



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:49 AM GMT

PDB ID : 3G4G  
Title : Crystal structure of human phosphodiesterase 4d with regulatory domain and d155871  
Authors : Staker, B.L.  
Deposited on : 2009-02-03  
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

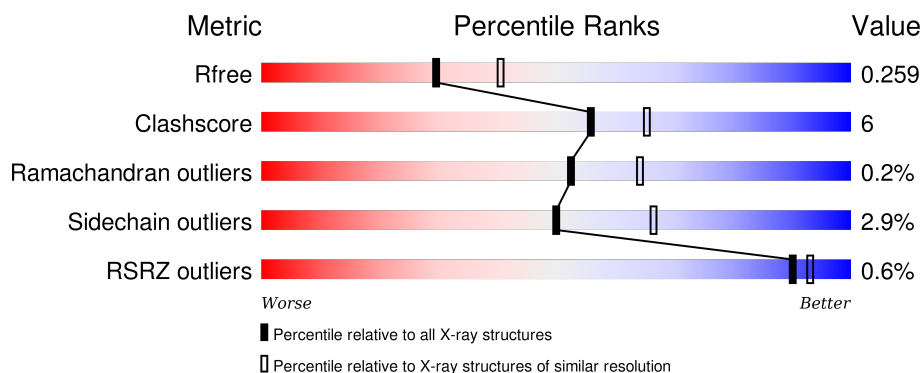
# 1 Overall quality at a glance

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	421	
1	B	421	
1	C	421	
1	D	421	

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MG	A	802	-	-	-	X
3	MG	B	804	-	-	-	X
3	MG	C	806	-	-	-	X
3	MG	D	808	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11183 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	338	Total	C	N	O	S	0	0	0
			2725	1724	464	523	14			
1	B	336	Total	C	N	O	S	0	0	0
			2712	1718	462	518	14			
1	C	339	Total	C	N	O	S	0	0	0
			2739	1733	468	524	14			
1	D	337	Total	C	N	O	S	0	0	0
			2716	1720	464	518	14			

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	162	MET	-	expression tag	UNP Q08499
A	215	LYS	-	linker	UNP Q08499
A	216	VAL	-	linker	UNP Q08499
A	217	THR	-	linker	UNP Q08499
A	218	ALA	-	linker	UNP Q08499
A	219	GLU	-	linker	UNP Q08499
A	220	GLU	-	linker	UNP Q08499
A	221	ALA	-	linker	UNP Q08499
A	222	PRO	-	linker	UNP Q08499
A	223	GLN	-	linker	UNP Q08499
A	579	ALA	-	expression tag	UNP Q08499
A	580	HIS	-	expression tag	UNP Q08499
A	581	HIS	-	expression tag	UNP Q08499
A	582	HIS	-	expression tag	UNP Q08499
A	583	HIS	-	expression tag	UNP Q08499
A	584	HIS	-	expression tag	UNP Q08499
A	585	HIS	-	expression tag	UNP Q08499
B	162	MET	-	expression tag	UNP Q08499
B	215	LYS	-	linker	UNP Q08499
B	216	VAL	-	linker	UNP Q08499
B	217	THR	-	linker	UNP Q08499

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Chain	Residue	Modelled	Actual	Comment	Reference
B	218	ALA	-	linker	UNP Q08499
B	219	GLU	-	linker	UNP Q08499
B	220	GLU	-	linker	UNP Q08499
B	221	ALA	-	linker	UNP Q08499
B	222	PRO	-	linker	UNP Q08499
B	223	GLN	-	linker	UNP Q08499
B	579	ALA	-	expression tag	UNP Q08499
B	580	HIS	-	expression tag	UNP Q08499
B	581	HIS	-	expression tag	UNP Q08499
B	582	HIS	-	expression tag	UNP Q08499
B	583	HIS	-	expression tag	UNP Q08499
B	584	HIS	-	expression tag	UNP Q08499
B	585	HIS	-	expression tag	UNP Q08499
C	162	MET	-	expression tag	UNP Q08499
C	215	LYS	-	linker	UNP Q08499
C	216	VAL	-	linker	UNP Q08499
C	217	THR	-	linker	UNP Q08499
C	218	ALA	-	linker	UNP Q08499
C	219	GLU	-	linker	UNP Q08499
C	220	GLU	-	linker	UNP Q08499
C	221	ALA	-	linker	UNP Q08499
C	222	PRO	-	linker	UNP Q08499
C	223	GLN	-	linker	UNP Q08499
C	579	ALA	-	expression tag	UNP Q08499
C	580	HIS	-	expression tag	UNP Q08499
C	581	HIS	-	expression tag	UNP Q08499
C	582	HIS	-	expression tag	UNP Q08499
C	583	HIS	-	expression tag	UNP Q08499
C	584	HIS	-	expression tag	UNP Q08499
C	585	HIS	-	expression tag	UNP Q08499
D	162	MET	-	expression tag	UNP Q08499
D	215	LYS	-	linker	UNP Q08499
D	216	VAL	-	linker	UNP Q08499
D	217	THR	-	linker	UNP Q08499
D	218	ALA	-	linker	UNP Q08499
D	219	GLU	-	linker	UNP Q08499
D	220	GLU	-	linker	UNP Q08499
D	221	ALA	-	linker	UNP Q08499
D	222	PRO	-	linker	UNP Q08499
D	223	GLN	-	linker	UNP Q08499
D	579	ALA	-	expression tag	UNP Q08499
D	580	HIS	-	expression tag	UNP Q08499

