



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:43 PM GMT

PDB ID : 4U2V  
Title : Bak BH3-in-Groove dimer (GFP)  
Authors : Brouwer, J.M.; Colman, P.M.; Czabotar, P.E.  
Deposited on : 2014-07-18  
Resolution : 2.30 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

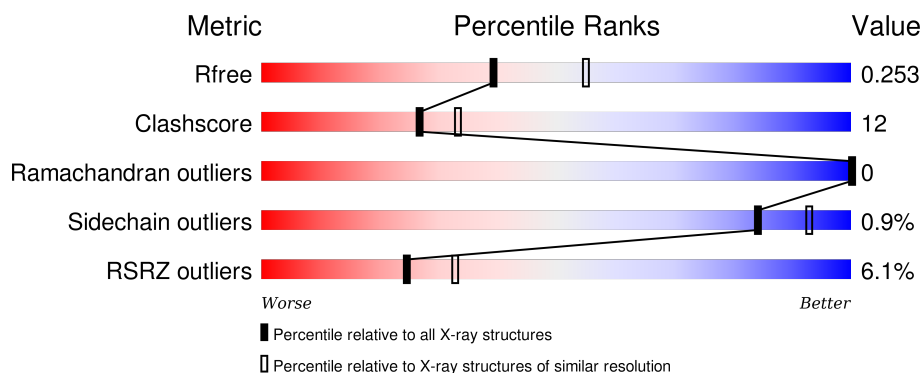
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	313	<div> <div>14%</div> <div>68%</div> <div>29%</div> <div>..</div> </div>
1	B	313	<div> <div>4%</div> <div>78%</div> <div>20%</div> <div>.</div> </div>
1	C	313	<div> <div>3%</div> <div>78%</div> <div>20%</div> <div>.</div> </div>
1	D	313	<div> <div>4%</div> <div>80%</div> <div>18%</div> <div>.</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
2	CAC	A	1202	-	-	-	X
2	CAC	B	1201	-	-	-	X
2	CAC	D	1203	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10100 atoms, of which 28 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 Green fluorescent protein,Bcl-2 homologous antagonist/killer.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	307	Total	C	N	O	S	0	0	0
			2458	1564	419	466	9			
1	D	307	Total	C	N	O	S	0	0	0
			2458	1564	419	466	9			
1	C	307	Total	C	N	O	S	0	0	0
			2458	1564	419	466	9			
1	A	306	Total	C	N	O	S	0	0	0
			2450	1559	418	465	8			

There are 36 discrepancies between the modelled and reference sequences:

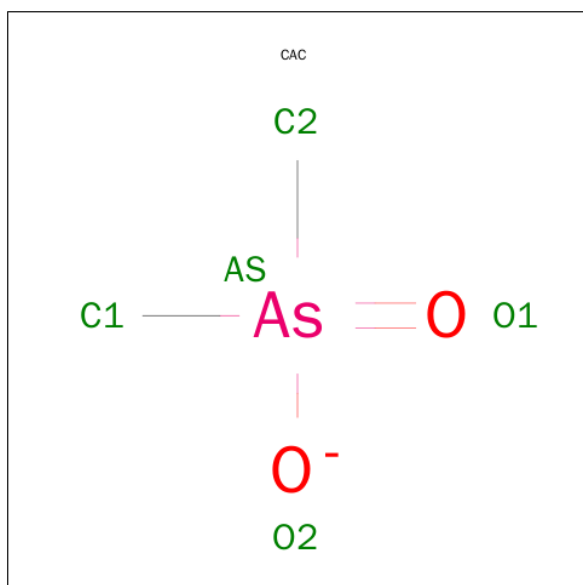
Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	expression tag	UNP P42212
B	-1	SER	-	expression tag	UNP P42212
B	0	HIS	-	expression tag	UNP P42212
B	?	CR2	SER	chromophore	UNP P42212
B	?	CR2	TYR	chromophore	UNP P42212
B	66	CR2	GLY	chromophore	UNP P42212
B	72	ALA	SER	engineered mutation	UNP P42212
B	206	ASN	ALA	engineered mutation	UNP P42212
B	231	GLY	-	linker	UNP P42212
D	-2	GLY	-	expression tag	UNP P42212
D	-1	SER	-	expression tag	UNP P42212
D	0	HIS	-	expression tag	UNP P42212
D	?	CR2	SER	chromophore	UNP P42212
D	?	CR2	TYR	chromophore	UNP P42212
D	66	CR2	GLY	chromophore	UNP P42212
D	72	ALA	SER	engineered mutation	UNP P42212
D	206	ASN	ALA	engineered mutation	UNP P42212
D	231	GLY	-	linker	UNP P42212
C	-2	GLY	-	expression tag	UNP P42212
C	-1	SER	-	expression tag	UNP P42212
C	0	HIS	-	expression tag	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	CR2	SER	chromophore	UNP P42212
C	?	CR2	TYR	chromophore	UNP P42212
C	66	CR2	GLY	chromophore	UNP P42212
C	72	ALA	SER	engineered mutation	UNP P42212
C	206	ASN	ALA	engineered mutation	UNP P42212
C	231	GLY	-	linker	UNP P42212
A	-2	GLY	-	expression tag	UNP P42212
A	-1	SER	-	expression tag	UNP P42212
A	0	HIS	-	expression tag	UNP P42212
A	?	CR2	SER	chromophore	UNP P42212
A	?	CR2	TYR	chromophore	UNP P42212
A	66	CR2	GLY	chromophore	UNP P42212
A	72	ALA	SER	engineered mutation	UNP P42212
A	206	ASN	ALA	engineered mutation	UNP P42212
A	231	GLY	-	linker	UNP P42212

- Molecule 2 is CACODYLATE ION (three-letter code: CAC) (formula:  $C_2H_6AsO_2$ ).



