Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:46 AM GMT

PDB ID	:	3C4C
Title	:	B-Raf Kinase in Complex with PLX4720
Authors	:	Zhang, K.Y.J.; Wang, W.
Deposited on	:	2008-01-29
Resolution	:	2.57 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
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:

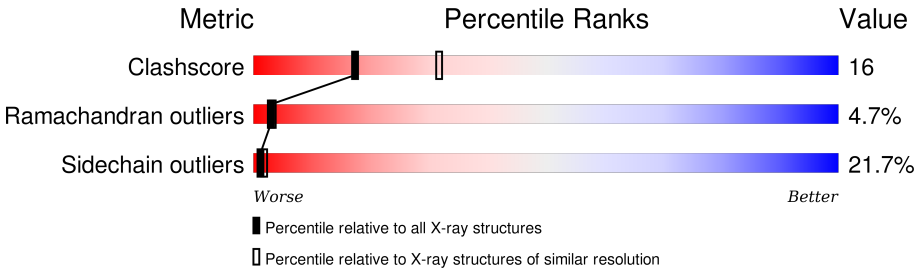
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.57 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))
Clashscore	102246	3003 (2.60-2.56)
Ramachandran outliers	100387	2956 (2.60-2.56)
Sidechain outliers	100360	2956 (2.60-2.56)

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 >=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 <=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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	280	52% 31% 7% • 8%
1	B	280	48% 34% 9% 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4319 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	258	Total	C	N	O	S	0	0	0
			2058	1301	366	378	13			
1	B	257	Total	C	N	O	S	0	0	0
			2054	1299	365	377	13			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	543	ALA	ILE	ENGINEERED	UNP P15056
A	544	SER	ILE	ENGINEERED	UNP P15056
A	551	LYS	ILE	ENGINEERED	UNP P15056
A	562	ARG	GLN	ENGINEERED	UNP P15056
A	588	ASN	LEU	ENGINEERED	UNP P15056
A	630	SER	LYS	ENGINEERED	UNP P15056
A	667	GLU	PHE	ENGINEERED	UNP P15056
A	673	SER	TYR	ENGINEERED	UNP P15056
A	688	ARG	ALA	ENGINEERED	UNP P15056
A	706	SER	LEU	ENGINEERED	UNP P15056
A	709	ARG	GLN	ENGINEERED	UNP P15056
A	713	GLU	SER	ENGINEERED	UNP P15056
A	716	GLU	LEU	ENGINEERED	UNP P15056
A	720	GLU	SER	ENGINEERED	UNP P15056
A	722	SER	-	EXPRESSION TAG	UNP P15056
A	723	GLY	-	EXPRESSION TAG	UNP P15056
B	543	ALA	ILE	ENGINEERED	UNP P15056
B	544	SER	ILE	ENGINEERED	UNP P15056
B	551	LYS	ILE	ENGINEERED	UNP P15056
B	562	ARG	GLN	ENGINEERED	UNP P15056
B	588	ASN	LEU	ENGINEERED	UNP P15056
B	630	SER	LYS	ENGINEERED	UNP P15056
B	667	GLU	PHE	ENGINEERED	UNP P15056
B	673	SER	TYR	ENGINEERED	UNP P15056
B	688	ARG	ALA	ENGINEERED	UNP P15056

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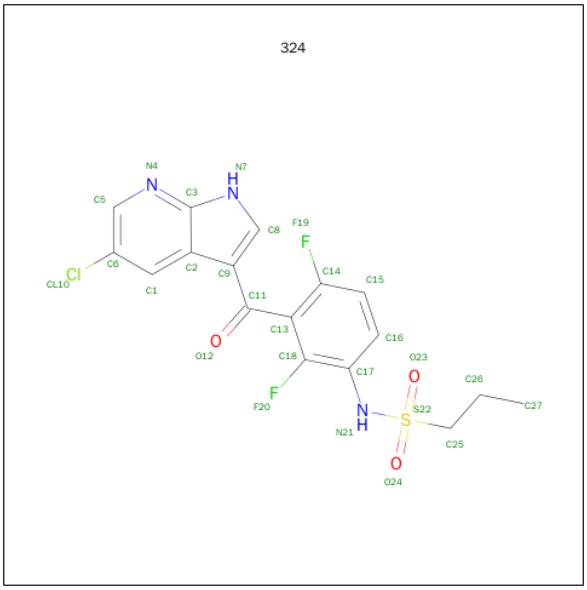
Chain	Residue	Modelled	Actual	Comment	Reference
B	706	SER	LEU	ENGINEERED	UNP P15056
B	709	ARG	GLN	ENGINEERED	UNP P15056
B	713	GLU	SER	ENGINEERED	UNP P15056
B	716	GLU	LEU	ENGINEERED	UNP P15056
B	720	GLU	SER	ENGINEERED	UNP P15056
B	722	SER	-	EXPRESSION TAG	UNP P15056
B	723	GLY	-	EXPRESSION TAG	UNP P15056

