2	1:C:494:SER:OG	2.37	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:N	1:A:473:ILE:HD12	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: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:H	1:C:489:LEU:HD22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:311:GLU:HG3	5:H:77:HOH:O	2.07	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:E:299:GLN:HB3	2:F:75:GLY:C	2.28	0.53
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
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: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:HA	1:E:312:ARG:HE	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: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:A:371:VAL:O	1:A:372:ASP:C	2.47	0.51
1:E:320:ARG:CD	1:E:363:LEU:O	2.57	0.51
1:G:379:LYS:O	1:G:450:LEU:HA	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:436:VAL:CG2	1:A:436:VAL:O	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:A:477:SER:O	1:A:478:VAL:C	2.51	0.49
1:E:433:ASN:OD1	2:F:14:THR:N	2.43	0.49
1:G:403:PRO:C	1:G:404:ILE:HD13	2.33	0.49
2:B:23:ILE:HG22	2:B:27:LYS:HE3	1.93	0.49
1:C:380:SER:HA	1:C:449:LYS:O	2.13	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
2:D:24:GLU:OE1	2:D:53:GLY:N	2.42	0.49
1:E:369:LYS:HE3	1:E:373:LEU:HD21	1.94	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: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:289:LYS:HZ1	1:E:315:LEU:HD21	1.79	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:C:403:PRO:C	1:C:404:ILE:HD13	2.35	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:CA	1:E:312:ARG:HE	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:A:222:PHE:C	1:A:222:PHE:CD1	2.88	0.46
1:C:401:SER:HA	1:C:462:HIS:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:373:LEU:HB2	1:E:374:PHE:HD1	1.79	0.46
2:D:27:LYS:HE2	2:D:43:LEU:CD2	2.46	0.46
1:E:313:LEU:HB3	1:E:370:ILE:CD1	2.45	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:E:403:PRO:C	1:E:404:ILE:HD13	2.36	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
2:B:43:LEU:HD22	2:B:43:LEU:N	2.30	0.46
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
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
2:B:27:LYS:HG2	2:B:43:LEU:HD21	1.98	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
1:A:401:SER:HA	1:A:462:HIS:HB3	1.97	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: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:A:299:GLN:HB3	2:B:75:GLY:C	2.37	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
2:F:23:ILE:O	2:F:27:LYS:HG3	2.17	0.44
1:G:312:ARG:HA	1:G:312:ARG:HE	1.82	0.44
2:H:27:LYS:HE2	2:H:43:LEU:CD2	2.45	0.44
1:E:299:GLN:HE22	1:E:517:GLY:H	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:234:ARG:O	1:G:235:PRO:C	2.54	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:CG2	1:G:436:VAL:O	2.67	0.43
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:473:ILE:HD13	2:F:40:GLN:HE22	1.84	0.43
1:E:455:PHE:CE1	1:E:493:ALA:HB2	2.54	0.43
1:C:216:ASN:HD22	1:C:216:ASN:C	2.22	0.43
1:C:464:ASN:HD22	1:C:464:ASN:HA	1.60	0.43
1:A:313:LEU:HB3	1:A:370:ILE:CD1	2.49	0.43
1:A:245:PHE:HB2	1:A:317:ILE:HG22	2.00	0.43
1:E:303:GLN:HE21	1:E:462:HIS:CG	2.37	0.43
1:G:275:CYS:O	1:G:276:GLU:C	2.56	0.43
1:A:369:LYS:HE3	1:A:373:LEU:HD21	2.01	0.43
1:C:262:PHE:O	1:C:263:ALA:C	2.55	0.43
1:E:464:ASN:HA	1:E:464:ASN:HD22	1.58	0.43
1:A:223:LEU:HD23	1:A:227:LEU:CD2	2.49	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:371:VAL:O	1:E:372:ASP:C	2.57	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:455:PHE:HE1	1:E:493:ALA:HB2	1.85	0.42
1:E:433:ASN:ND2	2:F:33:LYS:HE2	2.30	0.42
2:F:42:ARG:NE	2:F:49:GLN:OE1	2.39	0.42
1:A:312:ARG:CA	1:A:312:ARG:HE	2.31	0.42
1:C:280:PRO:O	1:C:281:THR:C	2.57	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:23:ILE:HD13	2:F:51:GLU:O	2.19	0.42
1:G:239:PHE:CE2	1:G:245:PHE:HB3	2.55	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
2:D:23:ILE:HD13	2:D:51:GLU:O	2.20	0.41
2:D:2:GLN:HG2	5:D:104:HOH:O	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
1:C:477:SER:O	1:C:478:VAL:C	2.59	0.41
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
2:D:27:LYS:CE	2:D:43:LEU:HD23	2.50	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:292:PRO:CB	1:E:290:TYR:HA	2.51	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
2:F:23:ILE:HG22	2:F:27:LYS:HE3	2.03	0.41
1:G:489:LEU:HD21	1:G:502:TYR:CD2	2.56	0.41
1:A:313:LEU:HB3	1:A:370:ILE:HD11	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:HA	1:E:461:LEU:HD23	1.84	0.41
1:G:312:ARG:CA	1:G:312:ARG:HE	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: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:299:GLN:HB3	2:D:75:GLY:C	2.41	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%)	41	64
1	C	303/355 (85%)	287 (95%)	14 (5%)	2 (1%)	22	43
1	E	302/355 (85%)	279 (92%)	22 (7%)	1 (0%)	41	64
1	G	295/355 (83%)	272 (92%)	21 (7%)	2 (1%)	22	43
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%)	34	57

