



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 10:20 PM GMT

PDB ID : 3CLX  
Title : Crystal structure of XIAP BIR3 domain in complex with a Smac-mimetic compound, Smac005  
Authors : Milani, M.; Mastrangelo, E.; Cossu, F.  
Deposited on : 2008-03-20  
Resolution : 2.70 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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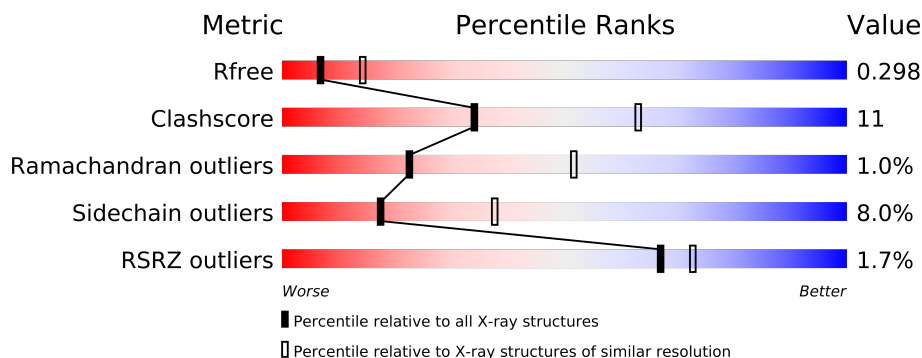
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.70 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))
$R_{free}$	66092	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (2.70-2.70)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	130	
1	B	130	
1	C	130	
1	D	130	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	X22	C	700	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3527 atoms, of which 0 are hydrogen and 0 are deuterium.

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	101	Total	C	N	O	S	0	0	0
			825	528	141	151	5			
1	A	99	Total	C	N	O	S	0	0	0
			804	517	135	147	5			
1	B	101	Total	C	N	O	S	0	1	0
			833	533	144	151	5			
1	C	98	Total	C	N	O	S	0	0	0
			799	514	134	146	5			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	227	MET	-	EXPRESSION TAG	UNP P98170
D	228	ALA	-	EXPRESSION TAG	UNP P98170
D	229	SER	-	EXPRESSION TAG	UNP P98170
D	230	MET	-	EXPRESSION TAG	UNP P98170
D	231	THR	-	EXPRESSION TAG	UNP P98170
D	232	GLY	-	EXPRESSION TAG	UNP P98170
D	233	GLY	-	EXPRESSION TAG	UNP P98170
D	234	GLN	-	EXPRESSION TAG	UNP P98170
D	235	GLN	-	EXPRESSION TAG	UNP P98170
D	236	MET	-	EXPRESSION TAG	UNP P98170
D	237	GLY	-	EXPRESSION TAG	UNP P98170
D	238	ARG	-	EXPRESSION TAG	UNP P98170
D	239	GLY	-	EXPRESSION TAG	UNP P98170
D	240	SER	-	EXPRESSION TAG	UNP P98170
A	227	MET	-	EXPRESSION TAG	UNP P98170
A	228	ALA	-	EXPRESSION TAG	UNP P98170
A	229	SER	-	EXPRESSION TAG	UNP P98170
A	230	MET	-	EXPRESSION TAG	UNP P98170
A	231	THR	-	EXPRESSION TAG	UNP P98170
A	232	GLY	-	EXPRESSION TAG	UNP P98170
A	233	GLY	-	EXPRESSION TAG	UNP P98170

