



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:35 PM GMT

PDB ID : 4CQE  
Title : B-Raf Kinase V600E mutant in complex with a diarylthiazole B-Raf Inhibitor  
Authors : Casale, E.; Fasolini, M.; Pulici, M.; Traquandi, G.; Marchionni, C.; Modugno, M.; Lupi, R.; Amboldi, N.; Colombo, N.; Corti, L.; Gasparri, F.; Pastori, W.; Sclaro, A.; Donati, D.; Felder, E.; Galvani, A.; Isacchi, A.; Pesenti, E.; Ciomei, M.  
Deposited on : 2014-02-14  
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

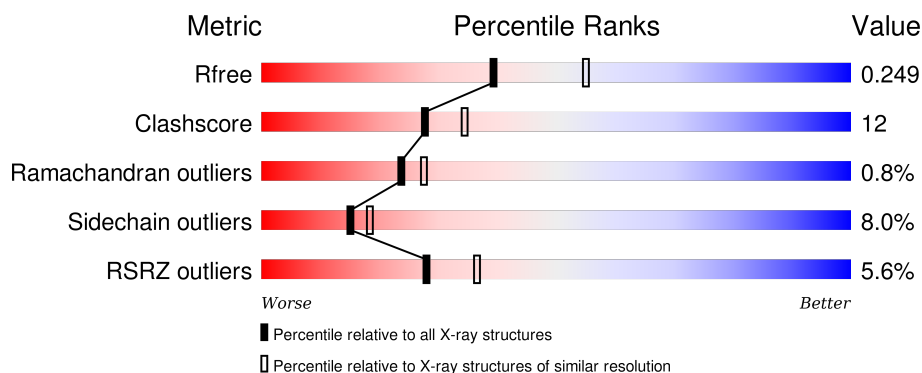
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	278	<div> <div>4%</div> <div>66%</div> <div>19%</div> <div>5%</div> <div>10%</div> </div>
1	B	278	<div> <div>6%</div> <div>69%</div> <div>16%</div> <div>•</div> <div>11%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4141 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 SLC45A3-BRAF FUSION PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	0	0
			2003	1269	359	362	13			
1	B	248	Total	C	N	O	S	0	0	0
			1989	1261	356	360	12			

There are 38 discrepancies between the modelled and reference sequences:

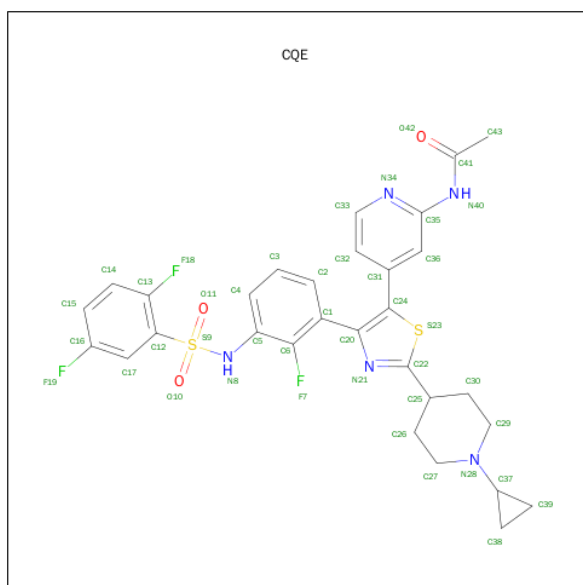
Chain	Residue	Modelled	Actual	Comment	Reference
A	446	GLY	-	EXPRESSION TAG	UNP D7PBN4
A	447	PRO	-	EXPRESSION TAG	UNP D7PBN4
A	543	ALA	ILE	ENGINEERED MUTATION	UNP D7PBN4
A	544	SER	ILE	ENGINEERED MUTATION	UNP D7PBN4
A	551	LYS	ILE	ENGINEERED MUTATION	UNP D7PBN4
A	562	ARG	GLN	ENGINEERED MUTATION	UNP D7PBN4
A	588	ASN	LEU	ENGINEERED MUTATION	UNP D7PBN4
A	600	GLU	VAL	ENGINEERED MUTATION	UNP D7PBN4
A	630	SER	LYS	ENGINEERED MUTATION	UNP D7PBN4
A	667	GLU	PHE	ENGINEERED MUTATION	UNP D7PBN4
A	673	SER	TYR	ENGINEERED MUTATION	UNP D7PBN4
A	688	ARG	ALA	ENGINEERED MUTATION	UNP D7PBN4
A	706	SER	LEU	ENGINEERED MUTATION	UNP D7PBN4
A	709	ARG	GLN	ENGINEERED MUTATION	UNP D7PBN4
A	713	GLU	SER	ENGINEERED MUTATION	UNP D7PBN4
A	716	GLU	LEU	ENGINEERED MUTATION	UNP D7PBN4
A	720	GLU	SER	ENGINEERED MUTATION	UNP D7PBN4
A	722	SER	PRO	ENGINEERED MUTATION	UNP D7PBN4
A	723	GLY	LYS	ENGINEERED MUTATION	UNP D7PBN4
B	446	GLY	-	EXPRESSION TAG	UNP D7PBN4
B	447	PRO	-	EXPRESSION TAG	UNP D7PBN4
B	543	ALA	ILE	ENGINEERED MUTATION	UNP D7PBN4
B	544	SER	ILE	ENGINEERED MUTATION	UNP D7PBN4
B	551	LYS	ILE	ENGINEERED MUTATION	UNP D7PBN4
B	562	ARG	GLN	ENGINEERED MUTATION	UNP D7PBN4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	588	ASN	LEU	ENGINEERED MUTATION	UNP D7PBN4
B	600	GLU	VAL	ENGINEERED MUTATION	UNP D7PBN4
B	630	SER	LYS	ENGINEERED MUTATION	UNP D7PBN4
B	667	GLU	PHE	ENGINEERED MUTATION	UNP D7PBN4
B	673	SER	TYR	ENGINEERED MUTATION	UNP D7PBN4
B	688	ARG	ALA	ENGINEERED MUTATION	UNP D7PBN4
B	706	SER	LEU	ENGINEERED MUTATION	UNP D7PBN4
B	709	ARG	GLN	ENGINEERED MUTATION	UNP D7PBN4
B	713	GLU	SER	ENGINEERED MUTATION	UNP D7PBN4
B	716	GLU	LEU	ENGINEERED MUTATION	UNP D7PBN4
B	720	GLU	SER	ENGINEERED MUTATION	UNP D7PBN4
B	722	SER	PRO	ENGINEERED MUTATION	UNP D7PBN4
B	723	GLY	LYS	ENGINEERED MUTATION	UNP D7PBN4

- Molecule 2 is N-{4-[2-(1-CYCLOPROPYLPYPERIDIN-4-YL)-4-(3-[(2,5-DIFLUOROPHENYL)SULFONYL]AMINO}-2-FLUOROPHENYL)-1,3-THIAZOL-5-YL]PYRIDIN-2-YL}A CETAMIDE (three-letter code: CQE) (formula: C<sub>30</sub>H<sub>28</sub>F<sub>3</sub>N<sub>5</sub>O<sub>3</sub>S<sub>2</sub>).



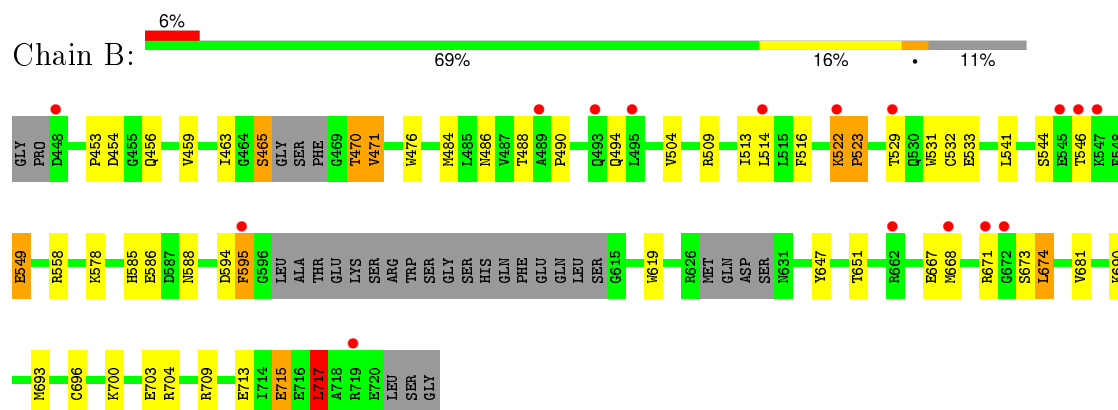
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	S	0	0
			43	30	3	5	3	2		
2	B	1	Total	C	F	N	O	S	0	0
			43	30	3	5	3	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	41	Total 41	O 41	0	0
3	B	22	Total 22	O 22	0	0



