



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:20 PM GMT

PDB ID : 4HY0  
Title : Crystal structure of XIAP BIR3 with T3256336  
Authors : Snell, G.S.; Dougan, D.R.  
Deposited on : 2012-11-12  
Resolution : 2.84 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

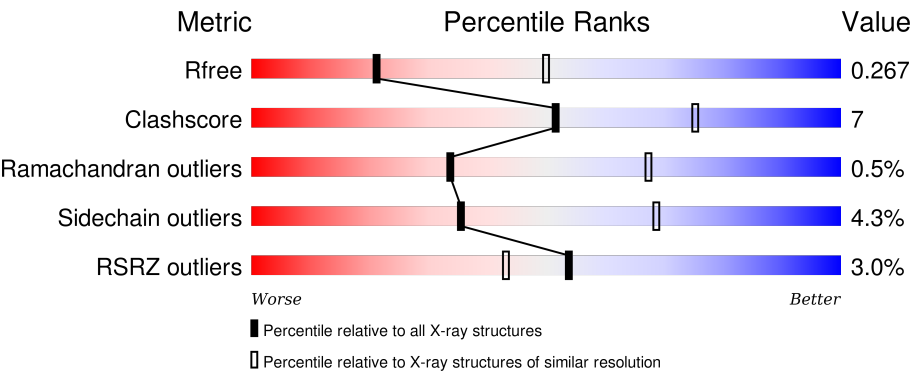
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.84 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 <sub>free</sub>	91344	3170 (2.88-2.80)
Clashscore	102246	3658 (2.88-2.80)
Ramachandran outliers	100387	3591 (2.88-2.80)
Sidechain outliers	100360	3594 (2.88-2.80)
RSRZ outliers	91569	3184 (2.88-2.80)

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. 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	125	<div><div></div><div>64%12%•23%</div></div>
1	B	125	<div>4%<div><div></div><div>64%12%•23%</div></div></div>
1	C	125	<div>2%<div><div></div><div>70%7%•22%</div></div></div>
1	D	125	<div>3%<div><div></div><div>54%22%•22%</div></div></div>
1	E	125	<div>2%<div><div></div><div>66%10%•23%</div></div></div>

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Mol	Chain	Length	Quality of chain
1	F	125	 3% 70% 6% 23%
1	G	125	 2% 66% 11% 22%
1	H	125	 2% 66% 11% 23%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6702 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 E3 ubiquitin-protein ligase XIAP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	96	Total	C	N	O	S	0	0	0
			784	503	133	144	4			
1	B	96	Total	C	N	O	S	0	0	0
			784	503	133	144	4			
1	C	97	Total	C	N	O	S	0	0	0
			793	508	134	147	4			
1	D	98	Total	C	N	O	S	0	0	0
			799	511	135	148	5			
1	E	96	Total	C	N	O	S	0	0	0
			784	503	133	144	4			
1	F	96	Total	C	N	O	S	0	0	0
			784	503	133	144	4			
1	G	98	Total	C	N	O	S	0	0	0
			799	511	135	148	5			
1	H	96	Total	C	N	O	S	0	0	0
			784	503	133	144	4			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	233	GLY	-	EXPRESSION TAG	UNP P98170
A	234	PRO	-	EXPRESSION TAG	UNP P98170
A	235	LEU	-	EXPRESSION TAG	UNP P98170
A	236	GLY	-	EXPRESSION TAG	UNP P98170
A	237	SER	-	EXPRESSION TAG	UNP P98170
B	233	GLY	-	EXPRESSION TAG	UNP P98170
B	234	PRO	-	EXPRESSION TAG	UNP P98170
B	235	LEU	-	EXPRESSION TAG	UNP P98170
B	236	GLY	-	EXPRESSION TAG	UNP P98170
B	237	SER	-	EXPRESSION TAG	UNP P98170
C	233	GLY	-	EXPRESSION TAG	UNP P98170
C	234	PRO	-	EXPRESSION TAG	UNP P98170
C	235	LEU	-	EXPRESSION TAG	UNP P98170

