



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 12:36 am GMT

PDB ID : 1Q9M  
Title : Three dimensional structures of PDE4D in complex with roliprams and implication on inhibitor selectivity  
Authors : Huai, Q.; Wang, H.; Sun, Y.; Kim, H.Y.; Liu, Y.; Ke, H.  
Deposited on : 2003-08-25  
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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
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

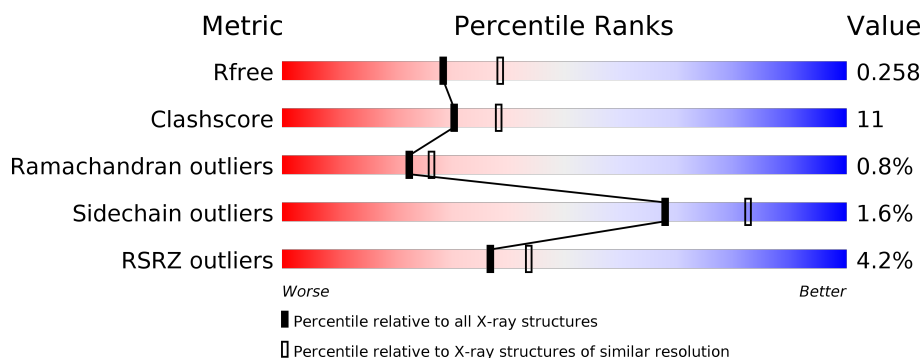
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
$R_{free}$	100719	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (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	360	<div> <div>4%</div> <div> <div></div> <div>72%</div> <div>20%</div> <div>• 7%</div> </div> </div>
1	B	360	<div> <div>6%</div> <div> <div></div> <div>66%</div> <div>24%</div> <div>• 9%</div> </div> </div>
1	C	360	<div> <div>4%</div> <div> <div></div> <div>71%</div> <div>19%</div> <div>• 9%</div> </div> </div>
1	D	360	<div> <div>2%</div> <div> <div></div> <div>76%</div> <div>16%</div> <div>• 7%</div> </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
3	ROL	A	503	-	-	-	X
3	ROL	C	507	-	-	-	X
3	ROL	D	509	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10972 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.

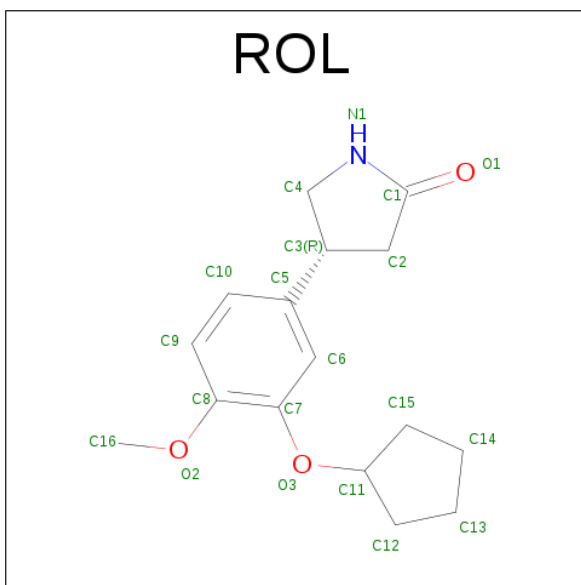
- Molecule 1 is a protein called cAMP-specific phosphodiesterase PDE4D2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	0	0
			2704	1712	463	515	14			
1	B	327	Total	C	N	O	S	0	0	0
			2647	1673	452	508	14			
1	C	329	Total	C	N	O	S	0	0	0
			2663	1684	455	510	14			
1	D	334	Total	C	N	O	S	0	0	0
			2704	1712	463	515	14			

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

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

- Molecule 3 is ROLIPRAM (three-letter code: ROL) (formula: C<sub>16</sub>H<sub>21</sub>NO<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			20	16	1	3		
3	B	1	Total	C	N	O	0	0
			20	16	1	3		
3	C	1	Total	C	N	O	0	0
			20	16	1	3		
3	D	1	Total	C	N	O	0	0
			20	16	1	3		

