



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 12:35 am GMT

PDB ID : 4WCU  
Title : PDE4 complexed with inhibitor  
Authors : Sorensen, M.D.  
Deposited on : 2014-09-05  
Resolution : 2.35 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28683  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

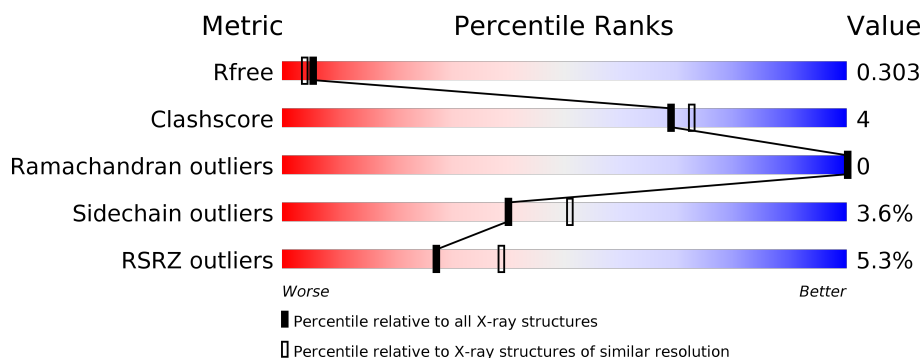
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 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))
$R_{free}$	100719	1522 (2.38-2.34)
Clashscore	112137	1626 (2.38-2.34)
Ramachandran outliers	110173	1605 (2.38-2.34)
Sidechain outliers	110143	1606 (2.38-2.34)
RSRZ outliers	101464	1528 (2.38-2.34)

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	359	<div> <div>3%</div> <div>84%</div> <div>8%</div> <div>8%</div> </div>
1	B	359	<div> <div>5%</div> <div>81%</div> <div>11%</div> <div>7%</div> </div>
1	C	359	<div> <div>6%</div> <div>75%</div> <div>14%</div> <div>10%</div> </div>
1	D	359	<div> <div>6%</div> <div>78%</div> <div>13%</div> <div>8%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MG	A	502	-	-	-	X
4	MG	B	502	-	-	-	X
4	MG	C	502	-	-	-	X
4	MG	D	502	-	-	-	X

## 2 Entry composition [i](#)

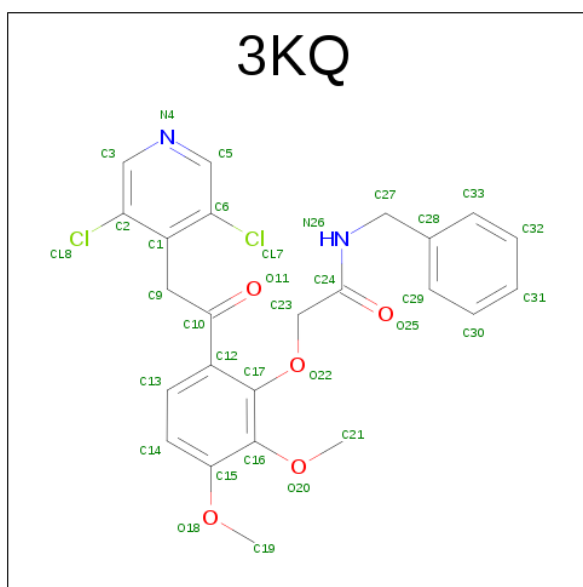
There are 5 unique types of molecules in this entry. The entry contains 11144 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 cAMP-specific 3',5'-cyclic phosphodiesterase 4D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	S	0	0	0
			2674	1696	454	510	14			
1	B	333	Total	C	N	O	S	0	0	0
			2702	1712	460	516	14			
1	C	322	Total	C	N	O	S	0	0	0
			2622	1664	447	497	14			
1	D	330	Total	C	N	O	S	0	0	0
			2671	1693	454	510	14			

