



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:43 PM GMT

PDB ID : 1UWJ  
Title : The complex of mutant V599E B-RAF and BAY439006  
Authors : Barford, D.; Roe, S.M.; Wan, P.T.C.; Project, Cancer Genome  
Deposited on : 2004-02-05  
Resolution : 3.50 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.

---

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

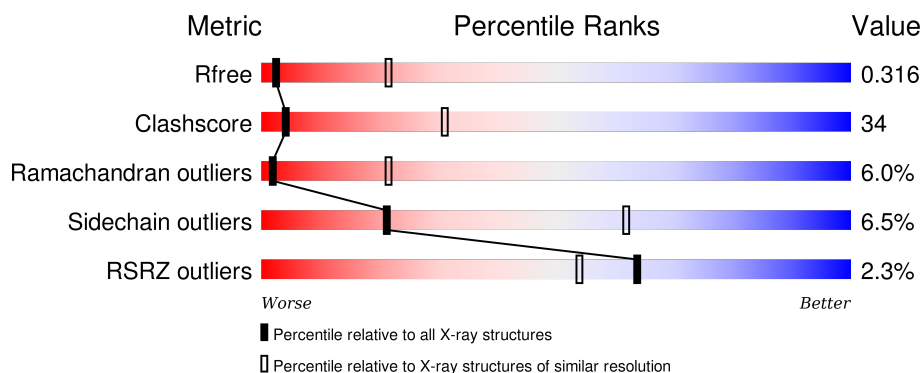
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 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	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

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	276	
1	B	276	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4281 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.

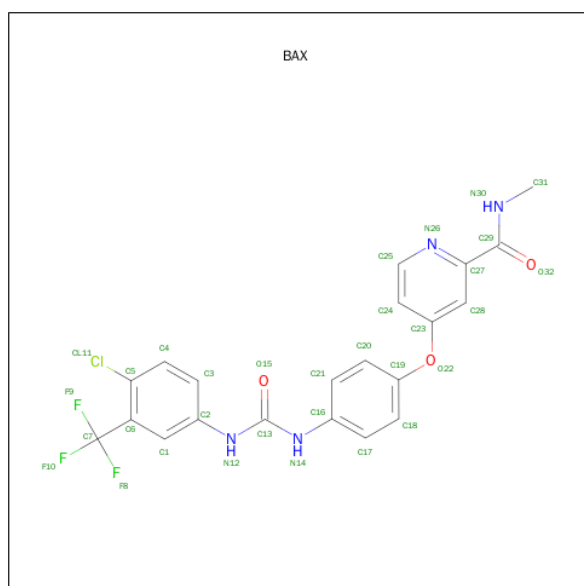
- Molecule 1 is a protein called B-RAF PROTO-ONCOGENE SERINE/THREONINE-PROTEIN KINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	0	0
			2111	1352	367	379	13			
1	B	263	Total	C	N	O	S	0	0	0
			2105	1349	366	377	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	599	GLU	VAL	ENGINEERED MUTATION	UNP P15056
B	599	GLU	VAL	ENGINEERED MUTATION	UNP P15056

- Molecule 2 is 4-{4-[(4-CHLORO-3-(TRIFLUOROMETHYL)PHENYL)AMINO]CARBONYL)AMINO]PHENOXY}-N-METHYLPYRIDINE-2-CARBOXAMIDE (three-letter code: BAX) (formula: C<sub>21</sub>H<sub>16</sub>ClF<sub>3</sub>N<sub>4</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Cl	F	N	O	0	0
			32	21	1	3	4	3		
2	B	1	Total	C	Cl	F	N	O	0	0
			32	21	1	3	4	3		

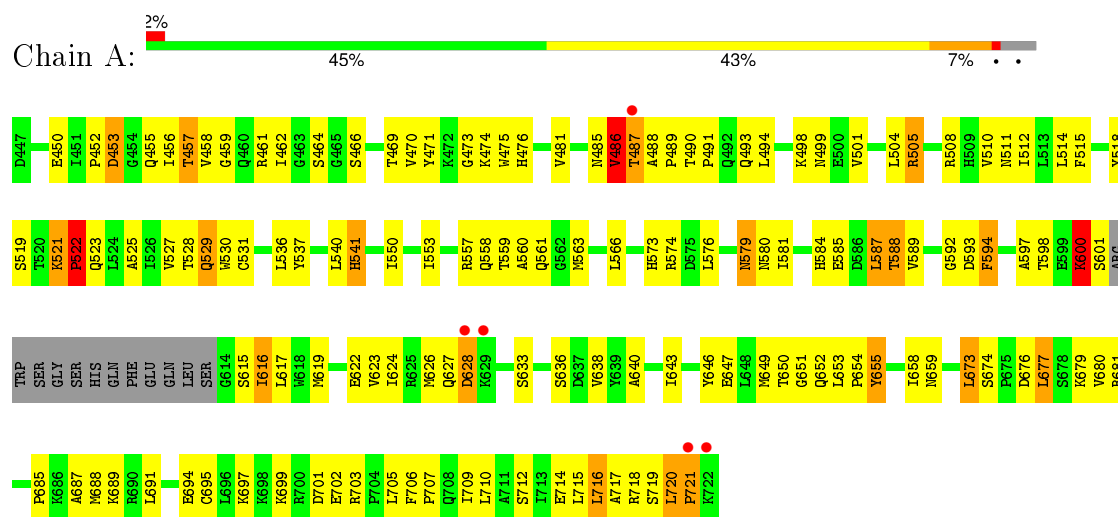
- Molecule 3 is water.