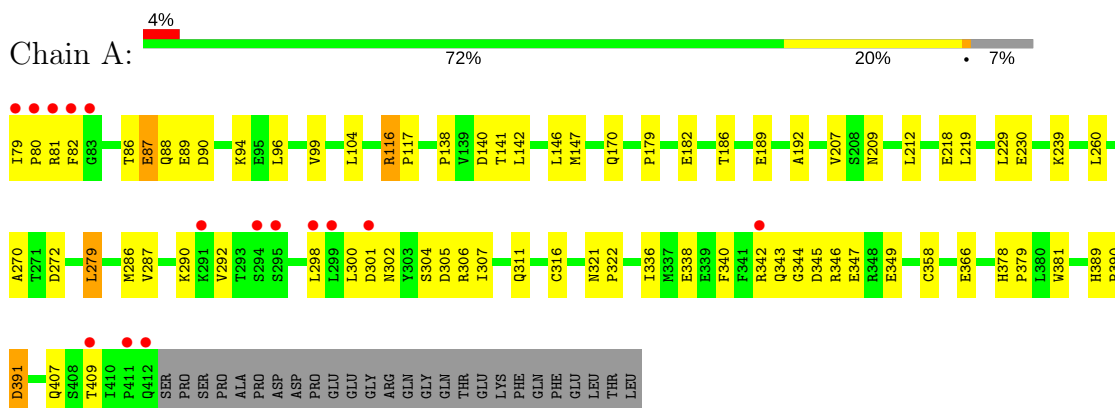
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	52	Total	O	0	0
			52	52		
4	B	36	Total	O	0	0
			36	36		
4	C	32	Total	O	0	0
			32	32		
4	D	46	Total	O	0	0
			46	46		

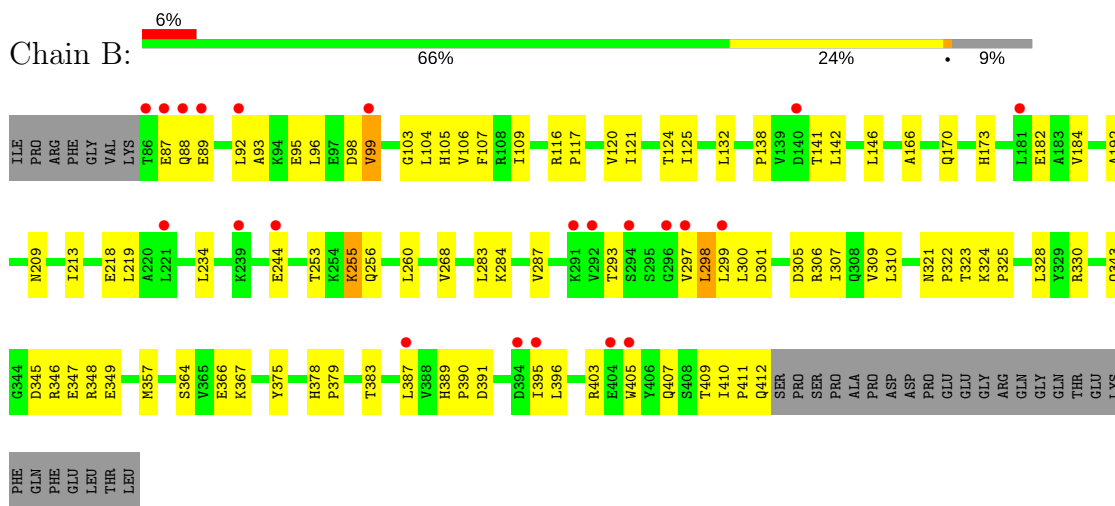
### 3 Residue-property plots [i](#)

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 ( $\text{RSRZ} > 2$ ). 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.

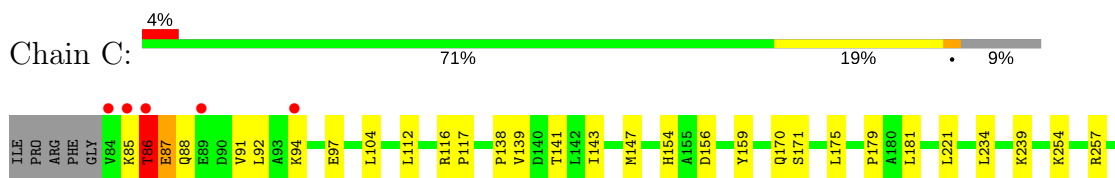
#### • Molecule 1: cAMP-specific phosphodiesterase PDE4D2



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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.27Å 112.49Å 160.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	99.00 – 2.30 92.20 – 2.30	Depositor EDS
% Data completeness (in resolution range)	93.9 (99.00-2.30) 93.6 (92.20-2.30)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.70 (at 2.29Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.224 , 0.259 0.223 , 0.258	Depositor DCC
$R_{free}$ test set	7639 reflections (10.09%)	DCC
Wilson B-factor (Å <sup>2</sup> )	31.7	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 37.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	10972	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% 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, ROL