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Chain	Residue	Modelled	Actual	Comment	Reference
C	236	GLY	-	EXPRESSION TAG	UNP P98170
C	237	SER	-	EXPRESSION TAG	UNP P98170
D	233	GLY	-	EXPRESSION TAG	UNP P98170
D	234	PRO	-	EXPRESSION TAG	UNP P98170
D	235	LEU	-	EXPRESSION TAG	UNP P98170
D	236	GLY	-	EXPRESSION TAG	UNP P98170
D	237	SER	-	EXPRESSION TAG	UNP P98170
E	233	GLY	-	EXPRESSION TAG	UNP P98170
E	234	PRO	-	EXPRESSION TAG	UNP P98170
E	235	LEU	-	EXPRESSION TAG	UNP P98170
E	236	GLY	-	EXPRESSION TAG	UNP P98170
E	237	SER	-	EXPRESSION TAG	UNP P98170
F	233	GLY	-	EXPRESSION TAG	UNP P98170
F	234	PRO	-	EXPRESSION TAG	UNP P98170
F	235	LEU	-	EXPRESSION TAG	UNP P98170
F	236	GLY	-	EXPRESSION TAG	UNP P98170
F	237	SER	-	EXPRESSION TAG	UNP P98170
G	233	GLY	-	EXPRESSION TAG	UNP P98170
G	234	PRO	-	EXPRESSION TAG	UNP P98170
G	235	LEU	-	EXPRESSION TAG	UNP P98170
G	236	GLY	-	EXPRESSION TAG	UNP P98170
G	237	SER	-	EXPRESSION TAG	UNP P98170
H	233	GLY	-	EXPRESSION TAG	UNP P98170
H	234	PRO	-	EXPRESSION TAG	UNP P98170
H	235	LEU	-	EXPRESSION TAG	UNP P98170
H	236	GLY	-	EXPRESSION TAG	UNP P98170
H	237	SER	-	EXPRESSION TAG	UNP P98170

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

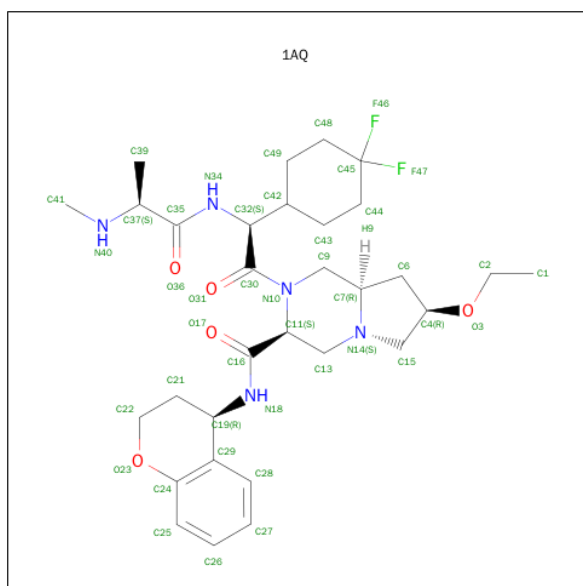
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	2	Total Zn 2 2	0	0
2	D	2	Total Zn 2 2	0	0
2	E	2	Total Zn 2 2	0	0
2	H	1	Total Zn 1 1	0	0
2	B	2	Total Zn 2 2	0	0
2	C	1	Total Zn 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	F	2	Total	Zn	0	0
			2	2		

- Molecule 3 is (3S,7R,8AR)-2-[(2S)-2-(4,4-DIFLUOROCYCLOHEXYL)-2-[(N-METHYL-L-ALANYL)AMINO]ACETYL}-N-[(4R)-3,4-DIHYDRO-2H-CHROMEN-4-YL]-7-ETHOXY OCTAHYDROPYRROLO[1,2-A]PYRAZINE-3-CARBOXAMIDE (three-letter code: 1AQ) (formula: C<sub>31</sub>H<sub>45</sub>F<sub>2</sub>N<sub>5</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			43	31	2	5	5		
3	B	1	Total	C	F	N	O	0	0
			43	31	2	5	5		
3	C	1	Total	C	F	N	O	0	0
			43	31	2	5	5		
3	D	1	Total	C	F	N	O	0	0
			43	31	2	5	5		
3	E	1	Total	C	F	N	O	0	0
			43	31	2	5	5		
3	F	1	Total	C	F	N	O	0	0
			43	31	2	5	5		
3	G	1	Total	C	F	N	O	0	0
			43	31	2	5	5		
3	H	1	Total	C	F	N	O	0	0
			43	31	2	5	5		

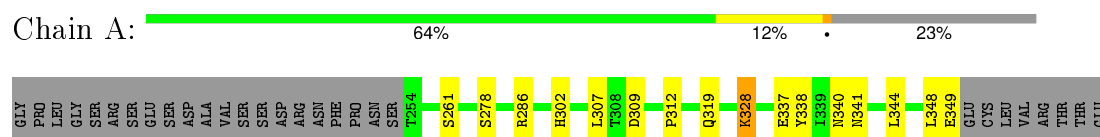
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	10	Total 10	O 10	0	0
4	B	2	Total 2	O 2	0	0
4	C	8	Total 8	O 8	0	0
4	D	3	Total 3	O 3	0	0
4	E	7	Total 7	O 7	0	0
4	F	2	Total 2	O 2	0	0
4	H	1	Total 1	O 1	0	0