- Molecule 2 is N-{3-[(5-CHLORO-1H-PYRROLO[2,3-B]PYRIDIN-3-YL)CARBONYL]-2,4-DIFLUOROPHENYL}PROPANE-1-SULFONAMIDE (three-letter code: 324) (formula: $C_{17}H_{14}ClF_2N_3O_3S$).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	A	1	Total	C	Cl	F	N	O	S	0	0
			27	17	1	2	3	3	1		
2	B	1	Total	C	Cl	F	N	O	S	0	0
			27	17	1	2	3	3	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	87	Total	O	0	0
			87	87		
3	B	66	Total	O	0	0
			66	66		

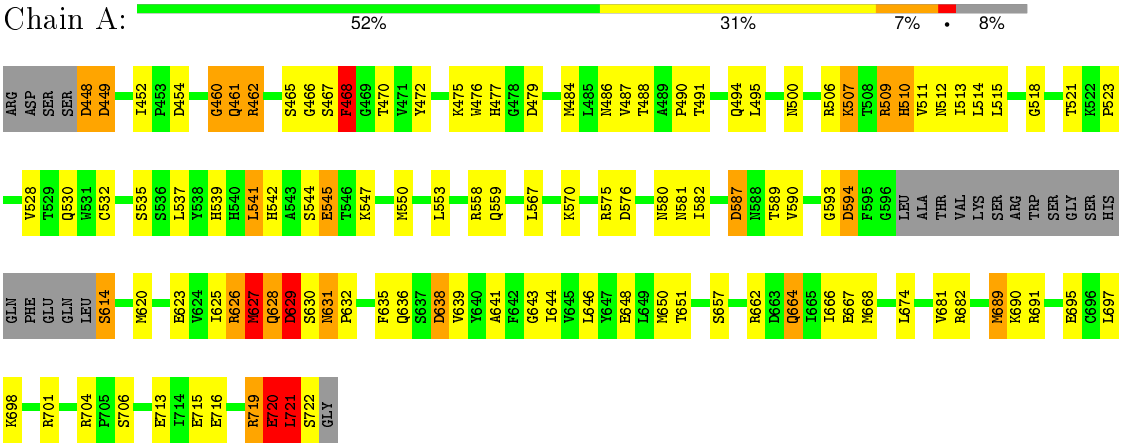
3 Residue-property plots (i)

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.

Note EDS was not executed.

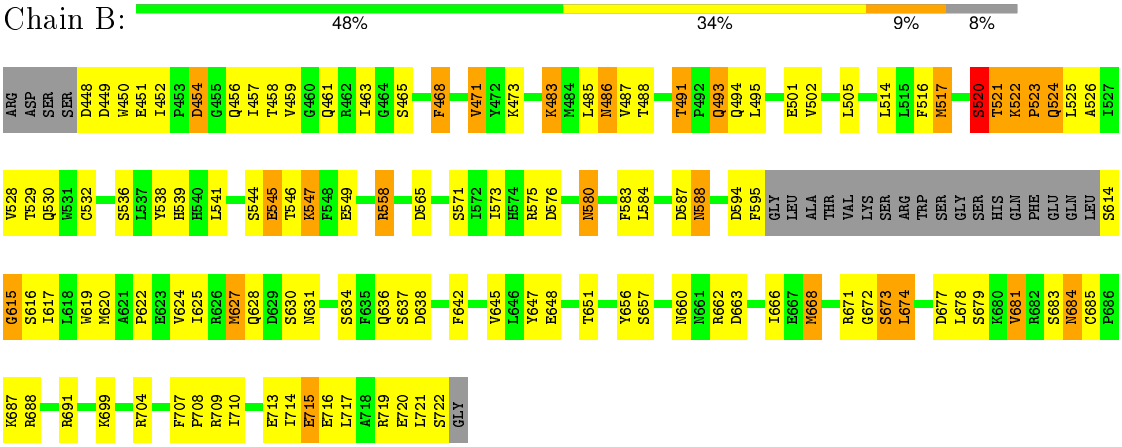
- Molecule 1: B-Raf proto-oncogene serine/threonine-protein kinase