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Chain	Residue	Modelled	Actual	Comment	Reference
D	581	HIS	-	expression tag	UNP Q08499
D	582	HIS	-	expression tag	UNP Q08499
D	583	HIS	-	expression tag	UNP Q08499
D	584	HIS	-	expression tag	UNP Q08499
D	585	HIS	-	expression tag	UNP Q08499

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

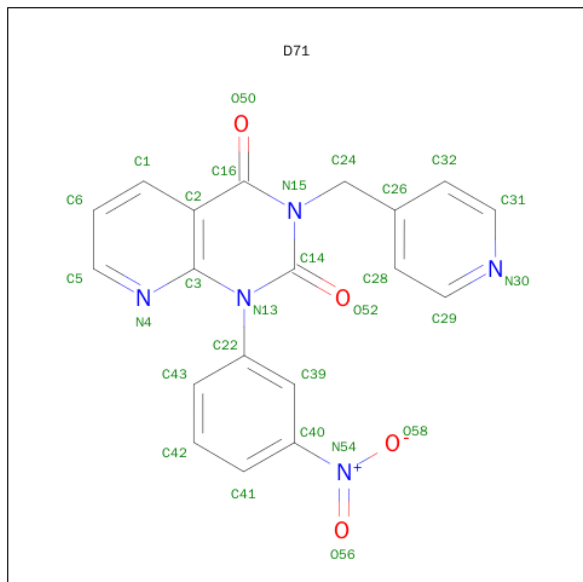
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 5 is 1-(3-NITROPHENYL)-3-(PYRIDIN-4-YLMETHYL)PYRIDO[2,3-D]PYRIMIDINE-2,4(1H,3H)-DIONE (three-letter code: D71) (formula: C<sub>19</sub>H<sub>13</sub>N<sub>5</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			28	19	5	4		
5	B	1	Total	C	N	O	0	0
			28	19	5	4		
5	C	1	Total	C	N	O	0	0
			28	19	5	4		
5	D	1	Total	C	N	O	0	0
			28	19	5	4		

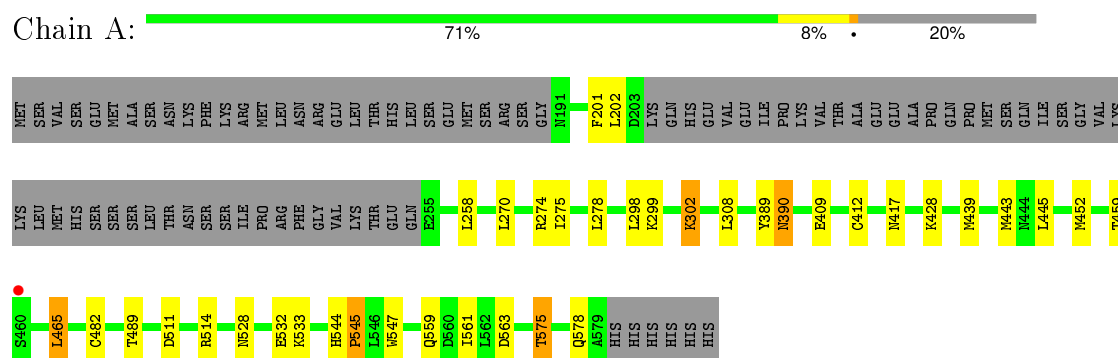
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	39	Total	O	0	0
			39	39		
6	B	35	Total	O	0	0
			35	35		
6	C	48	Total	O	0	0
			48	48		
6	D	45	Total	O	0	0
			45	45		