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Chain	Residue	Modelled	Actual	Comment	Reference
A	234	GLN	-	EXPRESSION TAG	UNP P98170
A	235	GLN	-	EXPRESSION TAG	UNP P98170
A	236	MET	-	EXPRESSION TAG	UNP P98170
A	237	GLY	-	EXPRESSION TAG	UNP P98170
A	238	ARG	-	EXPRESSION TAG	UNP P98170
A	239	GLY	-	EXPRESSION TAG	UNP P98170
A	240	SER	-	EXPRESSION TAG	UNP P98170
B	227	MET	-	EXPRESSION TAG	UNP P98170
B	228	ALA	-	EXPRESSION TAG	UNP P98170
B	229	SER	-	EXPRESSION TAG	UNP P98170
B	230	MET	-	EXPRESSION TAG	UNP P98170
B	231	THR	-	EXPRESSION TAG	UNP P98170
B	232	GLY	-	EXPRESSION TAG	UNP P98170
B	233	GLY	-	EXPRESSION TAG	UNP P98170
B	234	GLN	-	EXPRESSION TAG	UNP P98170
B	235	GLN	-	EXPRESSION TAG	UNP P98170
B	236	MET	-	EXPRESSION TAG	UNP P98170
B	237	GLY	-	EXPRESSION TAG	UNP P98170
B	238	ARG	-	EXPRESSION TAG	UNP P98170
B	239	GLY	-	EXPRESSION TAG	UNP P98170
B	240	SER	-	EXPRESSION TAG	UNP P98170
C	227	MET	-	EXPRESSION TAG	UNP P98170
C	228	ALA	-	EXPRESSION TAG	UNP P98170
C	229	SER	-	EXPRESSION TAG	UNP P98170
C	230	MET	-	EXPRESSION TAG	UNP P98170
C	231	THR	-	EXPRESSION TAG	UNP P98170
C	232	GLY	-	EXPRESSION TAG	UNP P98170
C	233	GLY	-	EXPRESSION TAG	UNP P98170
C	234	GLN	-	EXPRESSION TAG	UNP P98170
C	235	GLN	-	EXPRESSION TAG	UNP P98170
C	236	MET	-	EXPRESSION TAG	UNP P98170
C	237	GLY	-	EXPRESSION TAG	UNP P98170
C	238	ARG	-	EXPRESSION TAG	UNP P98170
C	239	GLY	-	EXPRESSION TAG	UNP P98170
C	240	SER	-	EXPRESSION TAG	UNP P98170

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

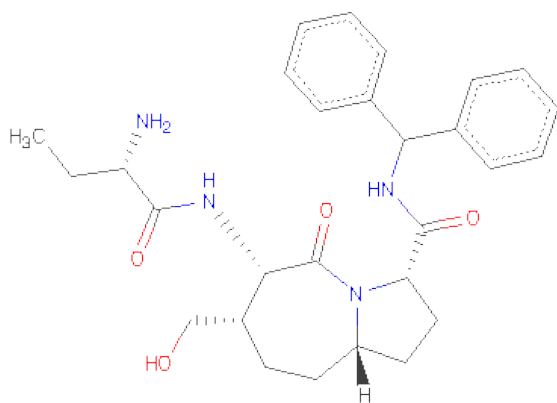
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Zn 1 1	0	0
2	A	1	Total Zn 1 1	0	0

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

- Molecule 3 is (3S,6S,7S,9AS)-6-{[(2S)-2-AMINO BUTANOYL]AMINO}-N-(DIPHENYL METHYL)-7-(HYDROXYMETHYL)-5-OXOOCTAHYDRO-1H-PYRROLO[1,2-A]AZEPINE-3-CARBOXAMIDE (three-letter code: X22) (formula: C<sub>28</sub>H<sub>36</sub>N<sub>4</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	D	1	Total	C	N	O	0	0
			36	28	4	4		
3	A	1	Total	C	N	O	0	0
			36	28	4	4		
3	B	1	Total	C	N	O	0	0
			36	28	4	4		
3	C	1	Total	C	N	O	0	0
			36	28	4	4		
3	C	1	Total	C	N	O	0	0
			36	28	4	4		
3	C	1	Total	C	N	O	0	0
			36	28	4	4		

- Molecule 4 is water.