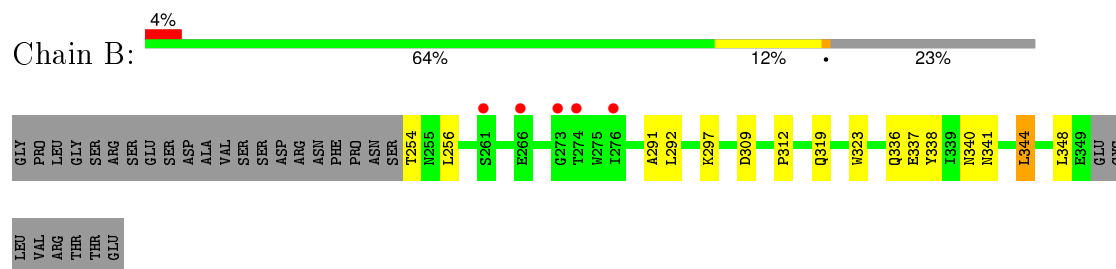
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

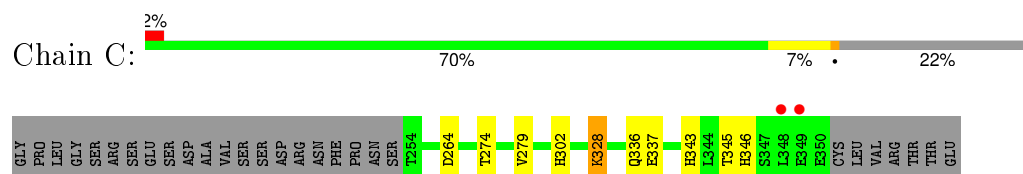
- Molecule 1: E3 ubiquitin-protein ligase XIAP



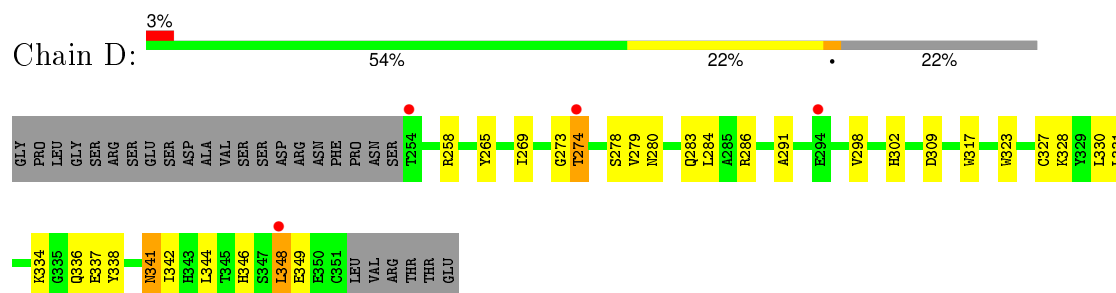
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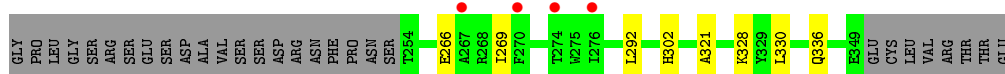


- Molecule 1: E3 ubiquitin-protein ligase XIAP

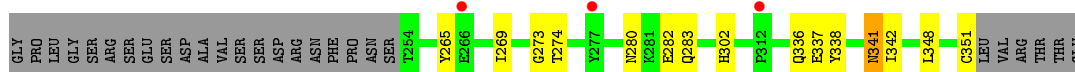




- Molecule 1: E3 ubiquitin-protein ligase XIAP



- Molecule 1: E3 ubiquitin-protein ligase XIAP



- Molecule 1: E3 ubiquitin-protein ligase XIAP



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.34Å 100.84Å 184.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.84 39.03 – 2.84	Depositor EDS
% Data completeness (in resolution range)	99.0 (40.00-2.84) 99.0 (39.03-2.84)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.80 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.208 , 0.262 0.211 , 0.267	Depositor DCC
$R_{free}$ test set	1342 reflections (5.39%)	DCC
Wilson B-factor (Å <sup>2</sup> )	75.7	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 51.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtriage
Outliers	2 of 26243 reflections (0.008%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6702	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.05 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 6.2026e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, 0.375 respectively for untwinned datasets, and 0.333, 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, 1AQ

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	0.58	0/810	0.55	0/1098
1	B	0.60	0/810	0.52	0/1098
1	C	0.60	0/819	0.55	0/1110
1	D	0.60	0/825	0.56	0/1118
1	E	0.59	1/810 (0.1%)	0.52	0/1098
1	F	0.58	0/810	0.52	0/1098
1	G	0.59	0/825	0.55	0/1118
1	H	0.60	0/810	0.55	0/1098
All	All	0.59	1/6519 (0.0%)	0.54	0/8836

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	323	TRP	CD2-CE2	5.05	1.47	1.41

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	784	0	731	15	0
1	B	784	0	731	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	793	0	737	15	0
1	D	799	0	742	27	0
1	E	784	0	731	17	0
1	F	784	0	731	5	0
1	G	799	0	742	11	0
1	H	784	0	731	14	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	1	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	1	0	0	0	0
3	A	43	0	45	6	0
3	B	43	0	45	2	0
3	C	43	0	45	0	0
3	D	43	0	45	4	0
3	E	43	0	45	3	0
3	F	43	0	45	2	0
3	G	43	0	45	1	0
3	H	43	0	45	2	0
4	A	10	0	0	0	0
4	B	2	0	0	0	0
4	C	8	0	0	1	0
4	D	3	0	0	0	0
4	E	7	0	0	0	0
4	F	2	0	0	0	0
4	H	1	0	0	0	0
All	All	6702	0	6236	88	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 7.