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%)	232 (84%)	44 (16%)	2	4
1	C	279/309 (90%)	239 (86%)	40 (14%)	3	5
1	E	278/309 (90%)	237 (85%)	41 (15%)	3	5
1	G	277/309 (90%)	229 (83%)	48 (17%)	2	3
2	B	68/68 (100%)	63 (93%)	5 (7%)	13	28
2	D	68/68 (100%)	61 (90%)	7 (10%)	7	13
2	F	68/68 (100%)	63 (93%)	5 (7%)	13	28
2	H	68/68 (100%)	65 (96%)	3 (4%)	28	53
All	All	1382/1508 (92%)	1189 (86%)	193 (14%)	3	6

All (193) 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	271	HIS
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	308	LEU
1	A	312	ARG
1	A	313	LEU
1	A	353	ASP
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	426	GLU
1	A	427	GLU
1	A	432	GLU

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Mol	Chain	Res	Type
1	A	433	ASN
1	A	436	VAL
1	A	446	SER
1	A	447	THR
1	A	459	LEU
1	A	464	ASN
1	A	470	ARG
1	A	473	ILE
1	A	486	ARG
1	A	489	LEU
1	A	509	ASN
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	216	ASN
1	C	227	LEU
1	C	231	SER
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	308	LEU
1	C	313	LEU
1	C	353	ASP
1	C	365	ARG
1	C	373	LEU
1	C	393	THR
1	C	396	VAL
1	C	399	ASP
1	C	400	LEU
1	C	406	LYS
1	C	427	GLU
1	C	432	GLU
1	C	436	VAL

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Mol	Chain	Res	Type
1	C	446	SER
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	509	ASN
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	216	ASN
1	E	227	LEU
1	E	231	SER
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	374	PHE
1	E	393	THR
1	E	396	VAL
1	E	400	LEU
1	E	406	LYS
1	E	427	GLU
1	E	432	GLU
1	E	433	ASN
1	E	436	VAL
1	E	446	SER

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Mol	Chain	Res	Type
1	E	459	LEU
1	E	464	ASN
1	E	470	ARG
1	E	473	ILE
1	E	486	ARG
1	E	489	LEU
1	E	509	ASN
1	E	514	VAL
1	E	524	ARG
1	E	540	VAL
1	E	542	GLU
1	E	543	ASN
1	E	545	VAL
1	E	558	MET
1	G	211	HIS
1	G	212	VAL
1	G	216	ASN
1	G	227	LEU
1	G	231	SER
1	G	260	GLU
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	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
1	G	426	GLU
1	G	427	GLU
1	G	432	GLU
1	G	433	ASN
1	G	436	VAL