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

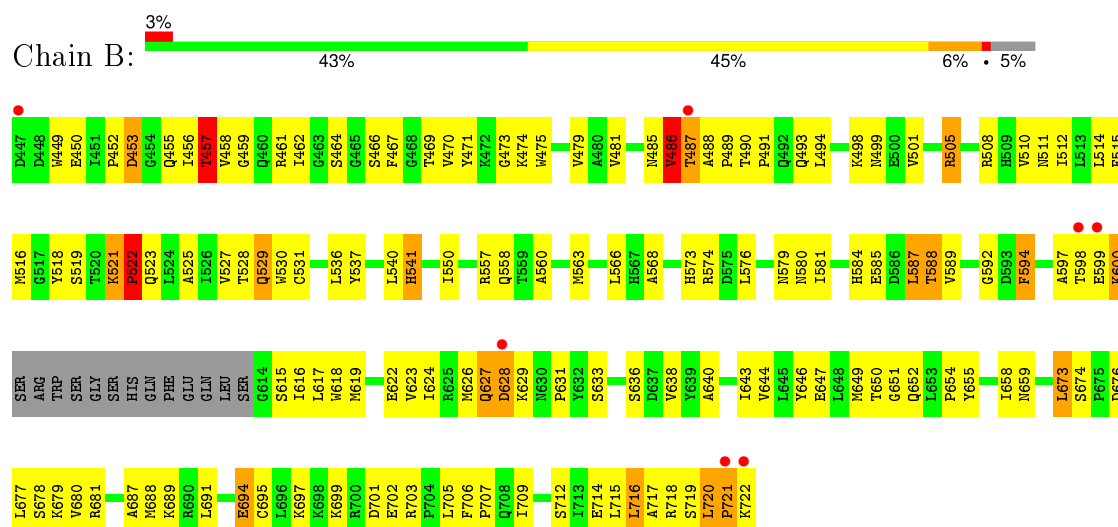
### 3 Residue-property plots

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: B-RAF PROTO-ONCOGENE SERINE/THREONINE-PROTEIN KINASE



#### • Molecule 1: B-RAF PROTO-ONCOGENE SERINE/THREONINE-PROTEIN KINASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	97.66 Å 97.66 Å 168.07 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.39 – 3.50 29.39 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.39-3.50) 99.9 (29.39-3.50)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.68 (at 3.47 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.275 , 0.357 0.251 , 0.316	Depositor DCC
$R_{free}$ test set	566 reflections (5.54%)	DCC
Wilson B-factor (Å <sup>2</sup> )	40.8	Xtriage
Anisotropy	0.615	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 16.0	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	2 of 10781 reflections (0.019%)	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	4281	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	5.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.21% 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

### 5.1 Standard geometry

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

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	0.50	0/2156	0.67	0/2907
1	B	0.50	0/2150	0.67	0/2899
All	All	0.50	0/4306	0.67	0/5806

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	2111	0	2150	146	0
1	B	2105	0	2145	151	0
2	A	32	0	16	0	0
2	B	32	0	16	0	0
3	A	1	0	0	0	0
All	All	4281	0	4327	290	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 34.