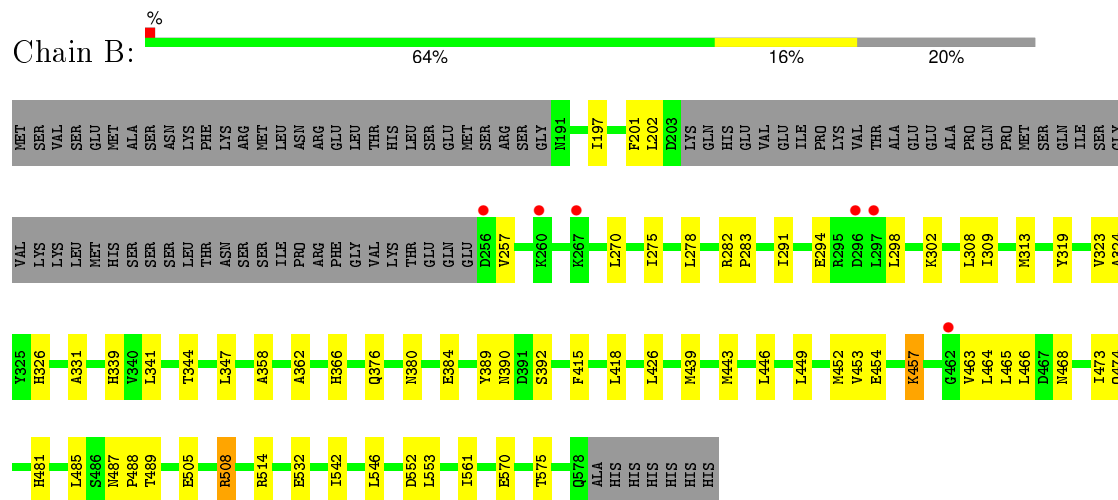
### 3 Residue-property plots [i](#)

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.

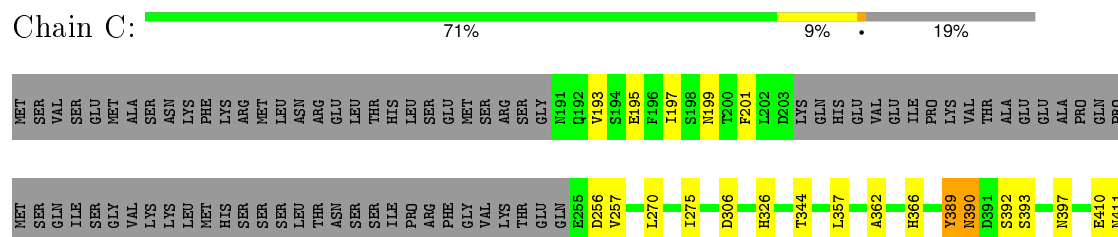
- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D



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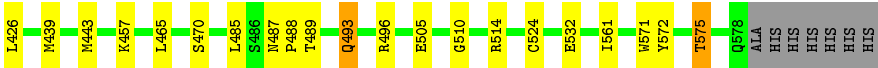
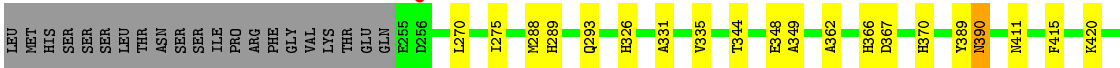
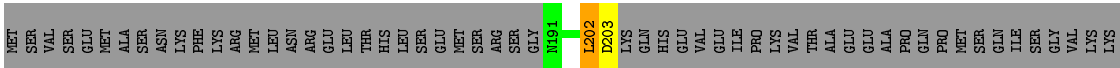
- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D







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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.13Å 75.31Å 162.56Å 90.00° 92.43° 90.00°	Depositor
Resolution (Å)	48.80 – 2.30 46.76 – 2.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (48.80-2.30) 95.0 (46.76-2.30)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.58 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.4.0067	Depositor
R, $R_{free}$	0.188 , 0.257 0.193 , 0.259	Depositor DCC
$R_{free}$ test set	3262 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.1	Xtriage
Anisotropy	0.117	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 41.3	EDS
Estimated twinning fraction	0.094 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 64569 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	11183	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 4.25% 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: MG, D71, CA, ZN

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	0.76	1/2780 (0.0%)	0.74	1/3778 (0.0%)
1	B	0.69	0/2767	0.72	4/3759 (0.1%)
1	C	0.75	0/2795	0.76	1/3797 (0.0%)
1	D	0.73	0/2771	0.73	2/3765 (0.1%)
All	All	0.73	1/11113 (0.0%)	0.74	8/15099 (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	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	412	CYS	CB-SG	-5.32	1.73	1.81

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	390	ASN	N-CA-C	-8.64	87.66	111.00
1	D	390	ASN	N-CA-C	-6.88	92.43	111.00
1	B	508	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	C	390	ASN	N-CA-C	-5.99	94.84	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	508	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	B	390	ASN	N-CA-C	-5.80	95.33	111.00
1	B	514	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	D	514	ARG	NE-CZ-NH2	-5.04	117.78	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	389	TYR	Peptide
1	B	389	TYR	Peptide
1	C	389	TYR	Peptide
1	D	389	TYR	Peptide

## 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	2725	0	2663	26	0
1	B	2712	0	2659	47	0
1	C	2739	0	2681	33	0
1	D	2716	0	2661	29	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
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	28	0	13	0	0
5	B	28	0	13	1	0
5	C	28	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	28	0	13	0	0
6	A	39	0	0	0	0
6	B	35	0	0	0	0
6	C	48	0	0	0	0
6	D	45	0	0	0	0
All	All	11183	0	10716	135	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 6.