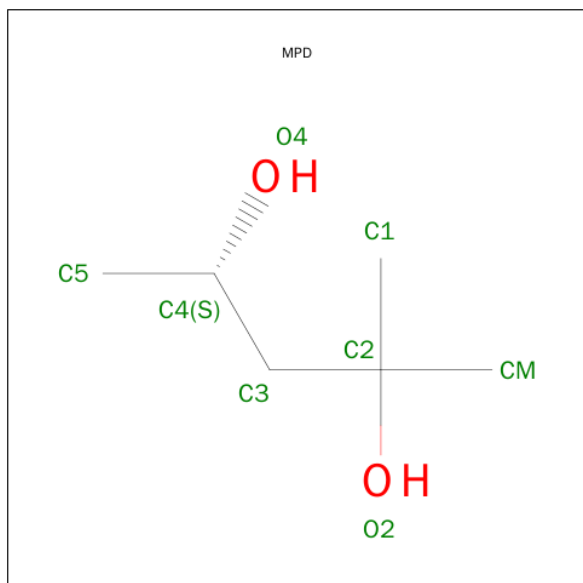
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	As	C	O	0	0
			5	1	2	2		
2	D	1	Total	As	C	O	0	0
			5	1	2	2		
2	D	1	Total	As	C	O	0	0
			5	1	2	2		
2	D	1	Total	As	C	O	0	0
			5	1	2	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	As	C	O	0	0
			5	1	2	2		
2	A	1	Total	As	C	O	0	0
			5	1	2	2		

- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:  $C_6H_{14}O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	H	O	0	0
			22	6	14	2		
3	A	1	Total	C	H	O	0	0
			22	6	14	2		

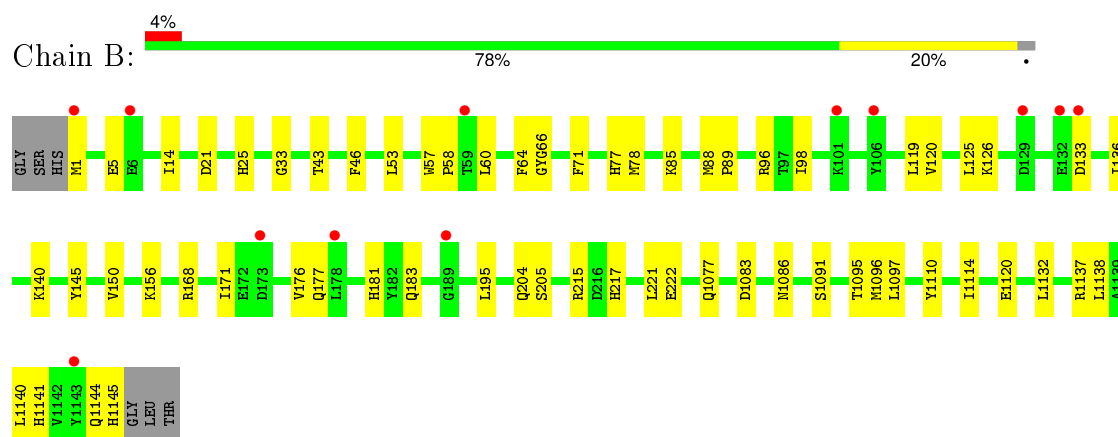
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	52	Total	O	0	0
			52	52		
4	D	56	Total	O	0	0
			56	56		
4	C	70	Total	O	0	0
			70	70		
4	A	24	Total	O	0	0
			24	24		

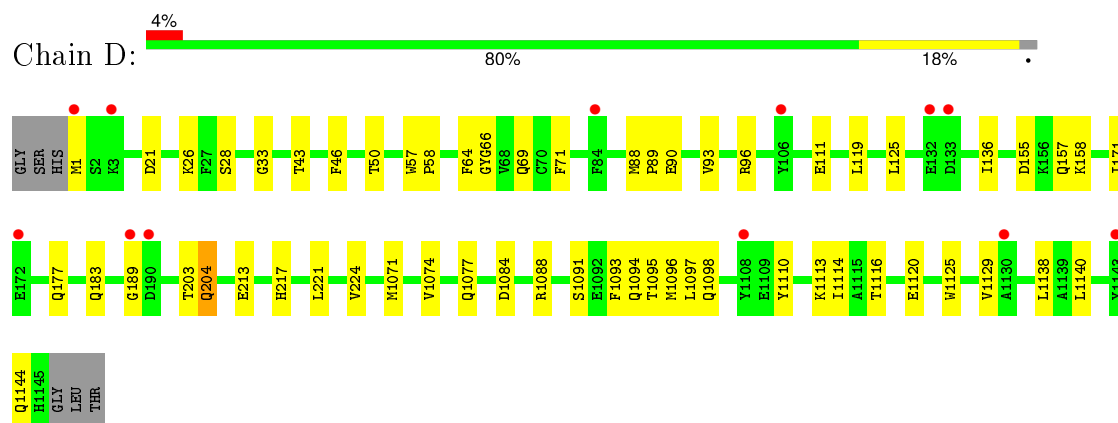
### 3 Residue-property plots [i](#)

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.

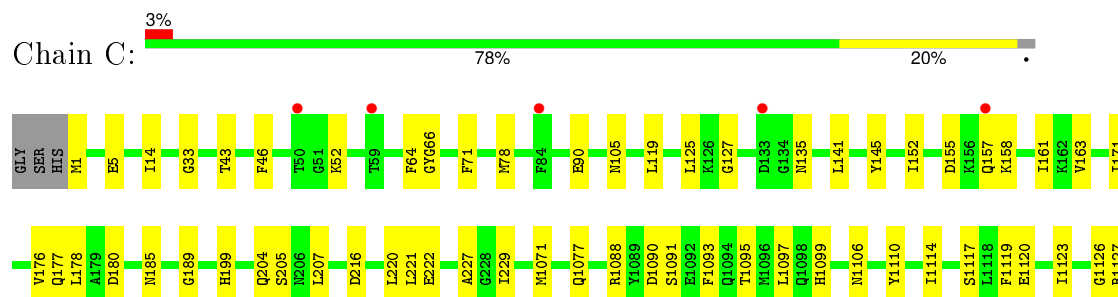
- Molecule 1: Green fluorescent protein,Bcl-2 homologous antagonist/killer

