



# Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 12:43 AM GMT

PDB ID : 2FB8  
Title : Structure of the B-Raf kinase domain bound to SB-590885  
Authors : Loughheed, J.C.; Lee, J.; Chau, D.C.; Stout, T.J.  
Deposited on : 2005-12-08  
Resolution : 2.90 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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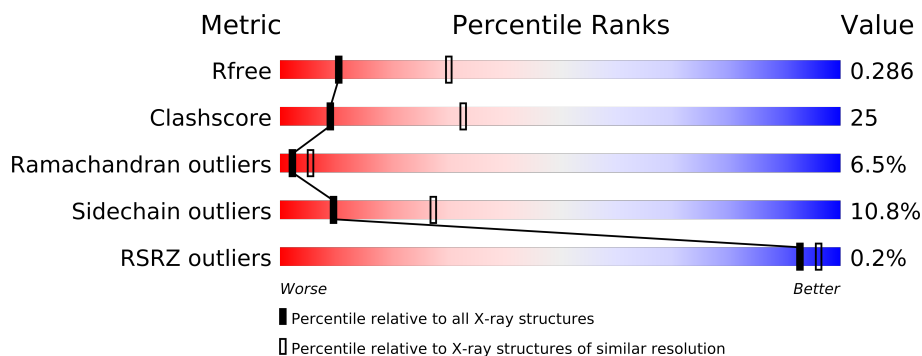
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.90 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	1053 (2.90-2.90)
Clashscore	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)
RSRZ outliers	66119	1054 (2.90-2.90)

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	281	
1	B	281	

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

Mol	Type	Chain	Res	Geometry	Electron density
2	215	A	102	-	X

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 4238 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.

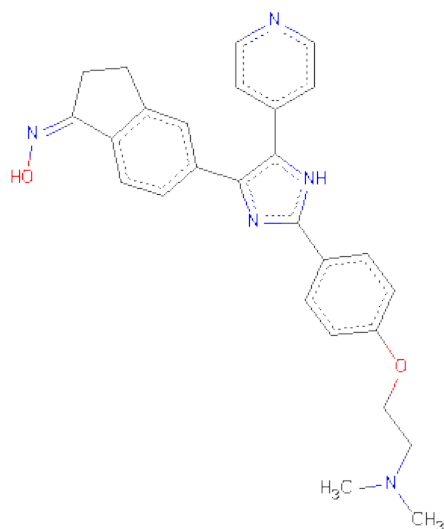
- Molecule 1 is a protein called B-Raf proto-oncogene serine/threonine-proteinkinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	259	Total	C	N	O	S	0	0	0
			2067	1325	360	369	13			
1	B	259	Total	C	N	O	S	0	0	0
			2067	1325	360	369	13			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	443	GLY	-	CLONING ARTIFACT	UNP P15056
A	444	SER	-	CLONING ARTIFACT	UNP P15056
B	443	GLY	-	CLONING ARTIFACT	UNP P15056
B	444	SER	-	CLONING ARTIFACT	UNP P15056

- Molecule 2 is (1Z)-5-(2-{4-[2-(DIMETHYLAMINO)ETHOXY]PHENYL}-5-PYRIDIN-4-YL-1H-IMIDAZOL-4-YL)INDAN-1-ONEOXIME (three-letter code: 215) (formula: C<sub>27</sub>H<sub>27</sub>N<sub>5</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			34	27	5	2		
2	A	1	Total	C	N	O	0	0
			34	27	5	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	22	Total	O	0	0
			22	22		
3	B	14	Total	O	0	0
			14	14		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	95.64Å 95.64Å 159.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.42 – 2.90 46.41 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.9 (46.42-2.90) 97.9 (46.41-2.90)	Depositor EDS
$R_{merge}$	0.23	Depositor
$R_{sym}$	0.23	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.08 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.199 , 0.291 0.198 , 0.286	Depositor DCC
$R_{free}$ test set	840 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	37.4	Xtriage
Anisotropy	0.121	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 10.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	0 of 16653 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	4238	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.42% 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:  
215

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	0.93	0/2111	1.01	3/2849 (0.1%)
1	B	0.94	1/2111 (0.0%)	1.04	3/2849 (0.1%)
All	All	0.93	1/4222 (0.0%)	1.03	6/5698 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	696	CYS	CB-SG	-5.30	1.73	1.81