All (135) 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:532:GLU:HG2	1:A:575:THR:HG22	1.51	0.92
1:D:532:GLU:HG2	1:D:575:THR:CG2	2.02	0.90
1:C:201:PHE:CE1	1:C:542:ILE:HD13	2.13	0.82
1:A:270:LEU:HD11	1:A:275:ILE:HD11	1.63	0.81
1:B:532:GLU:HG2	1:B:575:THR:HG22	1.65	0.79
1:D:532:GLU:HG2	1:D:575:THR:HG21	1.71	0.73
1:B:197:ILE:HG23	1:B:542:ILE:HD11	1.69	0.72
1:C:532:GLU:HG2	1:C:575:THR:HG22	1.73	0.71
1:D:439:MET:HE3	1:D:439:MET:HA	1.72	0.70
1:B:201:PHE:CE2	1:B:439:MET:HE2	2.26	0.69
1:A:298:LEU:HD21	1:A:308:LEU:HD22	1.75	0.69
1:C:532:GLU:CG	1:C:575:THR:HG22	2.23	0.69
1:D:202:LEU:HD22	1:D:443:MET:HG3	1.74	0.68
1:C:270:LEU:HD11	1:C:275:ILE:HD11	1.76	0.68
1:C:201:PHE:CD1	1:C:542:ILE:HD13	2.29	0.67
1:C:489:THR:HB	1:C:561:ILE:HG23	1.78	0.65
1:A:202:LEU:HD23	1:A:443:MET:HG3	1.79	0.64
1:B:532:GLU:CG	1:B:575:THR:HG22	2.28	0.64
1:A:459:THR:HG23	1:A:465:LEU:CD1	2.27	0.64
1:C:195:GLU:O	1:C:199:ASN:ND2	2.31	0.63
1:C:532:GLU:HG2	1:C:575:THR:CG2	2.28	0.63
1:B:376:GLN:NE2	1:B:380:ASN:OD1	2.32	0.62
1:A:202:LEU:CD2	1:A:443:MET:HG3	2.30	0.61
1:D:289:HIS:CE1	1:D:293:GLN:HE21	2.19	0.61
1:A:532:GLU:HG2	1:A:575:THR:CG2	2.30	0.61
1:B:201:PHE:HE2	1:B:439:MET:HE2	1.67	0.60
1:C:201:PHE:CD1	1:C:542:ILE:CD1	2.84	0.59
1:C:197:ILE:HG23	1:C:542:ILE:HD11	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:532:GLU:CG	1:C:575:THR:CG2	2.81	0.58
1:B:309:ILE:O	1:B:313:MET:HG2	2.05	0.57
1:D:510:GLY:HA3	1:D:524:CYS:O	2.05	0.57
1:D:489:THR:HB	1:D:561:ILE:HG23	1.87	0.56
1:C:270:LEU:HD11	1:C:275:ILE:CD1	2.35	0.56
1:B:202:LEU:CD2	1:B:443:MET:HG3	2.35	0.56
1:C:193:VAL:HG22	1:C:534:SER:HA	1.88	0.56
1:C:326:HIS:ND1	1:C:505:GLU:OE2	2.35	0.55
1:B:489:THR:HB	1:B:561:ILE:HG23	1.88	0.55
1:D:439:MET:HA	1:D:439:MET:CE	2.36	0.55
1:B:464:LEU:HD21	1:B:466:LEU:HD21	1.89	0.54
1:B:485:LEU:HD12	1:B:546:LEU:HD22	1.89	0.54
1:A:302:LYS:O	1:A:417:ASN:ND2	2.35	0.54
1:B:439:MET:HA	1:B:439:MET:HE3	1.90	0.53
1:B:449:LEU:O	1:B:453:VAL:HG23	2.09	0.53
1:A:270:LEU:HD11	1:A:275:ILE:CD1	2.36	0.52
1:A:459:THR:HG23	1:A:465:LEU:HD13	1.91	0.52
1:A:482:CYS:HB3	1:A:547:TRP:CZ2	2.44	0.52
1:A:459:THR:CG2	1:A:465:LEU:HD11	2.41	0.51
1:A:532:GLU:CG	1:A:575:THR:HG22	2.33	0.51
1:B:201:PHE:CD2	1:B:439:MET:HE2	2.46	0.51
1:A:459:THR:CG2	1:A:465:LEU:CD1	2.89	0.51
1:B:202:LEU:HD23	1:B:443:MET:CG	2.41	0.50
1:A:459:THR:HG22	1:A:465:LEU:HD11	1.94	0.50
1:D:496:ARG:HD3	1:D:571:TRP:CZ3	2.47	0.50
1:D:575:THR:CG2	1:D:575:THR:O	2.60	0.50
1:B:326:HIS:CE1	5:B:902:D71:H29	2.47	0.50
1:B:487:ASN:HB2	1:B:488:PRO:HD3	1.93	0.49
1:C:523:MET:CE	1:C:523:MET:HA	2.41	0.49
1:D:202:LEU:HD22	1:D:443:MET:CG	2.40	0.49
1:B:453:VAL:HG22	1:B:553:LEU:HD13	1.93	0.49
1:D:487:ASN:HB2	1:D:488:PRO:HD3	1.95	0.49
1:B:358:ALA:HB2	1:B:426:LEU:HD12	1.94	0.49
1:D:202:LEU:N	1:D:202:LEU:HD23	2.28	0.49
1:D:331:ALA:O	1:D:335:VAL:HG23	2.12	0.49
1:B:282:ARG:N	1:B:283:PRO:CD	2.75	0.48
1:D:532:GLU:HG2	1:D:575:THR:HG23	1.90	0.48
1:B:464:LEU:CD2	1:B:466:LEU:HD21	2.44	0.48
1:C:439:MET:HA	1:C:439:MET:HE3	1.95	0.48
1:C:362:ALA:O	1:C:366:HIS:HB3	2.14	0.48
1:A:258:LEU:HA	1:A:278:LEU:HD13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:ILE:HG12	1:B:542:ILE:CD1	2.43	0.48