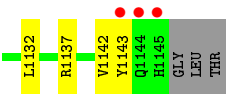


- Molecule 1: Green fluorescent protein,Bcl-2 homologous antagonist/killer

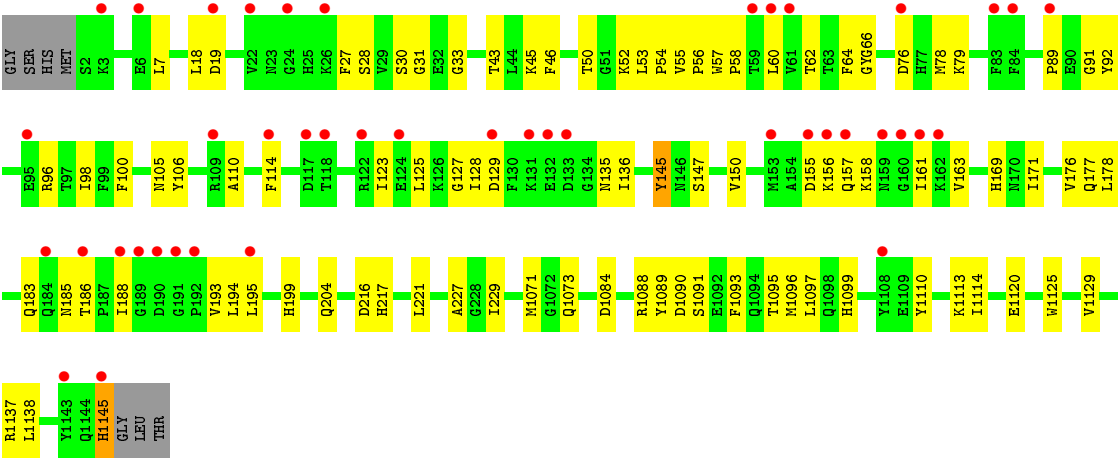


- Molecule 1: Green fluorescent protein,Bcl-2 homologous antagonist/killer





● Molecule 1: Green fluorescent protein,Bcl-2 homologous antagonist/killer





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	109.19Å 63.84Å 122.02Å 90.00° 98.35° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 20.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-2.30) 99.9 (20.00-2.30)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.39 (at 2.30Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, $R_{free}$	0.198 , 0.250 0.207 , 0.253	Depositor DCC
$R_{free}$ test set	3707 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	40.2	Xtriage
Anisotropy	0.407	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 57.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 74145 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	10100	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.41% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 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: CR2, CAC, MPD

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	0.46	0/2487	0.63	0/3362
1	B	0.48	0/2495	0.63	0/3372
1	C	0.45	0/2495	0.61	1/3372 (0.0%)
1	D	0.47	0/2495	0.61	0/3372
All	All	0.47	0/9972	0.62	1/13478 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	141	LEU	CA-CB-CG	5.18	127.21	115.30

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	2450	0	2369	106	0
1	B	2458	0	2381	53	0
1	C	2458	0	2381	56	0
1	D	2458	0	2381	55	0
2	A	10	0	0	1	0
2	B	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	15	0	0	0	0
3	A	8	14	14	2	0
3	C	8	14	14	0	0
4	A	24	0	0	3	0
4	B	52	0	0	4	0
4	C	70	0	0	4	0
4	D	56	0	0	1	0
All	All	10072	28	9540	235	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 12.

