Full wwPDB X-ray Structure Validation Report (i)

Oct 22, 2023 – 04:42 AM EDT

PDB ID	:	3G76
Title	:	Crystal structure of XIAP-BIR3 in complex with a bivalent compound
Authors	:	Cossu, F.; Milani, M.; Mastrangelo, E.; Bolognesi, M.
Deposited on	:	2009-02-09
Resolution	:	3.00 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 (i) 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 (1)) were used in the production of this report:

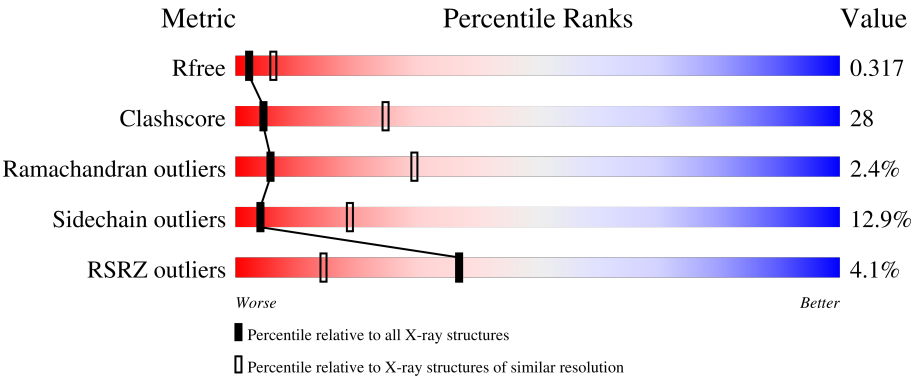
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 <=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	122	44% 25% 10% 20%
1	B	122	3% 43% 35% 7% 14%
1	C	122	2% 44% 30% 21%
1	D	122	39% 39% 7% 14%
1	E	122	2% 44% 28% 5% 22%

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Mol	Chain	Length	Quality of chain
1	F	122	7% 43% 37% 5% 15%
1	G	122	4% 48% 23% 7% 22%
1	H	122	7% 43% 30% 11% 14%

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
2	ZN	H	502	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7590 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 Baculoviral IAP repeat-containing protein 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	97	Total	C	N	O	S	0	0	0
			789	505	135	145	4			
1	B	105	Total	C	N	O	S	0	0	0
			855	545	147	158	5			
1	C	96	Total	C	N	O	S	0	0	0
			781	501	133	143	4			
1	D	105	Total	C	N	O	S	0	0	0
			855	545	147	158	5			
1	E	95	Total	C	N	O	S	0	0	0
			773	495	132	142	4			
1	F	104	Total	C	N	O	S	0	0	0
			852	544	148	155	5			
1	G	95	Total	C	N	O	S	0	0	0
			773	495	132	142	4			
1	H	105	Total	C	N	O	S	0	0	0
			855	545	147	158	5			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	357	HIS	-	expression tag	UNP P98170
A	358	HIS	-	expression tag	UNP P98170
A	359	HIS	-	expression tag	UNP P98170
A	360	HIS	-	expression tag	UNP P98170
A	361	HIS	-	expression tag	UNP P98170
A	362	HIS	-	expression tag	UNP P98170
B	357	HIS	-	expression tag	UNP P98170
B	358	HIS	-	expression tag	UNP P98170
B	359	HIS	-	expression tag	UNP P98170
B	360	HIS	-	expression tag	UNP P98170
B	361	HIS	-	expression tag	UNP P98170
B	362	HIS	-	expression tag	UNP P98170
C	357	HIS	-	expression tag	UNP P98170

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Chain	Residue	Modelled	Actual	Comment	Reference
C	358	HIS	-	expression tag	UNP P98170
C	359	HIS	-	expression tag	UNP P98170
C	360	HIS	-	expression tag	UNP P98170
C	361	HIS	-	expression tag	UNP P98170
C	362	HIS	-	expression tag	UNP P98170
D	357	HIS	-	expression tag	UNP P98170
D	358	HIS	-	expression tag	UNP P98170
D	359	HIS	-	expression tag	UNP P98170
D	360	HIS	-	expression tag	UNP P98170
D	361	HIS	-	expression tag	UNP P98170
D	362	HIS	-	expression tag	UNP P98170
E	357	HIS	-	expression tag	UNP P98170
E	358	HIS	-	expression tag	UNP P98170
E	359	HIS	-	expression tag	UNP P98170
E	360	HIS	-	expression tag	UNP P98170
E	361	HIS	-	expression tag	UNP P98170
E	362	HIS	-	expression tag	UNP P98170
F	357	HIS	-	expression tag	UNP P98170
F	358	HIS	-	expression tag	UNP P98170
F	359	HIS	-	expression tag	UNP P98170
F	360	HIS	-	expression tag	UNP P98170
F	361	HIS	-	expression tag	UNP P98170
F	362	HIS	-	expression tag	UNP P98170
G	357	HIS	-	expression tag	UNP P98170
G	358	HIS	-	expression tag	UNP P98170
G	359	HIS	-	expression tag	UNP P98170
G	360	HIS	-	expression tag	UNP P98170
G	361	HIS	-	expression tag	UNP P98170
G	362	HIS	-	expression tag	UNP P98170
H	357	HIS	-	expression tag	UNP P98170
H	358	HIS	-	expression tag	UNP P98170
H	359	HIS	-	expression tag	UNP P98170
H	360	HIS	-	expression tag	UNP P98170
H	361	HIS	-	expression tag	UNP P98170
H	362	HIS	-	expression tag	UNP P98170

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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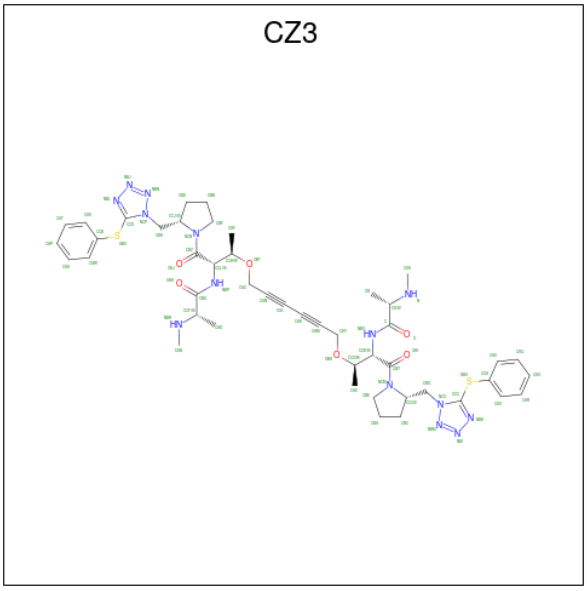
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0
2	E	1	Total Zn 1 1	0	0
2	F	1	Total Zn 1 1	0	0
2	G	1	Total Zn 1 1	0	0
2	H	1	Total Zn 1 1	0	0

- Molecule 3 is 1,1'-{hexa-2,4-diyne-1,6-diylbis[oxy{(2S,3R)-2-[(N-methyl-L-alanyl)amino]-1-oxobutane-3,1-diyl}(2S)pyrrolidine-1,2-diylmethanediyl]}bis[5-(phenylsulfanyl)-1H-tetrazole] (three-letter code: CZ3) (formula: $C_{46}H_{60}N_{14}O_6S_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O S 68 46 14 6 2	0	1
3	B	1	Total C N O S 68 46 14 6 2	0	1
3	C	1	Total C N O S 68 46 14 6 2	0	1
3	D	1	Total C N O S 68 46 14 6 2	0	1

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	E	1	Total	C	N	O	S	0	1
			68	46	14	6	2		
3	F	1	Total	C	N	O	S	0	1
			68	46	14	6	2		
3	G	1	Total	C	N	O	S	0	1
			68	46	14	6	2		
3	H	1	Total	C	N	O	S	0	1
			68	46	14	6	2		

- Molecule 4 is water.