1:B:298:LEU:HD21	1:B:308:LEU:HD22	1.96	0.48
1:B:298:LEU:O	1:B:302:LYS:HA	2.14	0.48
1:C:201:PHE:CE2	1:C:439:MET:HE2	2.50	0.47
1:B:324:ALA:HB2	1:B:508:ARG:HH22	1.80	0.47
1:A:559:GLN:NE2	1:A:563:ASP:OD1	2.47	0.47
1:A:201:PHE:CD2	1:A:439:MET:HE2	2.50	0.47
1:C:468:ASN:HD21	1:C:471:ASP:CG	2.18	0.46
1:D:439:MET:HE1	1:D:485:LEU:HD11	1.96	0.46
1:A:544:HIS:HB3	1:A:545:PRO:HD3	1.96	0.46
1:B:197:ILE:CG2	1:B:542:ILE:HD11	2.43	0.46
1:C:410:GLU:CD	1:C:410:GLU:H	2.18	0.46
1:D:457:LYS:HB2	1:D:465:LEU:HB3	1.98	0.46
1:B:453:VAL:HG11	1:B:552:ASP:HB3	1.97	0.46
1:D:493:GLN:HG2	1:D:493:GLN:O	2.16	0.46
1:D:575:THR:HG23	1:D:575:THR:O	2.15	0.45
1:C:357:LEU:HD23	1:C:426:LEU:CD1	2.46	0.45
1:B:257:VAL:HG12	1:B:278:LEU:CD1	2.47	0.45
1:A:489:THR:HB	1:A:561:ILE:HG23	1.98	0.45
1:C:306:ASP:OD2	1:C:306:ASP:N	2.44	0.45
1:D:572:TYR:O	1:D:575:THR:HB	2.17	0.45
1:D:348:GLU:O	1:D:349:ALA:HB3	2.16	0.44
1:C:201:PHE:CD2	1:C:439:MET:HE2	2.52	0.44
1:B:473:ILE:HA	1:B:473:ILE:HD12	1.89	0.44
1:B:202:LEU:HD23	1:B:443:MET:HG2	1.99	0.44
1:B:439:MET:HE3	1:B:481:HIS:HE1	1.82	0.44
1:B:323:VAL:CG1	1:B:505:GLU:OE1	2.65	0.44
1:B:457:LYS:CD	1:B:465:LEU:HD23	2.47	0.44
1:D:326:HIS:ND1	1:D:505:GLU:OE2	2.47	0.43
1:A:439:MET:HA	1:A:439:MET:HE3	2.00	0.43
1:D:415:PHE:CE1	1:D:426:LEU:HD21	2.54	0.43
1:C:344:THR:HG23	1:C:344:THR:O	2.18	0.43
1:B:446:LEU:HD13	1:B:546:LEU:HA	2.01	0.43
1:A:511:ASP:OD1	1:A:514:ARG:NH2	2.52	0.43
1:C:459:THR:HG23	1:C:465:LEU:HD13	1.99	0.43
1:B:319:TYR:CZ	1:B:331:ALA:HB2	2.54	0.43
1:C:532:GLU:HG3	1:C:575:THR:CG2	2.47	0.43
1:B:362:ALA:O	1:B:366:HIS:HB3	2.19	0.43
1:C:193:VAL:CG2	1:C:534:SER:HA	2.48	0.43
1:B:344:THR:CG2	1:B:347:LEU:HD12	2.48	0.43
1:C:389:TYR:CE1	1:C:397:ASN:HB3	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:415:PHE:CZ	1:D:426:LEU:HD21	2.54	0.42
1:A:202:LEU:HD23	1:A:443:MET:CG	2.49	0.42
1:A:439:MET:HE2	1:A:439:MET:HB3	1.92	0.42
1:B:341:LEU:O	1:B:344:THR:HG22	2.19	0.42
1:D:367:ASP:O	1:D:370:HIS:HB2	2.20	0.42
1:B:270:LEU:HD11	1:B:275:ILE:HD11	2.01	0.42
1:B:376:GLN:HE21	1:B:380:ASN:ND2	2.18	0.42
1:D:496:ARG:HD3	1:D:571:TRP:CH2	2.55	0.42
1:D:270:LEU:HD11	1:D:275:ILE:HD11	2.02	0.42
1:B:415:PHE:HB3	1:B:418:LEU:HD22	2.02	0.42
1:C:392:SER:O	1:C:393:SER:C	2.59	0.41
1:C:439:MET:HE1	1:C:485:LEU:HD11	2.02	0.41
1:B:464:LEU:HD23	1:B:466:LEU:HG	2.02	0.41
1:B:452:MET:HE1	1:B:474:GLN:HB3	2.02	0.41
1:B:376:GLN:HE21	1:B:380:ASN:CG	2.23	0.41
1:B:257:VAL:HG12	1:B:278:LEU:HD11	2.02	0.41
1:B:457:LYS:HD2	1:B:465:LEU:HD23	2.02	0.41
1:C:439:MET:HE2	1:C:439:MET:HB3	1.93	0.41
1:A:201:PHE:CE2	1:A:439:MET:HE2	2.56	0.41
1:D:362:ALA:O	1:D:366:HIS:HB3	2.20	0.41
1:D:288:MET:SD	1:D:335:VAL:HG11	2.61	0.40
1:C:456:LYS:NZ	1:C:553:LEU:O	2.48	0.40
1:B:291:ILE:HD13	1:B:339:HIS:HB2	2.03	0.40
1:C:439:MET:HA	1:C:439:MET:CE	2.52	0.40
1:A:274:ARG:HD2	1:A:274:ARG:O	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	334/421 (79%)	329 (98%)	4 (1%)	1 (0%)	46 57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	332/421 (79%)	326 (98%)	6 (2%)	0	100	100
1	C	335/421 (80%)	329 (98%)	5 (2%)	1 (0%)	46	57
1	D	333/421 (79%)	323 (97%)	9 (3%)	1 (0%)	46	57
All	All	1334/1684 (79%)	1307 (98%)	24 (2%)	3 (0%)	52	64

