



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:26 AM GMT

PDB ID : 2QRA  
Title : Crystal structure of XIAP BIR1 domain (P21 form)  
Authors : Lin, S.-C.  
Deposited on : 2007-07-27  
Resolution : 2.50 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

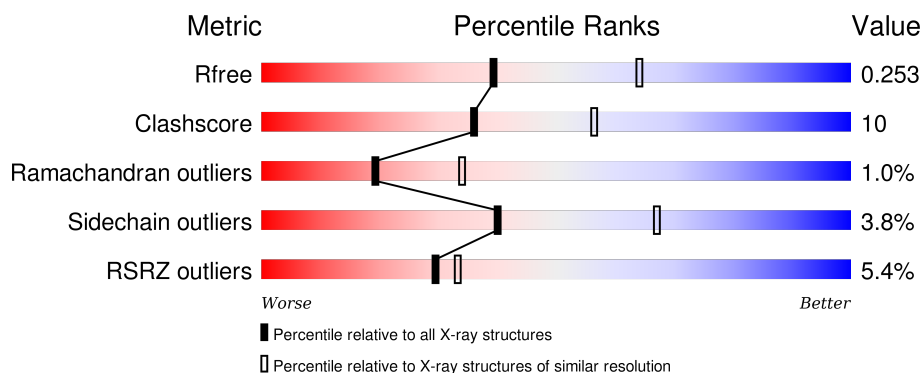
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	111	<div> <div>3%</div> <div>56% 14% • 28%</div> </div>
1	B	111	<div> <div>5%</div> <div>46% 22% •• 30%</div> </div>
1	C	111	<div> <div>3%</div> <div>59% 13% 28%</div> </div>
1	D	111	<div> <div>5%</div> <div>55% 15% 30%</div> </div>

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
3	EOH	A	5002	-	-	-	X
3	EOH	D	5001	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2595 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	D	78	Total	C	N	O	S	0	0	0
			618	390	111	114	3			
1	C	80	Total	C	N	O	S	0	0	0
			636	400	113	120	3			
1	B	78	Total	C	N	O	S	0	0	0
			618	390	111	114	3			
1	A	80	Total	C	N	O	S	0	0	0
			636	400	113	120	3			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	2989	MET	-	EXPRESSION TAG	UNP P98170
D	2990	GLY	-	EXPRESSION TAG	UNP P98170
D	2991	SER	-	EXPRESSION TAG	UNP P98170
D	2992	SER	-	EXPRESSION TAG	UNP P98170
D	2993	HIS	-	EXPRESSION TAG	UNP P98170
D	2994	HIS	-	EXPRESSION TAG	UNP P98170
D	2995	HIS	-	EXPRESSION TAG	UNP P98170
D	2996	HIS	-	EXPRESSION TAG	UNP P98170
D	2997	HIS	-	EXPRESSION TAG	UNP P98170
D	2998	HIS	-	EXPRESSION TAG	UNP P98170
D	2999	SER	-	EXPRESSION TAG	UNP P98170
D	3000	SER	-	EXPRESSION TAG	UNP P98170
D	3001	GLY	-	EXPRESSION TAG	UNP P98170
D	3002	LEU	-	EXPRESSION TAG	UNP P98170
D	3003	VAL	-	EXPRESSION TAG	UNP P98170
D	3004	PRO	-	EXPRESSION TAG	UNP P98170
D	3005	ARG	-	EXPRESSION TAG	UNP P98170
D	3006	GLY	-	EXPRESSION TAG	UNP P98170
D	3007	SER	-	EXPRESSION TAG	UNP P98170
D	3008	HIS	-	EXPRESSION TAG	UNP P98170
D	3009	MET	-	EXPRESSION TAG	UNP P98170