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	509	ARG	NE-CZ-NH1	7.77	124.19	120.30
1	A	594	ASP	CB-CG-OD1	-5.67	113.20	118.30
1	A	517	MET	CG-SD-CE	5.47	108.95	100.20
1	B	495	LEU	CA-CB-CG	5.14	127.13	115.30
1	B	696	CYS	CA-CB-SG	-5.13	104.76	114.00
1	A	693	MET	CB-CG-SD	-5.08	97.15	112.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	532	CYS	Peptide
1	A	614	SER	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	2067	0	2105	103	0
1	B	2067	0	2105	110	0
2	A	34	0	27	3	0
2	B	34	0	27	4	0
3	A	22	0	0	2	0
3	B	14	0	0	2	0
All	All	4238	0	4264	210	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 25.

All (210) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:491:THR:HG22	1:B:493:GLN:H	1.17	1.07
1:A:558:ARG:HH21	1:A:558:ARG:HG2	1.19	1.04
1:B:484:MET:HB3	1:B:526:ALA:HB2	1.41	1.02
1:B:538:TYR:CE2	2:B:101:215:H261	2.07	0.88
1:A:575:ARG:HD2	1:A:599:THR:HG22	1.62	0.82
1:B:491:THR:CG2	1:B:493:GLN:H	1.91	0.82
1:A:491:THR:HG22	1:A:493:GLN:H	1.45	0.80
1:A:516:PHE:O	1:B:509:ARG:HD3	1.81	0.80
1:B:521:THR:HA	1:B:525:LEU:HD23	1.64	0.80
1:B:491:THR:HG22	1:B:493:GLN:N	2.00	0.75
1:B:538:TYR:HE2	2:B:101:215:H261	1.52	0.75
1:B:575:ARG:NH1	1:B:599:THR:HB	2.02	0.75
1:B:661:ASN:O	1:B:662:ARG:C	2.24	0.74
1:A:504:VAL:HG13	1:A:572:ILE:HD12	1.71	0.73
1:A:578:LYS:HD2	1:A:580:ASN:HD22	1.55	0.71
1:A:575:ARG:HD3	1:A:597:LEU:O	1.91	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:491:THR:HB	1:A:494:GLN:H	1.54	0.71
1:A:501:GLU:HG2	1:A:505:LEU:CD1	2.21	0.71
1:A:485:LEU:O	1:A:485:LEU:HG	1.88	0.71
1:A:682:ARG:HB3	1:A:684:ASN:OD1	1.91	0.71
1:A:501:GLU:HG2	1:A:505:LEU:HD11	1.73	0.70
1:B:468:PHE:HD1	1:B:468:PHE:C	1.94	0.70
1:A:644:ILE:O	1:A:648:GLU:HG3	1.92	0.70
1:B:468:PHE:C	1:B:468:PHE:CD1	2.66	0.69
1:B:467:SER:OG	1:B:483:LYS:NZ	2.26	0.69
1:B:661:ASN:O	1:B:664:GLN:N	2.22	0.68
1:B:466:GLY:O	1:B:467:SER:HB3	1.94	0.68
1:B:500:ASN:O	1:B:504:VAL:HG23	1.94	0.68
1:B:691:ARG:NH1	1:B:691:ARG:HB2	2.08	0.68
1:B:710:ILE:O	1:B:714:ILE:HG13	1.95	0.66
1:B:661:ASN:OD1	1:B:663:ASP:HB3	1.95	0.66
1:A:707:PHE:HA	1:A:710:ILE:HD12	1.79	0.65
1:B:449:ASP:CG	1:B:450:TRP:H	1.99	0.65
1:A:552:LYS:O	1:A:556:ILE:HG13	1.97	0.65
1:B:552:LYS:O	1:B:556:ILE:HG12	1.98	0.64
1:B:578:LYS:NZ	1:B:616:SER:HB2	2.13	0.64
2:A:102:215:H16	2:A:102:215:C9	2.28	0.64
1:A:453:PRO:O	1:A:456:GLN:HB2	1.99	0.61
1:B:650:MET:HE2	1:B:685:CYS:HB2	1.82	0.61
1:B:523:PRO:HG2	1:B:524:GLN:H	1.65	0.61
1:A:584:LEU:HG	1:A:587:ASP:HA	1.81	0.61
1:A:496:GLN:OE1	1:A:496:GLN:HA	2.01	0.60