All (290) 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:B:626:MET:SD	1:B:631:PRO:HG2	2.10	0.91
1:A:550:ILE:HD12	1:A:550:ILE:H	1.38	0.89
1:B:550:ILE:H	1:B:550:ILE:HD12	1.37	0.89
1:B:598:THR:HG22	1:B:599:GLU:H	1.39	0.88
1:B:521:LYS:HB3	1:B:522:PRO:HD2	1.59	0.85
1:B:464:SER:HB3	1:B:469:THR:HG23	1.59	0.84
1:A:521:LYS:HB3	1:A:522:PRO:HD2	1.59	0.82
1:B:490:THR:HG22	1:B:493:GLN:H	1.46	0.81
1:A:490:THR:HG22	1:A:493:GLN:H	1.48	0.79
1:A:464:SER:HB3	1:A:469:THR:HG23	1.65	0.78
1:A:563:MET:CE	1:A:576:LEU:HD22	2.16	0.76
1:A:453:ASP:HB2	1:A:521:LYS:HB3	1.68	0.75
1:B:453:ASP:HB2	1:B:521:LYS:HB3	1.69	0.74
1:A:490:THR:HG23	1:A:491:PRO:HD2	1.69	0.74
1:A:550:ILE:CD1	1:A:550:ILE:H	2.03	0.72
1:A:452:PRO:HB2	1:A:455:GLN:HE21	1.53	0.72
1:B:563:MET:CE	1:B:576:LEU:HD22	2.20	0.72
1:B:550:ILE:H	1:B:550:ILE:CD1	2.01	0.71
1:B:680:VAL:HG21	1:B:689:LYS:HD2	1.71	0.71
1:A:680:VAL:HG21	1:A:689:LYS:HD2	1.72	0.71
1:A:600:LYS:HG3	1:A:601:SER:H	1.56	0.70
1:B:452:PRO:HB2	1:B:455:GLN:HE21	1.57	0.70
1:B:687:ALA:HB1	1:B:716:LEU:HD22	1.74	0.70
1:B:453:ASP:HB2	1:B:521:LYS:CB	2.22	0.69
1:B:490:THR:HG23	1:B:491:PRO:HD2	1.73	0.69
1:B:550:ILE:N	1:B:550:ILE:HD12	2.07	0.68
1:B:616:ILE:HD12	1:B:617:LEU:N	2.08	0.68
1:A:456:ILE:HG22	1:A:475:TRP:HB2	1.75	0.68
1:B:453:ASP:H	1:B:521:LYS:HE3	1.59	0.68
1:B:646:TYR:CE1	1:B:650:THR:HG21	2.29	0.68
1:A:453:ASP:HB2	1:A:521:LYS:CB	2.23	0.67
1:B:456:ILE:HG22	1:B:475:TRP:HB2	1.76	0.67
1:A:616:ILE:HD13	1:A:616:ILE:H	1.60	0.67
1:A:521:LYS:CB	1:A:522:PRO:HD2	2.24	0.67
1:B:719:SER:C	1:B:720:LEU:HD22	2.15	0.67
1:A:687:ALA:HB1	1:A:716:LEU:HD22	1.76	0.67
1:A:481:VAL:HG22	1:A:527:VAL:HG22	1.75	0.66
1:B:521:LYS:CB	1:B:522:PRO:HD2	2.23	0.66
1:A:646:TYR:CE1	1:A:650:THR:HG21	2.30	0.66
1:A:550:ILE:N	1:A:550:ILE:HD12	2.08	0.66
1:A:452:PRO:HD2	1:A:455:GLN:NE2	2.11	0.66
1:B:585:GLU:O	1:B:587:LEU:HD23	1.97	0.65

Continued on next page...



