



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 02:34 AM UTC

PDB ID : 4U2V / pdb_00004u2v
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 wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

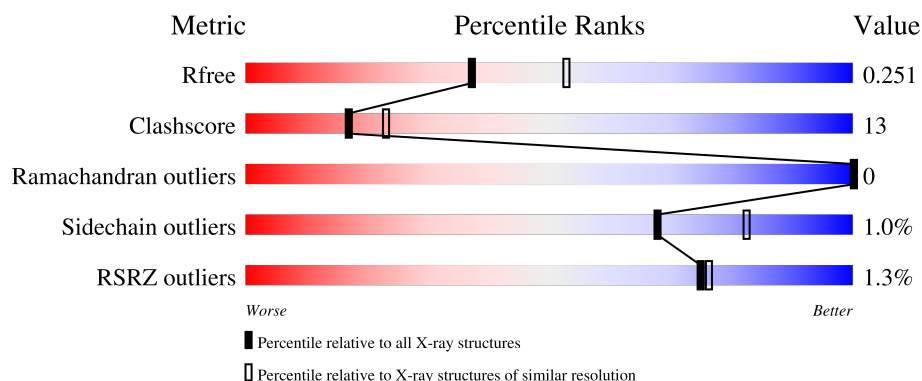
1 Overall quality at a glance

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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	5% 66% 30% ..
1	B	313	78% 19% ..
1	C	313	77% 21% ..
1	D	313	77% 20% .

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	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:

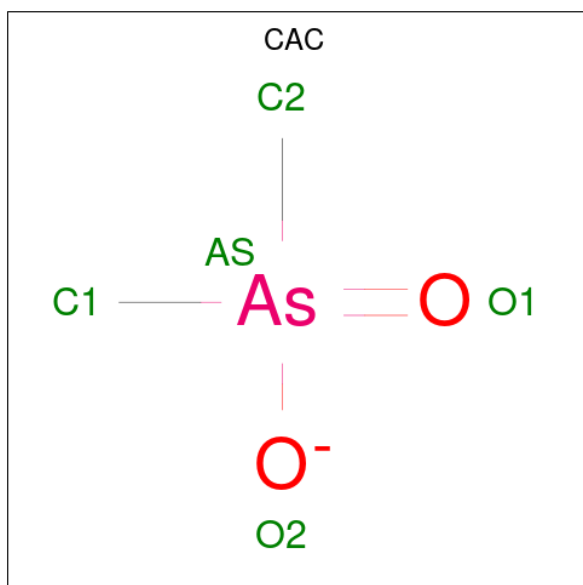
Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	expression tag	UNP P42212
B	-1	SER	-	expression tag	UNP P42212
B	0	HIS	-	expression tag	UNP P42212
B	?	CR2	SER	chromophore	UNP P42212
B	?	CR2	TYR	chromophore	UNP P42212
B	66	CR2	GLY	chromophore	UNP P42212
B	72	ALA	SER	engineered mutation	UNP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

Continued on next page...

Continued from previous page...

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 (CCD ID: CAC) (formula: $\text{C}_2\text{H}_6\text{AsO}_2$).



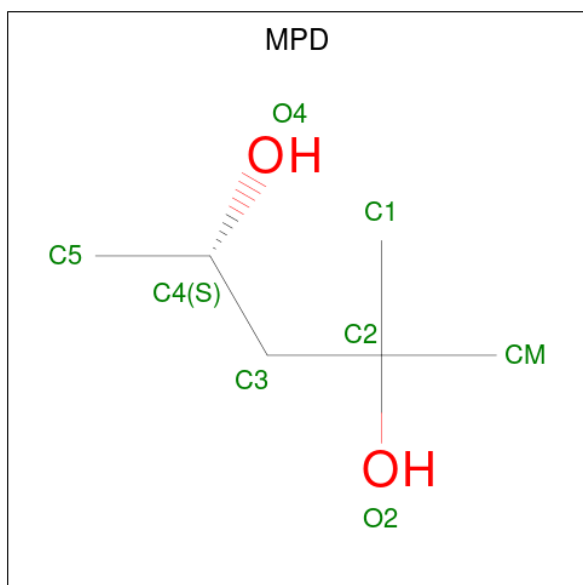
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	As	C	O	0	0
			5	1	2	2		
2	D	1	Total	As	C	O	0	0
			5	1	2	2		
2	D	1	Total	As	C	O	0	0
			5	1	2	2		
2	D	1	Total	As	C	O	0	0
			5	1	2	2		

Continued on next page...