● Molecule 1: SLC45A3-BRAF FUSION PROTEIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	52.60 Å 105.94 Å 109.89 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.30 38.13 – 2.29	Depositor EDS
% Data completeness (in resolution range)	99.7 (30.00-2.30) 99.5 (38.13-2.29)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.71 (at 2.29 Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.208 , 0.255 0.207 , 0.249	Depositor DCC
$R_{free}$ test set	1406 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	45.1	Xtriage
Anisotropy	0.605	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 41.2	EDS
Estimated twinning fraction	0.015 for -h,l,k	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 28099 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4141	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.75% 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: CQE

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	0.57	2/2042 (0.1%)	0.67	1/2747 (0.0%)
1	B	0.57	2/2028 (0.1%)	0.66	1/2729 (0.0%)
All	All	0.57	4/4070 (0.1%)	0.67	2/5476 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	531	TRP	CD2-CE2	5.22	1.47	1.41
1	B	476	TRP	CD2-CE2	5.04	1.47	1.41
1	B	619	TRP	CD2-CE2	5.03	1.47	1.41
1	A	450	TRP	CD2-CE2	5.01	1.47	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	717	LEU	CA-CB-CG	7.05	131.51	115.30
1	A	704	ARG	NE-CZ-NH2	-5.05	117.78	120.30