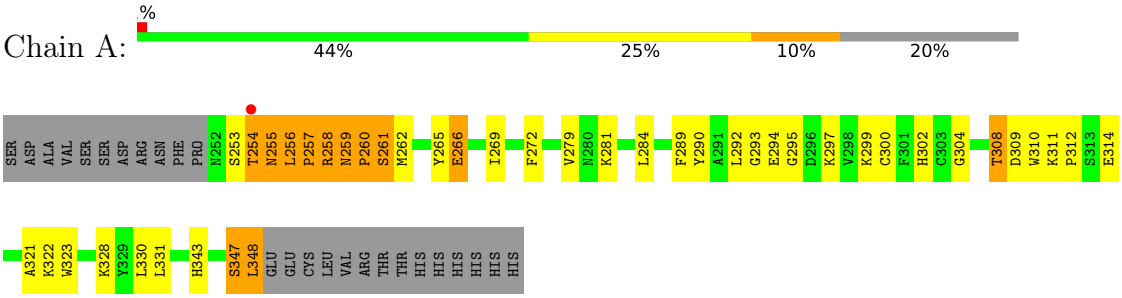
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	32	Total	O	0	0
			32	32		
4	B	34	Total	O	0	0
			34	34		
4	C	20	Total	O	0	0
			20	20		
4	D	48	Total	O	0	0
			48	48		
4	E	275	Total	O	0	0
			275	275		
4	F	23	Total	O	0	0
			23	23		
4	G	54	Total	O	0	0
			54	54		
4	H	19	Total	O	0	0
			19	19		

3 Residue-property plots (i)

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.

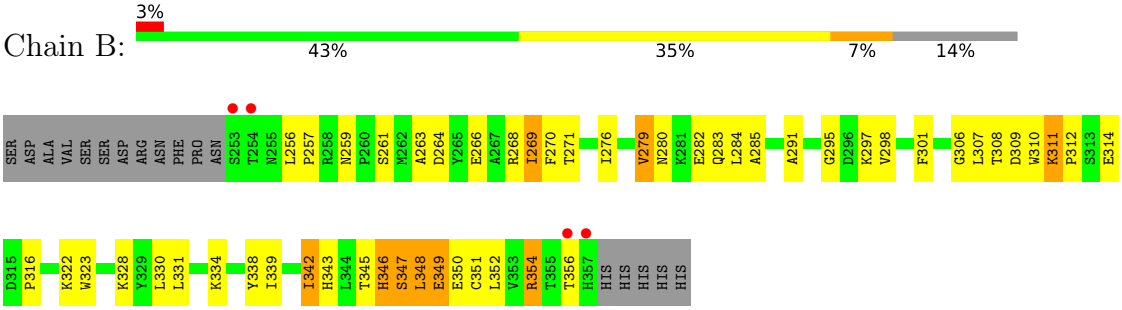
• Molecule 1: Baculoviral IAP repeat-containing protein 4

Chain A:



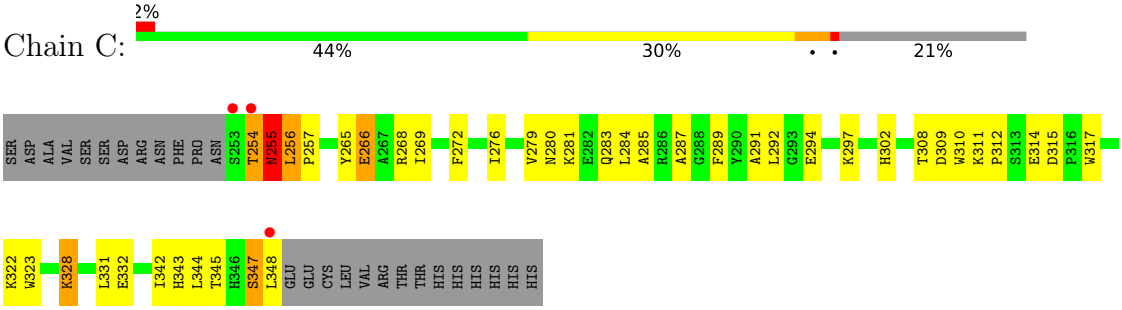
• Molecule 1: Baculoviral IAP repeat-containing protein 4

Chain B:



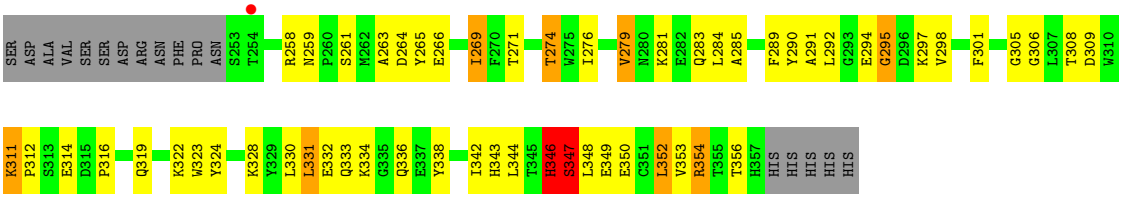
• Molecule 1: Baculoviral IAP repeat-containing protein 4

Chain C:



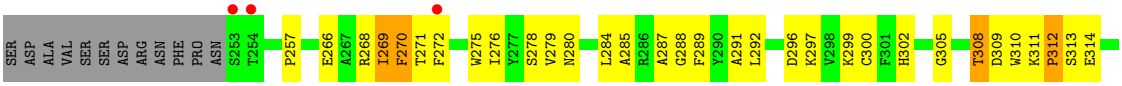
• Molecule 1: Baculoviral IAP repeat-containing protein 4

Chain D:



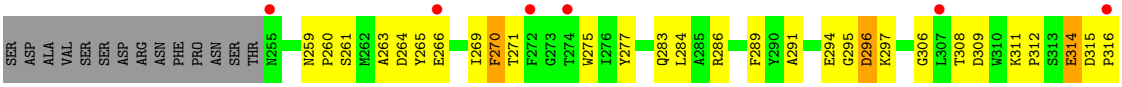
• Molecule 1: Baculoviral IAP repeat-containing protein 4

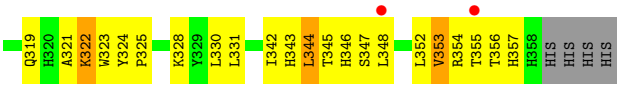
Chain E:



• Molecule 1: Baculoviral IAP repeat-containing protein 4

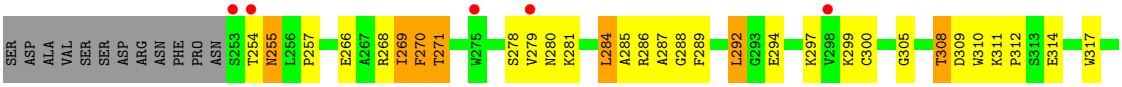
Chain F:

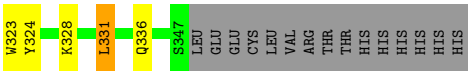




• Molecule 1: Baculoviral IAP repeat-containing protein 4

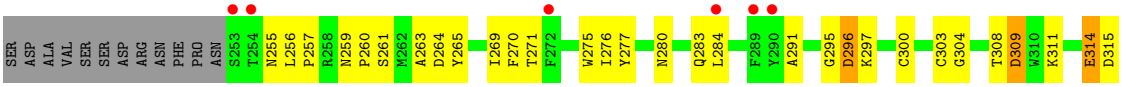
Chain G:

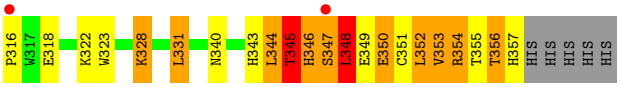




• Molecule 1: Baculoviral IAP repeat-containing protein 4

Chain H:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	119.08Å 119.08Å 105.59Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 3.00 39.50 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (40.00-3.00) 99.8 (39.50-3.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.16 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.231 , 0.311 0.243 , 0.317	Depositor DCC
R_{free} test set	1688 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	70.0	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 107.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.458 for -h,-k,l 0.309 for h,-h-k,-l 0.310 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	7590	wwPDB-VP
Average B, all atoms (Å^2)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.52% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, CZ3

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.78	5/815 (0.6%)	1.15	13/1105 (1.2%)
1	B	0.48	0/882	0.94	4/1196 (0.3%)
1	C	0.41	0/807	0.92	7/1094 (0.6%)
1	D	0.43	0/882	0.82	5/1196 (0.4%)
1	E	0.41	0/799	0.81	5/1083 (0.5%)
1	F	0.38	0/880	0.52	0/1193
1	G	0.39	0/799	0.50	0/1083
1	H	0.41	0/882	0.77	5/1196 (0.4%)
All	All	0.48	5/6746 (0.1%)	0.83	39/9146 (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	4
1	C	0	1
1	D	0	1
1	E	0	1
All	All	0	7

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	261	SER	C-N	12.35	1.62	1.34
1	A	260	PRO	N-CD	-9.06	1.35	1.47
1	A	256	LEU	C-N	-6.21	1.22	1.34
1	A	258	ARG	C-N	-5.68	1.21	1.34
1	A	260	PRO	C-N	5.54	1.46	1.34

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	258	ARG	O-C-N	-14.55	99.43	122.70
1	B	347	SER	N-CA-CB	-14.53	88.70	110.50
1	C	347	SER	N-CA-C	14.25	149.49	111.00
1	B	346	HIS	CB-CA-C	-14.09	82.22	110.40
1	A	347	SER	O-C-N	-13.23	101.54	122.70
1	E	346	HIS	O-C-N	-13.17	101.64	122.70
1	D	346	HIS	N-CA-C	11.59	142.29	111.00
1	A	347	SER	C-N-CA	11.36	150.10	121.70
1	H	345	THR	N-CA-C	11.03	140.77	111.00
1	A	258	ARG	CA-C-N	10.24	139.73	117.20
1	E	346	HIS	C-N-CA	10.19	147.16	121.70
1	B	346	HIS	N-CA-C	10.00	137.99	111.00
1	C	347	SER	C-N-CA	9.72	146.00	121.70
1	B	347	SER	N-CA-C	9.69	137.15	111.00
1	D	346	HIS	CB-CA-C	-9.23	91.94	110.40
1	C	347	SER	CA-C-N	-8.94	97.54	117.20
1	E	345	THR	CB-CA-C	8.85	135.50	111.60
1	C	347	SER	CB-CA-C	-8.53	93.90	110.10
1	C	255	ASN	N-CA-C	8.23	133.23	111.00
1	H	347	SER	CB-CA-C	7.99	125.28	110.10
1	A	347	SER	CA-C-N	7.71	134.15	117.20
1	H	348	LEU	N-CA-CB	-7.62	95.16	110.40
1	A	259	ASN	N-CA-C	-7.17	91.65	111.00
1	D	346	HIS	O-C-N	-7.13	111.29	122.70
1	H	346	HIS	N-CA-C	-6.46	93.55	111.00
1	A	260	PRO	CA-N-CD	6.44	120.71	111.70
1	A	258	ARG	CB-CA-C	-6.27	97.85	110.40
1	C	256	LEU	N-CA-CB	-6.24	97.92	110.40
1	E	346	HIS	CA-C-N	6.19	130.82	117.20
1	D	347	SER	N-CA-C	6.02	127.25	111.00
1	D	347	SER	N-CA-CB	-5.78	101.83	110.50
1	E	345	THR	N-CA-C	-5.68	95.68	111.00
1	A	254	THR	CB-CA-C	5.59	126.70	111.60
1	A	258	ARG	C-N-CA	5.56	135.61	121.70
1	A	260	PRO	O-C-N	-5.45	113.98	122.70
1	C	256	LEU	CB-CA-C	5.33	120.32	110.20
1	H	345	THR	CB-CA-C	-5.16	97.66	111.60
1	A	256	LEU	O-C-N	-5.13	111.34	121.10
1	A	261	SER	O-C-N	5.04	130.76	122.70

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	257	PRO	Mainchain,Peptide
1	A	347	SER	Mainchain,Peptide
1	C	347	SER	Mainchain
1	D	346	HIS	Mainchain
1	E	346	HIS	Mainchain

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	789	0	734	35	0
1	B	855	0	801	55	0
1	C	781	0	729	42	0
1	D	855	0	801	40	0
1	E	773	0	719	28	0
1	F	852	0	797	69	1
1	G	773	0	719	31	0
1	H	855	0	803	60	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	2	0
3	A	68	0	32	3	0
3	B	68	0	16	1	0
3	C	68	0	32	2	0
3	D	68	0	19	4	0
3	E	68	0	32	3	0
3	F	68	0	23	7	0
3	G	68	0	32	7	0
3	H	68	0	23	6	0
4	A	32	0	0	3	0
4	B	34	0	0	3	0
4	C	20	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	48	0	0	5	1
4	E	275	0	0	8	0
4	F	23	0	0	4	0
4	G	54	0	0	2	0
4	H	19	0	0	2	0
All	All	7590	0	6312	381	1

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 28.