Chain A:



- Molecule 1: B-Raf proto-oncogene serine/threonine-protein kinase

Chain B:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	51.57Å 105.50Å 110.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.57	Depositor
% Data completeness (in resolution range)	99.7 (50.00-2.57)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
Refinement program	REFMAC 5.1.25	Depositor
R, R_{free}	0.259 , 0.303	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4319	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 324

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	0.74	0/2100	0.97	10/2830 (0.4%)
1	B	0.72	0/2096	0.93	7/2825 (0.2%)
All	All	0.73	0/4196	0.95	17/5655 (0.3%)

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	1
1	B	0	3
All	All	0	4

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	587	ASP	CB-CG-OD2	7.66	125.20	118.30
1	B	704	ARG	NE-CZ-NH1	7.34	123.97	120.30
1	A	449	ASP	CB-CG-OD2	7.12	124.71	118.30
1	A	576	ASP	CB-CG-OD2	7.08	124.67	118.30
1	A	479	ASP	CB-CG-OD2	6.73	124.35	118.30
1	A	454	ASP	CB-CG-OD2	6.66	124.30	118.30
1	A	587	ASP	CB-CG-OD2	6.51	124.16	118.30
1	B	677	ASP	CB-CG-OD2	6.27	123.95	118.30
1	B	454	ASP	CB-CG-OD2	6.25	123.92	118.30
1	B	594	ASP	CB-CG-OD2	5.98	123.68	118.30
1	B	663	ASP	CB-CG-OD2	5.64	123.37	118.30
1	B	449	ASP	CB-CG-OD2	5.60	123.34	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	594	ASP	CB-CG-OD2	5.55	123.30	118.30
1	A	638	ASP	CB-CG-OD2	5.47	123.23	118.30
1	A	509	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	A	448	ASP	CB-CG-OD2	5.18	122.96	118.30
1	A	626	ARG	NE-CZ-NH1	5.08	122.84	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	460	GLY	Peptide
1	B	520	SER	Peptide
1	B	545	GLU	Peptide
1	B	615	GLY	Peptide

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	2058	0	2061	72	0
1	B	2054	0	2058	64	0
2	A	27	0	14	2	0
2	B	27	0	14	8	0
3	A	87	0	0	5	0
3	B	66	0	0	4	0
All	All	4319	0	4147	134	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 16.