All (235) 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:204:GLN:HG2	1:C:204:GLN:HG2	1.38	1.02
1:A:156:LYS:HG2	1:A:195:LEU:HD13	1.42	1.01
1:B:204:GLN:HG2	1:A:204:GLN:HG2	1.44	1.00
1:B:1097:LEU:HD11	1:B:1138:LEU:HA	1.53	0.90
1:A:18:LEU:HB2	1:A:123:ILE:HD11	1.54	0.86
1:A:76:ASP:HA	1:A:79:LYS:HE2	1.56	0.86
1:A:18:LEU:HD13	1:A:123:ILE:HG13	1.59	0.84
1:D:1071:MET:HE2	1:A:1113:LYS:HB2	1.59	0.84
1:A:28:SER:HB2	1:A:50:THR:HG23	1.60	0.81
1:A:1090:ASP:OD1	1:A:1137:ARG:NH2	2.13	0.81
1:D:1091:SER:O	1:D:1095:THR:HG23	1.81	0.80
1:C:1090:ASP:OD1	1:C:1137:ARG:NH2	2.14	0.80
1:D:1097:LEU:HD21	1:D:1138:LEU:HA	1.63	0.79
1:A:1145:HIS:ND1	4:A:1322:HOH:O	2.13	0.79
1:C:171:ILE:HD11	1:C:177:GLN:HB2	1.63	0.79
1:D:1077:GLN:HB3	1:A:1096:MET:CE	2.12	0.79
1:A:171:ILE:HD11	1:A:177:GLN:HB2	1.63	0.79
1:D:1113:LYS:HB2	1:A:1071:MET:HE1	1.65	0.78
1:B:1097:LEU:HD12	1:B:1137:ARG:HG3	1.66	0.78
1:D:1113:LYS:HB2	1:A:1071:MET:CE	2.13	0.78
1:D:1077:GLN:HB3	1:A:1096:MET:HE1	1.63	0.78
1:B:171:ILE:HD11	1:B:177:GLN:HB2	1.66	0.77
1:B:1091:SER:O	1:B:1095:THR:HG23	1.84	0.77
1:D:1093:PHE:HA	1:D:1096:MET:HE3	1.67	0.77
1:A:7:LEU:HD23	1:A:7:LEU:O	1.86	0.76
1:D:1071:MET:CE	1:A:1113:LYS:HB2	2.17	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:VAL:HG23	1:A:136:ILE:HG23	1.68	0.75
1:A:18:LEU:CD1	1:A:123:ILE:HG13	2.17	0.74
1:D:46:PHE:CZ	1:D:64:PHE:HB3	2.23	0.73
1:B:1077:GLN:HG3	3:A:1203:MPD:C1	2.20	0.72
1:D:28:SER:HB2	1:D:50:THR:HG23	1.70	0.72
1:D:171:ILE:HD11	1:D:177:GLN:HB2	1.73	0.70
1:A:161:ILE:HD11	1:A:185:ASN:HB2	1.74	0.70
1:B:215:ARG:NH2	4:B:1301:HOH:O	2.15	0.70
1:B:1110:TYR:HA	1:C:1071:MET:CE	2.23	0.69
1:A:1091:SER:O	1:A:1095:THR:HG23	1.94	0.68
1:C:1:MET:HB2	1:C:5:GLU:OE2	1.93	0.68
1:A:28:SER:HB2	1:A:50:THR:CG2	2.23	0.67
1:C:1091:SER:O	1:C:1095:THR:HG23	1.93	0.66
1:A:91:GLY:HA3	1:A:188:ILE:HD12	1.77	0.66
1:A:43:THR:HG23	1:A:221:LEU:HD21	1.76	0.66
1:B:1097:LEU:HD11	1:B:1138:LEU:CA	2.26	0.66
1:C:1110:TYR:O	1:C:1114:ILE:HG12	1.95	0.65
1:D:1097:LEU:CD2	1:D:1138:LEU:HA	2.26	0.65
1:B:1077:GLN:HG3	3:A:1203:MPD:H12	1.79	0.65
1:C:161:ILE:HG12	1:C:185:ASN:HB2	1.79	0.64
1:A:52:LYS:HD2	1:A:216:ASP:OD2	1.98	0.64
1:A:1073:GLN:HG3	4:A:1318:HOH:O	1.98	0.64
1:C:1099:HIS:CE1	1:A:176:VAL:HG22	2.34	0.63
1:D:90:GLU:OE1	1:D:189:GLY:HA3	1.98	0.63
1:D:1084:ASP:OD2	1:A:1089:TYR:OH	2.15	0.63
1:D:1084:ASP:O	1:D:1088:ARG:HG3	1.98	0.62
1:C:176:VAL:HG22	1:A:1099:HIS:CE1	2.34	0.62
1:A:96:ARG:HG2	1:A:183:GLN:HB2	1.81	0.62
1:C:155:ASP:OD2	1:C:158:LYS:HD2	1.98	0.62
1:D:1071:MET:HE2	1:A:1113:LYS:CB	2.28	0.62
1:A:43:THR:HG23	1:A:221:LEU:CD2	2.30	0.62
1:A:55:VAL:HG21	1:A:106:TYR:OH	2.00	0.62
1:C:43:THR:HG23	1:C:221:LEU:CD2	2.29	0.62
1:A:18:LEU:HB2	1:A:123:ILE:CD1	2.29	0.61
1:D:66:CR2:HB2	1:D:69:GLN:HE21	1.66	0.61
1:D:1093:PHE:HA	1:D:1096:MET:CE	2.30	0.61
1:A:128:ILE:HG22	1:A:129:ASP:CG	2.21	0.61
1:C:1097:LEU:HD12	1:C:1137:ARG:HG2	1.81	0.60
1:A:91:GLY:CA	1:A:188:ILE:HD12	2.32	0.60
1:B:1110:TYR:O	1:B:1114:ILE:HG12	2.01	0.60
1:A:155:ASP:OD1	1:A:157:GLN:NE2	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1117:SER:O	1:C:1120:GLU:HG2	2.02	0.59
1:B:156:LYS:HG2	1:B:195:LEU:HD13	1.85	0.59
1:B:156:LYS:HG2	1:B:195:LEU:CD1	2.32	0.59
1:D:155:ASP:OD2	1:D:158:LYS:HD2	2.03	0.59
1:B:85:LYS:NZ	4:B:1307:HOH:O	2.35	0.58
1:B:1097:LEU:CD1	1:B:1138:LEU:HA	2.32	0.58
1:B:66:CR2:N2	1:B:66:CR2:HD1	2.18	0.58
1:B:1096:MET:HE2	1:C:1077:GLN:HB3	1.85	0.58
1:C:46:PHE:CZ	1:C:64:PHE:HB3	2.38	0.58
1:C:43:THR:HG23	1:C:221:LEU:HD22	1.86	0.57
1:D:43:THR:HG23	1:D:221:LEU:CD2	2.34	0.57
1:D:1071:MET:CE	1:A:1110:TYR:HA	2.35	0.57
1:B:1:MET:HB2	1:B:5:GLU:OE2	2.05	0.57
1:A:1145:HIS:CD2	1:A:1145:HIS:N	2.73	0.56