- Molecule 2 is N-benzyl-2-{6-[(3,5-dichloropyridin-4-yl)acetyl]-2,3-dimethoxyphenoxy}acetamide (three-letter code: 3KQ) (formula: C<sub>24</sub>H<sub>22</sub>Cl<sub>2</sub>N<sub>2</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			33	24	2	2	5		
2	B	1	Total	C	Cl	N	O	0	0
			33	24	2	2	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	Cl	N	O	
			33	24	2	2	5	
2	D	1	Total	C	Cl	N	O	
			33	24	2	2	5	

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn		
			1	1	0	0
3	A	1	Total	Zn		
			1	1	0	0
3	D	1	Total	Zn		
			1	1	0	0
3	C	1	Total	Zn		
			1	1	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg		
			1	1	0	0
4	A	1	Total	Mg		
			1	1	0	0
4	D	1	Total	Mg		
			1	1	0	0
4	C	1	Total	Mg		
			1	1	0	0

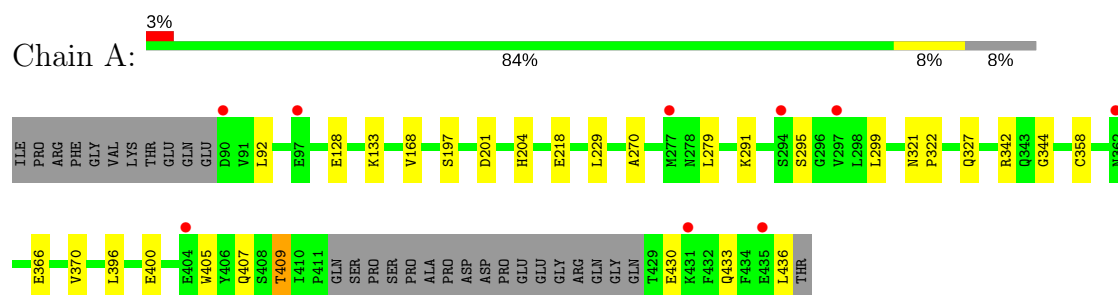
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	96	Total	O		
			96	96	0	0
5	B	92	Total	O		
			92	92	0	0
5	C	76	Total	O		
			76	76	0	0
5	D	71	Total	O		
			71	71	0	0

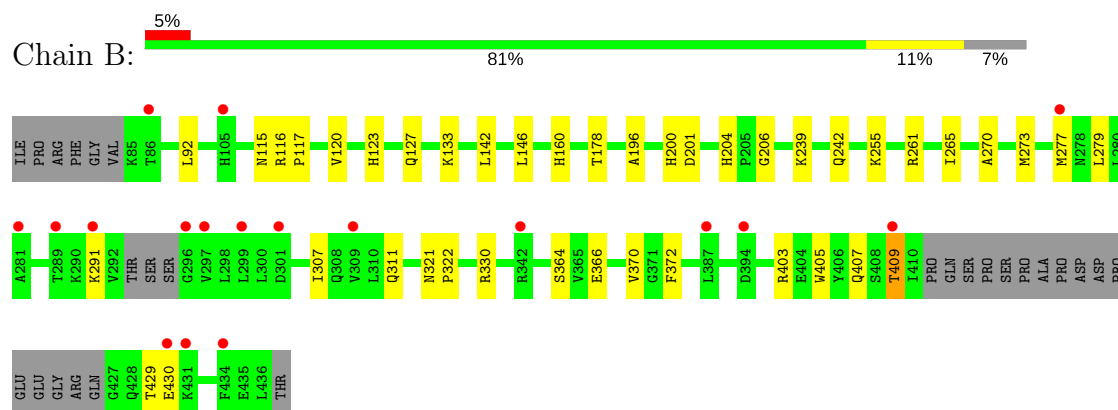
### 3 Residue-property plots [i](#)