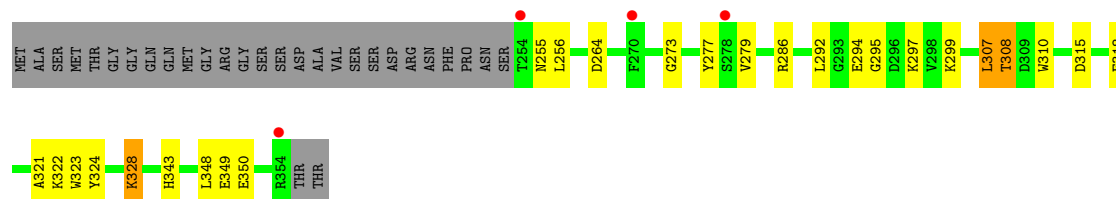
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	15	Total 15	O 15	0	0
4	A	10	Total 10	O 10	0	0
4	B	8	Total 8	O 8	0	0
4	C	13	Total 13	O 13	0	0

### 3 Residue-property plots

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.

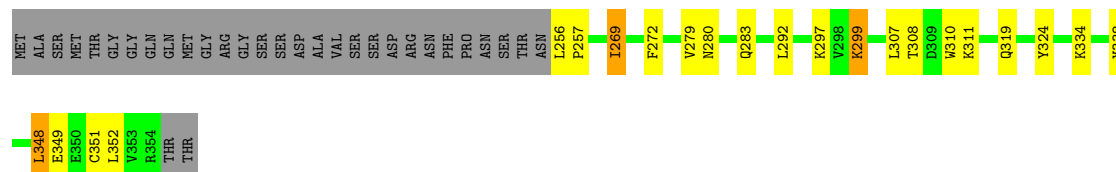
- Molecule 1: Baculoviral IAP repeat-containing protein 4

Chain D: 



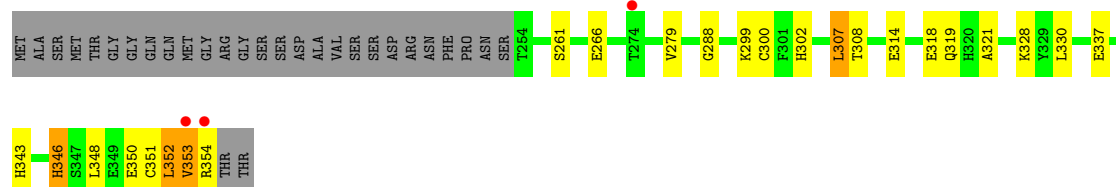
- Molecule 1: Baculoviral IAP repeat-containing protein 4

Chain A: 



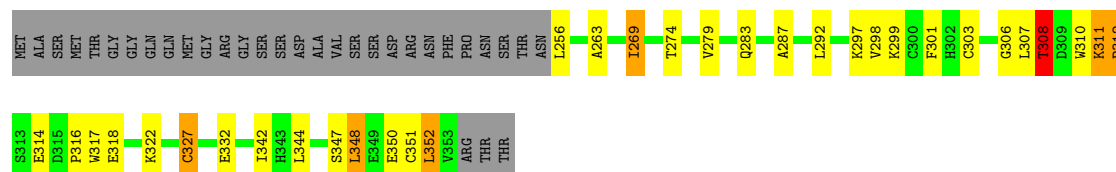
- Molecule 1: Baculoviral IAP repeat-containing protein 4

Chain B: 



- Molecule 1: Baculoviral IAP repeat-containing protein 4

Chain C: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.88Å 115.28Å 163.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.70 39.57 – 2.70	Depositor EDS
% Data completeness (in resolution range)	95.2 (40.00-2.70) 95.2 (39.57-2.70)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.44 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.221 , 0.306 0.216 , 0.298	Depositor DCC
$R_{free}$ test set	824 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	38.7	Xtriage
Anisotropy	0.193	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 18.2	EDS
Estimated twinning fraction	0.035 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.048 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	1 of 16397 reflections (0.006%)	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	3527	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.25% of the height of the origin peak. No significant pseudotranslation is detected.*