All (134) 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:A:719:ARG:HA	1:A:720:GLU:O	1.62	1.00
1:B:619:TRP:O	3:B:100:HOH:O	1.91	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:688:ARG:HD3	1:B:717:LEU:CD2	2.07	0.83
1:B:688:ARG:HD3	1:B:717:LEU:HD21	1.65	0.78
1:A:490:PRO:O	3:A:781:HOH:O	2.03	0.77
1:A:570:LYS:O	3:A:774:HOH:O	2.02	0.76
1:A:631:ASN:CB	1:A:632:PRO:HA	2.16	0.76
1:A:631:ASN:HD22	1:A:701:ARG:HH22	1.33	0.75
1:A:510:HIS:HD2	1:A:512:ASN:H	1.35	0.74
1:A:460:GLY:HA3	1:A:461:GLN:OE1	1.87	0.73
1:A:719:ARG:HA	1:A:720:GLU:C	2.09	0.72
1:A:628:GLN:O	1:A:629:ASP:HB2	1.87	0.72
1:B:501:GLU:HG2	2:B:3:324:H27	1.71	0.71
1:B:588:ASN:ND2	3:B:89:HOH:O	2.20	0.70
1:A:631:ASN:HD22	1:A:701:ARG:NH2	1.88	0.70
1:B:468:PHE:CE1	1:B:483:LYS:HD2	2.26	0.70
1:B:662:ARG:O	1:B:666:ILE:HD12	1.90	0.69
1:B:517:MET:HE1	1:B:530:GLN:HA	1.74	0.69
1:A:631:ASN:ND2	1:A:701:ARG:HH22	1.90	0.68
1:A:631:ASN:HB3	1:A:632:PRO:CA	2.25	0.66
1:A:631:ASN:HB3	1:A:632:PRO:HA	1.78	0.66
1:B:456:GLN:NE2	3:B:107:HOH:O	2.29	0.66
1:B:687:LYS:HB3	1:B:687:LYS:NZ	2.12	0.65
1:B:517:MET:CE	1:B:530:GLN:HA	2.27	0.65
1:B:678:LEU:O	1:B:681:VAL:CG2	2.45	0.64
1:B:539:HIS:CE1	1:B:544:SER:HB2	2.32	0.64
1:B:634:SER:OG	1:B:636:GLN:HB2	1.97	0.64
1:A:628:GLN:HG3	1:A:629:ASP:N	2.12	0.63
1:B:501:GLU:HB3	2:B:3:324:C27	2.29	0.63
1:B:620:MET:HG2	1:B:624:VAL:HB	1.80	0.63
1:A:691:ARG:O	1:A:695:GLU:HG2	1.99	0.62
1:A:620:MET:HE3	1:A:625:ILE:HA	1.82	0.61
1:A:491:THR:O	1:A:494:GLN:N	2.31	0.61
1:A:719:ARG:CA	1:A:720:GLU:O	2.44	0.60
1:B:501:GLU:CG	2:B:3:324:H27	2.32	0.59
1:B:468:PHE:HB2	1:B:485:LEU:HD11	1.84	0.59
1:A:628:GLN:HB3	1:A:632:PRO:HB3	1.83	0.59
1:A:664:GLN:O	1:A:668:MET:HG3	2.03	0.59
1:A:631:ASN:CB	1:A:632:PRO:CA	2.80	0.58
1:A:651:THR:HG22	1:A:681:VAL:HG12	1.85	0.58
1:B:716:GLU:O	1:B:720:GLU:N	2.37	0.57
1:A:720:GLU:CG	1:A:721:LEU:N	2.67	0.57
1:A:545:GLU:O	3:A:744:HOH:O	2.17	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:581:ASN:HB3	1:A:593:GLY:O	2.04	0.57
1:B:505:LEU:HD11	2:B:3:324:O24	2.04	0.57
1:B:687:LYS:CB	1:B:687:LYS:NZ	2.67	0.57
1:B:491:THR:OG1	1:B:493:GLN:OE1	2.11	0.56
1:B:647:TYR:CE1	1:B:651:THR:HG21	2.41	0.56
1:A:477:HIS:ND1	1:B:565:ASP:OD2	2.31	0.55
1:B:520:SER:HB2	1:B:526:ALA:HB3	1.88	0.55
1:B:545:GLU:HG3	1:B:546:THR:OG1	2.06	0.55
1:B:463:ILE:HG21	2:B:3:324:CL10	2.44	0.55
1:B:588:ASN:O	1:B:588:ASN:ND2	2.29	0.55
1:A:631:ASN:HB2	1:A:632:PRO:HA	1.89	0.54
1:B:501:GLU:HB3	2:B:3:324:H27A	1.89	0.53
1:B:468:PHE:CE1	1:B:483:LYS:CD	2.90	0.53
1:B:620:MET:HG2	1:B:624:VAL:CG1	2.37	0.53
1:B:707:PHE:N	1:B:708:PRO:CD	2.71	0.53
1:A:542:HIS:NE2	1:A:648:GLU:OE1	2.35	0.52
1:B:668:MET:HB3	1:B:674:LEU:HB2	1.92	0.52
1:B:687:LYS:CB	1:B:687:LYS:HZ2	2.22	0.52
1:A:594:ASP:H	2:A:2:324:HN21	1.57	0.51
1:B:622:PRO:O	1:B:625:ILE:HB	2.11	0.51
1:B:713:GLU:O	1:B:714:ILE:C	2.48	0.51
1:B:620:MET:HG2	1:B:624:VAL:CB	2.41	0.50
1:A:706:SER:HB2	3:A:734:HOH:O	2.12	0.50
1:A:650:MET:SD	1:A:689:MET:HG3	2.52	0.50
1:A:631:ASN:ND2	1:A:701:ARG:NH2	2.55	0.50
1:A:651:THR:HG22	1:A:681:VAL:HA	1.94	0.49