All (88) 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:D:336:GLN:HE22	1:E:302:HIS:CD2	1.82	0.97
1:A:302:HIS:CD2	1:B:336:GLN:HE22	1.86	0.94
1:C:336:GLN:HE22	1:H:302:HIS:CD2	2.00	0.80
1:D:336:GLN:HE22	1:E:302:HIS:HD2	1.32	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:ASN:HD22	1:D:341:ASN:ND2	1.84	0.74
1:D:302:HIS:HD2	1:E:336:GLN:HE22	1.37	0.72
1:C:336:GLN:HE22	1:H:302:HIS:HD2	1.38	0.71
1:C:343:HIS:ND1	4:C:508:HOH:O	2.23	0.71
1:D:302:HIS:CD2	1:E:336:GLN:HE22	2.09	0.70
1:A:302:HIS:CD2	1:B:336:GLN:NE2	2.59	0.68
1:C:337:GLU:HG2	1:E:338:TYR:HA	1.77	0.67
1:B:338:TYR:HA	1:D:337:GLU:HG2	1.77	0.65
1:A:338:TYR:HA	1:G:337:GLU:HG2	1.77	0.64
1:B:341:ASN:HD22	1:D:341:ASN:HD22	1.46	0.62
1:A:302:HIS:HD2	1:B:336:GLN:HE22	1.40	0.62
1:H:266:GLU:O	1:H:269:ILE:HG22	1.98	0.62
1:B:337:GLU:HB3	1:D:337:GLU:HB3	1.82	0.62
1:A:319:GLN:HE21	3:A:403:1AQ:H32	1.66	0.61
1:D:280:ASN:HB3	1:D:283:GLN:HG2	1.83	0.60
1:G:280:ASN:HB3	1:G:283:GLN:HE21	1.65	0.60
1:C:302:HIS:CD2	1:H:336:GLN:HE22	2.20	0.59
1:C:328:LYS:HB2	1:H:336:GLN:HE21	1.67	0.59
1:A:328:LYS:H	1:B:336:GLN:HE21	1.49	0.59
1:F:336:GLN:HE22	1:G:302:HIS:CD2	2.20	0.58
1:D:336:GLN:NE2	1:E:302:HIS:CD2	2.66	0.57
1:E:292:LEU:CD1	3:E:403:1AQ:H25	2.36	0.55
1:A:341:ASN:HD22	1:G:341:ASN:HD22	1.55	0.54
1:C:274:THR:O	1:C:274:THR:CG2	2.55	0.54
1:A:278:SER:HB2	1:A:312:PRO:HA	1.90	0.54
1:H:292:LEU:HD12	1:H:297:LYS:HB3	1.90	0.54
1:A:341:ASN:HD22	1:G:341:ASN:ND2	2.06	0.54
1:D:328:LYS:H	1:E:336:GLN:HE21	1.55	0.53
1:B:319:GLN:HE21	3:B:403:1AQ:H32	1.74	0.53
1:B:254:THR:HG23	1:B:256:LEU:HG	1.91	0.53
1:D:331:LEU:HD21	1:E:328:LYS:CG	2.40	0.52
1:G:338:TYR:CE2	1:G:342:ILE:HD12	2.45	0.51
1:B:340:ASN:O	1:B:344:LEU:HD22	2.12	0.49
3:A:403:1AQ:H1	1:B:348:LEU:HD21	1.94	0.49
1:E:266:GLU:O	1:E:269:ILE:HG22	2.12	0.49
1:C:336:GLN:HE21	1:H:328:LYS:HB2	1.78	0.49
1:F:266:GLU:O	1:F:269:ILE:HG22	2.13	0.49
1:F:321:ALA:HA	1:F:330:LEU:HD21	1.94	0.49
3:A:403:1AQ:H22	1:D:349:GLU:HB3	1.95	0.49
1:H:292:LEU:HD12	1:H:297:LYS:CB	2.43	0.49
3:A:403:1AQ:H20	1:D:348:LEU:CD1	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:279:VAL:HG23	1:D:284:LEU:HD11	1.96	0.48
1:C:336:GLN:NE2	1:H:328:LYS:H	2.12	0.48
1:H:311:LYS:HB3	1:H:312:PRO:HD2	1.96	0.48
1:A:337:GLU:HG2	1:G:338:TYR:HA	1.95	0.48
1:D:258:ARG:NH1	1:E:337:GLU:OE2	2.47	0.47
1:D:302:HIS:CD2	1:E:336:GLN:NE2	2.80	0.47
1:D:302:HIS:HD2	1:E:336:GLN:NE2	2.09	0.47
1:A:341:ASN:HB2	1:G:341:ASN:HD21	1.79	0.47
1:B:341:ASN:ND2	1:D:341:ASN:ND2	2.58	0.46
1:C:302:HIS:CD2	1:H:336:GLN:NE2	2.84	0.46
1:A:319:GLN:NE2	3:A:403:1AQ:H32	2.30	0.46
1:E:308:THR:HG22	3:E:403:1AQ:H27	1.98	0.46
1:A:340:ASN:O	1:A:344:LEU:HD23	2.16	0.45
1:C:345:THR:CG2	3:D:403:1AQ:H23	2.47	0.45
1:C:345:THR:HG22	3:D:403:1AQ:H23	1.99	0.45
1:D:323:TRP:CZ3	3:D:403:1AQ:H7	2.51	0.45
1:F:302:HIS:CD2	1:G:336:GLN:HE22	2.35	0.45
1:D:317:TRP:CG	1:D:334:LYS:HE3	2.52	0.44
1:F:292:LEU:HD11	3:F:403:1AQ:H25	1.99	0.44
1:B:341:ASN:ND2	1:D:341:ASN:HD22	2.13	0.43
1:E:292:LEU:HD11	1:E:299:LYS:HG3	2.00	0.43
1:B:292:LEU:HD12	1:B:297:LYS:HB3	2.00	0.43
1:C:274:THR:HG22	1:C:274:THR:O	2.18	0.43
3:H:402:1AQ:H28	3:H:402:1AQ:H10	1.79	0.43
1:E:269:ILE:HD11	1:E:282:GLU:HG3	2.01	0.42
1:D:291:ALA:HA	1:D:298:VAL:HG12	2.00	0.42
1:D:265:TYR:OH	1:D:269:ILE:HD13	2.20	0.42
1:D:327:CYS:HB3	1:D:330:LEU:HB3	2.00	0.42
1:C:345:THR:HG22	1:C:346:HIS:ND1	2.34	0.42
1:A:349:GLU:HG2	3:F:403:1AQ:H22	2.00	0.41
1:H:307:LEU:HD23	3:H:402:1AQ:H12	2.01	0.41
1:A:307:LEU:HD23	3:A:403:1AQ:H12	2.02	0.41
1:G:265:TYR:CZ	1:G:269:ILE:HD13	2.55	0.41
3:D:403:1AQ:H10	3:D:403:1AQ:H28	1.90	0.41
3:G:403:1AQ:H28	3:G:403:1AQ:H10	1.90	0.41
1:H:254:THR:HG23	1:H:254:THR:O	2.20	0.41
1:B:291:ALA:O	1:B:292:LEU:HD23	2.21	0.41
1:D:338:TYR:CZ	1:D:342:ILE:HD11	2.55	0.41
1:E:323:TRP:CH2	3:E:403:1AQ:H7	2.56	0.41
1:B:323:TRP:CZ3	3:B:403:1AQ:H7	2.56	0.41
1:D:317:TRP:CD1	1:D:334:LYS:HE3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:273:GLY:O	1:G:274:THR:HB	2.22	0.40
1:C:302:HIS:HD2	1:H:336:GLN:HE22	1.69	0.40