1:C:1099:HIS:CG	1:A:176:VAL:CG2	2.89	0.56
1:C:155:ASP:OD1	1:C:157:GLN:NE2	2.39	0.56
1:A:1120:GLU:HA	2:A:1201:CAC:C2	2.36	0.55
1:C:157:GLN:HB2	4:C:1302:HOH:O	2.05	0.55
1:A:96:ARG:NE	1:A:183:GLN:OE1	2.35	0.55
1:A:55:VAL:HG23	1:A:56:PRO:HD2	1.88	0.55
1:C:135:ASN:ND2	1:C:171:ILE:HD13	2.22	0.55
1:C:1099:HIS:ND1	1:A:176:VAL:HG22	2.22	0.55
1:B:1132:LEU:HD13	1:C:1132:LEU:HB3	1.87	0.54
1:D:1071:MET:HE1	1:A:1110:TYR:HA	1.89	0.54
1:D:66:CR2:HD1	1:D:66:CR2:N2	2.23	0.54
1:A:136:ILE:N	1:A:136:ILE:HD12	2.23	0.54
1:D:1077:GLN:HB3	1:A:1096:MET:HE2	1.89	0.53
1:A:161:ILE:CD1	1:A:185:ASN:HB2	2.38	0.53
1:B:126:LYS:NZ	4:B:1331:HOH:O	2.41	0.53
1:D:1113:LYS:HB2	1:A:1071:MET:HE2	1.88	0.53
1:A:55:VAL:CG2	1:A:56:PRO:HD2	2.38	0.53
1:A:91:GLY:C	1:A:188:ILE:HD12	2.29	0.53
1:A:1125:TRP:O	1:A:1129:VAL:HG23	2.09	0.53
1:C:1088:ARG:HG3	4:C:1330:HOH:O	2.08	0.53
1:A:66:CR2:HD2	1:A:150:VAL:HG21	1.91	0.52
1:A:105:ASN:O	1:A:127:GLY:HA2	2.09	0.52
1:C:1095:THR:HG21	1:A:178:LEU:HD11	1.91	0.52
1:B:64:PHE:O	1:B:66:CR2:HA31	2.10	0.52
1:D:64:PHE:O	1:D:66:CR2:HA31	2.09	0.52
1:C:1099:HIS:CG	1:A:176:VAL:HG22	2.45	0.52
1:D:1077:GLN:CB	1:A:1096:MET:HE2	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:ASP:HA	1:A:79:LYS:CE	2.37	0.51
1:B:88:MET:HB3	1:B:89:PRO:HA	1.91	0.51
1:D:1071:MET:HE1	1:A:1113:LYS:HD2	1.92	0.51
1:C:176:VAL:HG22	1:A:1099:HIS:ND1	2.24	0.51
1:A:106:TYR:CD2	1:A:125:LEU:HD11	2.45	0.51
1:D:43:THR:HG23	1:D:221:LEU:HD22	1.93	0.51
1:A:125:LEU:HD23	1:A:125:LEU:C	2.31	0.51
1:B:53:LEU:HD21	1:B:60:LEU:HD12	1.92	0.51
1:C:52:LYS:HD2	1:C:216:ASP:OD2	2.11	0.51
1:D:155:ASP:OD1	1:D:157:GLN:HG2	2.11	0.51
1:B:46:PHE:CZ	1:B:64:PHE:HB3	2.46	0.50
1:C:176:VAL:CG2	1:A:1099:HIS:CG	2.95	0.50
1:B:77:HIS:CD2	1:B:78:MET:HG3	2.46	0.50
1:C:1097:LEU:CD1	1:C:1137:ARG:HG2	2.42	0.50
1:D:1110:TYR:O	1:D:1114:ILE:HG12	2.11	0.50
1:A:1084:ASP:O	1:A:1088:ARG:HG3	2.12	0.50
1:A:161:ILE:HD13	1:A:163:VAL:HG23	1.94	0.50
1:A:171:ILE:CD1	1:A:177:GLN:HB2	2.37	0.49
1:B:1110:TYR:HA	1:C:1071:MET:HE1	1.91	0.49
1:B:46:PHE:O	1:B:217:HIS:HB2	2.12	0.49
1:A:169:HIS:HE1	4:A:1317:HOH:O	1.94	0.49
1:D:1097:LEU:HD21	1:D:1138:LEU:CA	2.38	0.49
1:B:125:LEU:C	1:B:125:LEU:HD23	2.33	0.49
1:B:168:ARG:HB3	1:B:176:VAL:HG11	1.93	0.49
1:B:1083:ASP:OD1	1:C:1127:ARG:NE	2.38	0.49
1:A:18:LEU:HD13	1:A:123:ILE:CG1	2.37	0.49
1:A:161:ILE:HD12	1:A:161:ILE:O	2.13	0.49
1:B:136:ILE:N	1:B:136:ILE:HD12	2.27	0.48
1:A:76:ASP:OD1	1:A:79:LYS:HE2	2.12	0.48
1:A:147:SER:OG	1:A:204:GLN:HG3	2.14	0.48
1:C:199:HIS:HB2	1:C:227:ALA:O	2.14	0.48
1:A:193:VAL:HG12	1:A:194:LEU:N	2.29	0.48
1:A:156:LYS:HG2	1:A:195:LEU:CD1	2.28	0.47
1:C:161:ILE:CG1	1:C:185:ASN:HB2	2.43	0.47
1:B:43:THR:HG23	1:B:221:LEU:CD2	2.44	0.47
1:A:46:PHE:CZ	1:A:64:PHE:HB3	2.49	0.47
1:D:125:LEU:C	1:D:125:LEU:HD23	2.34	0.47
1:D:93:VAL:HG22	1:D:111:GLU:HG2	1.97	0.47
1:B:21:ASP:HA	1:B:25:HIS:O	2.15	0.47
1:B:1097:LEU:HD13	1:B:1141:HIS:CB	2.44	0.47
1:B:71:PHE:CE2	1:B:119:LEU:HD22	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:LEU:HD21	1:A:114:PHE:CZ	2.50	0.47
1:A:135:ASN:CG	1:A:171:ILE:HD13	2.35	0.47
1:A:46:PHE:O	1:A:217:HIS:HB2	2.14	0.46
1:A:100:PHE:HB3	1:A:177:GLN:NE2	2.31	0.46
1:A:66:CR2:N2	1:A:66:CR2:HD1	2.30	0.46
1:D:21:ASP:OD2	1:D:26:LYS:NZ	2.49	0.46
1:A:27:PHE:CD2	1:A:54:PRO:HG3	2.51	0.46
1:C:33:GLY:HA3	1:C:43:THR:O	2.15	0.46
1:A:31:GLY:HA2	1:A:45:LYS:O	2.16	0.46
1:A:1097:LEU:HD12	1:A:1137:ARG:HG2	1.97	0.45
1:A:193:VAL:CG1	1:A:194:LEU:N	2.80	0.45
1:A:199:HIS:HB2	1:A:227:ALA:O	2.16	0.45
1:A:92:TYR:HA	1:A:188:ILE:HG13	1.98	0.45
1:C:1093:PHE:HB3	1:C:1137:ARG:HE	1.81	0.45
1:C:207:LEU:CD2	1:C:220:LEU:HD13	2.46	0.45
1:A:7:LEU:CD1	1:A:89:PRO:HB3	2.47	0.45