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	390	ASN
1	D	390	ASN
1	C	390	ASN

### 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	307/386 (80%)	295 (96%)	12 (4%)	39	53
1	B	306/386 (79%)	298 (97%)	8 (3%)	54	71
1	C	309/386 (80%)	302 (98%)	7 (2%)	58	75
1	D	306/386 (79%)	298 (97%)	8 (3%)	54	71
All	All	1228/1544 (80%)	1193 (97%)	35 (3%)	50	66

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

Mol	Chain	Res	Type
1	A	299	LYS
1	A	302	LYS
1	A	409	GLU
1	A	428	LYS
1	A	445	LEU
1	A	452	MET
1	A	465	LEU
1	A	528	ASN

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Mol	Chain	Res	Type
1	A	533	LYS
1	A	545	PRO
1	A	575	THR
1	A	578	GLN
1	B	294	GLU
1	B	384	GLU
1	B	392	SER
1	B	454	GLU
1	B	457	LYS
1	B	463	VAL
1	B	468	ASN
1	B	570	GLU
1	C	256	ASP
1	C	257	VAL
1	C	411	ASN
1	C	493	GLN
1	C	569	ARG
1	C	570	GLU
1	C	575	THR
1	D	202	LEU
1	D	203	ASP
1	D	344	THR
1	D	411	ASN
1	D	420	LYS
1	D	470	SER
1	D	493	GLN
1	D	575	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	289	HIS
1	A	411	ASN
1	B	289	HIS
1	B	376	GLN
1	B	380	ASN
1	B	411	ASN
1	B	573	GLN
1	C	192	GLN
1	C	271	HIS
1	C	411	ASN
1	C	424	GLN

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Mol	Chain	Res	Type
1	C	468	ASN
1	C	509	GLN
1	C	559	GLN
1	D	271	HIS
1	D	289	HIS
1	D	411	ASN
1	D	509	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 12 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	$\# Z  > 2$
5	D71	A	901	-	26,31,31	3.70	14 (53%)	30,44,44	1.90	9 (30%)
5	D71	B	902	-	26,31,31	3.41	16 (61%)	30,44,44	1.85	11 (36%)
5	D71	C	903	-	26,31,31	3.66	15 (57%)	30,44,44	2.24	10 (33%)
5	D71	D	904	-	26,31,31	3.29	15 (57%)	30,44,44	2.42	15 (50%)

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
5	D71	A	901	-	-	0/12/12/12	0/4/4/4
5	D71	B	902	-	-	0/12/12/12	0/4/4/4
5	D71	C	903	-	-	0/12/12/12	0/4/4/4
5	D71	D	904	-	-	0/12/12/12	0/4/4/4