There are no symmetry-related clashes.

## 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	94/125 (75%)	88 (94%)	6 (6%)	0	100	100
1	B	94/125 (75%)	86 (92%)	7 (7%)	1 (1%)	17	47
1	C	95/125 (76%)	93 (98%)	2 (2%)	0	100	100
1	D	96/125 (77%)	88 (92%)	6 (6%)	2 (2%)	9	27
1	E	94/125 (75%)	85 (90%)	9 (10%)	0	100	100
1	F	94/125 (75%)	90 (96%)	4 (4%)	0	100	100
1	G	96/125 (77%)	87 (91%)	9 (9%)	0	100	100
1	H	94/125 (75%)	83 (88%)	10 (11%)	1 (1%)	17	47
All	All	757/1000 (76%)	700 (92%)	53 (7%)	4 (0%)	34	67

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	274	THR
1	B	312	PRO
1	D	273	GLY
1	H	273	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	81/107 (76%)	76 (94%)	5 (6%)	23	52
1	B	81/107 (76%)	79 (98%)	2 (2%)	55	85
1	C	82/107 (77%)	79 (96%)	3 (4%)	41	74
1	D	83/107 (78%)	75 (90%)	8 (10%)	10	28
1	E	81/107 (76%)	78 (96%)	3 (4%)	41	74
1	F	81/107 (76%)	80 (99%)	1 (1%)	78	94
1	G	83/107 (78%)	79 (95%)	4 (5%)	31	64
1	H	81/107 (76%)	79 (98%)	2 (2%)	55	85
All	All	653/856 (76%)	625 (96%)	28 (4%)	35	69