1:B:486:ASN:HA	1:B:524:GLN:NE2	2.27	0.49
1:A:631:ASN:HB3	1:A:632:PRO:C	2.32	0.49
1:A:532:CYS:HB2	2:A:2:324:N4	2.28	0.49
1:A:720:GLU:CG	1:A:721:LEU:H	2.26	0.49
1:A:628:GLN:HG2	1:A:631:ASN:HB2	1.95	0.49
1:A:466:GLY:HA3	1:A:468:PHE:CE1	2.48	0.48
1:B:688:ARG:HB3	1:B:717:LEU:HD21	1.95	0.48
1:A:701:ARG:O	1:A:704:ARG:HB2	2.13	0.48
1:B:468:PHE:HB2	1:B:485:LEU:CD1	2.41	0.48
1:B:538:TYR:CD2	1:B:580:ASN:ND2	2.81	0.48
1:A:720:GLU:HG2	1:A:721:LEU:N	2.27	0.48
1:A:644:ILE:HD13	1:A:697:LEU:HD22	1.95	0.48
1:B:687:LYS:HZ3	1:B:687:LYS:HB3	1.79	0.47
1:B:521:THR:O	1:B:522:LYS:CB	2.62	0.47
2:B:3:324:H16	2:B:3:324:C25	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:491:THR:O	1:A:494:GLN:HB2	2.14	0.47
1:A:510:HIS:CD2	1:A:512:ASN:HD22	2.32	0.47
1:A:509:ARG:HD2	1:B:450:TRP:CZ3	2.50	0.47
1:B:452:ILE:HD12	1:B:528:VAL:HG21	1.97	0.47
1:B:471:VAL:HG13	1:B:483:LYS:HG3	1.96	0.46
1:A:462:ARG:HH21	1:A:465:SER:HB3	1.80	0.46
1:B:628:GLN:NE2	3:B:81:HOH:O	2.40	0.46
1:B:678:LEU:O	1:B:681:VAL:HG22	2.15	0.46
1:A:518:GLY:O	1:A:528:VAL:N	2.48	0.46
1:A:623:GLU:O	1:A:627:MET:N	2.49	0.46
1:A:623:GLU:O	1:A:627:MET:HA	2.16	0.45
1:A:643:GLY:O	1:A:646:LEU:HB2	2.16	0.45
1:B:625:ILE:HG23	1:B:666:ILE:HG23	1.99	0.45
1:B:539:HIS:ND1	1:B:544:SER:HB2	2.31	0.45
1:A:635:PHE:O	1:A:639:VAL:HG23	2.17	0.45
1:B:558:ARG:HD2	1:B:715:GLU:OE2	2.17	0.45
1:A:509:ARG:HD3	1:B:516:PHE:O	2.16	0.44
1:B:647:TYR:CZ	1:B:651:THR:HG21	2.51	0.44
1:A:507:LYS:O	1:A:570:LYS:NZ	2.49	0.44
1:B:684:ASN:O	1:B:685:CYS:C	2.56	0.44
1:A:638:ASP:O	1:A:641:ALA:HB3	2.17	0.44
1:B:529:THR:OG1	2:B:3:324:H8	2.18	0.44
1:B:717:LEU:HA	1:B:720:GLU:HB3	1.99	0.43
1:A:558:ARG:HD2	1:A:715:GLU:HG2	2.00	0.43
1:A:515:LEU:HB2	1:A:530:GLN:OE1	2.17	0.43
1:A:513:ILE:HD12	1:A:567:LEU:HD21	2.00	0.43
1:A:539:HIS:CE1	1:A:544:SER:HB2	2.54	0.43
1:A:537:LEU:HD11	1:A:541:LEU:HD22	2.00	0.43
1:B:487:VAL:O	1:B:488:THR:C	2.56	0.43
1:B:671:ARG:HB3	1:B:673:SER:OG	2.18	0.43
1:A:510:HIS:CD2	1:A:511:VAL:N	2.86	0.43
1:A:510:HIS:CD2	1:A:512:ASN:H	2.25	0.43
1:A:500:ASN:HB3	3:A:765:HOH:O	2.18	0.43
1:A:470:THR:HG22	1:A:472:TYR:CE1	2.55	0.42
1:B:468:PHE:CZ	1:B:483:LYS:HD2	2.52	0.42
1:B:522:LYS:CB	1:B:523:PRO:HD3	2.50	0.42
1:B:538:TYR:CG	1:B:580:ASN:ND2	2.87	0.42
1:A:626:ARG:O	1:A:627:MET:CB	2.67	0.42
1:B:493:GLN:H	1:B:493:GLN:HG3	1.74	0.42
1:A:559:GLN:HB3	1:A:590:VAL:HB	2.01	0.42
1:A:582:ILE:O	1:A:582:ILE:HG22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:ILE:HG12	1:A:476:TRP:CZ2	2.55	0.41
1:B:645:VAL:O	1:B:648:GLU:HB2	2.20	0.41
1:A:466:GLY:HA3	1:A:468:PHE:CD1	2.56	0.41
1:A:644:ILE:HD13	1:A:697:LEU:CD2	2.50	0.41
1:A:625:ILE:HG23	1:A:666:ILE:HG23	2.03	0.41
1:B:642:PHE:CE2	1:B:710:ILE:HG21	2.56	0.41
1:A:614:SER:HB2	1:A:662:ARG:NH2	2.36	0.41
1:A:486:ASN:O	1:A:487:VAL:HG23	2.21	0.40
1:A:650:MET:SD	1:A:689:MET:CG	3.10	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	254/280 (91%)	216 (85%)	26 (10%)	12 (5%)	3	3
1	B	253/280 (90%)	213 (84%)	28 (11%)	12 (5%)	3	3
All	All	507/560 (90%)	429 (85%)	54 (11%)	24 (5%)	3	3