All (381) 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:F:348:LEU:CD1	1:F:352:LEU:HD11	1.11	1.57
1:H:346:HIS:CB	1:H:347:SER:HB2	1.35	1.56
1:F:348:LEU:CD1	1:F:352:LEU:CD1	1.92	1.47
1:B:323:TRP:HA	1:B:348:LEU:CD2	1.59	1.32
1:H:346:HIS:HB3	1:H:347:SER:CB	1.65	1.26
1:F:342:ILE:O	1:F:346:HIS:CD2	1.89	1.25
1:F:342:ILE:O	1:F:346:HIS:HD2	1.24	1.19
1:C:344:LEU:O	1:C:348:LEU:HD13	1.42	1.19
1:B:348:LEU:HD12	1:B:348:LEU:O	1.46	1.11
1:B:348:LEU:HD13	1:B:351:CYS:CB	1.78	1.11
1:B:346:HIS:HE1	4:E:389:HOH:O	1.35	1.10
1:B:348:LEU:HD13	1:B:351:CYS:HB3	1.10	1.09
1:F:348:LEU:HD12	1:F:352:LEU:CD1	1.78	1.08
1:F:348:LEU:HD11	1:F:352:LEU:HD11	1.13	1.07
1:B:323:TRP:HA	1:B:348:LEU:HD23	1.34	1.06
1:F:348:LEU:HD13	1:F:352:LEU:HD11	1.04	1.01
1:H:346:HIS:CB	1:H:347:SER:CB	2.30	0.98
1:B:348:LEU:CD1	1:B:351:CYS:HB3	1.97	0.95
1:H:346:HIS:HB2	1:H:347:SER:HB2	1.48	0.94
3:H:600[B]:CZ3:HCF	3:H:600[B]:CZ3:HCH	1.49	0.94
1:B:323:TRP:CA	1:B:348:LEU:CD2	2.45	0.93
1:F:353:VAL:O	1:F:356:THR:OG1	1.87	0.91
1:H:355:THR:O	1:H:355:THR:HG23	1.67	0.90
1:H:355:THR:HG23	1:H:357:HIS:O	1.72	0.89
1:F:343:HIS:NE2	1:F:348:LEU:HD23	1.88	0.89
1:H:352:LEU:HD23	1:H:352:LEU:H	1.37	0.89
1:H:352:LEU:HD23	1:H:352:LEU:N	1.90	0.87
1:A:322:LYS:HD3	1:A:323:TRP:CE2	2.10	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:LEU:C	4:E:378:HOH:O	2.13	0.85
1:B:323:TRP:HA	1:B:348:LEU:HD22	1.60	0.84
1:F:322:LYS:HG2	1:F:346:HIS:CG	2.13	0.84
1:A:279:VAL:HG11	1:A:310:TRP:HB3	1.62	0.82
1:E:279:VAL:HG11	1:E:310:TRP:HB3	1.60	0.82
1:B:348:LEU:O	1:B:348:LEU:CD1	2.26	0.82
1:C:279:VAL:HG11	1:C:310:TRP:HB3	1.62	0.82
1:A:312:PRO:HD3	1:B:276:ILE:HG22	1.61	0.81
1:H:354:ARG:HD2	1:H:354:ARG:O	1.81	0.80
1:H:355:THR:O	1:H:355:THR:CG2	2.30	0.78
1:B:266:GLU:HA	1:B:269:ILE:HD11	1.66	0.78
1:H:346:HIS:HB3	1:H:347:SER:HB2	0.78	0.77
1:F:348:LEU:HD13	1:F:352:LEU:CD1	1.85	0.77
1:A:259:ASN:OD1	1:A:261:SER:OG	2.04	0.76
1:D:323:TRP:CH2	1:D:348:LEU:HD13	2.20	0.76
3:F:600[A]:CZ3:HBBA	3:F:600[A]:CZ3:NBN	2.01	0.76
1:E:279:VAL:HG23	1:E:284:LEU:HD11	1.68	0.75
1:F:348:LEU:HD12	1:F:352:LEU:HD12	1.69	0.74
1:H:322:LYS:HD3	1:H:346:HIS:HB2	1.71	0.72
1:F:325:PRO:HG3	1:F:348:LEU:CD2	2.20	0.71
1:F:348:LEU:HD11	1:F:352:LEU:CD1	1.87	0.71
1:G:297:LYS:HG2	1:G:308:THR:HG21	1.71	0.71
3:A:600[B]:CZ3:HBFA	3:A:600[B]:CZ3:HABA	1.72	0.71
1:C:322:LYS:HD3	1:C:323:TRP:CE2	2.24	0.71
1:D:266:GLU:HA	1:D:269:ILE:HD11	1.70	0.71
3:H:600[B]:CZ3:CBD	3:H:600[B]:CZ3:NBN	2.52	0.71
1:B:322:LYS:O	1:B:348:LEU:HD23	1.89	0.71
1:H:259:ASN:OD1	1:H:261:SER:HB3	1.90	0.71
1:G:279:VAL:HG11	1:G:310:TRP:HB3	1.72	0.69
1:D:291:ALA:HA	1:D:298:VAL:HG12	1.74	0.69
1:F:348:LEU:O	1:F:352:LEU:HG	1.91	0.69
4:E:416:HOH:O	1:F:347:SER:OG	2.11	0.69
1:H:323:TRP:CZ3	1:H:348:LEU:HB2	2.27	0.68
1:A:259:ASN:HD21	1:A:262:MET:HG2	1.57	0.68
1:H:303:CYS:SG	2:H:502:ZN:ZN	1.81	0.68
1:C:312:PRO:HD3	1:D:276:ILE:HG22	1.76	0.68
3:H:600[B]:CZ3:HCH	3:H:600[B]:CZ3:CCF	2.22	0.68
1:D:312:PRO:HD2	4:D:2:HOH:O	1.93	0.68
1:C:254:THR:O	1:C:255:ASN:HB2	1.93	0.68
1:C:302:HIS:CE1	1:C:328:LYS:HB3	2.28	0.67
1:D:352:LEU:O	1:D:356:THR:OG1	2.08	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:348:LEU:CD1	1:F:352:LEU:HD12	2.15	0.67
1:E:300:CYS:HB3	1:E:305:GLY:H	1.60	0.66
1:B:280:ASN:O	1:B:284:LEU:HG	1.96	0.66
1:D:330:LEU:O	1:D:334:LYS:HB2	1.95	0.66
3:G:600[B]:CZ3:HCJ	3:G:600[B]:CZ3:CAK	2.26	0.66
1:F:270:PHE:CE2	3:G:600[B]:CZ3:HBF	2.31	0.65
1:F:348:LEU:CD1	1:F:352:LEU:CG	2.72	0.65
1:A:311:LYS:HB2	1:A:314:GLU:HG3	1.77	0.65
1:B:284:LEU:HD23	1:B:316:PRO:HG3	1.79	0.65
1:B:312:PRO:HD2	4:B:45:HOH:O	1.96	0.65
1:B:323:TRP:C	1:B:348:LEU:HD21	2.17	0.65
1:D:283:GLN:HB3	1:D:316:PRO:HG2	1.78	0.65
1:D:349:GLU:HA	4:D:169:HOH:O	1.96	0.65
1:C:294:GLU:HB2	1:C:297:LYS:HD2	1.80	0.64
1:E:279:VAL:HG11	1:E:310:TRP:CB	2.27	0.64
1:D:259:ASN:OD1	1:D:261:SER:HB3	1.98	0.64
1:E:271:THR:HB	4:E:541:HOH:O	1.98	0.64
1:H:297:LYS:HG2	1:H:308:THR:CG2	2.28	0.64
1:H:353:VAL:HG12	1:H:354:ARG:N	2.12	0.64
1:F:259:ASN:OD1	1:F:261:SER:HB3	1.97	0.63
1:H:352:LEU:N	1:H:352:LEU:CD2	2.61	0.63
1:B:297:LYS:HA	1:B:308:THR:HG22	1.80	0.63
1:B:347:SER:O	1:B:349:GLU:N	2.31	0.63
1:E:268:ARG:NE	1:E:285:ALA:O	2.24	0.63
1:F:283:GLN:HB3	1:F:316:PRO:HG2	1.80	0.63
1:G:297:LYS:HG2	1:G:308:THR:CG2	2.28	0.63
1:H:297:LYS:HG2	1:H:308:THR:HG22	1.80	0.63
1:G:300:CYS:HB3	1:G:305:GLY:H	1.62	0.62
1:A:257:PRO:HG3	1:A:302:HIS:CD2	2.35	0.62
3:F:600[A]:CZ3:CAM	3:F:600[A]:CZ3:HBDB	2.30	0.62
1:A:322:LYS:HA	1:A:343:HIS:CE1	2.34	0.62
1:H:348:LEU:HD22	1:H:350:GLU:HB2	1.82	0.61
1:G:268:ARG:NE	1:G:285:ALA:O	2.33	0.61
1:C:272:PHE:CE2	1:C:291:ALA:HB2	2.34	0.61
1:E:288:GLY:O	1:E:300:CYS:HA	2.01	0.61
1:F:325:PRO:HG3	1:F:348:LEU:HD23	1.82	0.61
1:F:319:GLN:OE1	1:F:322:LYS:HE2	2.01	0.61
1:E:344:LEU:O	1:E:345:THR:C	2.39	0.61
1:F:322:LYS:HD3	1:F:346:HIS:ND1	2.16	0.60
3:E:600[B]:CZ3:OAJ	3:E:600[B]:CZ3:HBH	2.00	0.60
1:F:348:LEU:HD13	1:F:352:LEU:CG	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:600[B]:CZ3:NBN	3:H:600[B]:CZ3:HBDB	2.15	0.60
1:B:323:TRP:HA	1:B:348:LEU:HD21	1.75	0.60
1:F:323:TRP:HH2	4:F:190:HOH:O	1.84	0.60