1:A:619:TRP:CD1	1:A:644:ILE:HB	2.36	0.60
1:B:650:MET:CE	1:B:685:CYS:HB2	2.32	0.60
1:A:509:ARG:HD2	1:B:450:TRP:CH2	2.37	0.59
1:A:533:GLU:HB3	1:A:586:GLU:OE2	2.01	0.59
1:B:491:THR:HB	1:B:494:GLN:H	1.66	0.59
1:B:468:PHE:CE2	1:B:498:PHE:HB2	2.38	0.59
1:B:510:HIS:CE1	1:B:512:ASN:HB2	2.38	0.58
1:A:701:ARG:O	1:A:704:ARG:HG3	2.04	0.58
1:A:450:TRP:CE3	1:A:450:TRP:HA	2.39	0.58
1:A:711:LEU:O	1:A:715:GLU:HG3	2.02	0.58
1:B:647:TYR:O	1:B:651:THR:HG23	2.03	0.58
1:B:691:ARG:HH11	1:B:691:ARG:HB2	1.68	0.57
1:B:449:ASP:CG	1:B:450:TRP:N	2.58	0.57
1:A:576:ASP:HB2	1:A:597:LEU:HD12	1.88	0.56
1:A:512:ASN:HA	1:A:590:VAL:O	2.05	0.56
1:A:532:CYS:SG	1:A:585:HIS:HB2	2.46	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:558:ARG:HG2	1:A:558:ARG:NH2	2.00	0.56
1:A:651:THR:HG22	1:A:681:VAL:HA	1.87	0.56
1:A:575:ARG:HD2	1:A:599:THR:CG2	2.35	0.55
1:A:650:MET:CE	1:A:650:MET:HA	2.35	0.55
1:A:555:ASP:O	1:A:559:GLN:HG3	2.06	0.55
1:A:660:ASN:HB2	3:A:39:HOH:O	2.06	0.55
1:B:660:ASN:H	1:B:660:ASN:HD22	1.54	0.55
1:A:661:ASN:O	1:A:664:GLN:HB2	2.07	0.55
1:A:573:ILE:HG22	1:A:575:ARG:HG3	1.88	0.54
1:B:485:LEU:O	1:B:486:ASN:HB2	2.06	0.54
1:A:538:TYR:CG	1:A:580:ASN:OD1	2.60	0.54
1:B:626:ARG:O	1:B:627:MET:HB2	2.06	0.54
1:B:466:GLY:O	1:B:467:SER:CB	2.54	0.54
1:B:578:LYS:HZ3	1:B:616:SER:HB2	1.72	0.54
1:A:512:ASN:ND2	1:A:559:GLN:HB3	2.22	0.54
1:A:616:SER:HA	3:A:8:HOH:O	2.08	0.54
1:A:586:GLU:O	1:A:588:LEU:N	2.38	0.54
1:B:628:GLN:HG2	1:B:629:ASP:OD1	2.08	0.54
1:A:512:ASN:HD21	1:A:559:GLN:HB3	1.73	0.54
1:A:682:ARG:O	1:A:685:CYS:HB3	2.08	0.53
1:A:625:ILE:C	1:A:627:MET:H	2.11	0.53
1:A:509:ARG:HD3	1:B:516:PHE:O	2.09	0.53
1:A:700:LYS:O	1:A:701:ARG:C	2.46	0.53
1:A:578:LYS:HD3	1:A:616:SER:HB2	1.91	0.53
1:A:681:VAL:O	1:A:682:ARG:C	2.48	0.52
1:A:632:PRO:HD2	1:A:633:TYR:HD1	1.75	0.52
1:A:623:GLU:OE2	1:A:704:ARG:NH2	2.43	0.52
1:B:561:ALA:HB2	1:B:642:PHE:CZ	2.44	0.51
2:A:102:215:C9	2:A:102:215:C16	2.88	0.51
1:B:661:ASN:OD1	1:B:664:GLN:HG2	2.11	0.51
1:B:555:ASP:OD1	1:B:558:ARG:NH1	2.43	0.51
1:A:555:ASP:OD2	1:A:559:GLN:NE2	2.44	0.51
1:A:468:PHE:CE1	1:A:485:LEU:HB2	2.46	0.51
1:A:650:MET:HE3	1:A:650:MET:HA	1.94	0.51
1:B:468:PHE:HE2	1:B:498:PHE:HB2	1.75	0.50
1:A:473:LYS:HD2	1:A:531:TRP:CZ2	2.46	0.50
1:A:683:SER:C	1:A:685:CYS:H	2.15	0.50
1:B:578:LYS:HD3	1:B:580:ASN:ND2	2.26	0.50
1:A:491:THR:HG22	1:A:493:GLN:N	2.20	0.50
1:B:507:LYS:O	1:B:570:LYS:NZ	2.33	0.50
1:A:450:TRP:CH2	1:B:509:ARG:HG3	2.47	0.50