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1989	MET	-	EXPRESSION TAG	UNP P98170
C	1990	GLY	-	EXPRESSION TAG	UNP P98170
C	1991	SER	-	EXPRESSION TAG	UNP P98170
C	1992	SER	-	EXPRESSION TAG	UNP P98170
C	1993	HIS	-	EXPRESSION TAG	UNP P98170
C	1994	HIS	-	EXPRESSION TAG	UNP P98170
C	1995	HIS	-	EXPRESSION TAG	UNP P98170
C	1996	HIS	-	EXPRESSION TAG	UNP P98170
C	1997	HIS	-	EXPRESSION TAG	UNP P98170
C	1998	HIS	-	EXPRESSION TAG	UNP P98170
C	1999	SER	-	EXPRESSION TAG	UNP P98170
C	2000	SER	-	EXPRESSION TAG	UNP P98170
C	2001	GLY	-	EXPRESSION TAG	UNP P98170
C	2002	LEU	-	EXPRESSION TAG	UNP P98170
C	2003	VAL	-	EXPRESSION TAG	UNP P98170
C	2004	PRO	-	EXPRESSION TAG	UNP P98170
C	2005	ARG	-	EXPRESSION TAG	UNP P98170
C	2006	GLY	-	EXPRESSION TAG	UNP P98170
C	2007	SER	-	EXPRESSION TAG	UNP P98170
C	2008	HIS	-	EXPRESSION TAG	UNP P98170
C	2009	MET	-	EXPRESSION TAG	UNP P98170
B	989	MET	-	EXPRESSION TAG	UNP P98170
B	990	GLY	-	EXPRESSION TAG	UNP P98170
B	991	SER	-	EXPRESSION TAG	UNP P98170
B	992	SER	-	EXPRESSION TAG	UNP P98170
B	993	HIS	-	EXPRESSION TAG	UNP P98170
B	994	HIS	-	EXPRESSION TAG	UNP P98170
B	995	HIS	-	EXPRESSION TAG	UNP P98170
B	996	HIS	-	EXPRESSION TAG	UNP P98170
B	997	HIS	-	EXPRESSION TAG	UNP P98170
B	998	HIS	-	EXPRESSION TAG	UNP P98170
B	999	SER	-	EXPRESSION TAG	UNP P98170
B	1000	SER	-	EXPRESSION TAG	UNP P98170
B	1001	GLY	-	EXPRESSION TAG	UNP P98170
B	1002	LEU	-	EXPRESSION TAG	UNP P98170
B	1003	VAL	-	EXPRESSION TAG	UNP P98170
B	1004	PRO	-	EXPRESSION TAG	UNP P98170
B	1005	ARG	-	EXPRESSION TAG	UNP P98170
B	1006	GLY	-	EXPRESSION TAG	UNP P98170
B	1007	SER	-	EXPRESSION TAG	UNP P98170
B	1008	HIS	-	EXPRESSION TAG	UNP P98170
B	1009	MET	-	EXPRESSION TAG	UNP P98170

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	EXPRESSION TAG	UNP P98170
A	-10	GLY	-	EXPRESSION TAG	UNP P98170
A	-9	SER	-	EXPRESSION TAG	UNP P98170
A	-8	SER	-	EXPRESSION TAG	UNP P98170
A	-7	HIS	-	EXPRESSION TAG	UNP P98170
A	-6	HIS	-	EXPRESSION TAG	UNP P98170
A	-5	HIS	-	EXPRESSION TAG	UNP P98170
A	-4	HIS	-	EXPRESSION TAG	UNP P98170
A	-3	HIS	-	EXPRESSION TAG	UNP P98170
A	-2	HIS	-	EXPRESSION TAG	UNP P98170
A	-1	SER	-	EXPRESSION TAG	UNP P98170
A	0	SER	-	EXPRESSION TAG	UNP P98170
A	1	GLY	-	EXPRESSION TAG	UNP P98170
A	2	LEU	-	EXPRESSION TAG	UNP P98170
A	3	VAL	-	EXPRESSION TAG	UNP P98170
A	4	PRO	-	EXPRESSION TAG	UNP P98170
A	5	ARG	-	EXPRESSION TAG	UNP P98170
A	6	GLY	-	EXPRESSION TAG	UNP P98170
A	7	SER	-	EXPRESSION TAG	UNP P98170
A	8	HIS	-	EXPRESSION TAG	UNP P98170
A	9	MET	-	EXPRESSION TAG	UNP P98170

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

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

- Molecule 3 is ETHANOL (three-letter code: EOH) (formula: C<sub>2</sub>H<sub>6</sub>O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	C	O	0	0
			3	2	1		
3	A	1	Total	C	O	0	0
			3	2	1		
3	A	1	Total	C	O	0	0
			3	2	1		
3	C	1	Total	C	O	0	0
			3	2	1		
3	C	1	Total	C	O	0	0
			3	2	1		
3	C	1	Total	C	O	0	0
			3	2	1		