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



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, X22

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	0.44	0/830	0.58	0/1125
1	B	0.42	0/860	0.56	0/1165
1	C	0.44	0/825	0.59	0/1118
1	D	0.47	0/851	0.59	0/1153
All	All	0.45	0/3366	0.58	0/4561

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	B	0	2
1	C	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	350	GLU	Peptide
1	B	352	LEU	Peptide
1	C	308	THR	Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	804	0	751	17	0
1	B	833	0	776	15	0
1	C	799	0	749	25	0
1	D	825	0	775	17	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	36	0	36	2	0
3	B	36	0	36	2	0
3	C	108	0	107	10	0
3	D	36	0	36	3	0
4	A	10	0	0	0	0
4	B	8	0	0	4	0
4	C	13	0	0	1	0
4	D	15	0	0	3	0
All	All	3527	0	3266	72	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 11.

All (72) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:352:LEU:O	1:B:353:VAL:HG22	1.85	0.76
1:A:351:CYS:HG	1:C:351:CYS:HG	0.74	0.73
1:B:343:HIS:ND1	4:B:18:HOH:O	2.30	0.64
1:C:303:CYS:HB3	1:C:327:CYS:HB2	1.79	0.64
1:D:350:GLU:HG2	4:D:24:HOH:O	2.00	0.62
1:D:297:LYS:HG2	1:D:308:THR:HG23	1.80	0.61
1:B:314:GLU:CD	3:B:600:X22:HN	2.04	0.60
1:C:306:GLY:O	1:C:307:LEU:HD13	2.01	0.60
1:C:311:LYS:HB3	1:C:312:PRO:HD2	1.82	0.59
1:B:346[A]:HIS:NE2	4:B:8:HOH:O	2.32	0.59
1:D:286:ARG:HD2	4:D:23:HOH:O	2.02	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:352:LEU:O	1:B:353:VAL:CG2	2.52	0.58
4:D:33:HOH:O	3:C:701:X22:HAP	2.03	0.58
1:B:351:CYS:SG	1:B:351:CYS:O	2.61	0.58
1:B:352:LEU:N	1:B:353:VAL:O	2.37	0.57
1:A:279:VAL:HG21	1:A:310:TRP:CB	2.35	0.56
1:D:294:GLU:OE1	1:A:311:LYS:HB3	2.05	0.56
1:A:307:LEU:HD12	1:A:324:TYR:HE1	1.70	0.56
1:C:348:LEU:HD22	1:C:352:LEU:HD22	1.87	0.56
1:C:306:GLY:O	3:C:600:X22:OAD	2.24	0.56
1:A:280:ASN:HB3	1:A:283:GLN:HB2	1.88	0.55
1:D:297:LYS:CG	1:D:308:THR:HG23	2.37	0.54
1:A:292:LEU:HD21	1:A:299:LYS:HB2	1.91	0.53
1:A:256:LEU:N	1:A:257:PRO:HD3	2.23	0.53
1:D:322:LYS:O	3:C:700:X22:HAO	2.08	0.53
1:B:346[A]:HIS:CE1	4:B:1:HOH:O	2.63	0.51
1:D:297:LYS:HG2	3:D:600:X22:HAJ	1.91	0.51
1:A:348:LEU:HD22	1:A:352:LEU:HD22	1.93	0.50
1:C:303:CYS:CB	1:C:327:CYS:HB2	2.42	0.49
3:D:600:X22:HAR	1:A:349:GLU:HG3	1.93	0.49