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:ASP:H	1:A:521:LYS:HE3	1.62	0.65
1:B:485:ASN:ND2	1:B:489:PRO:HG3	2.12	0.65
1:A:453:ASP:OD2	1:A:522:PRO:HG2	1.97	0.64
1:A:580:ASN:HB3	1:A:592:GLY:O	1.96	0.64
1:B:452:PRO:HD2	1:B:455:GLN:NE2	2.12	0.64
1:A:490:THR:HG23	1:A:491:PRO:CD	2.27	0.64
1:A:720:LEU:H	1:A:721:PRO:CD	2.12	0.63
1:A:563:MET:HE3	1:A:576:LEU:HD22	1.79	0.63
1:B:563:MET:HE3	1:B:576:LEU:HD22	1.80	0.63
1:B:481:VAL:HG22	1:B:527:VAL:HG22	1.81	0.63
1:A:485:ASN:ND2	1:A:489:PRO:HG3	2.14	0.63
1:B:717:ALA:HA	1:B:720:LEU:HD23	1.79	0.63
1:B:580:ASN:HB3	1:B:592:GLY:O	1.98	0.62
1:B:490:THR:HG23	1:B:491:PRO:CD	2.30	0.62
1:A:563:MET:HE2	1:A:576:LEU:HD22	1.80	0.62
1:B:453:ASP:OD2	1:B:522:PRO:HG2	2.00	0.62
1:A:453:ASP:CG	1:A:522:PRO:HD2	2.20	0.61
1:B:514:LEU:HD12	1:B:515:PHE:H	1.65	0.61
1:A:466:SER:HB2	1:A:597:ALA:HA	1.82	0.61
1:B:616:ILE:HG22	1:B:619:MET:CE	2.30	0.61
1:A:587:LEU:O	1:A:588:THR:CB	2.48	0.61
1:B:453:ASP:CG	1:B:522:PRO:HD2	2.21	0.61
1:A:673:LEU:HD23	1:A:674:SER:H	1.66	0.60
1:B:466:SER:HB2	1:B:597:ALA:HA	1.82	0.60
1:A:537:TYR:HB3	1:A:579:ASN:ND2	2.17	0.60
1:A:453:ASP:OD1	1:A:521:LYS:HB2	2.01	0.60
1:B:587:LEU:O	1:B:588:THR:CB	2.50	0.60
1:B:537:TYR:HB3	1:B:579:ASN:ND2	2.18	0.59
1:B:453:ASP:OD1	1:B:521:LYS:HB2	2.03	0.59
1:B:646:TYR:O	1:B:650:THR:HG23	2.03	0.59
1:A:581:ILE:HG23	1:A:589:VAL:CG1	2.33	0.59
1:A:585:GLU:HG2	1:B:587:LEU:HD11	1.84	0.58
1:B:599:GLU:C	1:B:600:LYS:HD3	2.23	0.58
1:A:646:TYR:O	1:A:650:THR:HG23	2.04	0.58
1:B:587:LEU:O	1:B:587:LEU:HG	2.03	0.58
1:B:563:MET:HE2	1:B:576:LEU:HD22	1.86	0.58
1:B:494:LEU:O	1:B:498:LYS:HG3	2.03	0.58
1:A:587:LEU:O	1:A:587:LEU:HG	2.03	0.57
1:A:658:ILE:HD12	1:A:673:LEU:HD11	1.86	0.57
1:B:461:ARG:HE	1:B:471:TYR:HE2	1.52	0.57
1:A:716:LEU:O	1:A:716:LEU:HD12	2.05	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:633:SER:O	1:A:636:SER:HB3	2.05	0.57
1:B:522:PRO:O	1:B:523:GLN:HB2	2.05	0.57
1:A:522:PRO:O	1:A:523:GLN:HB2	2.05	0.57
1:B:581:ILE:HG23	1:B:589:VAL:CG1	2.35	0.57
1:A:514:LEU:HD12	1:A:515:PHE:H	1.69	0.56
1:B:514:LEU:HB3	1:B:529:GLN:HG2	1.87	0.56
1:B:673:LEU:HD23	1:B:674:SER:H	1.70	0.56
1:B:633:SER:O	1:B:636:SER:HB3	2.04	0.56
1:A:514:LEU:HB3	1:A:529:GLN:HG2	1.86	0.56
1:A:658:ILE:CD1	1:A:673:LEU:HD11	2.35	0.56
1:A:581:ILE:HG23	1:A:589:VAL:HG13	1.88	0.56
1:B:716:LEU:O	1:B:716:LEU:HD12	2.06	0.55
1:A:587:LEU:O	1:A:588:THR:HB	2.05	0.55
1:A:622:GLU:HG2	1:A:623:VAL:N	2.20	0.55
1:B:658:ILE:HD12	1:B:673:LEU:HD11	1.88	0.55
1:B:587:LEU:O	1:B:588:THR:HB	2.06	0.55
1:A:585:GLU:O	1:A:587:LEU:HD23	2.06	0.55
1:B:659:ASN:O	1:B:659:ASN:OD1	2.25	0.55
1:B:658:ILE:CD1	1:B:673:LEU:HD11	2.37	0.55
1:B:581:ILE:HG23	1:B:589:VAL:HG13	1.89	0.54
1:B:622:GLU:HG2	1:B:623:VAL:N	2.23	0.54
1:A:494:LEU:O	1:A:498:LYS:HG3	2.08	0.54
1:B:714:GLU:O	1:B:717:ALA:HB3	2.08	0.53
1:B:691:LEU:O	1:B:691:LEU:HD12	2.08	0.53
1:A:695:CYS:O	1:A:703:ARG:HD3	2.09	0.53
1:A:691:LEU:HD12	1:A:691:LEU:O	2.09	0.53
1:A:600:LYS:CG	1:A:601:SER:H	2.22	0.52
1:B:486:VAL:O	1:B:488:ALA:N	2.43	0.52
1:B:490:THR:HB	1:B:493:GLN:NE2	2.25	0.52
1:B:633:SER:H	1:B:636:SER:HB3	1.74	0.52
1:A:461:ARG:HE	1:A:471:TYR:HE2	1.56	0.52
1:A:553:ILE:HD11	1:A:685:PRO:HG2	1.92	0.52
1:B:699:LYS:HD2	1:B:702:GLU:OE2	2.09	0.52
1:A:519:SER:HB3	1:A:525:ALA:HB3	1.92	0.52
1:A:587:LEU:HD11	1:B:585:GLU:HG2	1.92	0.51
1:A:462:ILE:HB	1:A:470:VAL:HG12	1.93	0.51
1:B:453:ASP:HB2	1:B:521:LYS:CG	2.41	0.51
1:B:514:LEU:HD12	1:B:515:PHE:N	2.25	0.51
1:A:715:LEU:HG	1:A:716:LEU:N	2.26	0.50
1:A:699:LYS:HD2	1:A:702:GLU:OE2	2.11	0.50
1:B:654:PRO:HB2	1:B:655:TYR:CD2	2.45	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:490:THR:HB	1:B:493:GLN:CD	2.31	0.50