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	261	SER
1	A	286	ARG
1	A	309	ASP
1	A	328	LYS
1	A	348	LEU
1	B	309	ASP
1	B	344	LEU
1	C	264	ASP
1	C	279	VAL
1	C	328	LYS
1	D	274	THR
1	D	278	SER
1	D	286	ARG
1	D	309	ASP
1	D	341	ASN
1	D	344	LEU
1	D	346	HIS
1	D	348	LEU
1	E	328	LYS

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Mol	Chain	Res	Type
1	E	344	LEU
1	E	346	HIS
1	F	328	LYS
1	G	282	GLU
1	G	341	ASN
1	G	348	LEU
1	G	351	CYS
1	H	261	SER
1	H	349	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	302	HIS
1	A	319	GLN
1	B	302	HIS
1	B	319	GLN
1	B	336	GLN
1	C	302	HIS
1	C	336	GLN
1	D	283	GLN
1	D	302	HIS
1	D	341	ASN
1	E	302	HIS
1	E	336	GLN
1	F	336	GLN
1	F	341	ASN
1	G	283	GLN
1	G	302	HIS
1	G	336	GLN
1	G	341	ASN
1	H	302	HIS
1	H	336	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 22 ligands modelled in this entry, 14 are monoatomic - leaving 8 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$
3	1AQ	A	403	-	44,47,47	0.83	1 (2%)	54,68,68	1.77	13 (24%)
3	1AQ	B	403	-	44,47,47	0.90	2 (4%)	54,68,68	1.40	8 (14%)
3	1AQ	C	402	-	44,47,47	0.82	0	54,68,68	1.79	12 (22%)
3	1AQ	D	403	-	44,47,47	0.84	0	54,68,68	1.89	14 (25%)
3	1AQ	E	403	-	44,47,47	0.91	1 (2%)	54,68,68	1.56	8 (14%)
3	1AQ	F	403	-	44,47,47	0.82	0	54,68,68	1.83	13 (24%)
3	1AQ	G	403	-	44,47,47	0.81	0	54,68,68	1.76	13 (24%)
3	1AQ	H	402	-	44,47,47	0.82	1 (2%)	54,68,68	1.71	13 (24%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	1AQ	A	403	-	-	0/33/79/79	0/5/5/5
3	1AQ	B	403	-	-	0/33/79/79	0/5/5/5
3	1AQ	C	402	-	-	0/33/79/79	0/5/5/5
3	1AQ	D	403	-	-	0/33/79/79	0/5/5/5
3	1AQ	E	403	-	-	0/33/79/79	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	1AQ	F	403	-	-	0/33/79/79	0/5/5/5
3	1AQ	G	403	-	-	0/33/79/79	0/5/5/5
3	1AQ	H	402	-	-	0/33/79/79	0/5/5/5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	403	1AQ	C9-N10	2.00	1.49	1.46
3	H	402	1AQ	C9-N10	2.01	1.49	1.46
3	B	403	1AQ	C9-N10	2.01	1.49	1.46
3	B	403	1AQ	F47-C45	2.15	1.40	1.38
3	E	403	1AQ	F47-C45	2.34	1.41	1.38