Continued from previous page...

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 (CCD ID: MPD) (formula: C₆H₁₄O₂).



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		

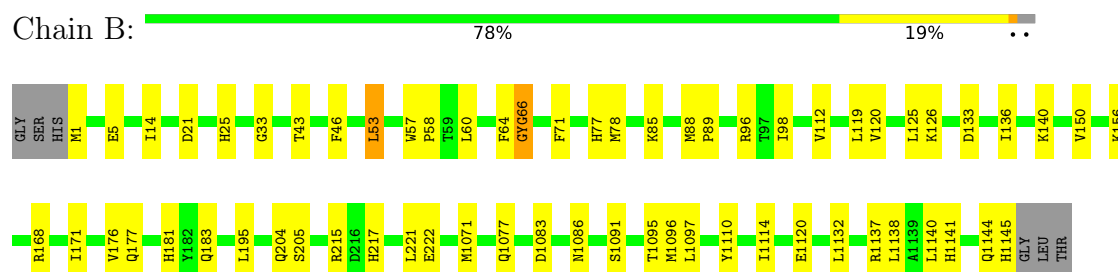
- Molecule 4 is water.

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		

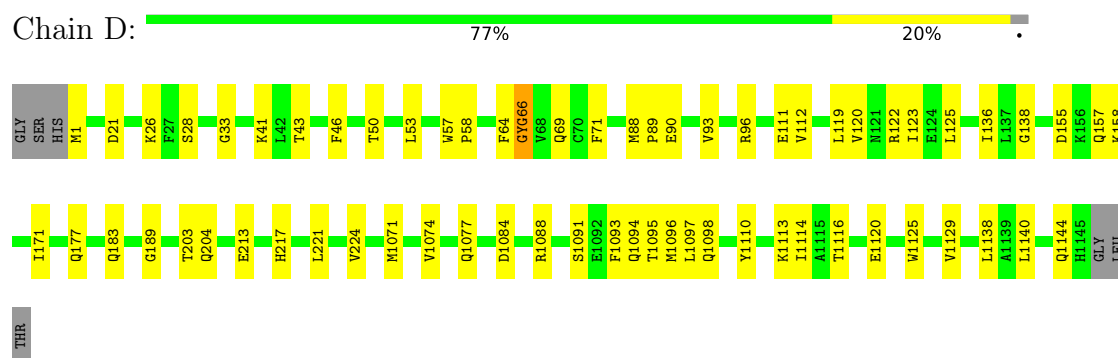
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

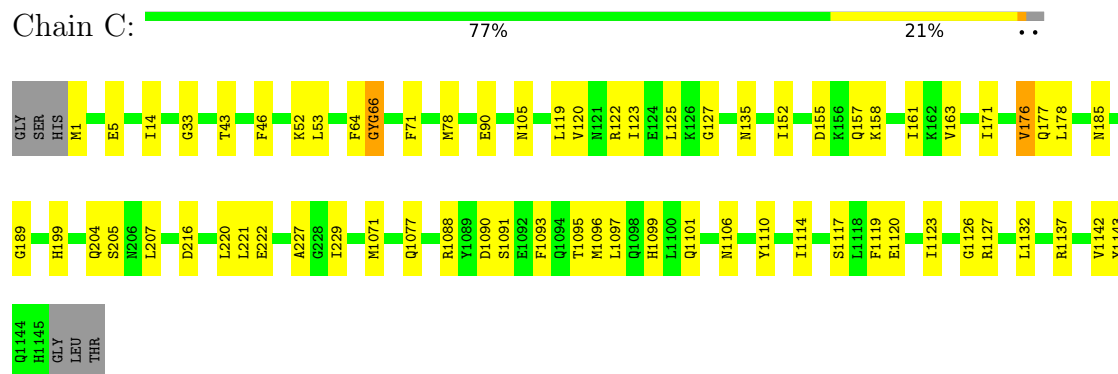
- Molecule 1: Green fluorescent protein,Bcl-2 homologous antagonist/killer