1:B:462:ILE:HB	1:B:470:VAL:HG12	1.93	0.50
1:B:462:ILE:HD11	1:B:530:TRP:HH2	1.76	0.50
1:A:462:ILE:CD1	1:A:530:TRP:HH2	2.25	0.50
1:B:695:CYS:O	1:B:703:ARG:HD3	2.12	0.50
1:B:519:SER:HB3	1:B:525:ALA:HB3	1.93	0.50
1:A:521:LYS:O	1:A:523:GLN:O	2.30	0.50
1:A:557:ARG:O	1:A:560:ALA:HB3	2.12	0.50
1:A:452:PRO:HA	1:A:521:LYS:HE3	1.92	0.50
1:A:633:SER:H	1:A:636:SER:HB3	1.77	0.49
1:A:462:ILE:HD11	1:A:530:TRP:HH2	1.77	0.49
1:A:619:MET:HB3	1:A:624:ILE:HD11	1.94	0.49
1:B:462:ILE:CD1	1:B:530:TRP:HH2	2.25	0.49
1:B:655:TYR:CE1	1:B:673:LEU:HD22	2.47	0.49
1:A:490:THR:HB	1:A:493:GLN:NE2	2.27	0.49
1:B:536:LEU:HG	1:B:540:LEU:HD13	1.95	0.49
1:A:616:ILE:H	1:A:616:ILE:CD1	2.24	0.49
1:A:655:TYR:CE1	1:A:673:LEU:HD22	2.48	0.49
1:A:511:ASN:ND2	1:A:558:GLN:HB3	2.27	0.49
1:A:453:ASP:HB2	1:A:521:LYS:CG	2.42	0.49
1:B:511:ASN:ND2	1:B:558:GLN:HB3	2.27	0.49
1:B:521:LYS:O	1:B:523:GLN:O	2.30	0.49
1:A:715:LEU:HD13	1:A:718:ARG:HH21	1.77	0.49
1:B:719:SER:O	1:B:720:LEU:HD13	2.12	0.49
1:A:486:VAL:O	1:A:488:ALA:N	2.45	0.49
1:A:490:THR:HB	1:A:493:GLN:CD	2.33	0.49
1:A:659:ASN:O	1:A:659:ASN:OD1	2.31	0.49
1:B:452:PRO:HA	1:B:521:LYS:HE3	1.95	0.48
1:B:640:ALA:O	1:B:643:ILE:N	2.46	0.48
1:B:541:HIS:N	1:B:541:HIS:ND1	2.60	0.48
1:B:717:ALA:CA	1:B:720:LEU:HD23	2.42	0.48
1:B:627:GLN:O	1:B:628:ASP:HB2	2.14	0.48
1:A:714:GLU:O	1:A:717:ALA:HB3	2.14	0.48
1:A:573:HIS:O	1:A:574:ARG:HB2	2.12	0.48
1:B:654:PRO:HB2	1:B:655:TYR:CE2	2.49	0.48
1:A:537:TYR:CB	1:A:579:ASN:ND2	2.76	0.48
1:A:508:ARG:NH2	1:B:505:ARG:HA	2.28	0.48
1:B:619:MET:HB3	1:B:624:ILE:HD11	1.95	0.48
1:B:697:LYS:HB2	1:B:703:ARG:HG2	1.96	0.48
1:A:541:HIS:N	1:A:541:HIS:ND1	2.61	0.47
1:A:536:LEU:HG	1:A:540:LEU:HD13	1.96	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:644:VAL:O	1:B:647:GLU:HB2	2.14	0.47
1:A:490:THR:HB	1:A:493:GLN:CG	2.44	0.47
1:B:461:ARG:HA	1:B:471:TYR:HD2	1.79	0.47
1:B:557:ARG:O	1:B:560:ALA:HB3	2.15	0.47
1:A:697:LYS:O	1:A:703:ARG:NH1	2.48	0.47
1:A:508:ARG:HB2	1:B:449:TRP:CH2	2.49	0.47
1:B:521:LYS:HB3	1:B:522:PRO:CD	2.37	0.47
1:B:537:TYR:CB	1:B:579:ASN:ND2	2.78	0.47
1:A:705:LEU:HB2	1:A:707:PRO:HD2	1.97	0.47
1:B:715:LEU:HD13	1:B:718:ARG:HH21	1.80	0.46
1:B:705:LEU:HB2	1:B:707:PRO:HD2	1.97	0.46
1:B:450:GLU:HG3	1:B:518:TYR:CE1	2.51	0.46
1:A:719:SER:O	1:A:720:LEU:HB2	2.16	0.46
1:A:720:LEU:N	1:A:721:PRO:CD	2.76	0.46
1:A:505:ARG:HA	1:B:508:ARG:NH2	2.31	0.46
1:A:521:LYS:HB3	1:A:522:PRO:CD	2.39	0.46
1:B:467:PHE:CD1	1:B:598:THR:O	2.69	0.46
1:A:501:VAL:O	1:A:505:ARG:HG2	2.16	0.46
1:B:720:LEU:O	1:B:722:LYS:N	2.49	0.46
1:B:616:ILE:HG22	1:B:619:MET:HE3	1.97	0.46
1:A:654:PRO:HB2	1:A:655:TYR:CD2	2.50	0.46
1:B:715:LEU:HG	1:B:716:LEU:N	2.31	0.46
1:A:461:ARG:HA	1:A:471:TYR:HD2	1.80	0.46
1:A:647:GLU:O	1:A:651:GLY:N	2.46	0.45
1:B:521:LYS:O	1:B:522:PRO:C	2.55	0.45
1:B:490:THR:HB	1:B:493:GLN:CG	2.47	0.45
1:A:486:VAL:O	1:A:487:THR:C	2.54	0.45
1:A:459:GLY:H	1:A:473:GLY:HA2	1.81	0.45
1:A:453:ASP:N	1:A:521:LYS:HG3	2.32	0.45
1:B:719:SER:O	1:B:720:LEU:HD22	2.17	0.45
1:A:512:ILE:CD1	1:A:566:LEU:HG	2.47	0.45
1:A:504:LEU:HD22	1:A:515:PHE:HB2	1.98	0.45
1:B:706:PHE:N	1:B:707:PRO:CD	2.80	0.45
1:A:452:PRO:HD2	1:A:455:GLN:HE22	1.82	0.45
1:B:521:LYS:CB	1:B:522:PRO:CD	2.92	0.44
1:A:688:MET:O	1:A:691:LEU:N	2.50	0.44
1:A:654:PRO:HB2	1:A:655:TYR:CE2	2.52	0.44
1:B:647:GLU:O	1:B:651:GLY:N	2.44	0.44
1:A:640:ALA:O	1:A:643:ILE:N	2.51	0.44
1:B:616:ILE:C	1:B:616:ILE:HD12	2.38	0.44
1:B:486:VAL:O	1:B:487:THR:C	2.55	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:594:PHE:CD1	1:A:594:PHE:N	2.86	0.44
1:B:563:MET:HE3	1:B:576:LEU:HB2	2.00	0.44
1:B:514:LEU:O	1:B:528:THR:HB	2.18	0.44
1:A:712:SER:O	1:A:716:LEU:HG	2.18	0.43