1:C:311:LYS:HB2	1:C:314:GLU:HG3	1.85	0.59
1:C:344:LEU:O	1:C:348:LEU:CD1	2.35	0.59
1:B:322:LYS:HD2	1:B:323:TRP:CE2	2.37	0.59
1:G:279:VAL:HG12	1:G:311:LYS:O	2.01	0.59
1:B:323:TRP:O	1:B:348:LEU:HD21	2.02	0.59
1:F:322:LYS:CG	1:F:346:HIS:ND1	2.66	0.58
1:B:291:ALA:HA	1:B:298:VAL:HG12	1.84	0.58
1:C:284:LEU:O	1:C:289:PHE:HB2	2.04	0.58
3:F:600[A]:CZ3:HBDB	3:F:600[A]:CZ3:CAK	2.34	0.57
1:H:265:TYR:O	1:H:269:ILE:HG13	2.04	0.57
1:F:346:HIS:CE1	4:F:113:HOH:O	2.56	0.57
1:G:266:GLU:OE2	1:G:269:ILE:HD11	2.03	0.57
1:A:294:GLU:HB2	1:A:297:LYS:HD2	1.87	0.57
1:D:284:LEU:HD23	1:D:316:PRO:HB3	1.87	0.57
1:F:297:LYS:HG2	1:F:308:THR:HG22	1.87	0.57
1:A:284:LEU:O	1:A:289:PHE:HB2	2.05	0.57
1:D:346:HIS:NE2	4:D:154:HOH:O	1.95	0.57
1:E:266:GLU:HA	1:E:269:ILE:HD11	1.87	0.57
1:F:275:TRP:CH2	1:F:296:ASP:HA	2.39	0.57
1:H:275:TRP:CH2	1:H:296:ASP:HA	2.39	0.56
1:C:256:LEU:HD23	1:C:257:PRO:HD2	1.87	0.56
3:H:600[B]:CZ3:NBP	3:H:600[B]:CZ3:CBF	2.68	0.56
1:D:297:LYS:HA	1:D:308:THR:HG22	1.88	0.56
1:H:323:TRP:HZ3	1:H:348:LEU:HB2	1.67	0.56
1:C:297:LYS:HG2	1:C:308:THR:HG21	1.88	0.56
1:A:255:ASN:OD1	4:A:70:HOH:O	2.18	0.56
1:F:343:HIS:NE2	1:F:348:LEU:CD2	2.65	0.56
1:F:348:LEU:HD13	1:F:352:LEU:HD21	1.88	0.55
1:E:257:PRO:HA	1:E:302:HIS:HA	1.89	0.55
1:B:323:TRP:CA	1:B:348:LEU:HD21	2.32	0.55
1:C:265:TYR:CE2	1:C:269:ILE:HG12	2.41	0.55
1:F:348:LEU:HD12	1:F:352:LEU:CG	2.36	0.55
1:E:311:LYS:HB3	1:E:312:PRO:HD2	1.87	0.55
1:H:354:ARG:O	1:H:354:ARG:CD	2.54	0.55
1:H:311:LYS:HB2	1:H:314:GLU:HG3	1.89	0.55
1:A:302:HIS:CE1	1:A:328:LYS:HB3	2.42	0.55
1:G:270:PHE:HA	4:G:57:HOH:O	2.06	0.55
1:H:346:HIS:CA	1:H:347:SER:HB2	2.26	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:ASN:OD1	1:B:261:SER:HB3	2.08	0.54
1:B:346:HIS:CE1	4:E:389:HOH:O	2.26	0.54
1:B:283:GLN:HB3	1:B:316:PRO:HG2	1.90	0.54
1:B:256:LEU:HB3	1:B:257:PRO:HD2	1.90	0.54
1:D:265:TYR:CE2	1:D:269:ILE:HG12	2.42	0.54
1:C:268:ARG:NE	1:C:285:ALA:O	2.35	0.53
4:E:530:HOH:O	1:G:271:THR:HB	2.07	0.53
1:B:348:LEU:HD13	1:B:351:CYS:HB2	1.82	0.53
1:C:297:LYS:HG2	1:C:308:THR:CG2	2.38	0.53
1:F:342:ILE:O	1:F:346:HIS:NE2	2.39	0.53
1:H:353:VAL:CG1	1:H:354:ARG:N	2.71	0.53
1:D:298:VAL:O	1:D:306:GLY:HA2	2.09	0.53
1:G:266:GLU:O	1:G:269:ILE:HG13	2.08	0.53
1:H:283:GLN:HB3	1:H:316:PRO:HG2	1.91	0.53
1:B:270:PHE:HE1	3:C:600[B]:CZ3:NBJ	2.06	0.53
1:H:346:HIS:HB3	4:H:23:HOH:O	2.07	0.53
1:E:272:PHE:CE2	1:E:291:ALA:HB2	2.43	0.52
1:G:279:VAL:HG11	1:G:310:TRP:CB	2.39	0.52
1:H:303:CYS:HG	2:H:502:ZN:ZN	1.22	0.52
1:D:350:GLU:O	1:D:354:ARG:HB2	2.10	0.52
1:C:257:PRO:HA	1:C:302:HIS:HA	1.91	0.52
1:G:328:LYS:HG2	4:G:85:HOH:O	2.10	0.52
1:F:325:PRO:CG	1:F:348:LEU:CD2	2.87	0.52
1:A:293:GLY:HA3	4:A:94:HOH:O	2.11	0.51
1:A:259:ASN:ND2	1:A:262:MET:HG2	2.24	0.51
1:F:325:PRO:CG	1:F:348:LEU:HD22	2.40	0.51
1:D:347:SER:O	1:D:348:LEU:C	2.48	0.51
1:D:332:GLU:OE1	1:D:333:GLN:NE2	2.43	0.51
1:F:322:LYS:HG2	1:F:346:HIS:ND1	2.24	0.51
3:G:600[B]:CZ3:HCJ	3:G:600[B]:CZ3:CAM	2.40	0.51
1:F:322:LYS:CG	1:F:346:HIS:CE1	2.94	0.51
1:C:312:PRO:HB3	1:D:276:ILE:HA	1.91	0.51
1:A:257:PRO:HG3	1:A:302:HIS:HD2	1.74	0.51
1:D:338:TYR:O	1:D:342:ILE:HD13	2.11	0.50
1:B:263:ALA:HA	1:B:301:PHE:CD1	2.46	0.50
1:H:345:THR:HB	1:H:346:HIS:CD2	2.47	0.50
1:A:290:TYR:CE2	1:A:299:LYS:HB2	2.45	0.50
1:F:321:ALA:HB2	1:F:330:LEU:HD11	1.93	0.50
1:F:297:LYS:HG2	1:F:308:THR:CG2	2.42	0.50
1:B:284:LEU:HD23	1:B:316:PRO:CG	2.41	0.50
1:A:266:GLU:HB2	4:A:53:HOH:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:323:TRP:HZ3	1:H:348:LEU:CB	2.24	0.49
1:H:328:LYS:HE2	1:H:331:LEU:HD12	1.93	0.49
1:A:322:LYS:HA	1:A:343:HIS:HE1	1.76	0.49
1:D:263:ALA:HA	1:D:301:PHE:CD1	2.46	0.49
1:E:279:VAL:HG12	1:E:311:LYS:O	2.12	0.49
1:B:330:LEU:HD21	1:B:339:ILE:HG12	1.95	0.49
1:F:311:LYS:HB2	1:F:314:GLU:HG3	1.93	0.49
1:G:311:LYS:HB3	1:G:312:PRO:HD2	1.94	0.49
1:A:266:GLU:HA	1:A:269:ILE:HD11	1.95	0.48
1:F:355:THR:C	1:F:357:HIS:H	2.16	0.48
1:B:268:ARG:O	1:B:271:THR:OG1	2.26	0.48
1:F:322:LYS:HG2	1:F:346:HIS:CD2	2.49	0.48
1:F:322:LYS:HG3	1:F:346:HIS:CE1	2.49	0.48
3:D:600[B]:CZ3:HAYA	3:D:600[B]:CZ3:HAW	1.96	0.48
1:E:270:PHE:HA	4:E:33:HOH:O	2.13	0.48
1:F:322:LYS:CD	1:F:346:HIS:ND1	2.76	0.48
1:F:354:ARG:HH11	1:F:357:HIS:CD2	2.31	0.48
3:G:600[B]:CZ3:HCL	3:G:600[B]:CZ3:HCF	1.66	0.48
1:G:331:LEU:HD21	1:G:336:GLN:HG2	1.96	0.48
1:D:269:ILE:HG23	1:D:285:ALA:CB	2.43	0.48
1:F:348:LEU:HD12	1:F:348:LEU:C	2.34	0.48
1:D:297:LYS:HG2	1:D:308:THR:CG2	2.44	0.48
1:C:294:GLU:CB	1:C:297:LYS:HD2	2.43	0.47
1:C:322:LYS:HA	1:C:343:HIS:CE1	2.49	0.47
1:F:266:GLU:HA	1:F:269:ILE:HD11	1.95	0.47
1:B:323:TRP:O	1:B:348:LEU:CD2	2.62	0.47
3:E:600[B]:CZ3:OAJ	3:E:600[B]:CZ3:CBH	2.62	0.47
1:A:322:LYS:HD3	1:A:323:TRP:CZ2	2.48	0.47
3:C:600[B]:CZ3:CBZ	3:C:600[B]:CZ3:HCF	2.44	0.47
1:D:271:THR:HG21	1:D:290:TYR:HB2	1.97	0.47
1:B:280:ASN:OD1	1:B:283:GLN:N	2.31	0.47
1:H:348:LEU:HG	4:H:37:HOH:O	2.14	0.47
1:E:280:ASN:O	1:E:284:LEU:HD12	2.14	0.47
1:E:297:LYS:HG2	1:E:308:THR:CG2	2.45	0.47
1:F:348:LEU:HD13	1:F:352:LEU:CD2	2.45	0.47
1:A:295:GLY:HA3	4:D:34:HOH:O	2.14	0.47
1:D:274:THR:O	1:D:274:THR:OG1	2.32	0.47
1:H:346:HIS:CA	1:H:347:SER:CB	2.91	0.47