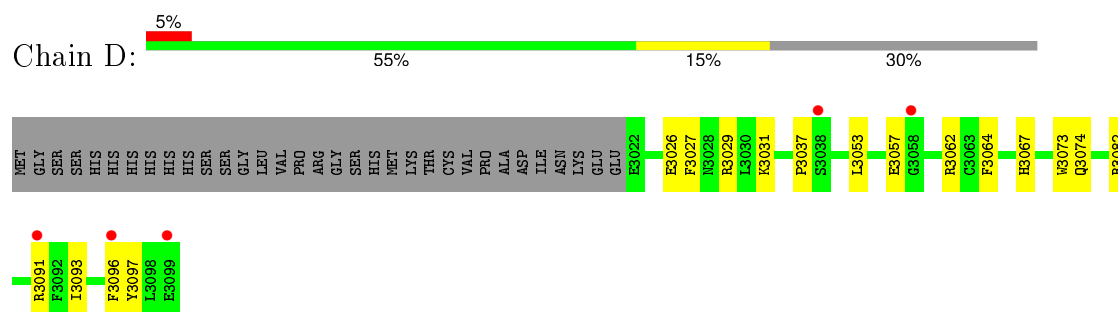
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	8	Total	O	0	0
			8	8		
4	C	27	Total	O	0	0
			27	27		
4	B	5	Total	O	0	0
			5	5		
4	A	25	Total	O	0	0
			25	25		

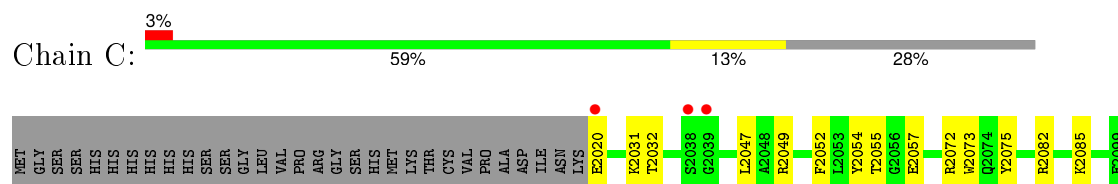
### 3 Residue-property plots [i](#)

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.

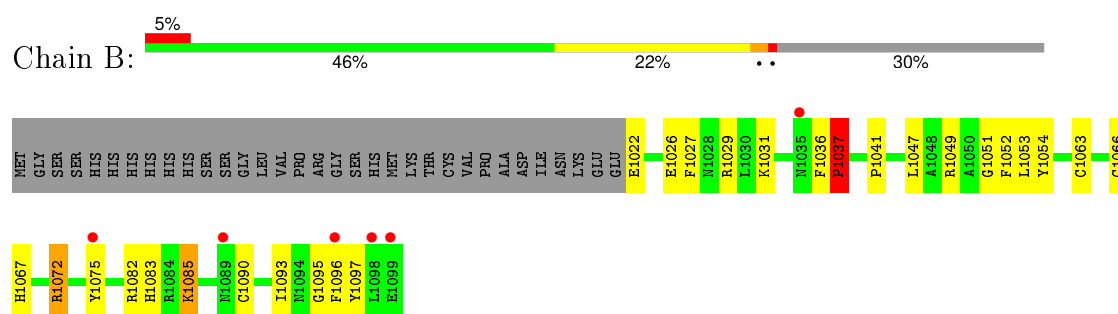
- Molecule 1: Baculoviral IAP repeat-containing protein 4



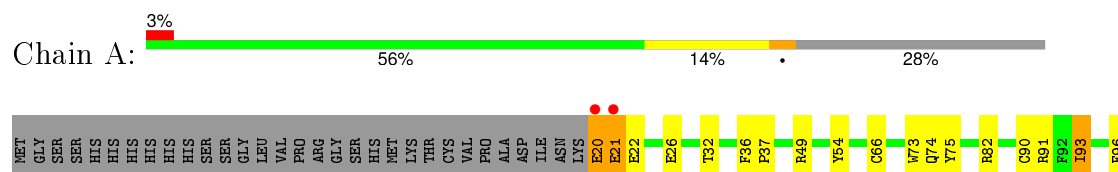
- Molecule 1: Baculoviral IAP repeat-containing protein 4



- Molecule 1: Baculoviral IAP repeat-containing protein 4



- Molecule 1: Baculoviral IAP repeat-containing protein 4







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	36.56Å 72.98Å 68.90Å 90.00° 95.69° 90.00°	Depositor
Resolution (Å)	30.00 – 2.50 26.29 – 2.46	Depositor EDS
% Data completeness (in resolution range)	97.6 (30.00-2.50) 95.9 (26.29-2.46)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.71 (at 2.47Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.196 , 0.253 0.196 , 0.253	Depositor DCC
$R_{free}$ test set	1266 reflections (10.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	38.0	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 49.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 12803 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	2595	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	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 20.38 % 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 8.7927e-03. 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

### 5.1 Standard geometry

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

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	0.62	0/653	0.74	0/880
1	B	0.49	0/635	0.66	1/856 (0.1%)
1	C	0.62	0/653	0.69	0/880
1	D	0.50	0/635	0.62	0/856
All	All	0.56	0/2576	0.68	1/3472 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1072	ARG	NE-CZ-NH2	-5.03	117.78	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	75	TYR	Sidechain

## 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	636	0	586	11	0
1	B	618	0	574	16	0
1	C	636	0	586	10	0
1	D	618	0	574	12	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
3	A	6	0	12	0	0
3	C	9	0	18	2	0
3	D	3	0	6	0	0
4	A	25	0	0	0	0
4	B	5	0	0	0	0
4	C	27	0	0	0	0
4	D	8	0	0	0	0
All	All	2595	0	2356	47	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 10.