1:A:514:LEU:HD12	1:A:515:PHE:N	2.30	0.43
1:B:499:ASN:C	1:B:501:VAL:H	2.20	0.43
1:B:617:LEU:HD13	1:B:654:PRO:HD2	2.00	0.43
1:A:514:LEU:O	1:A:528:THR:HB	2.17	0.43
1:B:499:ASN:C	1:B:501:VAL:N	2.71	0.43
1:B:457:THR:HB	1:B:474:LYS:HB2	1.99	0.43
1:B:573:HIS:O	1:B:574:ARG:HB2	2.18	0.43
1:B:501:VAL:O	1:B:505:ARG:HG2	2.18	0.43
1:A:499:ASN:C	1:A:501:VAL:H	2.21	0.43
1:A:521:LYS:O	1:A:522:PRO:C	2.56	0.43
1:A:697:LYS:HB2	1:A:703:ARG:HG2	2.00	0.43
1:A:499:ASN:C	1:A:501:VAL:N	2.71	0.43
1:B:594:PHE:CD1	1:B:594:PHE:N	2.86	0.43
1:B:453:ASP:CB	1:B:521:LYS:HB3	2.46	0.43
1:B:720:LEU:HB2	1:B:721:PRO:HD3	2.00	0.43
1:B:529:GLN:HB2	1:B:529:GLN:HE21	1.67	0.43
1:A:508:ARG:HB2	1:B:449:TRP:CZ3	2.54	0.43
1:A:521:LYS:CB	1:A:522:PRO:CD	2.94	0.43
1:B:655:TYR:CD1	1:B:673:LEU:HD22	2.54	0.43
1:B:584:HIS:O	1:B:587:LEU:O	2.37	0.43
1:B:691:LEU:HA	1:B:694:GLU:HB2	2.00	0.42
1:A:490:THR:CG2	1:A:491:PRO:N	2.82	0.42
1:B:712:SER:O	1:B:716:LEU:HG	2.20	0.42
1:A:695:CYS:O	1:A:703:ARG:CD	2.68	0.42
1:B:676:ASP:O	1:B:678:SER:N	2.53	0.42
1:A:649:MET:O	1:A:681:ARG:HG3	2.19	0.42
1:A:687:ALA:CB	1:A:716:LEU:HD22	2.46	0.42
1:B:697:LYS:O	1:B:703:ARG:NH1	2.52	0.42
1:B:453:ASP:N	1:B:521:LYS:HG3	2.34	0.42
1:B:522:PRO:O	1:B:523:GLN:CB	2.68	0.42
1:A:522:PRO:O	1:A:523:GLN:CB	2.68	0.42
1:A:706:PHE:N	1:A:707:PRO:CD	2.83	0.42
1:A:643:ILE:O	1:A:647:GLU:HG3	2.20	0.42
1:A:450:GLU:HG3	1:A:518:TYR:CE1	2.54	0.42
1:B:459:GLY:H	1:B:473:GLY:HA2	1.84	0.42
1:A:617:LEU:CD1	1:A:653:LEU:HD22	2.49	0.42
1:A:655:TYR:CD1	1:A:673:LEU:HD22	2.55	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:559:THR:HG23	1:A:581:ILE:HD11	2.01	0.42
1:B:715:LEU:C	1:B:717:ALA:H	2.20	0.42
1:A:715:LEU:HD13	1:A:718:ARG:NH2	2.35	0.42
1:A:650:THR:O	1:A:652:GLN:HG3	2.19	0.42
1:A:584:HIS:O	1:A:587:LEU:O	2.38	0.42
1:B:598:THR:HG22	1:B:599:GLU:N	2.19	0.41
1:B:687:ALA:CB	1:B:716:LEU:HD22	2.45	0.41
1:A:619:MET:CB	1:A:624:ILE:HD11	2.50	0.41
1:A:715:LEU:C	1:A:717:ALA:H	2.23	0.41
1:A:457:THR:HB	1:A:474:LYS:HB2	2.02	0.41
1:B:650:THR:O	1:B:652:GLN:HG3	2.20	0.41
1:B:479:VAL:HG12	1:B:516:MET:HE1	2.02	0.41
1:B:638:VAL:HG13	1:B:709:ILE:HD11	2.02	0.41
1:B:585:GLU:O	1:B:587:LEU:CD2	2.66	0.41
1:B:563:MET:CE	1:B:576:LEU:HB2	2.50	0.41
1:A:720:LEU:N	1:A:721:PRO:HD3	2.36	0.41
1:A:622:GLU:OE1	1:A:703:ARG:NH2	2.46	0.41
1:B:649:MET:O	1:B:681:ARG:HG3	2.20	0.41
1:A:616:ILE:HG22	1:A:619:MET:CE	2.51	0.41
1:A:529:GLN:HB2	1:A:529:GLN:HE21	1.70	0.41
1:A:563:MET:CE	1:A:576:LEU:HB2	2.51	0.41
1:B:531:CYS:HA	1:B:584:HIS:CE1	2.55	0.41
1:B:599:GLU:O	1:B:600:LYS:HD3	2.20	0.41
1:A:638:VAL:HG13	1:A:709:ILE:HD11	2.01	0.41
1:B:490:THR:CG2	1:B:491:PRO:N	2.84	0.41
1:A:563:MET:HE2	1:A:576:LEU:HD13	2.03	0.41
1:B:715:LEU:O	1:B:717:ALA:N	2.45	0.41
1:A:691:LEU:HA	1:A:694:GLU:HB2	2.02	0.41
1:B:512:ILE:CD1	1:B:566:LEU:HG	2.51	0.41
1:A:676:ASP:O	1:A:679:LYS:HG3	2.20	0.41
1:A:531:CYS:HA	1:A:584:HIS:CE1	2.56	0.41
1:B:615:SER:HG	1:B:618:TRP:HZ3	1.68	0.40
1:B:563:MET:HE2	1:B:576:LEU:HD13	2.02	0.40
1:A:677:LEU:O	1:A:689:LYS:HE3	2.22	0.40
1:A:561:GLN:HG3	1:A:710:LEU:HD11	2.03	0.40
1:A:593:ASP:OD2	1:A:600:LYS:NZ	2.54	0.40
1:B:688:MET:O	1:B:691:LEU:N	2.55	0.40
1:A:638:VAL:CG1	1:A:709:ILE:HD11	2.51	0.40
1:A:476:HIS:CE1	1:B:568:ALA:HB2	2.55	0.40
1:A:617:LEU:HD13	1:A:654:PRO:HD2	2.03	0.40
1:B:622:GLU:OE1	1:B:703:ARG:NH2	2.41	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:519:SER:N	1:B:525:ALA:O	2.55	0.40
1:B:676:ASP:O	1:B:679:LYS:HG3	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	260/276 (94%)	204 (78%)	40 (15%)	16 (6%)	2	21
1	B	259/276 (94%)	203 (78%)	41 (16%)	15 (6%)	2	23
All	All	519/552 (94%)	407 (78%)	81 (16%)	31 (6%)	2	21