1:A:458:THR:OG1	1:A:475:LYS:HB2	2.12	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:491:THR:HG21	1:B:493:GLN:HB2	1.92	0.49
1:A:501:GLU:HG2	1:A:505:LEU:HD12	1.93	0.49
1:A:503:GLY:O	1:A:507:LYS:NZ	2.28	0.49
1:A:493:GLN:O	1:A:496:GLN:HB3	2.12	0.49
1:B:468:PHE:HE2	1:B:498:PHE:HD1	1.59	0.49
1:B:682:ARG:HH11	1:B:682:ARG:CB	2.26	0.49
1:B:597:LEU:HD12	1:B:597:LEU:N	2.27	0.49
1:B:623:GLU:HG2	1:B:624:VAL:N	2.28	0.49
1:B:468:PHE:HD1	1:B:469:GLY:N	2.11	0.49
1:B:714:ILE:HA	1:B:717:LEU:CD2	2.43	0.49
1:B:513:ILE:O	1:B:514:LEU:C	2.51	0.49
1:A:558:ARG:HH21	1:A:558:ARG:CG	2.06	0.48
1:B:468:PHE:HE2	1:B:498:PHE:CD1	2.31	0.48
1:A:450:TRP:HE3	1:A:450:TRP:HA	1.78	0.48
1:A:509:ARG:O	1:A:510:HIS:HB2	2.13	0.48
1:B:580:ASN:ND2	1:B:580:ASN:N	2.61	0.47
1:A:461:GLN:HG2	1:A:462:ARG:N	2.29	0.47
1:A:622:PRO:O	1:A:625:ILE:HB	2.14	0.47
1:B:715:GLU:O	1:B:716:LEU:C	2.52	0.47
1:A:594:ASP:HA	2:A:102:215:O34	2.14	0.47
1:A:468:PHE:HD1	1:A:485:LEU:HD13	1.79	0.47
1:A:631:ASN:HA	1:A:632:PRO:HD3	1.64	0.47
1:A:632:PRO:HD2	1:A:633:TYR:CD1	2.50	0.47
1:B:533:GLU:HB3	1:B:586:GLU:OE2	2.13	0.47
1:B:462:ARG:NH1	1:B:464:GLY:HA2	2.30	0.47
1:A:485:LEU:CG	1:A:485:LEU:O	2.57	0.47
1:B:678:LEU:O	1:B:681:VAL:HG13	2.14	0.47
1:B:550:MET:HE3	1:B:684:ASN:OD1	2.15	0.47
1:B:505:LEU:O	1:B:507:LYS:N	2.48	0.47
1:B:707:PHE:HA	1:B:710:ILE:HB	1.97	0.47
1:A:532:CYS:HA	1:A:585:HIS:HD2	1.79	0.46
1:A:634:SER:OG	1:A:636:GLN:HB2	2.15	0.46
1:A:501:GLU:CG	1:A:505:LEU:HD11	2.44	0.46
1:A:486:ASN:O	1:A:487:VAL:C	2.53	0.46
1:B:660:ASN:N	1:B:660:ASN:HD22	2.12	0.46
1:B:644:ILE:O	1:B:648:GLU:HG3	2.16	0.46
1:A:586:GLU:C	1:A:588:LEU:H	2.18	0.46
1:B:671:ARG:HD3	3:B:32:HOH:O	2.16	0.46
1:A:676:PRO:HG3	1:A:697:LEU:HD13	1.98	0.46
1:B:484:MET:HB3	1:B:526:ALA:CB	2.28	0.45
1:A:491:THR:CG2	1:A:492:PRO:HD2	2.46	0.45
1:B:543:ILE:HG22	1:B:544:ILE:HG23	1.98	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:715:GLU:O	1:A:718:ALA:HB3	2.17	0.45
1:B:503:GLY:O	1:B:506:ARG:HG2	2.16	0.45
1:B:541:LEU:HD12	1:B:648:GLU:HB3	1.97	0.45
1:B:639:VAL:O	1:B:640:TYR:C	2.54	0.45
1:A:498:PHE:O	1:A:499:LYS:C	2.53	0.45
1:A:599:THR:OG1	1:A:600:VAL:N	2.50	0.45
1:B:485:LEU:HD12	1:B:525:LEU:HD12	1.99	0.45
1:A:619:TRP:HA	1:A:644:ILE:HG13	1.98	0.45
1:B:580:ASN:HD22	1:B:580:ASN:H	1.65	0.45
1:A:496:GLN:HE21	1:A:500:ASN:HD21	1.64	0.44
1:B:530:GLN:HG3	1:B:530:GLN:O	2.16	0.44
1:A:516:PHE:CE1	1:A:518:GLY:O	2.71	0.44
1:B:713:SER:O	1:B:717:LEU:HD23	2.18	0.44
1:A:697:LEU:O	1:A:698:LYS:C	2.55	0.44
1:B:625:ILE:O	1:B:626:ARG:C	2.54	0.44
1:B:575:ARG:HG2	1:B:633:TYR:CD2	2.53	0.44