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

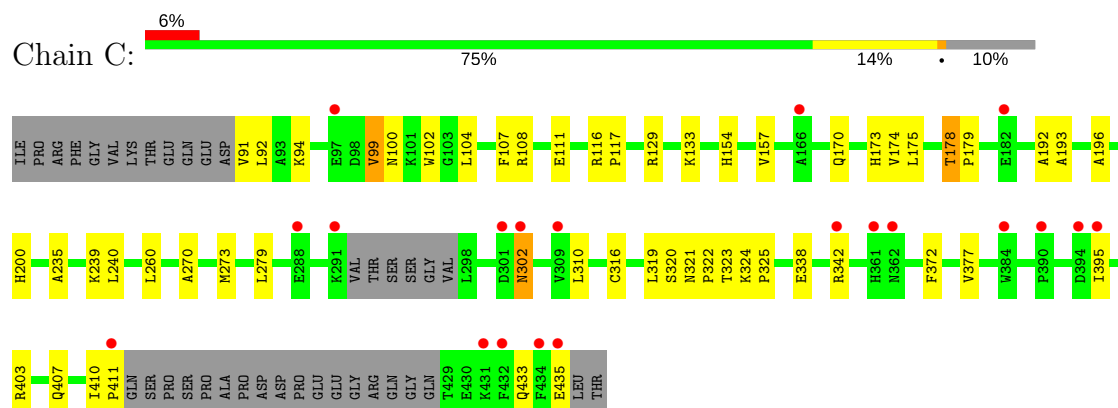
#### • Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D



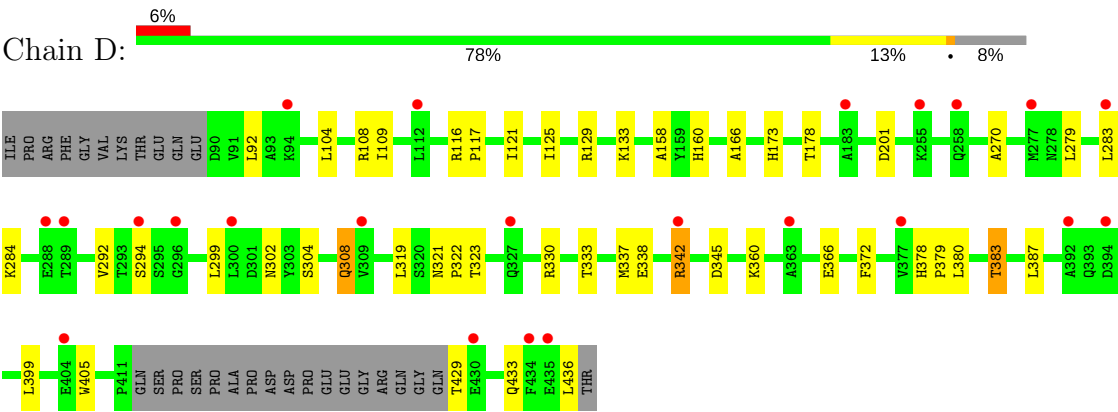
#### • Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D



#### • Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D



● Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.23Å 113.55Å 160.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	92.85 – 2.35 19.78 – 2.35	Depositor EDS
% Data completeness (in resolution range)	92.9 (92.85-2.35) 93.1 (19.78-2.35)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.31 (at 2.35Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.244 , 0.304 0.244 , 0.303	Depositor DCC
$R_{free}$ test set	3567 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	44.4	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 35.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.54$ , $\langle L^2 \rangle = 0.39$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	11144	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 3KQ, MG

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	0.49	0/2729	0.62	0/3706
1	B	0.47	0/2755	0.61	0/3736
1	C	0.46	0/2675	0.59	0/3629
1	D	0.46	0/2725	0.60	0/3702
All	All	0.47	0/10884	0.60	0/14773

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 [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	2674	0	2623	11	0
1	B	2702	0	2647	26	0
1	C	2622	0	2569	30	0
1	D	2671	0	2612	23	0
2	A	33	0	22	0	0
2	B	33	0	22	3	0
2	C	33	0	22	2	0
2	D	33	0	22	4	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	96	0	0	0	0
5	B	92	0	0	1	0
5	C	76	0	0	0	0
5	D	71	0	0	0	0
All	All	11144	0	10539	91	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 4.