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Mol	Chain	Res	Type
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	509	ASN
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	11	LYS
2	B	50	LEU
2	B	56	LEU
2	B	67	LEU
2	D	8	LEU
2	D	11	LYS
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	11	LYS
2	F	50	LEU
2	F	56	LEU
2	F	63	LYS
2	H	8	LEU
2	H	50	LEU
2	H	56	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	216	ASN
1	A	219	ASN
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	377	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	G	216	ASN
1	G	219	ASN
1	G	299	GLN
1	G	377	GLN
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	40	GLN
2	D	2	GLN
2	D	40	GLN
2	F	2	GLN
2	F	40	GLN
2	F	68	HIS

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Mol	Chain	Res	Type
2	H	2	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 carbohydrates 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	H	76	2	2,2,2	0.55	0	0,1,1	0.00	-
4	NEH	F	76	2	2,2,2	0.29	0	0,1,1	0.00	-
4	NEH	D	76	2	2,2,2	0.61	0	0,1,1	0.00	-
4	NEH	B	76	2	2,2,2	0.45	0	0,1,1	0.00	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	76	NEH	1	0
4	B	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	303/355 (85%)	0.85	39 (12%) 3 2	22, 39, 70, 83	0
1	C	310/355 (87%)	0.80	22 (7%) 16 11	19, 39, 70, 83	0
1	E	310/355 (87%)	0.82	19 (6%) 21 16	22, 39, 70, 83	0
1	G	304/355 (85%)	0.80	32 (10%) 6 4	22, 39, 70, 83	0
2	B	75/75 (100%)	1.16	12 (16%) 1 1	27, 49, 61, 62	0
2	D	75/75 (100%)	0.91	8 (10%) 6 3	26, 49, 61, 61	0
2	F	75/75 (100%)	0.75	3 (4%) 38 31	27, 49, 61, 62	1 (1%)
2	H	75/75 (100%)	0.96	12 (16%) 1 1	27, 49, 61, 62	1 (1%)
All	All	1527/1720 (88%)	0.84	147 (9%) 8 5	19, 42, 67, 83	2 (0%)

All (147) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	436	VAL	7.6
2	B	32	ASP	7.2
1	A	440	CYS	6.7
1	A	451	THR	6.5
1	C	471	GLY	6.5
2	B	1	MET	6.1
1	A	441	ARG	5.5
1	C	386	ALA	5.4
2	D	32	ASP	5.3
1	G	263	ALA	5.0
2	B	3	ILE	4.7
2	H	54	ARG	4.5
1	E	429	LEU	4.4
1	A	430	GLU	4.3
1	G	388	GLY	4.2
2	D	61	ILE	4.2