1:B:505:LEU:HD21	1:B:595:PHE:CD1	2.53	0.44
1:B:529:THR:HG23	2:B:101:215:H311	1.99	0.44
1:A:651:THR:O	1:A:653:GLN:N	2.50	0.44
1:A:684:ASN:N	1:A:684:ASN:OD1	2.49	0.43
1:B:644:ILE:HD13	1:B:697:LEU:HD21	2.00	0.43
1:B:661:ASN:O	1:B:663:ASP:N	2.50	0.43
1:A:646:LEU:HD12	1:A:693:MET:HG2	2.00	0.43
1:B:473:LYS:HD2	1:B:531:TRP:CZ2	2.53	0.43
1:A:468:PHE:CD1	1:A:485:LEU:HD13	2.54	0.43
1:B:660:ASN:ND2	1:B:660:ASN:H	2.14	0.43
1:B:585:HIS:CG	1:B:586:GLU:N	2.86	0.43
1:B:483:LYS:HB3	2:B:101:215:H312	2.00	0.43
1:B:505:LEU:O	1:B:506:ARG:C	2.56	0.43
1:B:517:MET:HB2	1:B:528:VAL:O	2.19	0.43
1:B:537:LEU:HD21	1:B:649:LEU:HD21	2.01	0.43
1:A:584:LEU:HD11	1:A:587:ASP:O	2.18	0.42
1:A:634:SER:OG	1:A:636:GLN:N	2.52	0.42
1:B:578:LYS:HB3	1:B:619:TRP:CD2	2.55	0.42
1:A:676:PRO:CG	1:A:697:LEU:HD13	2.50	0.42
1:B:523:PRO:CG	1:B:524:GLN:H	2.31	0.42
1:A:578:LYS:NZ	1:A:616:SER:HB2	2.35	0.42
1:A:683:SER:C	1:A:685:CYS:N	2.73	0.42
1:B:586:GLU:OE2	1:B:586:GLU:HA	2.19	0.42
1:A:468:PHE:CD1	1:A:469:GLY:N	2.88	0.42
1:A:654:LEU:HD23	1:A:654:LEU:HA	1.61	0.42
1:A:619:TRP:HD1	1:A:644:ILE:HB	1.82	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:660:ASN:ND2	1:B:660:ASN:N	2.68	0.42
1:A:625:ILE:C	1:A:627:MET:N	2.72	0.42
1:B:587:ASP:C	1:B:588:LEU:HD23	2.39	0.41
1:B:718:ALA:O	1:B:719:ARG:C	2.59	0.41
1:A:481:ALA:HB3	1:A:529:THR:OG1	2.20	0.41
1:B:583:PHE:HE1	1:B:593:GLY:HA3	1.86	0.41
1:B:571:SER:O	1:B:600:VAL:HA	2.20	0.41
1:B:482:VAL:HG22	1:B:528:VAL:HG22	2.03	0.41
1:B:539:HIS:O	1:B:543:ILE:HB	2.20	0.41
1:A:628:GLN:HB3	1:A:628:GLN:HE21	1.68	0.41
1:B:514:LEU:HA	1:B:514:LEU:HD12	1.80	0.41
1:B:572:ILE:HA	1:B:599:THR:O	2.21	0.41
1:A:539:HIS:O	1:A:543:ILE:HB	2.20	0.41
1:B:707:PHE:HA	1:B:710:ILE:HD12	2.02	0.41
1:B:641:ALA:O	1:B:642:PHE:C	2.58	0.41
1:B:535:SER:HB2	1:B:539:HIS:HB3	2.02	0.41
1:B:573:ILE:HG23	1:B:638:ASP:OD2	2.21	0.41
1:B:504:VAL:O	1:B:505:LEU:C	2.60	0.41
1:A:642:PHE:CZ	1:A:646:LEU:HD21	2.56	0.41
1:B:706:LEU:HA	1:B:706:LEU:HD23	1.79	0.41
1:A:509:ARG:HD2	1:B:450:TRP:CZ2	2.56	0.40
1:B:695:GLU:HG3	3:B:21:HOH:O	2.21	0.40
1:B:578:LYS:HZ2	1:B:616:SER:HB2	1.86	0.40
1:B:682:ARG:CG	1:B:682:ARG:HH11	2.34	0.40
1:A:502:VAL:O	1:A:503:GLY:C	2.59	0.40
1:A:667:PHE:CZ	1:A:671:ARG:HD3	2.55	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	255/281 (91%)	201 (79%)	37 (14%)	17 (7%)	2	5
1	B	255/281 (91%)	215 (84%)	24 (9%)	16 (6%)	2	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	510/562 (91%)	416 (82%)	61 (12%)	33 (6%)	<b>2</b> <b>5</b>