All (47) 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:C:2075:TYR:HB2	3:C:5006:EOH:H11	1.50	0.91
1:C:2049:ARG:HB2	1:C:2049:ARG:HH11	1.52	0.73
1:C:2049:ARG:NH1	1:C:2049:ARG:HB2	2.06	0.69
1:A:20:GLU:HB3	1:A:22:GLU:HG2	1.74	0.69
1:D:3091:ARG:HH11	1:D:3091:ARG:HG3	1.63	0.64
1:B:1047:LEU:O	1:B:1052:PHE:HB2	2.04	0.58
1:B:1063:CYS:O	1:B:1067:HIS:HA	2.03	0.57
1:B:1083:HIS:ND1	1:B:1093:ILE:HD11	2.21	0.56
1:B:1027:PHE:CE2	1:B:1031:LYS:HE3	2.41	0.55
1:A:21:GLU:HA	1:A:21:GLU:OE1	2.06	0.55
1:A:73:TRP:CZ3	1:A:82:ARG:HD3	2.43	0.54
1:B:1063:CYS:HB3	1:B:1066:CYS:SG	2.48	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3073:TRP:CZ3	1:D:3082:ARG:HD3	2.43	0.53
1:D:3091:ARG:NH1	1:D:3091:ARG:HG3	2.25	0.52
1:C:2055:THR:HG21	3:C:5004:EOH:H11	1.93	0.50
1:C:2082:ARG:O	1:C:2085:LYS:HB3	2.12	0.49
1:C:2049:ARG:CB	1:C:2049:ARG:HH11	2.25	0.49
1:B:1049:ARG:C	1:B:1051:GLY:H	2.17	0.48
1:C:2073:TRP:CZ3	1:C:2082:ARG:HD3	2.50	0.47
1:A:32:THR:O	1:A:54:TYR:HB3	2.14	0.47
1:B:1029:ARG:HG2	1:B:1053:LEU:HD21	1.98	0.46
1:B:1036:PHE:O	1:B:1037:PRO:C	2.52	0.46
1:B:1022:GLU:OE2	1:B:1022:GLU:O	2.33	0.45
1:D:3062:ARG:HG3	1:D:3067:HIS:O	2.16	0.45
1:B:1041:PRO:HB3	1:B:1075:TYR:CD1	2.52	0.45
1:C:2072:ARG:NH1	1:A:74:GLN:HG3	2.31	0.45
1:D:3026:GLU:O	1:D:3029:ARG:HB2	2.17	0.45
1:D:3096:PHE:C	1:D:3096:PHE:CD1	2.90	0.45
1:B:1036:PHE:HA	1:B:1054:TYR:CE1	2.52	0.44
1:B:1026:GLU:O	1:B:1029:ARG:N	2.39	0.44
1:B:1082:ARG:O	1:B:1085:LYS:HB2	2.17	0.44
1:D:3074:GLN:HG2	1:B:1072:ARG:NH1	2.33	0.44
1:C:2032:THR:O	1:C:2054:TYR:HB3	2.19	0.42
1:A:96:PHE:CD1	1:A:96:PHE:C	2.92	0.42
1:C:2047:LEU:O	1:C:2052:PHE:HB2	2.20	0.42
1:A:66:CYS:HB3	1:A:90:CYS:SG	2.58	0.42
1:B:1036:PHE:CD1	1:B:1037:PRO:HD2	2.55	0.42
1:A:93:ILE:HA	1:A:93:ILE:HD12	1.91	0.42
1:D:3097:TYR:N	1:D:3097:TYR:CD1	2.88	0.41
1:D:3029:ARG:HD3	1:D:3064:PHE:CD2	2.55	0.41
1:A:36:PHE:CD1	1:A:37:PRO:HD2	2.55	0.41
1:B:1095:GLY:O	1:B:1097:TYR:N	2.54	0.41
1:A:26:GLU:OE2	1:A:49:ARG:HB2	2.21	0.40
1:A:91:ARG:O	1:A:96:PHE:HB3	2.21	0.40
1:D:3093:ILE:HD13	1:D:3093:ILE:HA	1.94	0.40
1:D:3029:ARG:HG2	1:D:3053:LEU:HD21	2.04	0.40
1:D:3027:PHE:CE2	1:D:3031:LYS:HE3	2.56	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	78/111 (70%)	74 (95%)	4 (5%)	0	100	100
1	B	76/111 (68%)	65 (86%)	9 (12%)	2 (3%)	7	10
1	C	78/111 (70%)	78 (100%)	0	0	100	100
1	D	76/111 (68%)	67 (88%)	8 (10%)	1 (1%)	15	26
All	All	308/444 (69%)	284 (92%)	21 (7%)	3 (1%)	19	34