1:A:279:VAL:HG11	1:A:310:TRP:CB	2.40	0.47
1:B:338:TYR:O	1:B:342:ILE:HD13	2.15	0.47
1:G:280:ASN:O	1:G:284:LEU:HD12	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:294:GLU:HB2	1:G:297:LYS:HD2	1.96	0.46
1:B:323:TRP:C	1:B:348:LEU:CD2	2.77	0.46
1:C:280:ASN:CG	1:C:283:GLN:HG3	2.36	0.46
1:G:292:LEU:HD21	1:G:299:LYS:HB2	1.96	0.46
1:D:258:ARG:NH1	4:D:3:HOH:O	2.48	0.46
4:E:448:HOH:O	1:G:271:THR:HG21	2.15	0.46
1:F:265:TYR:O	1:F:269:ILE:HG13	2.14	0.46
1:F:271:THR:HB	1:F:291:ALA:HB3	1.98	0.46
1:A:265:TYR:O	1:A:269:ILE:HG13	2.15	0.46
1:D:305:GLY:HA3	1:D:324:TYR:CE1	2.50	0.46
1:E:296:ASP:OD1	1:E:308:THR:HG22	2.16	0.46
1:E:297:LYS:HG2	1:E:308:THR:HG23	1.98	0.46
1:B:330:LEU:O	1:B:334:LYS:HB2	2.15	0.46
1:D:311:LYS:HA	1:D:311:LYS:HD3	1.60	0.46
1:F:270:PHE:CD2	3:G:600[B]:CZ3:HBF	2.51	0.46
1:G:288:GLY:O	1:G:300:CYS:HA	2.16	0.46
1:F:315:ASP:HA	4:F:20:HOH:O	2.16	0.46
1:B:284:LEU:HD23	1:B:316:PRO:HB3	1.97	0.45
1:G:266:GLU:HA	1:G:269:ILE:HD11	1.96	0.45
1:H:260:PRO:HA	1:H:263:ALA:HB2	1.98	0.45
1:H:351:CYS:HB2	1:H:352:LEU:HD23	1.98	0.45
1:F:283:GLN:HG2	1:F:286:ARG:HH12	1.81	0.45
1:D:294:GLU:O	1:D:295:GLY:C	2.55	0.45
1:F:275:TRP:HH2	1:F:296:ASP:HA	1.81	0.45
1:H:275:TRP:CE2	1:H:277:TYR:HB2	2.51	0.45
1:C:287:ALA:HA	1:C:317:TRP:CZ2	2.51	0.45
1:D:331:LEU:HD21	1:D:336:GLN:HG2	1.98	0.45
1:B:352:LEU:HD22	4:B:38:HOH:O	2.16	0.45
1:C:332:GLU:HB2	4:C:10:HOH:O	2.16	0.45
1:D:348:LEU:C	1:D:350:GLU:H	2.20	0.45
1:G:297:LYS:HA	1:G:308:THR:HG23	1.99	0.45
3:G:600[B]:CZ3:HBHA	3:G:600[B]:CZ3:OAJ	2.16	0.45
3:A:600[B]:CZ3:HCF	3:A:600[B]:CZ3:HCL	1.73	0.45
1:F:269:ILE:HG13	1:F:269:ILE:H	1.66	0.45
1:A:321:ALA:HA	1:A:330:LEU:HD21	1.99	0.44
1:C:302:HIS:HE1	1:C:328:LYS:HB3	1.76	0.44
1:C:322:LYS:CD	1:C:323:TRP:CE2	2.98	0.44
1:E:276:ILE:HD12	1:F:277:TYR:CD2	2.53	0.44
1:E:289:PHE:HA	1:E:299:LYS:O	2.17	0.44
1:B:350:GLU:O	1:B:354:ARG:HB2	2.18	0.44
1:E:302:HIS:CE1	1:E:328:LYS:HB3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:600[B]:CZ3:HBFA	3:A:600[B]:CZ3:HCF	1.99	0.44
1:C:257:PRO:HG3	1:C:302:HIS:HD2	1.82	0.44
1:B:311:LYS:HG2	1:B:314:GLU:OE2	2.18	0.44
1:H:297:LYS:HA	1:H:308:THR:HG22	2.00	0.44
1:H:297:LYS:HG2	1:H:308:THR:HG21	1.99	0.44
1:A:269:ILE:HG13	1:A:269:ILE:H	1.71	0.43
1:C:279:VAL:HG23	1:C:279:VAL:O	2.17	0.43
1:B:322:LYS:HE3	1:B:323:TRP:NE1	2.34	0.43
1:B:346:HIS:HB3	4:B:70:HOH:O	2.17	0.43
1:C:254:THR:O	1:C:255:ASN:CB	2.60	0.43
1:B:352:LEU:O	1:B:356:THR:HG23	2.19	0.43
1:A:294:GLU:CB	1:A:297:LYS:HD2	2.48	0.43
1:H:340:ASN:O	1:H:344:LEU:HD13	2.19	0.43
1:E:275:TRP:O	1:F:312:PRO:HG3	2.18	0.43
1:H:352:LEU:H	1:H:352:LEU:CD2	2.11	0.43
1:C:266:GLU:HA	1:C:269:ILE:HD11	2.00	0.43
1:A:279:VAL:HG23	1:A:284:LEU:HD11	2.01	0.42
1:A:300:CYS:O	1:A:304:GLY:HA2	2.19	0.42
3:F:600[A]:CZ3:HAFA	3:F:600[A]:CZ3:HAZA	1.80	0.42
1:D:284:LEU:O	1:D:289:PHE:HB2	2.18	0.42
1:G:287:ALA:HA	1:G:317:TRP:CH2	2.55	0.42
1:D:297:LYS:HG2	1:D:308:THR:HG22	2.02	0.42
1:F:284:LEU:O	1:F:289:PHE:HB2	2.18	0.42
1:F:297:LYS:NZ	4:F:172:HOH:O	2.52	0.42
1:F:315:ASP:O	1:F:319:GLN:HG2	2.18	0.42
1:H:300:CYS:O	1:H:304:GLY:HA2	2.19	0.42
1:E:276:ILE:HD12	1:F:277:TYR:CE2	2.55	0.42
1:H:354:ARG:HA	1:H:354:ARG:HD3	1.63	0.42
1:B:345:THR:O	1:B:346:HIS:HB2	2.20	0.42
1:C:268:ARG:HD2	1:C:289:PHE:O	2.18	0.42
1:C:276:ILE:HA	1:D:312:PRO:HG3	2.00	0.42
1:E:279:VAL:HG23	1:E:284:LEU:CD1	2.44	0.42
1:H:355:THR:O	1:H:357:HIS:N	2.53	0.42
1:G:286:ARG:NH1	1:G:317:TRP:HE1	2.18	0.42
1:B:322:LYS:HE3	1:B:323:TRP:HE1	1.85	0.42
3:F:600[A]:CZ3:CBF	3:F:600[A]:CZ3:NBP	2.83	0.42
1:G:254:THR:HG22	1:G:255:ASN:H	1.85	0.42
1:G:317:TRP:HA	1:G:317:TRP:CE3	2.54	0.42
1:B:269:ILE:HG23	1:B:285:ALA:CB	2.50	0.41
1:H:308:THR:OG1	3:H:600[B]:CZ3:HAY	2.20	0.41
1:H:315:ASP:HB3	1:H:318:GLU:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:269:ILE:HG13	1:H:269:ILE:H	1.70	0.41
1:D:311:LYS:HG2	1:D:314:GLU:OE2	2.20	0.41
1:E:287:ALA:HA	1:E:317:TRP:CH2	2.55	0.41
1:E:342:ILE:O	1:E:345:THR:OG1	2.37	0.41
1:B:280:ASN:OD1	1:B:282:GLU:N	2.53	0.41
1:H:275:TRP:HH2	1:H:296:ASP:HA	1.82	0.41
1:D:283:GLN:CB	1:D:316:PRO:HG2	2.46	0.41
1:G:312:PRO:HD3	1:H:276:ILE:HG22	2.03	0.41
1:H:271:THR:HB	1:H:291:ALA:HB3	2.03	0.41
1:H:343:HIS:C	1:H:345:THR:H	2.24	0.41
1:H:280:ASN:O	1:H:284:LEU:HG	2.20	0.41
1:A:272:PHE:O	1:A:281:LYS:HE3	2.20	0.41
1:A:297:LYS:HG2	1:A:308:THR:CG2	2.51	0.41
1:C:322:LYS:HD3	1:C:323:TRP:CZ2	2.56	0.41
3:E:600[B]:CZ3:HCF	3:E:600[B]:CZ3:HCL	1.84	0.41
1:H:256:LEU:HB3	1:H:257:PRO:HD2	2.02	0.41
1:H:349:GLU:HG3	1:H:352:LEU:HG	2.01	0.41
1:B:298:VAL:O	1:B:306:GLY:HA2	2.20	0.41
1:G:305:GLY:HA2	1:G:324:TYR:CE2	2.56	0.41
1:G:297:LYS:HA	1:G:308:THR:CG2	2.51	0.40
1:C:265:TYR:O	1:C:269:ILE:HG13	2.21	0.40
1:E:329:TYR:CZ	1:E:333:GLN:HG3	2.57	0.40
1:F:297:LYS:HA	1:F:308:THR:HG22	2.03	0.40
1:A:259:ASN:N	1:A:260:PRO:CD	2.82	0.40
1:C:281:LYS:H	1:C:281:LYS:HG2	1.68	0.40
1:F:260:PRO:HA	1:F:263:ALA:HB2	2.02	0.40
1:G:284:LEU:O	1:G:289:PHE:HB2	2.22	0.40
1:A:279:VAL:HG12	1:A:311:LYS:O	2.22	0.40
1:B:310:TRP:O	1:B:311:LYS:HD3	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:344:LEU:O	4:D:17:HOH:O[1_556]	2.09	0.11