- 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, α , β , γ	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) 99.7 (20.00-2.30)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 2.30Å)	Xtriage
Refinement program	PHENIX, PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.198 , 0.250 0.201 , 0.251	Depositor DCC
R_{free} test set	3707 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	40.2	Xtriage
Anisotropy	0.407	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 64.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10100	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.59	0/2487	0.93	5/3362 (0.1%)
1	B	0.60	0/2495	0.87	2/3372 (0.1%)
1	C	0.56	0/2495	0.84	4/3372 (0.1%)
1	D	0.58	0/2495	0.83	3/3372 (0.1%)
All	All	0.58	0/9972	0.87	14/13478 (0.1%)

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1101	GLN	CA-C-N	-6.36	113.40	120.14
1	A	1101	GLN	C-N-CA	-6.36	113.40	120.14
1	B	53	LEU	CA-C-N	5.54	126.02	120.04
1	B	53	LEU	C-N-CA	5.54	126.02	120.04
1	D	53	LEU	CA-C-N	5.51	125.60	119.87

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	111	0
1	B	2458	0	2381	55	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2458	0	2381	59	0
1	D	2458	0	2381	59	0
2	A	10	0	0	1	0
2	B	5	0	0	0	0
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	2	0
All	All	10072	28	9540	247	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 13.

The worst 5 of 247 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:1093:PHE:HA	1:D:1096:MET:HE3	1.33	1.06
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:D:1113:LYS:HB2	1:A:1071:MET:HE1	1.44	0.99

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	301/313 (96%)	296 (98%)	5 (2%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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 ⓘ

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%)	257 (98%)	6 (2%)	44	63
1	B	264/268 (98%)	263 (100%)	1 (0%)	84	92
1	C	264/268 (98%)	262 (99%)	2 (1%)	73	86
1	D	264/268 (98%)	262 (99%)	2 (1%)	73	86
All	All	1055/1072 (98%)	1044 (99%)	11 (1%)	68	82

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	176	VAL
1	A	186	THR
1	A	1145	HIS
1	A	1095	THR
1	C	176	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	139	HIS
1	C	206	ASN
1	A	1145	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	206	ASN
1	D	105	ASN

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	B	66	1	20,20,21	3.47	5 (25%)	25,27,29	3.25	9 (36%)
1	CR2	D	66	1	20,20,21	3.63	5 (25%)	25,27,29	3.34	9 (36%)
1	CR2	C	66	1	20,20,21	3.51	6 (30%)	25,27,29	3.67	9 (36%)
1	CR2	A	66	1	20,20,21	3.66	4 (20%)	25,27,29	3.53	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	B	66	1	-	1/6/25/26	0/2/2/2
1	CR2	D	66	1	-	1/6/25/26	0/2/2/2
1	CR2	C	66	1	-	1/6/25/26	0/2/2/2
1	CR2	A	66	1	-	2/6/25/26	0/2/2/2

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	66	CR2	CB2-CA2	15.34	1.49	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	66	CR2	CB2-CA2	14.84	1.49	1.35
1	B	66	CR2	CB2-CA2	14.33	1.48	1.35
1	C	66	CR2	CB2-CA2	14.27	1.48	1.35
1	D	66	CR2	O2-C2	3.49	1.30	1.23

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	66	CR2	O2-C2-CA2	-12.92	122.78	131.02
1	D	66	CR2	O2-C2-CA2	-11.49	123.69	131.02
1	A	66	CR2	O2-C2-CA2	-11.11	123.93	131.02
1	B	66	CR2	O2-C2-CA2	-10.86	124.09	131.02
1	C	66	CR2	CA2-C2-N3	7.59	109.87	103.50

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	66	CR2	C3-CA3-N3-C2
1	C	66	CR2	C3-CA3-N3-C2
1	A	66	CR2	C3-CA3-N3-C1
1	A	66	CR2	C3-CA3-N3-C2
1	B	66	CR2	C3-CA3-N3-C2

There are no ring outliers.