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	904	D71	C3-N4	-4.22	1.29	1.35
5	D	904	D71	C1-C2	-3.71	1.33	1.41
5	D	904	D71	C28-C29	-2.80	1.32	1.38
5	B	902	D71	C1-C2	-2.68	1.35	1.41
5	A	901	D71	C1-C2	-2.65	1.35	1.41
5	C	903	D71	C3-N4	-2.48	1.31	1.35
5	B	902	D71	C42-C41	-2.36	1.34	1.38
5	C	903	D71	C42-C41	-2.25	1.34	1.38
5	C	903	D71	C1-C2	-2.18	1.36	1.41
5	B	902	D71	C28-C29	-2.10	1.34	1.38
5	C	903	D71	C28-C29	-2.07	1.34	1.38
5	B	902	D71	C3-N4	-2.04	1.32	1.35
5	A	901	D71	C42-C41	-2.02	1.34	1.38
5	B	902	D71	C3-N13	2.05	1.43	1.39
5	D	904	D71	C16-N15	2.09	1.41	1.38
5	D	904	D71	C16-C2	2.44	1.45	1.41
5	D	904	D71	C29-N30	2.70	1.41	1.33
5	D	904	D71	C3-N13	2.71	1.45	1.39
5	A	901	D71	C16-N15	2.89	1.42	1.38
5	C	903	D71	C29-N30	2.90	1.42	1.33
5	A	901	D71	C3-N13	2.97	1.46	1.39
5	B	902	D71	C29-N30	3.06	1.42	1.33
5	B	902	D71	C16-N15	3.07	1.42	1.38
5	B	902	D71	C16-C2	3.17	1.46	1.41
5	A	901	D71	C16-C2	3.31	1.47	1.41
5	A	901	D71	C29-N30	3.32	1.43	1.33
5	C	903	D71	C3-N13	3.38	1.46	1.39
5	C	903	D71	C16-C2	3.55	1.47	1.41
5	D	904	D71	C6-C1	3.91	1.45	1.36
5	D	904	D71	C5-N4	4.00	1.40	1.32
5	D	904	D71	C42-C43	4.06	1.47	1.38
5	B	902	D71	C42-C43	4.24	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	903	D71	C28-C26	4.26	1.47	1.38
5	D	904	D71	C32-C31	4.30	1.47	1.38
5	A	901	D71	C28-C26	4.34	1.48	1.38
5	D	904	D71	C28-C26	4.48	1.48	1.38
5	C	903	D71	C6-C1	4.49	1.47	1.36
5	B	902	D71	C5-N4	4.49	1.41	1.32
5	A	901	D71	C6-C1	4.64	1.47	1.36
5	B	902	D71	C41-C40	4.64	1.48	1.38
5	C	903	D71	C41-C40	4.66	1.48	1.38
5	B	902	D71	C28-C26	4.81	1.49	1.38
5	C	903	D71	C42-C43	4.90	1.49	1.38
5	B	902	D71	C32-C31	4.90	1.48	1.38
5	D	904	D71	C41-C40	4.91	1.48	1.38
5	A	901	D71	C42-C43	4.93	1.49	1.38
5	C	903	D71	C32-C31	4.96	1.48	1.38
5	A	901	D71	C41-C40	4.99	1.48	1.38
5	B	902	D71	C6-C1	5.19	1.48	1.36
5	C	903	D71	C5-N4	5.44	1.43	1.32
5	A	901	D71	C5-N4	5.64	1.43	1.32
5	A	901	D71	C32-C31	5.85	1.50	1.38
5	D	904	D71	C39-C22	6.72	1.47	1.38
5	B	902	D71	C39-C22	6.84	1.47	1.38
5	D	904	D71	C2-C3	6.99	1.47	1.40
5	A	901	D71	C39-C22	7.52	1.48	1.38
5	B	902	D71	C2-C3	7.64	1.48	1.40
5	C	903	D71	C39-C22	7.86	1.49	1.38
5	A	901	D71	C2-C3	8.78	1.49	1.40
5	C	903	D71	C2-C3	9.05	1.49	1.40