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	95/122 (78%)	83 (87%)	11 (12%)	1 (1%)	14	50
1	B	103/122 (84%)	91 (88%)	9 (9%)	3 (3%)	4	24
1	C	94/122 (77%)	79 (84%)	13 (14%)	2 (2%)	7	33
1	D	103/122 (84%)	88 (85%)	11 (11%)	4 (4%)	3	17
1	E	93/122 (76%)	81 (87%)	11 (12%)	1 (1%)	14	50
1	F	102/122 (84%)	91 (89%)	9 (9%)	2 (2%)	7	34
1	G	93/122 (76%)	81 (87%)	11 (12%)	1 (1%)	14	50
1	H	103/122 (84%)	86 (84%)	12 (12%)	5 (5%)	2	13
All	All	786/976 (80%)	680 (86%)	87 (11%)	19 (2%)	6	29

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	353	VAL
1	A	258	ARG
1	B	348	LEU
1	C	255	ASN
1	D	295	GLY
1	F	295	GLY
1	F	314	GLU
1	H	255	ASN
1	H	295	GLY
1	H	314	GLU
1	B	279	VAL
1	D	279	VAL
1	D	347	SER
1	H	344	LEU
1	H	356	THR
1	B	295	GLY
1	C	342	ILE

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Mol	Chain	Res	Type
1	G	257	PRO
1	E	312	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	82/106 (77%)	73 (89%)	9 (11%)	6	25
1	B	90/106 (85%)	79 (88%)	11 (12%)	5	21
1	C	81/106 (76%)	73 (90%)	8 (10%)	8	30
1	D	90/106 (85%)	75 (83%)	15 (17%)	2	11
1	E	80/106 (76%)	70 (88%)	10 (12%)	4	20
1	F	89/106 (84%)	78 (88%)	11 (12%)	4	20
1	G	80/106 (76%)	69 (86%)	11 (14%)	3	17
1	H	90/106 (85%)	77 (86%)	13 (14%)	3	15
All	All	682/848 (80%)	594 (87%)	88 (13%)	4	19