1:B:321:ALA:HA	1:B:330:LEU:HD21	1.95	0.49
1:C:279:VAL:HG21	1:C:310:TRP:HB3	1.94	0.49
1:B:343:HIS:CE1	4:B:18:HOH:O	2.65	0.49
1:B:307:LEU:HG	3:B:600:X22:HAAA	1.94	0.49
1:C:318:GLU:HG3	1:C:342:ILE:HD12	1.94	0.48
1:D:307:LEU:HD13	1:D:324:TYR:HE1	1.78	0.48
1:C:322:LYS:O	3:C:701:X22:HAI	2.15	0.47
1:A:334:LYS:HB3	1:A:338:TYR:CD2	2.50	0.47
1:C:297:LYS:HG2	3:C:600:X22:HAJ	1.97	0.46
1:D:350:GLU:CD	1:C:350:GLU:HG2	2.36	0.46
1:C:318:GLU:HB2	4:C:25:HOH:O	2.15	0.46
1:C:263:ALA:HA	1:C:301:PHE:CD1	2.51	0.46
1:C:307:LEU:HB3	3:C:600:X22:CAA	2.45	0.46
1:C:298:VAL:O	1:C:306:GLY:HA2	2.16	0.45
1:C:303:CYS:HB3	1:C:327:CYS:CB	2.45	0.45
1:D:315:ASP:HB3	1:D:318:GLU:HB2	1.98	0.45
1:A:307:LEU:HD23	3:A:600:X22:HAA	2.00	0.44
1:A:269:ILE:HA	1:A:272:PHE:HD1	1.80	0.44
1:C:297:LYS:HG2	1:C:308:THR:HG23	1.99	0.43
1:C:283:GLN:HB3	1:C:316:PRO:HG2	1.99	0.43
1:A:279:VAL:HG21	1:A:310:TRP:HB3	1.99	0.43
1:C:344:LEU:HA	3:C:700:X22:HAL	2.00	0.43
1:D:292:LEU:HD21	1:D:299:LYS:HB2	1.99	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:287:ALA:HA	1:C:317:TRP:CZ2	2.53	0.43
1:D:279:VAL:HG21	1:D:310:TRP:HB3	2.01	0.43
1:C:292:LEU:HD21	1:C:299:LYS:HB2	1.99	0.43
1:D:255:ASN:HD22	1:D:328:LYS:HB2	1.84	0.42
1:D:321:ALA:O	1:D:343:HIS:HE1	2.03	0.42
1:C:269:ILE:HG13	1:C:269:ILE:H	1.68	0.42
1:A:307:LEU:CD1	1:A:324:TYR:HE1	2.33	0.41
1:D:277:TYR:OH	1:D:295:GLY:HA2	2.20	0.41
1:C:314:GLU:CD	3:C:600:X22:HN	2.23	0.41
1:B:288:GLY:O	1:B:300:CYS:HA	2.20	0.41
1:B:302:HIS:CE1	1:B:328:LYS:HB3	2.56	0.41
1:C:347:SER:OG	3:C:700:X22:HAH	2.20	0.41
1:D:323:TRP:O	3:C:700:X22:NAW	2.50	0.41
1:A:352:LEU:HA	1:A:352:LEU:HD12	1.84	0.41
1:B:318:GLU:CD	1:B:319:GLN:HE21	2.24	0.41
1:A:297:LYS:HG2	1:A:308:THR:HB	2.03	0.41
1:B:353:VAL:HB	1:B:354:ARG:H	1.67	0.40
1:D:308:THR:OG1	3:D:600:X22:HAN	2.20	0.40
1:A:319:GLN:OE1	3:A:600:X22:HBA	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	97/130 (75%)	95 (98%)	2 (2%)	0	100	100
1	B	100/130 (77%)	95 (95%)	4 (4%)	1 (1%)	22	51
1	C	96/130 (74%)	90 (94%)	4 (4%)	2 (2%)	11	27
1	D	99/130 (76%)	95 (96%)	3 (3%)	1 (1%)	22	51
All	All	392/520 (75%)	375 (96%)	13 (3%)	4 (1%)	22	51

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	273	GLY
1	B	353	VAL
1	C	312	PRO
1	C	332	GLU