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	522	PRO
1	A	628	ASP
1	A	720	LEU
1	B	486	VAL
1	B	487	THR
1	B	522	PRO
1	B	628	ASP
1	A	486	VAL
1	A	487	THR
1	A	588	THR
1	A	600	LYS
1	B	588	THR
1	B	677	LEU
1	B	721	PRO
1	A	677	LEU
1	B	594	PHE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	629	LYS
1	B	720	LEU
1	A	521	LYS
1	A	594	PHE
1	A	615	SER
1	A	655	TYR
1	B	521	LYS
1	A	587	LEU
1	B	587	LEU
1	B	716	LEU
1	A	716	LEU
1	B	457	THR
1	A	721	PRO
1	A	458	VAL
1	B	458	VAL

### 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	232/243 (96%)	215 (93%)	17 (7%)	17	57
1	B	231/243 (95%)	218 (94%)	13 (6%)	26	66
All	All	463/486 (95%)	433 (94%)	30 (6%)	21	62

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	453	ASP
1	A	457	THR
1	A	486	VAL
1	A	505	ARG
1	A	510	VAL
1	A	522	PRO
1	A	529	GLN
1	A	541	HIS

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	579	ASN
1	A	598	THR
1	A	600	LYS
1	A	616	ILE
1	A	626	MET
1	A	627	GLN
1	A	628	ASP
1	A	673	LEU
1	A	701	ASP
1	B	453	ASP
1	B	457	THR
1	B	486	VAL
1	B	505	ARG
1	B	510	VAL
1	B	522	PRO
1	B	529	GLN
1	B	541	HIS
1	B	600	LYS
1	B	627	GLN
1	B	673	LEU
1	B	694	GLU
1	B	701	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	455	GLN
1	A	476	HIS
1	A	499	ASN
1	A	509	HIS
1	A	511	ASN
1	A	529	GLN
1	A	579	ASN
1	A	659	ASN
1	B	455	GLN
1	B	476	HIS
1	B	499	ASN
1	B	509	HIS
1	B	511	ASN
1	B	529	GLN
1	B	579	ASN
1	B	659	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

2 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	BAX	A	1723	-	34,34,34	3.96	13 (38%)	45,48,48	3.35	15 (33%)
2	BAX	B	1723	-	34,34,34	4.17	14 (41%)	45,48,48	3.34	14 (31%)

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	BAX	A	1723	-	-	0/24/24/24	0/3/3/3
2	BAX	B	1723	-	-	0/24/24/24	0/3/3/3

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1723	BAX	C7-C6	-4.84	1.39	1.50