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	0.35	0/2760	0.56	0/3749
1	B	0.32	0/2701	0.54	0/3670
1	C	0.33	0/2717	0.54	0/3691
1	D	0.36	0/2760	0.57	0/3749
All	All	0.34	0/10938	0.55	0/14859

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	2704	0	2664	54	0
1	B	2647	0	2599	74	0
1	C	2663	0	2621	61	0
1	D	2704	0	2664	42	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	20	0	21	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	20	0	21	3	0
3	C	20	0	21	1	0
3	D	20	0	21	1	0
4	A	52	0	0	0	0
4	B	36	0	0	1	0
4	C	32	0	0	1	0
4	D	46	0	0	0	0
All	All	10972	0	10632	226	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 11.

All (226) 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:255:LYS:H	1:B:255:LYS:HD2	1.29	0.95
1:C:293:THR:HG23	1:C:295:SER:H	1.46	0.80
1:B:364:SER:HB3	1:B:367:LYS:HD3	1.64	0.79
1:B:330:ARG:HD3	1:B:405:TRP:CH2	2.19	0.77
1:B:244:GLU:HG3	1:C:254:LYS:NZ	2.02	0.74
1:D:79:ILE:N	1:D:80:PRO:HD2	2.03	0.73
1:C:306:ARG:HH11	1:C:306:ARG:HB3	1.55	0.72
1:B:98:ASP:HB2	1:B:104:LEU:HD13	1.72	0.71
1:B:255:LYS:H	1:B:255:LYS:CD	2.04	0.69
1:C:293:THR:HG22	1:C:297:VAL:H	1.57	0.69
1:A:87:GLU:HG3	1:A:88:GLN:N	2.09	0.68
1:B:96:LEU:O	1:B:99:VAL:HG23	1.94	0.68
1:D:302:ASN:ND2	1:D:302:ASN:H	1.90	0.67
1:A:96:LEU:O	1:A:99:VAL:HG23	1.94	0.67
1:C:85:LYS:O	1:C:86:THR:HG23	1.94	0.67
1:B:300:LEU:HB3	1:B:306:ARG:HG2	1.78	0.66
1:B:283:LEU:O	1:B:287:VAL:HG23	1.95	0.66
1:B:324:LYS:HB3	1:B:325:PRO:HD2	1.77	0.65
1:B:378:HIS:HB3	1:B:379:PRO:HD3	1.78	0.65
1:D:79:ILE:N	1:D:80:PRO:CD	2.60	0.65
1:A:116:ARG:HE	1:A:147:MET:HE2	1.62	0.65
1:D:138:PRO:HG2	1:D:141:THR:OG1	1.97	0.64
1:B:411:PRO:O	1:B:412:GLN:HB2	1.97	0.64
1:C:254:LYS:HG2	1:C:257:ARG:HH22	1.62	0.64
1:B:366:GLU:HG2	1:B:409:THR:HG22	1.79	0.63
1:A:344:GLY:HA3	1:A:358:CYS:O	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:181:LEU:HD21	1:C:298:LEU:HD12	1.80	0.63
1:D:407:GLN:NE2	1:D:410:ILE:HD12	2.13	0.63
1:B:389:HIS:CE1	1:B:390:PRO:HB3	2.34	0.62
1:D:79:ILE:N	1:D:79:ILE:HD12	2.15	0.62
1:B:284:LYS:HE2	1:B:383:THR:OG1	2.00	0.62
1:A:79:ILE:N	1:A:80:PRO:HD2	2.14	0.61
1:C:321:ASN:HB2	1:C:322:PRO:HD3	1.82	0.61
1:C:86:THR:O	1:C:88:GLN:N	2.34	0.61
1:B:293:THR:HG22	1:B:299:LEU:HD23	1.82	0.61
1:B:321:ASN:HB2	1:B:322:PRO:HD3	1.83	0.61
1:D:302:ASN:OD1	1:D:304:SER:HB3	2.01	0.60
1:A:321:ASN:HB2	1:A:322:PRO:HD3	1.82	0.60
1:C:403:ARG:HD2	1:C:404:GLU:OE1	2.01	0.59