### 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	83/109 (76%)	80 (96%)	3 (4%)	47	79
1	B	86/109 (79%)	76 (88%)	10 (12%)	8	18
1	C	83/109 (76%)	75 (90%)	8 (10%)	12	27
1	D	86/109 (79%)	79 (92%)	7 (8%)	17	36
All	All	338/436 (78%)	310 (92%)	28 (8%)	17	35

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

Mol	Chain	Res	Type
1	D	256	LEU
1	D	264	ASP
1	D	307	LEU
1	D	308	THR
1	D	328	LYS
1	D	348	LEU
1	D	349	GLU
1	A	269	ILE
1	A	299	LYS
1	A	348	LEU
1	B	261	SER
1	B	266	GLU
1	B	279	VAL
1	B	299	LYS
1	B	307	LEU
1	B	308	THR
1	B	337	GLU
1	B	346[A]	HIS
1	B	346[B]	HIS

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Mol	Chain	Res	Type
1	B	348	LEU
1	C	256	LEU
1	C	269	ILE
1	C	274	THR
1	C	308	THR
1	C	311	LYS
1	C	327	CYS
1	C	348	LEU
1	C	352	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	255	ASN
1	D	343	HIS
1	B	255	ASN
1	B	302	HIS
1	C	259	ASN
1	C	283	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 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	X22	A	600	-	39,39,39	0.90	2 (5%)	54,54,54	1.98	11 (20%)
3	X22	B	600	-	39,39,39	0.88	1 (2%)	54,54,54	2.03	15 (27%)
3	X22	C	600	-	39,39,39	1.04	3 (7%)	54,54,54	3.18	15 (27%)
3	X22	C	700	-	39,39,39	0.77	2 (5%)	54,54,54	2.13	13 (24%)
3	X22	C	701	-	39,39,39	0.98	2 (5%)	54,54,54	1.81	14 (25%)
3	X22	D	600	-	39,39,39	0.73	0	54,54,54	2.41	15 (27%)

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	X22	A	600	-	-	0/28/58/58	0/2/4/4
3	X22	B	600	-	-	0/28/58/58	0/2/4/4
3	X22	C	600	-	-	0/28/58/58	0/2/4/4
3	X22	C	700	-	-	0/28/58/58	0/2/4/4
3	X22	C	701	-	-	0/28/58/58	0/2/4/4
3	X22	D	600	-	-	0/28/58/58	0/2/4/4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	600	X22	CBI-CBA	3.21	1.57	1.53
3	A	600	X22	CBI-CBA	2.67	1.56	1.53
3	C	600	X22	CBC-CBH	2.61	1.56	1.52
3	A	600	X22	CBG-NBJ	2.61	1.50	1.46
3	C	701	X22	CBA-NBJ	-2.58	1.32	1.35
3	C	600	X22	CBF-NBJ	2.38	1.50	1.47
3	B	600	X22	CBI-CBA	2.28	1.56	1.53
3	C	701	X22	CB-CA	2.22	1.55	1.53
3	C	700	X22	CBA-NBJ	-2.17	1.32	1.35
3	C	700	X22	CB-CA	2.06	1.55	1.53