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	2003	0	2022	59	0
1	B	1989	0	2006	36	0
2	A	43	0	28	3	0
2	B	43	0	28	4	0
3	A	41	0	0	0	0
3	B	22	0	0	1	0
All	All	4141	0	4084	96	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (96) 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:684:ASN:N	1:A:684:ASN:HD22	1.55	1.03
1:A:628:GLN:HG2	1:A:632:PRO:HG3	1.03	1.00
1:A:628:GLN:CG	1:A:632:PRO:HG3	1.93	0.98
1:A:684:ASN:HD22	1:A:684:ASN:H	1.03	0.94
1:A:664:GLN:HG2	1:A:668:MET:CE	1.97	0.93
1:B:522:LYS:HB2	1:B:523:PRO:HD3	1.53	0.91
1:A:684:ASN:ND2	1:A:684:ASN:H	1.67	0.89
1:A:700:LYS:H	1:A:700:LYS:HD2	1.37	0.89
1:A:628:GLN:HG2	1:A:632:PRO:CG	1.99	0.87
1:A:558:ARG:HG2	1:A:558:ARG:HH11	1.40	0.86
1:A:664:GLN:HG2	1:A:668:MET:HE2	1.57	0.83
1:B:667:GLU:O	1:B:671:ARG:HB2	1.82	0.80
1:A:684:ASN:N	1:A:684:ASN:ND2	2.29	0.79
1:A:510:HIS:HD2	1:A:512:ASN:H	1.28	0.78
1:B:454:ASP:HB2	1:B:522:LYS:HG3	1.68	0.75
1:A:625:ILE:C	1:A:627:MET:H	1.90	0.75
1:A:664:GLN:HG2	1:A:668:MET:HE1	1.66	0.75
1:A:647:TYR:HD2	1:A:693:MET:HE3	1.50	0.74
1:A:647:TYR:HD2	1:A:693:MET:CE	2.04	0.70
1:B:533:GLU:H	1:B:585:HIS:HD2	1.40	0.69
1:A:647:TYR:CD2	1:A:693:MET:HE3	2.28	0.69
1:A:510:HIS:CD2	1:A:512:ASN:H	2.11	0.68
1:A:531:TRP:CZ2	2:A:1721:CQE:H433	2.30	0.67
1:B:531:TRP:CZ2	2:B:1721:CQE:H433	2.28	0.67
1:A:631:ASN:N	1:A:632:PRO:CD	2.58	0.66
1:B:533:GLU:H	1:B:585:HIS:CD2	2.14	0.64
1:A:625:ILE:O	1:A:627:MET:N	2.30	0.64
1:A:594:ASP:H	2:A:1721:CQE:H8	1.45	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:681:VAL:HG21	1:A:690:LYS:HD2	1.81	0.63
1:A:713:GLU:O	1:A:717:LEU:HD23	1.97	0.63
1:B:522:LYS:CB	1:B:523:PRO:HD3	2.28	0.62
1:B:558:ARG:HD3	1:B:715:GLU:HG3	1.83	0.61
1:B:549:GLU:CD	1:B:549:GLU:H	2.04	0.60
1:A:706:SER:HB3	1:A:708:PRO:HD2	1.85	0.59
1:B:594:ASP:H	2:B:1721:CQE:H8	1.51	0.58
1:B:454:ASP:HB2	1:B:522:LYS:CG	2.33	0.58
1:A:558:ARG:HG2	1:A:558:ARG:NH1	2.15	0.58
1:A:631:ASN:N	1:A:632:PRO:HD3	2.18	0.58
1:B:453:PRO:HG2	1:B:456:GLN:NE2	2.19	0.57
1:A:678:LEU:HD22	1:A:693:MET:HE2	1.86	0.57
1:A:506:ARG:HG2	1:A:516:PHE:CE2	2.39	0.57
1:A:555:ASP:OD1	1:A:558:ARG:NH1	2.34	0.56
1:A:627:MET:O	1:A:628:GLN:HB2	2.04	0.56
1:B:668:MET:HG2	1:B:671:ARG:HH12	1.70	0.56
1:B:595:PHE:CD1	1:B:595:PHE:N	2.74	0.56
1:A:490:PRO:HG3	1:A:525:LEU:HD21	1.89	0.55
1:A:625:ILE:C	1:A:627:MET:N	2.60	0.55
1:B:696:CYS:O	1:B:704:ARG:HD2	2.08	0.54
1:A:574:HIS:O	1:A:575:ARG:HB2	2.08	0.54
1:A:462:ARG:NH1	1:A:465:SER:OG	2.41	0.53
1:B:595:PHE:HD1	1:B:595:PHE:N	2.07	0.52
1:B:700:LYS:HE3	1:B:703:GLU:OE2	2.09	0.52
1:A:558:ARG:HD3	1:A:715:GLU:HG3	1.92	0.52
1:A:462:ARG:HD2	1:A:470:THR:HG21	1.92	0.52
1:A:620:MET:CE	1:A:624:VAL:HG12	2.40	0.52
1:A:647:TYR:CD2	1:A:693:MET:CE	2.88	0.51
1:B:463:ILE:HB	1:B:471:VAL:HG22	1.92	0.51
1:B:681:VAL:HG21	1:B:690:LYS:HD2	1.92	0.51
1:A:541:LEU:HD23	1:A:648:GLU:HB3	1.93	0.51
1:A:642:PHE:CE2	1:A:646:LEU:HD11	2.46	0.51
1:A:626:ARG:C	1:A:628:GLN:H	2.13	0.50
2:A:1721:CQE:H36	2:A:1721:CQE:O42	2.12	0.50
1:A:681:VAL:CG2	1:A:690:LYS:HD2	2.42	0.50
1:B:532:CYS:HA	1:B:585:HIS:CD2	2.47	0.50
1:A:469:GLY:HA3	1:A:484:MET:O	2.12	0.50
1:B:713:GLU:O	1:B:717:LEU:HB3	2.10	0.50
1:A:668:MET:HB3	1:A:674:LEU:HB2	1.92	0.49
1:A:619:TRP:HA	1:A:644:ILE:HG13	1.95	0.49
1:B:522:LYS:HB2	1:B:523:PRO:CD	2.34	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:620:MET:HE2	1:A:624:VAL:HG12	1.95	0.48
2:B:1721:CQE:H36	2:B:1721:CQE:O42	2.13	0.48
1:B:544:SER:OG	1:B:546:THR:OG1	2.32	0.47
1:B:667:GLU:HG3	1:B:671:ARG:HH11	1.79	0.47
1:B:465:SER:HB3	1:B:470:THR:HB	1.97	0.46
1:B:490:PRO:HA	1:B:494:GLN:NE2	2.30	0.46
1:A:548:PHE:CB	1:A:553:LEU:HD13	2.46	0.46
1:A:678:LEU:O	1:A:681:VAL:HG13	2.16	0.46
1:A:509:ARG:HD3	1:B:516:PHE:O	2.16	0.45
1:A:522:LYS:HG3	1:A:523:PRO:HA	1.98	0.44
1:B:647:TYR:CZ	1:B:651:THR:HG21	2.53	0.44
1:A:691:ARG:O	1:A:695:GLU:HG2	2.18	0.44
1:B:532:CYS:HA	1:B:585:HIS:HD2	1.82	0.43
1:A:516:PHE:O	1:B:509:ARG:HD3	2.18	0.43
1:A:634:SER:H	1:A:637:SER:HG	1.65	0.42
1:B:647:TYR:HD1	1:B:693:MET:HE1	1.85	0.42
1:B:522:LYS:HG2	3:B:2002:HOH:O	2.19	0.42
1:A:548:PHE:HB3	1:A:553:LEU:HD13	2.02	0.42
1:A:568:HIS:HE1	1:A:638:ASP:OD2	2.02	0.42
1:B:668:MET:HB3	1:B:674:LEU:HB2	2.00	0.42
1:B:558:ARG:CD	1:B:715:GLU:HG3	2.47	0.42
1:A:651:THR:HG22	1:A:681:VAL:HA	2.03	0.41
1:B:513:ILE:O	1:B:514:LEU:C	2.58	0.41
2:B:1721:CQE:C1	2:B:1721:CQE:H32	2.51	0.41
1:A:685:CYS:O	1:A:686:PRO:C	2.60	0.41
1:B:522:LYS:CB	1:B:523:PRO:CD	2.98	0.40
1:A:626:ARG:C	1:A:628:GLN:N	2.75	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	242/278 (87%)	227 (94%)	13 (5%)	2 (1%)	24	27
1	B	240/278 (86%)	233 (97%)	5 (2%)	2 (1%)	24	27
All	All	482/556 (87%)	460 (95%)	18 (4%)	4 (1%)	24	27