All (91) 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:204:HIS:HD2	1:B:206:GLY:H	1.24	0.84
1:B:273:MET:HE3	2:B:500:3KQ:H5	1.62	0.82
1:C:175:LEU:O	1:C:178:THR:HG22	1.81	0.80
1:C:270:ALA:HB1	1:C:279:LEU:HD11	1.73	0.71
1:A:321:ASN:HB2	1:A:322:PRO:HD3	1.75	0.69
1:D:330:ARG:HD3	1:D:405:TRP:CH2	2.29	0.67
1:A:396:LEU:O	1:A:400:GLU:HG3	1.95	0.67
1:B:330:ARG:NH1	1:B:405:TRP:HH2	1.93	0.65
1:A:366:GLU:HG2	1:A:409:THR:HG23	1.78	0.65
1:B:372:PHE:CD1	2:B:500:3KQ:H11	2.33	0.64
1:B:196:ALA:O	1:B:200:HIS:HB3	1.98	0.63
1:D:378:HIS:HB3	1:D:379:PRO:HD3	1.81	0.63
1:B:261:ARG:O	1:B:265:ILE:HG13	1.99	0.63
1:A:295:SER:HB2	1:B:255:LYS:HG3	1.81	0.62
1:B:366:GLU:HG2	1:B:409:THR:HG23	1.80	0.62
1:C:99:VAL:HG12	1:C:100:ASN:HD22	1.65	0.61
1:B:270:ALA:HB1	1:B:279:LEU:HD11	1.81	0.61
1:D:436:LEU:HD11	2:D:500:3KQ:H6	1.83	0.61
1:A:405:TRP:O	1:A:409:THR:HG22	2.03	0.58
1:B:403:ARG:NH1	1:B:407:GLN:HG3	2.19	0.58
1:A:270:ALA:HB1	1:A:279:LEU:HD11	1.86	0.56
1:C:99:VAL:HG12	1:C:100:ASN:ND2	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:129:ARG:HE	1:C:173:HIS:HD1	1.54	0.55
1:D:338:GLU:O	1:D:342:ARG:HD2	2.06	0.55
1:D:284:LYS:HG2	1:D:383:THR:HG21	1.90	0.54
1:B:370:VAL:HG11	1:B:407:GLN:HE21	1.73	0.54
1:D:116:ARG:N	1:D:117:PRO:CD	2.71	0.54
1:A:370:VAL:HG11	1:A:407:GLN:HE21	1.73	0.53
1:A:344:GLY:HA3	1:A:358:CYS:O	2.08	0.53
1:A:201:ASP:O	1:A:204:HIS:HB2	2.09	0.52
1:B:160:HIS:HD2	1:B:201:ASP:OD2	1.93	0.52
1:D:321:ASN:HB2	1:D:322:PRO:HD3	1.91	0.52
1:D:270:ALA:HB1	1:D:279:LEU:HD11	1.92	0.51
1:B:273:MET:CE	2:B:500:3KQ:H5	2.38	0.51
1:B:123:HIS:CE1	1:B:127:GLN:HE21	2.28	0.51
1:B:405:TRP:O	1:B:409:THR:HG22	2.11	0.51
1:C:235:ALA:O	1:C:239:LYS:HB2	2.11	0.50
1:D:104:LEU:HD11	1:D:109:ILE:HD11	1.93	0.50
1:C:319:LEU:HD22	1:C:372:PHE:HZ	1.76	0.50
2:D:500:3KQ:H9	2:D:500:3KQ:C5	2.42	0.50
1:D:129:ARG:HE	1:D:173:HIS:HD2	1.58	0.50
1:A:168:VAL:HG12	1:A:197:SER:HB3	1.94	0.50
1:B:307:ILE:O	1:B:311:GLN:HG3	2.13	0.49
1:B:204:HIS:CD2	1:B:206:GLY:H	2.16	0.49
1:D:283:LEU:HD11	1:D:387:LEU:HD22	1.95	0.49
1:C:192:ALA:HB2	1:C:260:LEU:HD12	1.94	0.48
1:D:160:HIS:HD2	1:D:201:ASP:OD2	1.96	0.48
1:B:330:ARG:HH11	1:B:405:TRP:HH2	1.62	0.48
1:C:302:ASN:HD22	1:C:302:ASN:N	2.11	0.48
1:C:322:PRO:HG2	1:C:377:VAL:HG21	1.95	0.48
1:C:273:MET:CE	2:C:500:3KQ:H5	2.44	0.48