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	403	1AQ	F47-C45-C48	-4.22	106.94	109.41
3	A	403	1AQ	F46-C45-C48	-4.09	107.02	109.41
3	F	403	1AQ	F46-C45-C44	-4.07	107.03	109.41
3	G	403	1AQ	C44-C43-C42	-4.06	104.73	111.89
3	C	402	1AQ	C48-C49-C42	-3.96	104.92	111.89
3	D	403	1AQ	C48-C49-C42	-3.81	105.17	111.89
3	F	403	1AQ	C44-C43-C42	-3.81	105.18	111.89
3	H	402	1AQ	F47-C45-C48	-3.77	107.21	109.41
3	C	402	1AQ	F46-C45-C48	-3.76	107.22	109.41
3	A	403	1AQ	C44-C43-C42	-3.75	105.28	111.89
3	F	403	1AQ	C48-C49-C42	-3.74	105.29	111.89
3	G	403	1AQ	F46-C45-C48	-3.74	107.22	109.41
3	D	403	1AQ	F46-C45-C44	-3.66	107.27	109.41
3	G	403	1AQ	C21-C19-N18	-3.65	106.34	111.71
3	F	403	1AQ	C21-C19-N18	-3.63	106.37	111.71
3	A	403	1AQ	C21-C19-N18	-3.62	106.39	111.71
3	C	402	1AQ	C44-C43-C42	-3.48	105.75	111.89
3	H	402	1AQ	C48-C49-C42	-3.40	105.91	111.89
3	A	403	1AQ	C48-C49-C42	-3.30	106.07	111.89
3	D	403	1AQ	C44-C43-C42	-3.22	106.21	111.89
3	G	403	1AQ	F47-C45-C44	-3.12	107.59	109.41
3	H	402	1AQ	F46-C45-C44	-2.95	107.69	109.41
3	H	402	1AQ	C21-C19-N18	-2.93	107.40	111.71
3	D	403	1AQ	O23-C24-C29	-2.82	119.73	122.80
3	G	403	1AQ	O23-C24-C29	-2.81	119.73	122.80
3	C	402	1AQ	O23-C24-C29	-2.74	119.82	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	403	1AQ	C21-C19-N18	-2.72	107.72	111.71
3	D	403	1AQ	C21-C19-N18	-2.67	107.78	111.71
3	F	403	1AQ	F47-C45-C48	-2.65	107.86	109.41
3	E	403	1AQ	O23-C24-C29	-2.61	119.95	122.80
3	E	403	1AQ	F46-C45-C44	-2.60	107.89	109.41
3	G	403	1AQ	C48-C49-C42	-2.54	107.42	111.89
3	B	403	1AQ	C21-C19-N18	-2.53	107.99	111.71
3	C	402	1AQ	C21-C19-N18	-2.42	108.16	111.71
3	B	403	1AQ	O23-C24-C29	-2.41	120.18	122.80
3	F	403	1AQ	F46-C45-C48	-2.38	108.02	109.41
3	H	402	1AQ	O23-C24-C29	-2.36	120.23	122.80
3	F	403	1AQ	O23-C24-C29	-2.33	120.27	122.80
3	H	402	1AQ	C29-C19-N18	-2.29	105.36	111.28
3	A	403	1AQ	F47-C45-C48	-2.19	108.13	109.41
3	B	403	1AQ	O31-C30-C32	-2.15	115.91	120.12
3	G	403	1AQ	F46-C45-C44	-2.14	108.16	109.41
3	A	403	1AQ	O23-C24-C29	-2.12	120.50	122.80
3	C	402	1AQ	C35-C37-N40	-2.09	107.97	112.35
3	C	402	1AQ	F47-C45-C44	-2.03	108.22	109.41
3	D	403	1AQ	C2-O3-C4	2.09	116.73	113.89
3	A	403	1AQ	C2-O3-C4	2.12	116.77	113.89
3	D	403	1AQ	C32-C30-N10	2.16	124.29	118.62
3	F	403	1AQ	C9-N10-C11	2.18	120.69	115.95
3	H	402	1AQ	C42-C32-C30	2.22	115.62	110.86
3	G	403	1AQ	C42-C32-C30	2.23	115.64	110.86
3	B	403	1AQ	C2-O3-C4	2.24	116.93	113.89
3	F	403	1AQ	C2-O3-C4	2.27	116.97	113.89
3	D	403	1AQ	C6-C4-C15	2.28	105.69	103.64
3	H	402	1AQ	C9-N10-C11	2.29	120.92	115.95
3	B	403	1AQ	C32-C30-N10	2.30	124.65	118.62
3	G	403	1AQ	C9-N10-C11	2.30	120.94	115.95
3	D	403	1AQ	C42-C32-C30	2.30	115.80	110.86
3	A	403	1AQ	C32-C30-N10	2.31	124.69	118.62
3	B	403	1AQ	C9-N10-C11	2.32	120.99	115.95
3	E	403	1AQ	C32-C30-N10	2.36	124.81	118.62
3	E	403	1AQ	C2-O3-C4	2.40	117.14	113.89
3	A	403	1AQ	C42-C32-C30	2.41	116.02	110.86
3	E	403	1AQ	C9-N10-C11	2.42	121.21	115.95
3	H	402	1AQ	C2-O3-C4	2.46	117.23	113.89
3	H	402	1AQ	F47-C45-C44	2.47	110.85	109.41
3	G	403	1AQ	C6-C4-C15	2.57	105.95	103.64
3	F	403	1AQ	F46-C45-F47	2.67	108.60	105.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	403	1AQ	C9-N10-C11	2.67	121.75	115.95
3	D	403	1AQ	C9-N10-C11	2.69	121.78	115.95
3	H	402	1AQ	F46-C45-F47	2.86	108.85	105.11
3	G	403	1AQ	C43-C42-C32	2.89	115.79	111.98
3	A	403	1AQ	F46-C45-F47	2.91	108.91	105.11