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	626	ARG
1	B	522	LYS
1	B	523	PRO
1	A	493	GLN

### 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	219/243 (90%)	204 (93%)	15 (7%)	20	25
1	B	218/243 (90%)	198 (91%)	20 (9%)	11	13
All	All	437/486 (90%)	402 (92%)	35 (8%)	15	18

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	500	ASN
1	A	520	SER
1	A	541	LEU
1	A	553	LEU
1	A	558	ARG
1	A	625	ILE
1	A	637	SER
1	A	674	LEU
1	A	681	VAL
1	A	684	ASN
1	A	700	LYS
1	A	701	ARG

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Mol	Chain	Res	Type
1	A	706	SER
1	A	709	ARG
1	A	717	LEU
1	B	459	VAL
1	B	465	SER
1	B	470	THR
1	B	471	VAL
1	B	484	MET
1	B	486	ASN
1	B	488	THR
1	B	504	VAL
1	B	529	THR
1	B	541	LEU
1	B	549	GLU
1	B	578	LYS
1	B	586	GLU
1	B	588	ASN
1	B	595	PHE
1	B	673	SER
1	B	674	LEU
1	B	709	ARG
1	B	715	GLU
1	B	717	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	486	ASN
1	A	493	GLN
1	A	500	ASN
1	A	510	HIS
1	A	568	HIS
1	A	684	ASN
1	B	486	ASN
1	B	494	GLN
1	B	580	ASN
1	B	585	HIS

### 5.3.3 RNA ⓘ

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	CQE	A	1721	-	44,48,48	3.48	12 (27%)	52,71,71	2.10	14 (26%)
2	CQE	B	1721	-	44,48,48	3.68	14 (31%)	52,71,71	1.82	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	CQE	A	1721	-	-	0/25/43/43	0/5/6/6
2	CQE	B	1721	-	-	0/25/43/43	0/5/6/6

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1721	CQE	C31-C24	-13.83	1.34	1.48
2	B	1721	CQE	C1-C20	-13.11	1.36	1.49
2	A	1721	CQE	C31-C24	-12.12	1.36	1.48
2	A	1721	CQE	C1-C20	-12.06	1.37	1.49
2	A	1721	CQE	C22-S23	-4.42	1.59	1.73
2	A	1721	CQE	F7-C6	-4.33	1.28	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1721	CQE	S9-N8	-3.96	1.56	1.63
2	B	1721	CQE	C5-N8	-3.91	1.35	1.42
2	A	1721	CQE	C5-N8	-3.88	1.35	1.42
2	B	1721	CQE	F19-C16	-3.18	1.29	1.36
2	B	1721	CQE	F7-C6	-3.04	1.30	1.35
2	B	1721	CQE	C38-C37	2.29	1.53	1.48
2	B	1721	CQE	C43-C41	2.31	1.55	1.50
2	A	1721	CQE	C43-C41	2.47	1.55	1.50
2	B	1721	CQE	C12-S9	2.51	1.81	1.77
2	B	1721	CQE	C39-C37	2.56	1.54	1.48
2	A	1721	CQE	C38-C37	2.58	1.54	1.48
2	A	1721	CQE	C39-C37	2.70	1.54	1.48
2	A	1721	CQE	F19-C16	2.78	1.42	1.36
2	B	1721	CQE	C33-N34	2.84	1.40	1.34
2	A	1721	CQE	C33-N34	2.92	1.41	1.34
2	B	1721	CQE	C22-C25	3.99	1.57	1.50
2	A	1721	CQE	O11-S9	6.83	1.51	1.43
2	B	1721	CQE	O10-S9	7.05	1.51	1.43
2	B	1721	CQE	O11-S9	7.59	1.51	1.43
2	A	1721	CQE	O10-S9	8.22	1.52	1.43