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	903	D71	C2-C3-N4	-4.74	117.89	123.53
5	A	901	D71	C2-C3-N4	-4.05	118.72	123.53
5	C	903	D71	C43-C22-C39	-3.95	117.93	121.50
5	D	904	D71	C2-C3-N4	-3.71	119.12	123.53
5	A	901	D71	C43-C22-C39	-3.30	118.52	121.50
5	D	904	D71	C6-C5-N4	-3.01	119.23	123.94
5	D	904	D71	C24-C26-C28	-2.98	114.40	120.40
5	C	903	D71	C24-C26-C28	-2.94	114.50	120.40
5	D	904	D71	C28-C29-N30	-2.83	118.71	123.64
5	B	902	D71	C32-C31-N30	-2.37	119.52	123.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	904	D71	C32-C31-N30	-2.31	119.62	123.64
5	D	904	D71	C31-C32-C26	-2.30	116.09	119.63
5	A	901	D71	C24-C26-C28	-2.28	115.81	120.40
5	A	901	D71	C32-C31-N30	-2.24	119.75	123.64
5	B	902	D71	C6-C5-N4	-2.22	120.46	123.94
5	B	902	D71	C2-C3-N4	-2.21	120.91	123.53
5	B	902	D71	C24-C26-C28	-2.18	116.01	120.40
5	C	903	D71	C32-C31-N30	-2.14	119.92	123.64
5	B	902	D71	C2-C3-N13	-2.11	118.24	122.21
5	B	902	D71	C39-C22-N13	2.01	121.36	119.27
5	B	902	D71	N4-C3-N13	2.04	120.86	114.99
5	D	904	D71	N4-C3-N13	2.09	121.01	114.99
5	C	903	D71	C24-C26-C32	2.11	124.65	120.40
5	D	904	D71	C1-C2-C3	2.23	119.08	117.00
5	C	903	D71	C29-N30-C31	2.24	122.23	116.83
5	A	901	D71	C1-C2-C3	2.30	119.15	117.00
5	A	901	D71	N4-C3-N13	2.40	121.88	114.99
5	B	902	D71	C39-C40-N54	2.50	121.00	118.80
5	B	902	D71	C29-N30-C31	2.54	122.96	116.83
5	D	904	D71	C28-C26-C32	2.58	122.26	118.13
5	D	904	D71	C24-N15-C14	2.63	121.17	118.05
5	C	903	D71	N4-C3-N13	2.65	122.61	114.99
5	A	901	D71	C39-C22-N13	3.18	122.57	119.27
5	C	903	D71	C1-C2-C3	3.23	120.02	117.00
5	D	904	D71	C29-N30-C31	3.26	124.70	116.83
5	A	901	D71	C2-C16-N15	3.43	118.93	116.09
5	D	904	D71	C39-C40-N54	3.48	121.85	118.80
5	A	901	D71	C5-N4-C3	3.56	121.35	116.93
5	B	902	D71	C5-N4-C3	3.66	121.47	116.93
5	D	904	D71	C39-C22-N13	4.02	123.44	119.27
5	C	903	D71	C5-N4-C3	4.39	122.37	116.93
5	D	904	D71	C2-C16-N15	4.83	120.08	116.09
5	D	904	D71	C5-N4-C3	5.01	123.15	116.93
5	B	902	D71	C2-C16-N15	5.09	120.29	116.09
5	C	903	D71	C2-C16-N15	5.09	120.30	116.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	902	D71	1	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	338/421 (80%)	-0.12	1 (0%) 94 96	11, 23, 38, 47	0
1	B	336/421 (79%)	0.02	6 (1%) 71 78	14, 30, 46, 54	0
1	C	339/421 (80%)	-0.08	0 100 100	11, 25, 41, 49	0
1	D	337/421 (80%)	-0.17	1 (0%) 94 96	14, 26, 38, 45	0
All	All	1350/1684 (80%)	-0.09	8 (0%) 90 93	11, 26, 42, 54	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	260	LYS	2.5
1	B	267	LYS	2.4
1	B	462	GLY	2.2
1	B	297	LEU	2.2
1	A	460	SER	2.2
1	B	256	ASP	2.2
1	D	256	ASP	2.2
1	B	296	ASP	2.0

### 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	MG	B	804	1/1	0.94	0.24	12.82	17,17,17,17	0
3	MG	A	802	1/1	0.92	0.29	8.62	12,12,12,12	0
3	MG	D	808	1/1	0.99	0.15	4.96	10,10,10,10	0
3	MG	C	806	1/1	0.95	0.20	3.19	14,14,14,14	0
2	ZN	B	803	1/1	1.00	0.12	0.93	25,25,25,25	0
5	D71	D	904	28/28	0.95	0.13	0.66	14,16,21,24	0
4	CA	D	3	1/1	0.98	0.20	0.52	35,35,35,35	0
5	D71	A	901	28/28	0.95	0.13	0.43	14,19,31,36	0
5	D71	B	902	28/28	0.95	0.12	0.41	16,19,24,27	0
5	D71	C	903	28/28	0.94	0.13	0.27	14,20,31,36	0
4	CA	B	1	1/1	0.94	0.18	0.26	41,41,41,41	0
2	ZN	A	801	1/1	0.99	0.14	-0.02	21,21,21,21	0
2	ZN	D	807	1/1	0.99	0.09	-0.58	22,22,22,22	0
2	ZN	C	805	1/1	1.00	0.12	-0.85	20,20,20,20	0
4	CA	A	4	1/1	0.93	0.10	-1.46	53,53,53,53	0
4	CA	C	2	1/1	0.97	0.08	-1.52	52,52,52,52	0

## 6.5 Other polymers

There are no such residues in this entry.