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	486	ASN
1	A	487	VAL
1	A	545	GLU
1	A	587	ASP
1	A	701	ARG
1	B	467	SER
1	B	587	ASP
1	B	629	ASP
1	A	629	ASP
1	A	684	ASN
1	B	487	VAL
1	B	594	ASP
1	B	662	ARG
1	B	663	ASP
1	A	627	MET
1	A	663	ASP
1	B	514	LEU
1	B	586	GLU
1	B	716	LEU
1	A	510	HIS
1	A	652	GLY
1	B	489	ALA
1	B	627	MET
1	B	717	LEU
1	A	489	ALA
1	A	511	VAL
1	A	662	ARG
1	A	682	ARG
1	B	506	ARG
1	B	511	VAL
1	A	594	ASP
1	A	490	PRO
1	B	523	PRO

### 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	227/247 (92%)	202 (89%)	25 (11%)	9	26
1	B	227/247 (92%)	203 (89%)	24 (11%)	10	28
All	All	454/494 (92%)	405 (89%)	49 (11%)	9	27

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	451	GLU
1	A	454	ASP
1	A	456	GLN
1	A	468	PHE
1	A	495	LEU
1	A	498	PHE
1	A	511	VAL
1	A	520	SER
1	A	523	PRO
1	A	533	GLU
1	A	535	SER
1	A	545	GLU
1	A	558	ARG
1	A	586	GLU
1	A	614	SER
1	A	628	GLN
1	A	650	MET
1	A	657	SER
1	A	663	ASP
1	A	671	ARG
1	A	689	MET
1	A	698	LYS
1	A	701	ARG
1	A	709	GLN
1	A	717	LEU
1	B	468	PHE
1	B	480	VAL
1	B	484	MET
1	B	495	LEU