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	253	SER
1	A	254	THR
1	A	255	ASN
1	A	256	LEU
1	A	266	GLU
1	A	308	THR
1	A	309	ASP
1	A	331	LEU
1	A	348	LEU
1	B	264	ASP
1	B	269	ILE
1	B	279	VAL
1	B	309	ASP

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Mol	Chain	Res	Type
1	B	311	LYS
1	B	328	LYS
1	B	331	LEU
1	B	342	ILE
1	B	343	HIS
1	B	349	GLU
1	B	354	ARG
1	C	254	THR
1	C	255	ASN
1	C	266	GLU
1	C	309	ASP
1	C	315	ASP
1	C	328	LYS
1	C	331	LEU
1	C	345	THR
1	D	264	ASP
1	D	269	ILE
1	D	274	THR
1	D	279	VAL
1	D	281	LYS
1	D	309	ASP
1	D	311	LYS
1	D	322	LYS
1	D	328	LYS
1	D	331	LEU
1	D	343	HIS
1	D	344	LEU
1	D	347	SER
1	D	352	LEU
1	D	354	ARG
1	E	269	ILE
1	E	270	PHE
1	E	278	SER
1	E	292	LEU
1	E	308	THR
1	E	309	ASP
1	E	313	SER
1	E	328	LYS
1	E	331	LEU
1	E	345	THR
1	F	264	ASP
1	F	270	PHE

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Mol	Chain	Res	Type
1	F	294	GLU
1	F	296	ASP
1	F	309	ASP
1	F	322	LYS
1	F	328	LYS
1	F	331	LEU
1	F	344	LEU
1	F	345	THR
1	F	353	VAL
1	G	255	ASN
1	G	269	ILE
1	G	270	PHE
1	G	271	THR
1	G	278	SER
1	G	281	LYS
1	G	284	LEU
1	G	292	LEU
1	G	308	THR
1	G	309	ASP
1	G	331	LEU
1	H	264	ASP
1	H	270	PHE
1	H	296	ASP
1	H	309	ASP
1	H	328	LYS
1	H	331	LEU
1	H	345	THR
1	H	348	LEU
1	H	350	GLU
1	H	352	LEU
1	H	353	VAL
1	H	354	ARG
1	H	356	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	255	ASN
1	A	283	GLN
1	A	302	HIS
1	A	343	HIS
1	B	255	ASN

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Mol	Chain	Res	Type
1	C	255	ASN
1	C	283	GLN
1	C	302	HIS
1	D	255	ASN
1	E	283	GLN
1	E	302	HIS
1	E	346	HIS
1	F	255	ASN
1	F	346	HIS
1	F	357	HIS
1	G	283	GLN
1	G	302	HIS
1	H	255	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	261:SER	C	262:MET	N	1.62

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^{th} 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	97/122 (79%)	0.12	1 (1%)	82	59	34, 56, 96, 128	1 (1%)
1	B	105/122 (86%)	0.21	4 (3%)	40	16	34, 54, 92, 134	1 (0%)
1	C	96/122 (78%)	0.27	3 (3%)	49	21	34, 57, 99, 128	1 (1%)
1	D	105/122 (86%)	0.15	1 (0%)	82	59	33, 53, 85, 117	1 (0%)
1	E	95/122 (77%)	0.34	3 (3%)	47	20	52, 81, 121, 141	1 (1%)
1	F	104/122 (85%)	0.51	8 (7%)	13	4	54, 95, 118, 140	1 (0%)
1	G	95/122 (77%)	0.46	5 (5%)	26	10	60, 83, 118, 150	1 (1%)
1	H	105/122 (86%)	0.49	8 (7%)	13	4	45, 92, 121, 149	1 (0%)
All	All	802/976 (82%)	0.32	33 (4%)	37	14	33, 75, 115, 150	8 (0%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	253	SER	7.0
1	B	253	SER	6.8
1	G	254	THR	6.2
1	E	254	THR	5.5
1	G	253	SER	5.2
1	H	254	THR	5.1
1	H	272	PHE	4.2
1	E	253	SER	4.0
1	B	254	THR	3.7
1	H	316	PRO	3.6
1	C	348	LEU	3.5
1	D	254	THR	3.4
1	G	275	TRP	3.3
1	H	289	PHE	3.2
1	C	254	THR	2.9
1	H	347	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	272	PHE	2.8
1	F	272	PHE	2.8
1	H	284	LEU	2.6
1	H	290	TYR	2.6
1	C	253	SER	2.6
1	G	298	VAL	2.5
1	F	274	THR	2.5
1	F	316	PRO	2.5
1	F	255	ASN	2.4
1	G	279	VAL	2.4
1	A	254	THR	2.3
1	F	355	THR	2.2
1	B	357	HIS	2.2
1	B	356	THR	2.1
1	F	307	LEU	2.1
1	F	266	GLU	2.0
1	F	348	LEU	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 monosaccharides 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^{th} 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(Å^2)	Q<0.9
3	CZ3	G	600[B]	68/68	0.83	0.35	40,73,113,125	36
3	CZ3	E	600[B]	68/68	0.84	0.35	31,73,105,114	36
3	CZ3	A	600[B]	68/68	0.90	0.32	21,57,83,133	36
3	CZ3	C	600[B]	68/68	0.90	0.34	15,57,94,172	36
3	CZ3	H	600[B]	68/68	0.92	0.29	10,65,100,116	36
3	CZ3	F	600[A]	68/68	0.93	0.29	14,61,102,123	36

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	D	502	1/1	0.96	0.23	41,41,41,41	0
2	ZN	B	502	1/1	0.97	0.23	44,44,44,44	0
3	CZ3	D	600[B]	68/68	0.97	0.24	4,32,69,124	36
3	CZ3	B	600[A]	68/68	0.97	0.23	7,34,57,88	36
2	ZN	F	502	1/1	0.98	0.18	92,92,92,92	0
2	ZN	E	502	1/1	0.99	0.12	75,75,75,75	0
2	ZN	C	502	1/1	0.99	0.19	46,46,46,46	0
2	ZN	G	502	1/1	0.99	0.12	80,80,80,80	0
2	ZN	H	502	1/1	0.99	0.16	108,108,108,108	0
2	ZN	A	502	1/1	1.00	0.18	41,41,41,41	0

6.5 Other polymers (i)

There are no such residues in this entry.