1:B:53:LEU:HD22	1:B:57:TRP:CE2	2.52	0.45
1:A:53:LEU:HD21	1:A:60:LEU:HD12	1.99	0.45
1:A:18:LEU:HB2	1:A:123:ILE:CG1	2.46	0.45
1:C:66:CR2:N2	1:C:66:CR2:HD1	2.32	0.45
1:D:1116:THR:O	1:D:1120:GLU:HG3	2.16	0.44
1:A:55:VAL:CG2	1:A:56:PRO:CD	2.95	0.44
1:C:1088:ARG:HD3	4:C:1352:HOH:O	2.17	0.44
1:D:136:ILE:N	1:D:136:ILE:HD12	2.31	0.44
1:C:105:ASN:O	1:C:127:GLY:HA2	2.16	0.44
1:C:14:ILE:HD11	1:C:71:PHE:CE2	2.52	0.44
1:D:1125:TRP:O	1:D:1129:VAL:HG23	2.18	0.44
1:A:76:ASP:HA	1:A:79:LYS:HG3	1.99	0.44
1:A:57:TRP:N	1:A:58:PRO:CD	2.80	0.44
1:D:66:CR2:HB2	1:D:69:GLN:NE2	2.31	0.44
1:A:18:LEU:HD12	1:A:19:ASP:N	2.33	0.44
1:C:1106:ASN:HB3	4:C:1360:HOH:O	2.18	0.44
1:B:1096:MET:CE	1:C:1077:GLN:HB3	2.48	0.43
1:B:53:LEU:HD22	1:B:57:TRP:CD2	2.52	0.43
1:A:62:THR:HG23	1:A:145:TYR:OH	2.18	0.43
1:D:1094:GLN:O	1:D:1098:GLN:HG2	2.18	0.43
1:D:1140:LEU:O	1:D:1144:GLN:HG3	2.17	0.43
1:C:176:VAL:HG22	1:A:1099:HIS:CG	2.53	0.43
1:B:33:GLY:HA3	1:B:43:THR:O	2.19	0.43
1:D:88:MET:HB3	1:D:89:PRO:HA	2.00	0.43
1:B:1096:MET:HE2	1:C:1077:GLN:CB	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1144:GLN:O	1:B:1145:HIS:HB2	2.18	0.43
1:B:1086:ASN:HB2	1:C:1126:GLY:HA3	2.01	0.43
1:C:135:ASN:ND2	1:C:171:ILE:CD1	2.82	0.43
1:D:1074:VAL:HB	1:A:1114:ILE:HD12	2.00	0.43
1:D:213:GLU:HB3	1:D:217:HIS:CE1	2.54	0.43
1:A:33:GLY:HA3	1:A:43:THR:O	2.18	0.42
1:B:14:ILE:HD11	1:B:71:PHE:CE2	2.54	0.42
1:B:1120:GLU:HG3	4:B:1322:HOH:O	2.19	0.42
1:C:78:MET:HE3	1:C:229:ILE:HG13	2.01	0.42
1:C:178:LEU:HD11	1:A:1095:THR:HG21	2.01	0.42
1:C:1119:PHE:CD1	1:C:1123:ILE:HG12	2.54	0.42
1:B:98:ILE:HD13	1:B:181:HIS:NE2	2.35	0.42
1:D:71:PHE:CE2	1:D:119:LEU:HD22	2.55	0.42
1:C:90:GLU:OE1	1:C:189:GLY:HA3	2.20	0.42
1:D:33:GLY:HA3	1:D:43:THR:O	2.19	0.42
1:C:71:PHE:CE2	1:C:119:LEU:HD22	2.55	0.42
1:A:30:SER:O	1:A:46:PHE:HA	2.20	0.42
1:D:57:TRP:N	1:D:58:PRO:CD	2.83	0.42
1:C:1142:VAL:HG23	1:C:1143:TYR:N	2.35	0.42
1:C:152:ILE:HG12	1:C:163:VAL:HG22	2.01	0.42
1:A:1097:LEU:HD11	1:A:1138:LEU:HA	2.01	0.41
1:D:66:CR2:CB2	1:D:69:GLN:HE21	2.32	0.41
1:D:96:ARG:HG2	1:D:183:GLN:HB2	2.02	0.41
1:B:66:CR2:HD2	1:B:150:VAL:HG21	2.01	0.41
1:A:66:CR2:HD2	1:A:150:VAL:CG2	2.50	0.41
1:B:205:SER:OG	1:B:222:GLU:HG2	2.21	0.41
1:A:161:ILE:HD13	1:A:163:VAL:CG2	2.50	0.41
1:A:110:ALA:CB	1:A:123:ILE:HG22	2.50	0.41
1:A:1093:PHE:HB3	1:A:1137:ARG:HE	1.85	0.41
1:D:1084:ASP:OD2	1:D:1088:ARG:HD2	2.21	0.41
1:B:133:ASP:O	1:B:140:LYS:NZ	2.39	0.41
1:C:125:LEU:C	1:C:125:LEU:HD23	2.41	0.41
1:A:78:MET:HE3	1:A:229:ILE:HG13	2.02	0.41
1:B:1097:LEU:HD23	1:B:1097:LEU:HA	1.74	0.41
1:C:205:SER:OG	1:C:222:GLU:HG2	2.20	0.41
1:D:203:THR:HG23	1:D:224:VAL:HG22	2.02	0.41
1:D:28:SER:HB2	1:D:50:THR:CG2	2.45	0.41
1:A:128:ILE:N	1:A:128:ILE:HD12	2.36	0.41
1:B:1140:LEU:O	1:B:1144:GLN:HG3	2.21	0.40
1:B:96:ARG:HG2	1:B:183:GLN:HB2	2.03	0.40
1:A:155:ASP:OD2	1:A:158:LYS:HD2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:ILE:O	1:A:105:ASN:HA	2.21	0.40
1:B:66:CR2:HD2	1:B:150:VAL:CG2	2.51	0.40
1:B:57:TRP:N	1:B:58:PRO:CD	2.85	0.40
1:D:96:ARG:HD2	4:D:1311:HOH:O	2.21	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	301/313 (96%)	296 (98%)	5 (2%)	0	100	100
1	B	302/313 (96%)	296 (98%)	6 (2%)	0	100	100
1	C	302/313 (96%)	297 (98%)	5 (2%)	0	100	100
1	D	302/313 (96%)	295 (98%)	7 (2%)	0	100	100
All	All	1207/1252 (96%)	1184 (98%)	23 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	263/268 (98%)	260 (99%)	3 (1%)	80	90
1	B	264/268 (98%)	262 (99%)	2 (1%)	86	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	264/268 (98%)	262 (99%)	2 (1%)	86	94
1	D	264/268 (98%)	262 (99%)	2 (1%)	86	94
All	All	1055/1072 (98%)	1046 (99%)	9 (1%)	84	93