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Mol	Chain	Res	Type
1	B	500	ASN
1	B	506	ARG
1	B	511	VAL
1	B	521	THR
1	B	524	GLN
1	B	535	SER
1	B	546	THR
1	B	578	LYS
1	B	580	ASN
1	B	586	GLU
1	B	616	SER
1	B	617	ILE
1	B	660	ASN
1	B	675	SER
1	B	682	ARG
1	B	691	ARG
1	B	698	LYS
1	B	709	GLN
1	B	717	LEU
1	B	720	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	496	GLN
1	A	512	ASN
1	A	580	ASN
1	A	585	HIS
1	A	628	GLN
1	B	477	HIS
1	B	512	ASN
1	B	539	HIS
1	B	562	GLN
1	B	580	ASN
1	B	585	HIS
1	B	660	ASN

### 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 ⓘ

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	215	A	102	-	37,38,38	1.41	4 (10%)	53,53,53	2.28	15 (28%)
2	215	B	101	-	37,38,38	1.00	3 (8%)	53,53,53	1.99	14 (26%)

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	215	A	102	-	-	0/19/29/29	0/3/5/5
2	215	B	101	-	-	0/19/29/29	0/3/5/5

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	102	215	C6-C5	4.40	1.53	1.47
2	A	102	215	C7-C2	4.27	1.53	1.47
2	B	101	215	C28-C32	2.62	1.51	1.44
2	A	102	215	C28-C32	2.32	1.50	1.44
2	B	101	215	C32-N33	-2.11	1.26	1.28
2	A	102	215	C20-C21	2.10	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	101	215	C27-N25	2.02	1.52	1.46

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	102	215	O34-N33-C32	8.45	124.17	112.57
2	B	101	215	O34-N33-C32	6.58	121.61	112.57
2	B	101	215	C31-C32-N33	-5.20	118.78	129.09
2	A	102	215	C23-O22-C19	5.17	131.10	117.94
2	A	102	215	C31-C32-N33	-4.78	119.59	129.09
2	A	102	215	C30-C29-C28	3.98	113.58	111.36
2	A	102	215	C7-C2-N1	3.72	126.47	121.45
2	B	101	215	C12-C13-N14	-3.68	116.97	123.63
2	A	102	215	C6-C5-N1	3.65	127.77	121.22
2	B	101	215	C11-C10-C28	-3.63	115.68	121.12
2	A	102	215	C16-C7-C2	3.62	123.34	120.65
2	B	101	215	C8-C9-C29	-3.59	116.44	121.98
2	A	102	215	N1-C5-N4	-3.28	105.50	112.31
2	B	101	215	C30-C29-C9	-3.04	124.71	129.67
2	A	102	215	O22-C23-C24	-3.04	100.57	107.50
2	A	102	215	C17-C18-C19	2.87	123.60	119.76
2	B	101	215	C6-C5-N1	2.84	126.32	121.22
2	A	102	215	C2-N1-C5	2.77	112.12	108.03
2	A	102	215	C6-C5-N4	2.69	126.67	122.85
2	B	101	215	C13-N14-C15	2.66	123.60	116.84
2	B	101	215	C15-C16-C7	-2.54	115.48	119.56
2	B	101	215	C18-C17-C6	-2.30	117.64	121.16
2	A	102	215	C18-C19-C20	-2.21	116.42	120.21
2	B	101	215	C17-C18-C19	2.20	122.71	119.76
2	B	101	215	N1-C5-N4	-2.17	107.81	112.31
2	A	102	215	C30-C29-C9	-2.16	126.15	129.67
2	B	101	215	C12-C7-C2	-2.15	119.06	120.65
2	B	101	215	C6-C5-N4	2.13	125.87	122.85
2	A	102	215	C27-N25-C24	2.00	119.01	110.76

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	259/281 (92%)	-0.40	1 (0%) 90 94	9, 26, 49, 61	9 (3%)
1	B	259/281 (92%)	-0.45	0 100 100	8, 24, 40, 55	9 (3%)
All	All	518/562 (92%)	-0.43	1 (0%) 93 96	8, 25, 45, 61	18 (3%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	630	LYS	2.2

### 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
2	215	A	102	34/34	0.22	3.10	18,28,36,38	0
2	215	B	101	34/34	0.17	1.13	19,21,24,32	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.