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1723	BAX	C7-C6	-4.25	1.41	1.50
2	A	1723	BAX	C28-C23	-3.58	1.32	1.38
2	A	1723	BAX	C28-C27	-2.72	1.32	1.40
2	B	1723	BAX	C28-C23	-2.66	1.34	1.38
2	B	1723	BAX	C28-C27	-2.65	1.32	1.40
2	B	1723	BAX	C13-N14	2.14	1.41	1.37
2	A	1723	BAX	C27-C29	2.38	1.56	1.50
2	B	1723	BAX	C5-CL11	2.48	1.79	1.73
2	A	1723	BAX	C13-N14	2.48	1.41	1.37
2	B	1723	BAX	C27-C29	2.49	1.56	1.50
2	A	1723	BAX	C5-C6	2.85	1.45	1.39
2	B	1723	BAX	C5-C6	3.88	1.47	1.39
2	A	1723	BAX	C27-N26	4.37	1.42	1.34
2	A	1723	BAX	C17-C16	4.45	1.46	1.39
2	A	1723	BAX	C24-C23	4.59	1.47	1.38
2	B	1723	BAX	C24-C23	4.77	1.48	1.38
2	B	1723	BAX	C27-N26	4.81	1.42	1.34
2	B	1723	BAX	C17-C16	4.99	1.47	1.39
2	A	1723	BAX	C25-N26	5.18	1.45	1.34
2	B	1723	BAX	C25-N26	5.49	1.46	1.34
2	A	1723	BAX	C16-N14	8.98	1.58	1.41
2	B	1723	BAX	C16-N14	9.15	1.59	1.41
2	A	1723	BAX	C13-N12	9.50	1.54	1.37
2	B	1723	BAX	C13-N12	9.89	1.55	1.37
2	A	1723	BAX	C29-N30	14.10	1.49	1.33
2	B	1723	BAX	C29-N30	14.83	1.50	1.33

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1723	BAX	O15-C13-N12	-8.86	110.13	123.58
2	B	1723	BAX	O15-C13-N12	-8.84	110.16	123.58
2	A	1723	BAX	C31-N30-C29	-8.73	111.39	121.80
2	B	1723	BAX	C31-N30-C29	-8.28	111.92	121.80
2	B	1723	BAX	O32-C29-N30	-5.59	113.24	122.47
2	A	1723	BAX	O32-C29-N30	-5.36	113.61	122.47
2	A	1723	BAX	C24-C25-N26	-5.30	117.85	123.90
2	B	1723	BAX	C24-C25-N26	-4.99	118.20	123.90
2	B	1723	BAX	O15-C13-N14	-4.08	117.39	123.58
2	A	1723	BAX	O15-C13-N14	-3.68	118.00	123.58
2	B	1723	BAX	O32-C29-C27	-3.57	113.64	121.23
2	B	1723	BAX	C28-C27-N26	-3.04	119.73	123.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1723	BAX	O32-C29-C27	-2.96	114.94	121.23
2	A	1723	BAX	C28-C27-N26	-2.90	119.89	123.30
2	A	1723	BAX	O22-C23-C28	-2.76	110.69	119.04
2	A	1723	BAX	C16-N14-C13	-2.76	121.33	126.65
2	B	1723	BAX	O22-C23-C28	-2.69	110.89	119.04
2	B	1723	BAX	F8-C7-C6	-2.34	108.57	112.68
2	A	1723	BAX	F8-C7-C6	-2.00	109.16	112.68
2	A	1723	BAX	C25-N26-C27	2.24	119.92	116.92
2	B	1723	BAX	C25-N26-C27	2.26	119.96	116.92
2	B	1723	BAX	O22-C23-C24	2.47	128.26	119.42
2	A	1723	BAX	O22-C23-C24	2.54	128.53	119.42
2	B	1723	BAX	N14-C13-N12	7.20	123.86	112.53
2	B	1723	BAX	C29-C27-N26	7.50	126.56	117.67
2	A	1723	BAX	C29-C27-N26	7.61	126.69	117.67
2	A	1723	BAX	N14-C13-N12	8.63	126.10	112.53
2	A	1723	BAX	C2-N12-C13	8.66	143.37	126.65
2	B	1723	BAX	C2-N12-C13	9.97	145.89	126.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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 [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, 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	264/276 (95%)	-0.32	5 (1%) 70 60	4, 4, 4, 4	0
1	B	263/276 (95%)	-0.27	7 (2%) 58 47	7, 7, 7, 7	0
All	All	527/552 (95%)	-0.29	12 (2%) 64 54	4, 4, 7, 7	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	721	PRO	3.0
1	A	628	ASP	2.7
1	B	721	PRO	2.7
1	B	447	ASP	2.5
1	B	722	LYS	2.4
1	A	722	LYS	2.4
1	B	599	GLU	2.3
1	A	487	THR	2.2
1	A	629	LYS	2.1
1	B	628	ASP	2.1
1	B	598	THR	2.0
1	B	487	THR	2.0

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	BAX	A	1723	32/32	0.92	0.23	0.05	2,2,2,2	0
2	BAX	B	1723	32/32	0.92	0.21	-0.21	2,2,2,2	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.