4 monomers are involved in 13 short contacts:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	-	2,4,4	2.58	2 (100%)	4,6,6	2.49	2 (50%)
3	MPD	A	1203	-	7,7,7	0.36	0	9,10,10	0.51	0
3	MPD	C	1201	-	7,7,7	0.31	0	9,10,10	0.53	0
2	CAC	D	1201	-	2,4,4	2.45	2 (100%)	4,6,6	1.28	1 (25%)
2	CAC	A	1202	-	2,4,4	2.48	2 (100%)	4,6,6	1.71	1 (25%)
2	CAC	B	1201	-	2,4,4	2.60	2 (100%)	4,6,6	1.44	1 (25%)
2	CAC	D	1202	-	2,4,4	2.63	2 (100%)	4,6,6	1.81	1 (25%)
2	CAC	D	1203	-	2,4,4	2.72	2 (100%)	4,6,6	2.04	2 (50%)

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	MPD	A	1203	-	-	1/5/5/5	-
3	MPD	C	1201	-	-	0/5/5/5	-

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1203	CAC	AS-C1	2.82	1.97	1.90
2	A	1201	CAC	AS-C2	2.77	1.96	1.90
2	D	1202	CAC	AS-C1	2.72	1.96	1.90
2	B	1201	CAC	AS-C2	2.71	1.96	1.90
2	D	1203	CAC	AS-C2	2.62	1.96	1.90

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	CAC	O1-AS-C1	-3.92	106.63	111.50
2	A	1202	CAC	O1-AS-C1	-2.76	108.07	111.50
2	D	1203	CAC	O1-AS-C1	-2.43	108.47	111.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	A	1201	CAC	O2-AS-C1	2.43	111.74	105.84
2	D	1203	CAC	O1-AS-C2	-2.38	108.54	111.50

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1203	MPD	C2-C3-C4-O4

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	305/313 (97%)	0.38	16 (5%) 33 34	32, 75, 117, 145	0
1	B	306/313 (97%)	-0.52	0 100 100	26, 50, 85, 120	0
1	C	306/313 (97%)	-0.46	0 100 100	31, 52, 88, 122	0
1	D	306/313 (97%)	-0.47	0 100 100	30, 52, 92, 119	0
All	All	1223/1252 (97%)	-0.27	16 (1%) 75 76	26, 56, 103, 145	0

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	160	GLY	4.6
1	A	114	PHE	4.4
1	A	22	VAL	3.4
1	A	188	ILE	2.9
1	A	195	LEU	2.7

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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	CR2	A	66	19/20	0.85	0.11	59,73,98,114	0
1	CR2	C	66	19/20	0.89	0.08	37,48,69,79	0
1	CR2	D	66	19/20	0.93	0.06	44,48,57,57	0
1	CR2	B	66	19/20	0.96	0.05	27,37,52,64	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MPD	A	1203	8/8	0.81	0.15	70,90,104,114	0
2	CAC	D	1203	5/5	0.89	0.14	78,78,146,199	0
2	CAC	D	1201	5/5	0.90	0.12	57,62,92,192	0
2	CAC	A	1202	5/5	0.94	0.17	57,60,236,297	0
2	CAC	A	1201	5/5	0.94	0.12	88,91,155,197	0
2	CAC	B	1201	5/5	0.95	0.12	42,53,190,293	0
3	MPD	C	1201	8/8	0.95	0.08	42,56,68,73	0
2	CAC	D	1202	5/5	0.95	0.12	64,84,128,223	0

6.5 Other polymers [i](#)

There are no such residues in this entry.