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1037	PRO
1	B	1096	PHE
1	D	3037	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	66/93 (71%)	63 (96%)	3 (4%)	34	59
1	B	64/93 (69%)	61 (95%)	3 (5%)	32	56
1	C	66/93 (71%)	63 (96%)	3 (4%)	34	59
1	D	64/93 (69%)	63 (98%)	1 (2%)	70	90
All	All	260/372 (70%)	250 (96%)	10 (4%)	40	67

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	3057	GLU
1	C	2020	GLU
1	C	2031	LYS
1	C	2057	GLU
1	B	1037	PRO
1	B	1085	LYS
1	B	1090	CYS
1	A	20	GLU
1	A	21	GLU
1	A	93	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	2074	GLN
1	B	1035	ASN

### 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 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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	EOH	A	5002	-	2,2,2	0.47	0	1,1,1	0.30	0
3	EOH	A	5003	-	2,2,2	0.43	0	1,1,1	0.46	0
3	EOH	C	5004	-	2,2,2	0.55	0	1,1,1	0.32	0
3	EOH	C	5005	-	2,2,2	0.58	0	1,1,1	0.36	0
3	EOH	C	5006	-	2,2,2	0.53	0	1,1,1	0.37	0
3	EOH	D	5001	-	2,2,2	0.54	0	1,1,1	0.34	0

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	EOH	A	5002	-	-	0/0/0/0	0/0/0/0
3	EOH	A	5003	-	-	0/0/0/0	0/0/0/0
3	EOH	C	5004	-	-	0/0/0/0	0/0/0/0
3	EOH	C	5005	-	-	0/0/0/0	0/0/0/0
3	EOH	C	5006	-	-	0/0/0/0	0/0/0/0
3	EOH	D	5001	-	-	0/0/0/0	0/0/0/0

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
3	C	5004	EOH	1	0
3	C	5006	EOH	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	80/111 (72%)	-0.03	3 (3%)	44	49	20, 30, 63, 108	0
1	B	78/111 (70%)	0.39	6 (7%)	16	18	26, 54, 83, 113	0
1	C	80/111 (72%)	0.04	3 (3%)	44	49	20, 32, 68, 112	0
1	D	78/111 (70%)	0.29	5 (6%)	23	25	24, 54, 83, 120	0
All	All	316/444 (71%)	0.17	17 (5%)	29	33	20, 40, 80, 120	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2020	GLU	4.8
1	B	1098	LEU	4.5
1	D	3099	GLU	4.2
1	A	20	GLU	4.2
1	B	1096	PHE	4.2
1	A	99	GLU	3.4
1	B	1099	GLU	3.2
1	D	3096	PHE	3.2
1	A	21	GLU	2.8
1	B	1075	TYR	2.8
1	D	3038	SER	2.5
1	C	2038	SER	2.5
1	C	2039	GLY	2.3
1	B	1035	ASN	2.3
1	D	3091	ARG	2.3
1	B	1089	ASN	2.1
1	D	3058	GLY	2.0

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

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	EOH	A	5002	3/3	0.92	0.36	7.46	48,48,48,48	0
3	EOH	D	5001	3/3	0.93	0.39	5.78	48,48,48,48	0
2	ZN	A	100	1/1	1.00	0.11	-0.86	26,26,26,26	0
2	ZN	C	2100	1/1	1.00	0.10	-1.61	26,26,26,26	0
2	ZN	B	1100	1/1	0.99	0.07	-1.79	47,47,47,47	0
2	ZN	D	3100	1/1	0.99	0.07	-2.70	51,51,51,51	0
3	EOH	C	5005	3/3	0.87	0.25	-	48,48,48,48	0
3	EOH	A	5003	3/3	0.94	0.26	-	48,48,48,48	0
3	EOH	C	5004	3/3	0.72	0.28	-	48,48,48,48	0
3	EOH	C	5006	3/3	0.90	0.26	-	48,48,48,48	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.