1:B:115:ASN:HB2	5:B:670:HOH:O	2.14	0.47
1:D:304:SER:O	1:D:308:GLN:HB2	2.15	0.47
1:C:196:ALA:O	1:C:200:HIS:HB3	2.14	0.47
1:D:330:ARG:HD3	1:D:405:TRP:CZ3	2.50	0.46
1:B:321:ASN:HB2	1:B:322:PRO:HD3	1.97	0.46
1:D:323:THR:HG22	1:D:399:LEU:HB2	1.97	0.46
1:B:116:ARG:O	1:B:120:VAL:HG22	2.16	0.45
1:B:330:ARG:HD3	1:B:405:TRP:CH2	2.52	0.45
1:C:403:ARG:NH1	1:C:407:GLN:HG3	2.32	0.45
1:C:154:HIS:HB2	1:C:157:VAL:HG23	1.98	0.45
1:D:319:LEU:HD12	1:D:380:LEU:HD22	2.00	0.44
1:B:116:ARG:N	1:B:117:PRO:CD	2.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:LEU:O	1:B:146:LEU:HG	2.18	0.44
1:C:104:LEU:HD22	1:C:170:GLN:HG3	2.00	0.44
1:D:333:THR:O	1:D:337:MET:HG2	2.18	0.43
1:C:107:PHE:O	1:C:111:GLU:HG3	2.18	0.43
1:C:116:ARG:N	1:C:117:PRO:CD	2.81	0.43
1:C:91:VAL:CG1	1:C:94:LYS:HB2	2.47	0.43
1:C:100:ASN:HD22	1:C:100:ASN:N	2.17	0.43
1:B:239:LYS:NZ	1:B:242:GLN:HE22	2.17	0.43
1:C:102:TRP:HE3	1:C:174:VAL:HG11	1.84	0.42
1:D:345:ASP:OD1	1:D:360:LYS:HE2	2.18	0.42
1:B:239:LYS:HD2	1:B:239:LYS:HA	1.86	0.42
1:C:273:MET:HE2	2:C:500:3KQ:H5	2.01	0.42
2:D:500:3KQ:H9	2:D:500:3KQ:H2	2.01	0.42
1:D:366:GLU:CD	1:D:366:GLU:H	2.23	0.42
1:D:158:ALA:H	1:D:342:ARG:HH12	1.68	0.42
1:C:193:ALA:HB2	1:C:310:LEU:HD22	2.01	0.41
1:A:229:LEU:HA	1:A:229:LEU:HD23	1.91	0.41
1:C:338:GLU:OE2	1:C:342:ARG:NH2	2.54	0.41
1:C:321:ASN:HB2	1:C:322:PRO:HD3	2.02	0.41
1:C:410:ILE:HA	1:C:411:PRO:HD3	1.87	0.41
1:C:316:CYS:O	1:C:320:SER:HB3	2.21	0.41
1:D:372:PHE:CD1	2:D:500:3KQ:H11	2.56	0.41
1:C:324:LYS:O	1:C:325:PRO:C	2.59	0.41
1:D:125:ILE:HD13	1:D:173:HIS:HB2	2.03	0.41
1:C:178:THR:HA	1:C:179:PRO:HD3	1.96	0.41
1:C:323:THR:HB	1:C:395:ILE:HG23	2.02	0.41
1:D:121:ILE:HD12	1:D:166:ALA:HB1	2.04	0.40
1:C:319:LEU:HD22	1:C:372:PHE:CZ	2.56	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	326/359 (91%)	316 (97%)	10 (3%)	0	100	100
1	B	327/359 (91%)	316 (97%)	11 (3%)	0	100	100
1	C	316/359 (88%)	304 (96%)	12 (4%)	0	100	100
1	D	326/359 (91%)	307 (94%)	19 (6%)	0	100	100
All	All	1295/1436 (90%)	1243 (96%)	52 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	301/327 (92%)	289 (96%)	12 (4%)	36	46
1	B	303/327 (93%)	294 (97%)	9 (3%)	46	58
1	C	294/327 (90%)	285 (97%)	9 (3%)	45	56
1	D	300/327 (92%)	287 (96%)	13 (4%)	33	42
All	All	1198/1308 (92%)	1155 (96%)	43 (4%)	40	51