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	627	MET
1	A	628	GLN
1	A	629	ASP
1	A	631	ASN
1	A	720	GLU
1	B	522	LYS
1	B	630	SER
1	B	656	TYR
1	B	523	PRO

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Mol	Chain	Res	Type
1	B	547	LYS
1	A	575	ARG
1	A	721	LEU
1	B	473	LYS
1	B	524	GLN
1	B	571	SER
1	B	576	ASP
1	A	468	PHE
1	A	630	SER
1	A	514	LEU
1	B	627	MET
1	A	510	HIS
1	B	615	GLY
1	A	523	PRO
1	B	672	GLY

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	226/246 (92%)	186 (82%)	40 (18%)	2 3
1	B	226/246 (92%)	168 (74%)	58 (26%)	0 1
All	All	452/492 (92%)	354 (78%)	98 (22%)	1 2

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	448	ASP
1	A	449	ASP
1	A	461	GLN
1	A	462	ARG
1	A	467	SER
1	A	468	PHE
1	A	475	LYS
1	A	484	MET

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Mol	Chain	Res	Type
1	A	488	THR
1	A	495	LEU
1	A	506	ARG
1	A	507	LYS
1	A	521	THR
1	A	535	SER
1	A	541	LEU
1	A	545	GLU
1	A	547	LYS
1	A	550	MET
1	A	553	LEU
1	A	580	ASN
1	A	587	ASP
1	A	589	THR
1	A	614	SER
1	A	627	MET
1	A	629	ASP
1	A	636	GLN
1	A	657	SER
1	A	664	GLN
1	A	667	GLU
1	A	674	LEU
1	A	682	ARG
1	A	689	MET
1	A	690	LYS
1	A	698	LYS
1	A	713	GLU
1	A	716	GLU
1	A	719	ARG
1	A	720	GLU
1	A	721	LEU
1	A	722	SER
1	B	448	ASP
1	B	451	GLU
1	B	454	ASP
1	B	457	ILE
1	B	458	THR
1	B	459	VAL
1	B	461	GLN
1	B	465	SER
1	B	468	PHE
1	B	471	VAL