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	600	X22	CBE-CBI-CBA	10.64	120.70	110.59
3	C	600	X22	CBG-NBJ-CBA	10.35	131.26	118.34
3	C	600	X22	CBG-NBJ-CBF	-9.52	102.33	112.73
3	C	600	X22	CAZ-CBG-NBJ	9.45	131.13	112.12
3	C	600	X22	CBB-CBH-NAW	8.20	127.93	111.18
3	A	600	X22	CBE-CBI-CBA	7.78	117.99	110.59
3	C	701	X22	CBE-CBI-NAX	6.90	119.46	110.72
3	B	600	X22	CBE-CBI-CBA	6.64	116.90	110.59
3	C	700	X22	CBH-NAW-CAZ	6.42	134.95	121.28
3	C	600	X22	CBE-CBI-CBA	6.02	116.31	110.59
3	C	700	X22	CBE-CBI-NAX	5.81	118.08	110.72
3	D	600	X22	CBH-NAW-CAZ	5.70	133.41	121.28
3	B	600	X22	CBH-NAW-CAZ	5.40	132.78	121.28
3	A	600	X22	CBG-NBJ-CBA	5.29	124.94	118.34
3	C	600	X22	CAU-CAV-CBG	-5.05	96.18	103.96
3	C	701	X22	CBG-NBJ-CBA	4.94	124.50	118.34
3	C	700	X22	CAZ-CBG-NBJ	4.84	121.85	112.12
3	A	600	X22	CAU-CBF-NBJ	4.80	106.93	101.69
3	C	600	X22	CBH-NAW-CAZ	-4.75	111.17	121.28
3	A	600	X22	CAZ-CBG-NBJ	4.68	121.53	112.12
3	C	700	X22	CBG-CAZ-NAW	-4.64	106.47	116.70
3	C	700	X22	CBE-CBI-CBA	4.57	114.93	110.59
3	B	600	X22	CBG-NBJ-CBA	4.41	123.84	118.34
3	C	600	X22	CAU-CBF-NBJ	4.36	106.46	101.69
3	C	700	X22	CBG-NBJ-CBA	4.36	123.77	118.34
3	D	600	X22	CAZ-CBG-NBJ	4.10	120.37	112.12
3	B	600	X22	CAU-CBF-NBJ	4.09	106.16	101.69
3	D	600	X22	CBG-NBJ-CBA	4.03	123.36	118.34
3	C	701	X22	CBE-CBI-CBA	3.96	114.35	110.59
3	C	700	X22	CBB-CBH-NAW	3.79	118.92	111.18
3	B	600	X22	CBI-CBA-NBJ	3.75	122.90	116.70
3	D	600	X22	CBI-CBA-NBJ	3.66	122.75	116.70
3	D	600	X22	CAT-CBF-NBJ	-3.58	104.86	111.33
3	C	600	X22	CBA-CBI-NAX	3.57	115.48	108.13
3	D	600	X22	CBG-CAZ-NAW	-3.54	108.90	116.70
3	D	600	X22	OAE-CBA-NBJ	-3.48	117.46	121.68
3	B	600	X22	CAZ-CBG-NBJ	3.24	118.64	112.12
3	C	600	X22	CBG-CAZ-NAW	3.16	123.68	116.70
3	C	701	X22	CAZ-CBG-NBJ	3.16	118.47	112.12
3	C	700	X22	CBB-CBH-CBC	3.14	120.15	112.45
3	B	600	X22	OAE-CBA-CBI	-3.13	118.56	121.81
3	B	600	X22	CBG-CAZ-NAW	-3.10	109.87	116.70
3	D	600	X22	CAU-CBF-NBJ	3.03	105.00	101.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	700	X22	CAU-CBF-NBJ	2.93	104.89	101.69
3	C	700	X22	OAD-CAZ-NAW	2.87	128.46	122.93
3	C	701	X22	CAV-CBG-NBJ	-2.83	100.53	103.03
3	A	600	X22	CAV-CBG-NBJ	2.82	105.52	103.03
3	A	600	X22	CBI-CBA-NBJ	2.77	121.28	116.70
3	D	600	X22	CAO-CBC-CBH	-2.71	115.80	120.71
3	D	600	X22	CAP-CBC-CAO	2.69	121.90	118.33
3	C	701	X22	CBB-CBH-NAW	-2.69	105.69	111.18
3	A	600	X22	CAT-CBF-NBJ	2.67	116.15	111.33
3	D	600	X22	CBB-CBH-NAW	2.65	116.60	111.18
3	B	600	X22	OAE-CBA-NBJ	-2.61	118.51	121.68
3	C	600	X22	CBC-CBH-NAW	-2.60	105.87	111.18
3	B	600	X22	CBC-CBH-NAW	2.58	116.44	111.18
3	C	701	X22	CBA-CBI-NAX	2.56	113.40	108.13
3	B	600	X22	CB-CA-C	2.56	115.06	110.46
3	A	600	X22	CBB-CBH-NAW	2.51	116.29	111.18
3	C	600	X22	OAD-CAZ-CBG	-2.49	114.83	120.38
3	C	700	X22	CBI-CBA-NBJ	2.48	120.80	116.70
3	B	600	X22	CAA-CB-CA	2.43	115.90	113.15
3	A	600	X22	OAE-CBA-NBJ	-2.38	118.79	121.68
3	C	701	X22	OAE-CBA-NBJ	-2.35	118.83	121.68
3	C	701	X22	CBI-NAX-C	2.35	127.89	121.81
3	C	701	X22	CBC-CBH-NAW	2.30	115.87	111.18
3	C	701	X22	OAD-CAZ-NAW	2.22	127.19	122.93
3	B	600	X22	CBG-NBJ-CBF	-2.21	110.32	112.73
3	C	700	X22	OAE-CBA-NBJ	-2.18	119.03	121.68
3	C	701	X22	OAE-CBA-CBI	2.18	124.06	121.81
3	B	600	X22	CA-C-NAX	-2.17	113.43	116.31
3	A	600	X22	CAV-CBG-CAZ	-2.16	107.27	111.15
3	D	600	X22	CAV-CBG-NBJ	-2.15	101.13	103.03
3	C	600	X22	CB-CA-C	2.14	114.31	110.46
3	A	600	X22	CBE-CBI-NAX	2.13	113.42	110.72
3	C	600	X22	CAM-CBB-CBH	-2.12	116.87	120.71
3	D	600	X22	OAD-CAZ-NAW	2.12	127.00	122.93
3	C	700	X22	OAD-CAZ-CBG	2.11	125.08	120.38
3	B	600	X22	CAT-CBF-NBJ	-2.11	107.52	111.33
3	C	600	X22	CAV-CAU-CBF	-2.11	100.89	103.96
3	D	600	X22	OAE-CBA-CBI	-2.06	119.68	121.81
3	C	701	X22	CAV-CBG-CAZ	-2.03	107.51	111.15
3	C	701	X22	CBG-CAZ-NAW	-2.02	112.26	116.70