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	LEU
1	A	128	GLU
1	A	133	LYS
1	A	218	GLU
1	A	291	LYS
1	A	299	LEU
1	A	327	GLN
1	A	342	ARG
1	A	409	THR
1	A	430	GLU
1	A	433	GLN
1	A	436	LEU
1	B	92	LEU

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Mol	Chain	Res	Type
1	B	133	LYS
1	B	178	THR
1	B	277	MET
1	B	291	LYS
1	B	364	SER
1	B	409	THR
1	B	429	THR
1	B	430	GLU
1	C	92	LEU
1	C	99	VAL
1	C	108	ARG
1	C	133	LYS
1	C	178	THR
1	C	240	LEU
1	C	302	ASN
1	C	433	GLN
1	C	435	GLU
1	D	92	LEU
1	D	108	ARG
1	D	133	LYS
1	D	178	THR
1	D	292	VAL
1	D	294	SER
1	D	299	LEU
1	D	302	ASN
1	D	308	GLN
1	D	342	ARG
1	D	383	THR
1	D	429	THR
1	D	433	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	ASN
1	A	210	GLN
1	A	214	ASN
1	A	242	GLN
1	A	362	ASN
1	A	407	GLN
1	B	123	HIS
1	B	160	HIS

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Mol	Chain	Res	Type
1	B	204	HIS
1	B	242	GLN
1	B	407	GLN
1	C	100	ASN
1	C	127	GLN
1	C	242	GLN
1	C	278	ASN
1	C	302	ASN
1	C	389	HIS
1	D	100	ASN
1	D	173	HIS
1	D	242	GLN
1	D	278	ASN
1	D	302	ASN
1	D	308	GLN
1	D	433	GLN

### 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](#)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 for Mogul analysis.

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	3KQ	A	500	-	35,35,35	2.00	6 (17%)	43,47,47	1.45	6 (13%)
2	3KQ	B	500	-	35,35,35	1.97	6 (17%)	43,47,47	1.29	5 (11%)
2	3KQ	C	500	-	35,35,35	1.93	7 (20%)	43,47,47	1.51	8 (18%)
2	3KQ	D	500	-	35,35,35	1.96	6 (17%)	43,47,47	1.45	9 (20%)

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	3KQ	A	500	-	-	0/22/22/22	0/3/3/3
2	3KQ	B	500	-	-	0/22/22/22	0/3/3/3
2	3KQ	C	500	-	-	0/22/22/22	0/3/3/3
2	3KQ	D	500	-	-	0/22/22/22	0/3/3/3