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	120	VAL
1	B	145	TYR
1	D	1	MET
1	D	204	GLN
1	C	145	TYR
1	C	180	ASP
1	A	145	TYR
1	A	186	THR
1	A	1145	HIS

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	135	ASN
1	A	1145	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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
1	CR2	A	66	1	20,20,21	3.90	3 (15%)	25,27,29	3.92	7 (28%)
1	CR2	B	66	1	20,20,21	3.70	5 (25%)	25,27,29	3.65	7 (28%)
1	CR2	C	66	1	20,20,21	3.73	6 (30%)	25,27,29	4.27	6 (24%)
1	CR2	D	66	1	20,20,21	3.85	5 (25%)	25,27,29	3.81	9 (36%)

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
1	CR2	A	66	1	-	0/6/25/26	0/2/2/2
1	CR2	B	66	1	-	0/6/25/26	0/2/2/2
1	CR2	C	66	1	-	0/6/25/26	0/2/2/2
1	CR2	D	66	1	-	0/6/25/26	0/2/2/2

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	66	CR2	CA2-C2	-2.83	1.45	1.48
1	A	66	CR2	C2-N3	-2.51	1.34	1.39
1	C	66	CR2	C2-N3	-2.45	1.34	1.39
1	B	66	CR2	C2-N3	-2.29	1.34	1.39
1	D	66	CR2	C2-N3	-2.22	1.35	1.39
1	B	66	CR2	CA2-C2	-2.05	1.46	1.48
1	B	66	CR2	C1-N2	2.08	1.37	1.33
1	C	66	CR2	CA1-C1	2.19	1.51	1.49
1	D	66	CR2	C1-N2	2.30	1.38	1.33
1	C	66	CR2	C1-N2	2.42	1.38	1.33
1	D	66	CR2	CA1-C1	2.50	1.52	1.49
1	C	66	CR2	O2-C2	2.54	1.28	1.23
1	A	66	CR2	O2-C2	2.81	1.29	1.23
1	B	66	CR2	O2-C2	3.24	1.30	1.23
1	D	66	CR2	O2-C2	3.34	1.30	1.23
1	C	66	CR2	CB2-CA2	15.51	1.48	1.35
1	B	66	CR2	CB2-CA2	15.58	1.48	1.35
1	D	66	CR2	CB2-CA2	16.13	1.49	1.35
1	A	66	CR2	CB2-CA2	16.66	1.49	1.35

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	66	CR2	O2-C2-CA2	-15.13	122.78	130.95
1	D	66	CR2	O2-C2-CA2	-13.44	123.69	130.95
1	A	66	CR2	O2-C2-CA2	-12.99	123.93	130.95
1	B	66	CR2	O2-C2-CA2	-12.70	124.09	130.95
1	B	66	CR2	CG2-CB2-CA2	-4.83	123.94	130.22
1	A	66	CR2	C2-CA2-N2	-3.75	105.92	108.91
1	C	66	CR2	C2-CA2-N2	-3.42	106.19	108.91
1	D	66	CR2	CG2-CB2-CA2	-3.03	126.28	130.22
1	A	66	CR2	CG2-CB2-CA2	-2.99	126.33	130.22
1	D	66	CR2	C2-CA2-N2	-2.72	106.74	108.91
1	B	66	CR2	C2-CA2-N2	-2.51	106.90	108.91
1	B	66	CR2	CB2-CA2-N2	-2.47	124.25	128.67
1	A	66	CR2	CB2-CA2-N2	-2.32	124.53	128.67
1	C	66	CR2	CG2-CB2-CA2	-2.22	127.33	130.22
1	D	66	CR2	CB2-CA2-N2	-2.20	124.74	128.67
1	D	66	CR2	CA3-N3-C1	-2.02	124.89	127.91
1	B	66	CR2	CA3-N3-C2	2.65	128.30	123.99
1	C	66	CR2	CA3-N3-C2	2.92	128.75	123.99
1	D	66	CR2	C3-CA3-N3	3.01	119.58	113.00
1	D	66	CR2	CA3-N3-C2	3.31	129.38	123.99
1	A	66	CR2	CA3-N3-C2	3.63	129.90	123.99
1	C	66	CR2	CB2-CA2-C2	3.78	127.90	122.36
1	D	66	CR2	CB2-CA2-C2	4.19	128.50	122.36
1	B	66	CR2	CB2-CA2-C2	4.42	128.84	122.36
1	A	66	CR2	CB2-CA2-C2	4.91	129.55	122.36
1	B	66	CR2	CA2-C2-N3	9.61	108.22	103.40
1	D	66	CR2	CA2-C2-N3	10.44	108.63	103.40
1	A	66	CR2	CA2-C2-N3	11.63	109.23	103.40
1	C	66	CR2	CA2-C2-N3	12.91	109.87	103.40

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	66	CR2	3	0
1	B	66	CR2	4	0
1	C	66	CR2	1	0
1	D	66	CR2	5	0

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

8 ligands are modelled in this entry.