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1721	CQE	O11-S9-O10	-5.20	112.64	119.54
2	A	1721	CQE	C35-N40-C41	-5.04	122.66	128.16
2	A	1721	CQE	C36-C35-N34	-5.03	117.43	123.06
2	B	1721	CQE	C36-C35-N34	-4.99	117.48	123.06
2	A	1721	CQE	O11-S9-O10	-4.00	114.24	119.54
2	A	1721	CQE	C32-C33-N34	-3.48	119.93	123.90
2	B	1721	CQE	C35-N40-C41	-3.43	124.42	128.16
2	B	1721	CQE	C32-C33-N34	-2.74	120.77	123.90
2	A	1721	CQE	C15-C16-C17	-2.54	120.07	123.35
2	B	1721	CQE	C38-C37-N28	-2.15	115.72	118.53
2	B	1721	CQE	C6-C5-N8	-2.07	113.33	117.92
2	B	1721	CQE	F7-C6-C5	-2.06	115.02	118.08
2	B	1721	CQE	C1-C6-C5	2.01	123.23	120.73
2	B	1721	CQE	C27-N28-C29	2.12	113.07	109.23
2	A	1721	CQE	F19-C16-C17	2.17	121.11	118.22
2	A	1721	CQE	C1-C6-C5	2.22	123.49	120.73
2	A	1721	CQE	C27-N28-C37	2.45	117.16	112.37
2	A	1721	CQE	C12-S9-N8	2.54	110.05	107.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1721	CQE	O10-S9-N8	2.58	113.23	106.69
2	A	1721	CQE	C4-C5-N8	2.60	126.54	120.94
2	B	1721	CQE	C4-C5-N8	2.99	127.37	120.94
2	B	1721	CQE	C31-C36-C35	3.11	121.53	118.57
2	B	1721	CQE	C12-S9-N8	3.12	110.69	107.25
2	B	1721	CQE	C33-N34-C35	3.42	122.00	117.28
2	A	1721	CQE	C29-N28-C37	3.75	119.72	112.37
2	A	1721	CQE	C33-N34-C35	3.79	122.50	117.28
2	A	1721	CQE	C31-C36-C35	4.31	122.68	118.57
2	A	1721	CQE	C27-N28-C29	4.47	117.34	109.23

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1721	CQE	3	0
2	B	1721	CQE	4	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	250/278 (89%)	0.39	12 (4%) 34 43	29, 47, 80, 96	0
1	B	248/278 (89%)	0.46	16 (6%) 22 30	27, 49, 81, 103	0
All	All	498/556 (89%)	0.42	28 (5%) 28 36	27, 48, 81, 103	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	631	ASN	4.5
1	B	545	GLU	4.4
1	B	719	ARG	4.2
1	B	546	THR	4.1
1	B	522	LYS	3.8
1	B	493	GLN	3.7
1	A	495	LEU	3.6
1	B	671	ARG	3.4
1	A	628	GLN	3.3
1	B	495	LEU	3.2
1	B	448	ASP	3.0
1	A	492	PRO	2.9
1	B	547	LYS	2.9
1	A	493	GLN	2.9
1	A	488	THR	2.8
1	B	662	ARG	2.7
1	A	461	GLN	2.5
1	B	529	THR	2.4
1	A	497	ALA	2.4
1	B	489	ALA	2.4
1	A	515	LEU	2.3
1	A	513	ILE	2.2
1	A	547	LYS	2.2
1	B	595	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	672	GLY	2.1
1	B	514	LEU	2.0
1	B	668	MET	2.0
1	A	514	LEU	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	CQE	B	1721	43/43	0.94	0.15	-0.43	33,43,75,81	0
2	CQE	A	1721	43/43	0.97	0.15	-0.66	28,33,70,80	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.