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	500	3KQ	C6-CL7	2.17	1.78	1.73
2	B	500	3KQ	C6-CL7	2.19	1.78	1.73
2	C	500	3KQ	C2-CL8	2.23	1.79	1.73
2	D	500	3KQ	C6-CL7	2.24	1.79	1.73
2	A	500	3KQ	C6-CL7	2.52	1.79	1.73
2	B	500	3KQ	C15-C16	3.66	1.48	1.40
2	D	500	3KQ	C15-C16	4.27	1.49	1.40
2	D	500	3KQ	C6-C1	4.30	1.47	1.39
2	C	500	3KQ	C12-C17	4.44	1.49	1.40
2	A	500	3KQ	C12-C17	4.49	1.49	1.40
2	C	500	3KQ	C15-C16	4.51	1.50	1.40
2	A	500	3KQ	C15-C16	4.52	1.50	1.40
2	B	500	3KQ	C12-C17	4.63	1.50	1.40
2	C	500	3KQ	C6-C1	4.66	1.48	1.39
2	C	500	3KQ	C2-C1	4.73	1.48	1.39
2	D	500	3KQ	C12-C17	4.76	1.50	1.40
2	A	500	3KQ	C2-C1	4.78	1.48	1.39
2	A	500	3KQ	C6-C1	4.79	1.48	1.39
2	D	500	3KQ	C2-C1	4.93	1.48	1.39
2	B	500	3KQ	C2-C1	4.95	1.48	1.39
2	B	500	3KQ	C6-C1	4.96	1.48	1.39
2	C	500	3KQ	C17-C16	5.07	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	500	3KQ	C17-C16	5.64	1.49	1.39
2	B	500	3KQ	C17-C16	5.75	1.50	1.39
2	A	500	3KQ	C17-C16	5.81	1.50	1.39

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	500	3KQ	C1-C9-C10	-3.57	109.63	114.25
2	B	500	3KQ	C1-C9-C10	-2.87	110.54	114.25
2	A	500	3KQ	O18-C15-C14	-2.73	119.78	124.37
2	C	500	3KQ	O18-C15-C14	-2.53	120.12	124.37
2	D	500	3KQ	C1-C9-C10	-2.32	111.25	114.25
2	D	500	3KQ	C12-C17-C16	-2.27	117.34	120.73
2	C	500	3KQ	C2-C3-N4	-2.14	120.65	122.86
2	C	500	3KQ	C5-C6-CL7	2.03	121.34	118.47
2	D	500	3KQ	O18-C15-C16	2.10	118.91	115.22
2	B	500	3KQ	O18-C15-C16	2.17	119.04	115.22
2	D	500	3KQ	C21-O20-C16	2.23	120.93	114.81
2	B	500	3KQ	C19-O18-C15	2.23	120.75	117.54
2	B	500	3KQ	C5-C6-CL7	2.28	121.69	118.47
2	D	500	3KQ	C23-O22-C17	2.32	121.46	114.74
2	A	500	3KQ	C21-O20-C16	2.32	121.18	114.81
2	C	500	3KQ	C3-C2-CL8	2.44	121.92	118.47
2	D	500	3KQ	C3-C2-CL8	2.49	121.99	118.47
2	D	500	3KQ	C19-O18-C15	2.56	121.22	117.54
2	A	500	3KQ	O18-C15-C16	2.89	120.30	115.22
2	A	500	3KQ	C23-O22-C17	2.92	123.20	114.74
2	C	500	3KQ	C23-O22-C17	3.13	123.81	114.74
2	C	500	3KQ	O18-C15-C16	3.16	120.78	115.22
2	D	500	3KQ	C5-C6-CL7	3.26	123.08	118.47
2	A	500	3KQ	C3-N4-C5	3.60	122.53	117.45
2	D	500	3KQ	C3-N4-C5	3.76	122.77	117.45
2	A	500	3KQ	C19-O18-C15	3.88	123.11	117.54
2	B	500	3KQ	C3-N4-C5	4.12	123.28	117.45
2	C	500	3KQ	C3-N4-C5	4.22	123.41	117.45