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Mol	Chain	Res	Type
1	B	483	LYS
1	B	486	ASN
1	B	491	THR
1	B	493	GLN
1	B	494	GLN
1	B	495	LEU
1	B	502	VAL
1	B	514	LEU
1	B	517	MET
1	B	520	SER
1	B	521	THR
1	B	525	LEU
1	B	532	CYS
1	B	536	SER
1	B	541	LEU
1	B	547	LYS
1	B	549	GLU
1	B	558	ARG
1	B	573	ILE
1	B	575	ARG
1	B	580	ASN
1	B	583	PHE
1	B	584	LEU
1	B	588	ASN
1	B	595	PHE
1	B	614	SER
1	B	616	SER
1	B	617	ILE
1	B	627	MET
1	B	631	ASN
1	B	637	SER
1	B	638	ASP
1	B	657	SER
1	B	660	ASN
1	B	668	MET
1	B	673	SER
1	B	674	LEU
1	B	679	SER
1	B	681	VAL
1	B	683	SER
1	B	684	ASN
1	B	691	ARG

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Mol	Chain	Res	Type
1	B	699	LYS
1	B	709	ARG
1	B	715	GLU
1	B	719	ARG
1	B	721	LEU
1	B	722	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	510	HIS
1	A	512	ASN
1	A	628	GLN
1	A	631	ASN
1	B	539	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

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	324	A	2	-	28,29,29	2.63	7 (25%)	31,43,43	2.69	12 (38%)
2	324	B	3	-	28,29,29	2.59	8 (28%)	31,43,43	2.29	10 (32%)

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	324	A	2	-	-	0/13/17/17	0/3/3/3
2	324	B	3	-	-	0/13/17/17	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3	324	C25-S22	-5.00	1.66	1.78
2	A	2	324	C25-S22	-4.34	1.67	1.78
2	A	2	324	C17-N21	-4.22	1.35	1.42
2	B	3	324	C17-N21	-3.69	1.36	1.42
2	B	3	324	C1-C2	-2.54	1.37	1.42
2	B	3	324	C5-N4	2.30	1.35	1.31
2	A	2	324	C1-C6	2.73	1.42	1.36
2	A	2	324	C13-C18	3.14	1.44	1.38
2	A	2	324	C17-C18	4.65	1.47	1.38
2	A	2	324	C13-C14	4.75	1.46	1.39
2	B	3	324	C13-C18	4.84	1.47	1.38
2	B	3	324	C17-C18	5.31	1.49	1.38
2	B	3	324	C9-C2	5.70	1.47	1.42
2	B	3	324	C13-C14	6.13	1.48	1.39
2	A	2	324	C9-C2	8.59	1.49	1.42

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	2	324	O23-S22-O24	-8.49	104.68	119.34
2	B	3	324	C13-C18-C17	-7.02	116.45	121.20
2	B	3	324	O23-S22-O24	-5.32	110.16	119.34
2	A	2	324	C18-C13-C11	-4.00	114.22	121.47
2	A	2	324	C13-C18-C17	-4.00	118.50	121.20
2	B	3	324	C1-C6-CL10	-3.41	114.88	119.74
2	A	2	324	F20-C18-C13	-3.27	115.48	119.93
2	B	3	324	C6-C1-C2	-2.92	115.36	120.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	3	324	C15-C14-C13	-2.53	119.05	123.42
2	A	2	324	C15-C14-C13	-2.45	119.18	123.42
2	B	3	324	O23-S22-C25	2.00	111.50	107.73
2	A	2	324	C15-C16-C17	2.04	123.77	119.79
2	B	3	324	C15-C16-C17	2.04	123.77	119.79
2	B	3	324	C16-C15-C14	2.14	121.33	119.00
2	A	2	324	O23-S22-N21	2.59	115.53	107.66
2	A	2	324	O24-S22-C25	2.93	113.24	107.73
2	A	2	324	C5-N4-C3	2.97	120.42	116.93
2	A	2	324	C1-C6-CL10	3.10	124.16	119.74
2	B	3	324	O12-C11-C9	3.10	126.87	120.70
2	A	2	324	O12-C11-C9	3.73	128.11	120.70
2	B	3	324	F20-C18-C17	3.92	123.92	118.08
2	A	2	324	F20-C18-C17	5.33	126.01	118.08

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2	324	2	0
2	B	3	324	8	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

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.