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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	99/130 (76%)	-0.09	0 100 100	15, 32, 46, 53	0
1	B	101/130 (77%)	-0.02	3 (2%) 48 54	23, 37, 55, 71	1 (0%)
1	C	98/130 (75%)	-0.19	0 100 100	15, 34, 50, 57	3 (3%)
1	D	101/130 (77%)	-0.04	4 (3%) 36 41	13, 34, 56, 75	2 (1%)
All	All	399/520 (76%)	-0.08	7 (1%) 67 71	13, 34, 54, 75	6 (1%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	354	ARG	4.1
1	D	270	PHE	3.8
1	B	353	VAL	2.9
1	D	254	THR	2.6
1	B	274	THR	2.4
1	D	278	SER	2.1
1	D	354	ARG	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 ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	X22	C	700	36/36	0.21	2.04	23,34,53,57	0
3	X22	B	600	36/36	0.20	1.60	35,48,58,62	0
3	X22	C	701	36/36	0.17	1.08	10,26,36,39	0
3	X22	D	600	36/36	0.19	0.40	13,28,40,41	0
3	X22	A	600	36/36	0.16	0.13	17,30,39,49	0
3	X22	C	600	36/36	0.18	0.03	16,30,42,54	0
2	ZN	B	502	1/1	0.10	-1.31	33,33,33,33	0
2	ZN	D	502	1/1	0.08	-2.00	27,27,27,27	0
2	ZN	C	502	1/1	0.08	-2.83	23,23,23,23	0
2	ZN	A	502	1/1	0.08	-3.28	27,27,27,27	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.