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	500	3KQ	3	0
2	C	500	3KQ	2	0
2	D	500	3KQ	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	330/359 (91%)	0.14	9 (2%) 55 65	26, 42, 60, 67	0
1	B	333/359 (92%)	0.22	18 (5%) 26 37	29, 41, 64, 76	0
1	C	322/359 (89%)	0.31	20 (6%) 21 30	29, 44, 73, 83	0
1	D	330/359 (91%)	0.40	23 (6%) 17 24	30, 48, 68, 76	0
All	All	1315/1436 (91%)	0.27	70 (5%) 27 39	26, 43, 66, 83	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	434	PHE	9.0
1	D	434	PHE	5.1
1	B	297	VAL	5.0
1	D	289	THR	4.3
1	D	377	VAL	4.2
1	C	301	ASP	4.1
1	C	431	LYS	4.0
1	B	434	PHE	4.0
1	A	431	LYS	3.7
1	C	394	ASP	3.6
1	B	301	ASP	3.5
1	D	296	GLY	3.4
1	D	363	ALA	3.3
1	B	281	ALA	3.2
1	D	435	GLU	3.2
1	C	411	PRO	3.2
1	C	390	PRO	3.1
1	B	277	MET	3.0
1	D	309	VAL	3.0
1	C	432	PHE	2.9
1	C	309	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	288	GLU	2.8
1	C	291	LYS	2.8
1	A	90	ASP	2.8
1	D	283	LEU	2.8
1	B	291	LYS	2.7
1	B	409	THR	2.7
1	D	342	ARG	2.6
1	A	277	MET	2.6
1	D	327	GLN	2.6
1	C	288	GLU	2.5
1	B	86	THR	2.5
1	D	404	GLU	2.5
1	B	430	GLU	2.5
1	B	342	ARG	2.5
1	D	183	ALA	2.4
1	B	387	LEU	2.4
1	D	294	SER	2.4
1	C	302	ASN	2.4
1	B	296	GLY	2.4
1	A	294	SER	2.4
1	C	435	GLU	2.4
1	C	395	ILE	2.4
1	B	105	HIS	2.4
1	B	299	LEU	2.3
1	A	297	VAL	2.3
1	C	362	ASN	2.3
1	D	255	LYS	2.3
1	B	289	THR	2.3
1	B	309	VAL	2.3
1	D	300	LEU	2.2
1	B	431	LYS	2.2
1	C	384	TRP	2.2
1	A	97	GLU	2.2
1	C	361	HIS	2.2
1	C	182	GLU	2.2
1	A	362	ASN	2.2
1	C	97	GLU	2.2
1	D	94	LYS	2.1
1	D	394	ASP	2.1
1	D	277	MET	2.1
1	D	258	GLN	2.1
1	A	404	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	394	ASP	2.1
1	D	112	LEU	2.1
1	C	342	ARG	2.1
1	D	392	ALA	2.1
1	D	430	GLU	2.0
1	A	435	GLU	2.0
1	C	166	ALA	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(Å <sup>2</sup> )	Q<0.9
4	MG	B	502	1/1	0.97	0.47	34.03	29,29,29,29	0
4	MG	D	502	1/1	0.98	0.45	20.44	30,30,30,30	0
4	MG	C	502	1/1	0.98	0.43	19.70	26,26,26,26	0
4	MG	A	502	1/1	0.92	0.36	11.26	20,20,20,20	0
2	3KQ	C	500	33/33	0.86	0.20	0.82	43,45,52,53	0
2	3KQ	D	500	33/33	0.87	0.19	0.73	47,52,58,58	0
2	3KQ	A	500	33/33	0.93	0.18	0.59	46,47,53,53	0
2	3KQ	B	500	33/33	0.89	0.18	0.41	40,43,52,53	0
3	ZN	C	501	1/1	0.96	0.12	0.05	48,48,48,48	0
3	ZN	A	501	1/1	0.94	0.11	-0.78	45,45,45,45	0
3	ZN	D	501	1/1	0.95	0.11	-0.93	50,50,50,50	0
3	ZN	B	501	1/1	0.98	0.10	-1.86	43,43,43,43	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.