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	$\# Z  > 2$
2	CAC	A	1201	-	0,4,4	0.00	-	0,6,6	0.00	-
2	CAC	A	1202	-	0,4,4	0.00	-	0,6,6	0.00	-
3	MPD	A	1203	-	6,7,7	0.37	0	7,10,10	0.46	0
2	CAC	B	1201	-	0,4,4	0.00	-	0,6,6	0.00	-
3	MPD	C	1201	-	6,7,7	0.31	0	7,10,10	0.40	0
2	CAC	D	1201	-	0,4,4	0.00	-	0,6,6	0.00	-
2	CAC	D	1202	-	0,4,4	0.00	-	0,6,6	0.00	-
2	CAC	D	1203	-	0,4,4	0.00	-	0,6,6	0.00	-

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
2	CAC	A	1201	-	-	0/0/0/0	0/0/0/0
2	CAC	A	1202	-	-	0/0/0/0	0/0/0/0
3	MPD	A	1203	-	-	0/5/5/5	0/0/0/0
2	CAC	B	1201	-	-	0/0/0/0	0/0/0/0
3	MPD	C	1201	-	-	0/5/5/5	0/0/0/0
2	CAC	D	1201	-	-	0/0/0/0	0/0/0/0
2	CAC	D	1202	-	-	0/0/0/0	0/0/0/0
2	CAC	D	1203	-	-	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 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1201	CAC	1	0
3	A	1203	MPD	2	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	305/313 (97%)	0.74	43 (14%) 4 6	32, 75, 117, 145	0
1	B	306/313 (97%)	-0.03	12 (3%) 43 52	26, 50, 85, 120	0
1	C	306/313 (97%)	-0.10	8 (2%) 59 68	31, 52, 88, 122	0
1	D	306/313 (97%)	-0.02	12 (3%) 43 52	30, 52, 92, 119	0
All	All	1223/1252 (97%)	0.15	75 (6%) 25 33	26, 56, 103, 145	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	160	GLY	6.0
1	C	1143	TYR	5.9
1	A	1143	TYR	5.4
1	A	114	PHE	5.2
1	A	157	GLN	4.8
1	A	132	GLU	4.5
1	A	195	LEU	4.4
1	A	109	ARG	4.2
1	A	59	THR	4.1
1	A	162	LYS	3.9
1	D	1	MET	3.9
1	A	6	GLU	3.8
1	A	76	ASP	3.7
1	A	24	GLY	3.7
1	A	22	VAL	3.6
1	A	188	ILE	3.5
1	A	131	LYS	3.4
1	A	190	ASP	3.4
1	A	192	PRO	3.3
1	B	173	ASP	3.3
1	A	156	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	133	ASP	3.2
1	A	118	THR	3.2
1	A	84	PHE	3.2
1	C	133	ASP	3.1
1	A	133	ASP	3.0
1	A	161	ILE	3.0
1	D	132	GLU	3.0
1	A	129	ASP	2.9
1	A	83	PHE	2.9
1	A	3	LYS	2.9
1	A	189	GLY	2.9
1	A	60	LEU	2.9
1	A	1145	HIS	2.8
1	A	155	ASP	2.7
1	B	1143	TYR	2.7
1	B	132	GLU	2.7
1	C	1145	HIS	2.7
1	A	1108	TYR	2.6
1	A	19	ASP	2.6
1	D	172	GLU	2.6
1	C	157	GLN	2.6
1	B	1	MET	2.5
1	B	189	GLY	2.4
1	A	95	GLU	2.4
1	A	26	LYS	2.4
1	A	153	MET	2.4
1	D	1108	TYR	2.4
1	D	1143	TYR	2.4
1	A	186	THR	2.3
1	A	159	ASN	2.3
1	B	59	THR	2.3
1	C	50	THR	2.3
1	B	133	ASP	2.3
1	C	59	THR	2.3
1	B	101	LYS	2.3
1	D	3	LYS	2.2
1	B	6	GLU	2.2
1	A	89	PRO	2.2
1	D	190	ASP	2.2
1	B	178	LEU	2.2
1	B	129	ASP	2.1
1	D	189	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	117	ASP	2.1
1	A	184	GLN	2.1
1	D	1130	ALA	2.1
1	A	61	VAL	2.1
1	A	124	GLU	2.1
1	D	84	PHE	2.0
1	D	106	TYR	2.0
1	A	191	GLY	2.0
1	C	84	PHE	2.0
1	C	1144	GLN	2.0
1	B	106	TYR	2.0
1	A	122	ARG	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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
1	CR2	B	66	19/20	0.97	0.13	-	27,37,52,64	0
1	CR2	A	66	19/20	0.90	0.18	-	59,73,98,114	0
1	CR2	D	66	19/20	0.96	0.11	-	44,48,57,57	0
1	CR2	C	66	19/20	0.93	0.13	-	37,48,69,79	0

## 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( $\text{\AA}^2$ )	Q<0.9
2	CAC	D	1203	5/5	0.90	0.26	9.67	78,78,146,199	0
2	CAC	A	1202	5/5	0.92	0.31	6.73	57,60,236,297	0
2	CAC	B	1201	5/5	0.97	0.24	3.35	42,53,190,293	0
2	CAC	D	1202	5/5	0.94	0.22	2.00	64,84,128,223	0
2	CAC	D	1201	5/5	0.92	0.22	1.91	57,62,92,192	0
2	CAC	A	1201	5/5	0.94	0.19	1.38	88,91,155,197	0
3	MPD	A	1203	8/8	0.92	0.18	1.36	70,90,104,114	0
3	MPD	C	1201	8/8	0.96	0.10	-0.65	42,56,68,73	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.