3	F	403	1AQ	C42-C32-C30	2.99	117.27	110.86
3	C	402	1AQ	C2-O3-C4	3.00	117.96	113.89
3	C	402	1AQ	C9-N10-C11	3.01	122.48	115.95
3	C	402	1AQ	F46-C45-F47	3.08	109.14	105.11
3	D	403	1AQ	F46-C45-F47	3.08	109.14	105.11
3	G	403	1AQ	F46-C45-F47	3.36	109.50	105.11
3	B	403	1AQ	F46-C45-F47	3.37	109.52	105.11
3	H	402	1AQ	C43-C42-C32	3.39	116.45	111.98
3	A	403	1AQ	C43-C42-C32	3.70	116.87	111.98
3	F	403	1AQ	C43-C42-C32	3.92	117.15	111.98
3	C	402	1AQ	C13-C11-N10	4.01	113.51	109.44
3	A	403	1AQ	C13-C11-N10	4.26	113.76	109.44
3	C	402	1AQ	C43-C42-C32	4.29	117.64	111.98
3	D	403	1AQ	C43-C42-C32	4.33	117.69	111.98
3	E	403	1AQ	F46-C45-F47	4.40	110.85	105.11
3	G	403	1AQ	C13-C11-N10	4.75	114.26	109.44
3	F	403	1AQ	C13-C11-N10	5.00	114.51	109.44
3	B	403	1AQ	C13-C11-N10	5.12	114.63	109.44
3	H	402	1AQ	C13-C11-N10	5.12	114.63	109.44
3	E	403	1AQ	C13-C11-N10	5.45	114.97	109.44
3	D	403	1AQ	C13-C11-N10	5.50	115.02	109.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	403	1AQ	6	0
3	B	403	1AQ	2	0
3	D	403	1AQ	4	0
3	E	403	1AQ	3	0
3	F	403	1AQ	2	0
3	G	403	1AQ	1	0
3	H	402	1AQ	2	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	96/125 (76%)	-0.31	0 100 100	47, 64, 106, 114	0
1	B	96/125 (76%)	0.34	5 (5%) 31 21	47, 90, 131, 156	0
1	C	97/125 (77%)	-0.17	2 (2%) 67 57	46, 62, 96, 153	0
1	D	98/125 (78%)	-0.02	4 (4%) 41 30	45, 77, 115, 143	0
1	E	96/125 (76%)	0.10	3 (3%) 52 41	48, 91, 133, 163	0
1	F	96/125 (76%)	0.21	4 (4%) 40 29	48, 86, 134, 152	0
1	G	98/125 (78%)	0.07	3 (3%) 52 41	56, 93, 138, 151	0
1	H	96/125 (76%)	0.34	2 (2%) 67 57	48, 95, 140, 158	0
All	All	773/1000 (77%)	0.07	23 (2%) 54 43	45, 80, 132, 163	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	274	THR	4.7
1	C	348	LEU	4.6
1	B	273	GLY	3.8
1	B	274	THR	3.1
1	F	274	THR	2.9
1	E	275	TRP	2.8
1	D	254	THR	2.7
1	B	266	GLU	2.7
1	G	312	PRO	2.7
1	G	277	TYR	2.6
1	D	274	THR	2.5
1	D	294	GLU	2.5
1	H	279	VAL	2.5
1	E	279	VAL	2.4
1	F	267	ALA	2.4
1	C	349	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	270	PHE	2.1
1	B	261	SER	2.1
1	D	348	LEU	2.1
1	F	276	ILE	2.1
1	E	278	SER	2.1
1	B	276	ILE	2.0
1	G	266	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 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	1AQ	C	402	43/43	0.93	0.27	1.93	56,65,81,91	0
3	1AQ	D	403	43/43	0.91	0.23	0.36	65,80,92,98	0
3	1AQ	A	403	43/43	0.94	0.22	0.33	66,72,90,93	0
3	1AQ	F	403	43/43	0.93	0.23	0.21	57,74,86,101	0
3	1AQ	G	403	43/43	0.92	0.19	0.20	69,80,87,98	0
3	1AQ	H	402	43/43	0.89	0.22	-0.13	82,90,108,118	0
3	1AQ	E	403	43/43	0.93	0.21	-0.14	62,75,97,105	0
3	1AQ	B	403	43/43	0.93	0.19	-0.53	70,85,105,108	0
2	ZN	H	401	1/1	0.99	0.12	-1.03	69,69,69,69	0
2	ZN	B	401	1/1	0.99	0.11	-1.18	64,64,64,64	0
2	ZN	G	401	1/1	0.98	0.11	-1.48	71,71,71,71	0
2	ZN	F	402	1/1	0.86	0.14	-1.49	110,110,110,110	0
2	ZN	G	402	1/1	0.98	0.16	-1.57	100,100,100,100	0
2	ZN	A	401	1/1	1.00	0.11	-1.96	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ZN	C	401	1/1	0.99	0.10	-2.11	47,47,47,47	0
2	ZN	D	402	1/1	0.89	0.11	-2.15	116,116,116,116	0
2	ZN	F	401	1/1	1.00	0.11	-2.19	67,67,67,67	0
2	ZN	D	401	1/1	1.00	0.08	-2.51	59,59,59,59	0
2	ZN	E	402	1/1	0.93	0.09	-2.74	115,115,115,115	0
2	ZN	E	401	1/1	1.00	0.10	-2.83	66,66,66,66	0
2	ZN	A	402	1/1	0.95	0.09	-3.01	94,94,94,94	0
2	ZN	B	402	1/1	0.91	0.10	-3.31	99,99,99,99	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.