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Mol	Chain	Res	Type	RSRZ
2	D	1	MET	4.2
1	A	388	GLY	4.0
1	G	428	GLU	4.0
1	G	357	LEU	4.0
2	H	64	GLU	4.0
1	G	476	SER	4.0
1	C	412	GLY	3.9
1	A	471	GLY	3.9
1	A	383	LYS	3.8
1	E	471	GLY	3.8
1	C	354	ARG	3.8
2	B	13	ILE	3.8
1	A	470	ARG	3.7
1	A	469	SER	3.7
1	E	388	GLY	3.7
1	C	473	ILE	3.6
1	E	386	ALA	3.6
2	H	4	PHE	3.6
1	A	363	LEU	3.4
1	A	365	ARG	3.4
1	A	389	TYR	3.4
1	G	349	LEU	3.4
1	G	433	ASN	3.4
1	A	385	GLN	3.4
2	H	50	LEU	3.4
1	A	375	VAL	3.4
1	A	445	ARG	3.4
1	C	389	TYR	3.4
1	A	379	LYS	3.3
1	A	382	LEU	3.2
1	C	358	MET	3.2
1	A	442	GLN	3.2
2	H	59	TYR	3.2
1	A	359	TRP	3.2
1	C	390	ARG	3.2
2	B	17	VAL	3.1
1	G	390	ARG	3.1
2	F	2	GLN	3.1
1	C	438	ASP	3.0
2	B	16	GLU	3.0
1	G	447	THR	3.0
2	H	15	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	G	430	GLU	3.0
1	A	356	ASN	3.0
1	E	450	LEU	2.9
1	A	354	ARG	2.9
2	D	11	LYS	2.9
2	B	52	ASP	2.8
2	D	2	GLN	2.8
1	C	441	ARG	2.8
1	G	432	GLU	2.8
2	H	32	ASP	2.8
1	G	359	TRP	2.8
2	B	4	PHE	2.8
1	A	433	ASN	2.8
2	F	15	LEU	2.8
1	G	470	ARG	2.8
1	A	429	LEU	2.7
1	E	445	ARG	2.7
1	A	446	SER	2.7
2	H	3	ILE	2.7
1	C	362	TYR	2.7
1	A	493	ALA	2.6
1	G	501	VAL	2.6
1	G	365	ARG	2.6
1	G	415	SER	2.6
2	H	16	GLU	2.6
1	G	419	CYS	2.5
1	A	431	SER	2.5
2	D	36	ILE	2.5
1	C	431	SER	2.5
1	E	391	SER	2.5
1	G	499	SER	2.4
1	A	386	ALA	2.4
1	G	386	ALA	2.4
1	E	382	LEU	2.4
1	G	320	ARG	2.4
1	A	361	ARG	2.4
1	E	409	PHE	2.4
1	C	375	VAL	2.4
1	C	411	GLY	2.4
2	D	17	VAL	2.4
1	G	383	LYS	2.4
1	G	442	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	426	GLU	2.3
1	E	437	CYS	2.3
1	E	486	ARG	2.3
1	E	265	VAL	2.3
1	A	358	MET	2.3
1	E	357	LEU	2.3
2	F	74	ARG	2.3
1	G	364	GLU	2.3
1	A	234	ARG	2.3
1	A	557	LEU	2.3
1	A	357	LEU	2.3
1	A	428	GLU	2.3
2	H	40	GLN	2.2
2	B	36	ILE	2.2
1	E	271	HIS	2.2
1	C	508	CYS	2.2
1	G	414	VAL	2.2
1	C	269	LEU	2.2
1	C	378	LEU	2.2
1	E	432	GLU	2.2
1	E	390	ARG	2.2
1	A	258	LEU	2.2
2	H	21	ASP	2.2
1	A	534	ASP	2.2
1	C	486	ARG	2.1
1	G	459	LEU	2.1
1	C	430	GLU	2.1
1	E	387	CYS	2.1
2	D	28	ALA	2.1
1	G	382	LEU	2.1
1	G	429	LEU	2.1
1	C	472	SER	2.1
2	H	10	GLY	2.1
1	G	445	ARG	2.1
1	G	407	LYS	2.1
2	B	14	THR	2.1
1	A	547	SER	2.1
1	G	527	THR	2.1
2	B	23	ILE	2.1
1	C	357	LEU	2.0
1	A	443	LYS	2.0
1	G	449	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	G	441	ARG	2.0
1	C	480	VAL	2.0
2	B	54	ARG	2.0
1	E	370	ILE	2.0
1	A	455	PHE	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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
3	ZN	A	700	1/1	0.94	0.06	74,74,74,74	0
3	ZN	E	700	1/1	0.96	0.06	68,68,68,68	0
4	NEH	H	76	3/3	0.98	0.14	29,29,30,31	0
3	ZN	G	700	1/1	0.98	0.03	74,74,74,74	0
3	ZN	C	700	1/1	0.98	0.05	71,71,71,71	0
4	NEH	B	76	3/3	0.98	0.17	23,23,24,24	0
4	NEH	F	76	3/3	0.98	0.20	21,21,22,24	0
4	NEH	D	76	3/3	0.98	0.22	22,22,22,23	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.