1:D:344:GLY:HA3	1:D:358:CYS:O	2.02	0.59
1:A:179:PRO:HD2	1:A:391:ASP:OD2	2.03	0.59
1:D:321:ASN:HB2	1:D:322:PRO:HD3	1.83	0.59
1:C:291:LYS:O	1:C:299:LEU:HB3	2.02	0.58
1:D:298:LEU:HD23	1:D:299:LEU:H	1.68	0.58
1:D:403:ARG:HD2	1:D:404:GLU:OE1	2.03	0.58
1:B:409:THR:O	1:B:409:THR:HG22	2.03	0.58
1:A:306:ARG:HG3	1:A:306:ARG:HH11	1.69	0.57
1:B:184:VAL:HG11	1:B:300:LEU:HD12	1.86	0.57
1:D:307:ILE:O	1:D:311:GLN:HG3	2.04	0.57
1:C:290:LYS:HG2	1:C:292:VAL:HG13	1.86	0.57
1:A:389:HIS:CE1	1:A:390:PRO:HB3	2.40	0.56
1:B:298:LEU:HD23	1:B:299:LEU:N	2.21	0.56
1:A:116:ARG:NE	1:A:147:MET:HE2	2.21	0.56
1:B:218:GLU:OE2	1:D:239:LYS:HE2	2.05	0.56
1:B:244:GLU:HG3	1:C:254:LYS:HZ2	1.71	0.56
1:C:254:LYS:CG	1:C:257:ARG:HH22	2.20	0.55
1:A:186:THR:OG1	1:A:189:GLU:HG3	2.06	0.55
1:B:192:ALA:HB2	1:B:260:LEU:HD12	1.87	0.55
1:A:307:ILE:O	1:A:311:GLN:HG3	2.06	0.55
1:B:293:THR:CG2	1:B:299:LEU:HD23	2.37	0.55
1:B:325:PRO:HG2	1:B:328:LEU:HD12	1.89	0.55
1:C:221:LEU:HD23	1:C:221:LEU:O	2.07	0.55
1:D:298:LEU:HD11	1:D:387:LEU:HD11	1.89	0.55
1:A:81:ARG:HG3	1:A:81:ARG:O	2.06	0.54
1:B:345:ASP:O	1:B:349:GLU:HG3	2.07	0.54
1:C:181:LEU:CD2	1:C:298:LEU:HD12	2.38	0.54
1:D:84:VAL:HG11	1:D:116:ARG:HD2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:330:ARG:HD3	1:C:405:TRP:CH2	2.43	0.53
1:C:293:THR:HG22	1:C:297:VAL:N	2.22	0.53
1:B:170:GLN:O	1:B:173:HIS:HB3	2.09	0.53
1:B:234:LEU:HD21	1:B:268:VAL:HB	1.90	0.53
1:C:307:ILE:O	1:C:311:GLN:HG3	2.09	0.53
1:C:234:LEU:HD21	1:C:268:VAL:HB	1.89	0.53
1:D:107:PHE:O	1:D:111:GLU:HG3	2.08	0.53
1:B:300:LEU:HD21	1:B:309:VAL:HG21	1.91	0.53
1:B:305:ASP:O	1:B:309:VAL:HG23	2.09	0.53
1:C:290:LYS:HE2	1:C:292:VAL:HG11	1.90	0.52
1:C:289:THR:HG22	1:C:289:THR:O	2.08	0.52
1:D:298:LEU:HD23	1:D:299:LEU:N	2.23	0.52
1:A:81:ARG:O	1:A:82:PHE:HB2	2.09	0.52
1:C:139:VAL:HG23	4:C:531:HOH:O	2.08	0.52
1:D:345:ASP:O	1:D:349:GLU:HG3	2.10	0.52
1:A:306:ARG:HG3	1:A:306:ARG:NH1	2.24	0.51
1:B:184:VAL:CG1	1:B:300:LEU:HD12	2.40	0.51
1:C:290:LYS:HE2	1:C:292:VAL:CG1	2.41	0.51
1:A:138:PRO:HG2	1:A:141:THR:OG1	2.11	0.51
1:A:79:ILE:N	1:A:80:PRO:CD	2.74	0.51
1:C:357:MET:SD	3:C:507:ROL:H131	2.51	0.51
1:B:87:GLU:HG3	1:B:88:GLN:HG3	1.93	0.51
1:D:104:LEU:HD22	1:D:170:GLN:HG3	1.91	0.51
1:B:138:PRO:HG2	1:B:141:THR:OG1	2.11	0.51
1:C:302:ASN:O	1:C:306:ARG:HG3	2.11	0.51
1:D:121:ILE:HD12	1:D:166:ALA:HB1	1.93	0.51
1:B:346:ARG:HD2	4:B:509:HOH:O	2.11	0.50
1:A:349:GLU:HB3	1:C:147:MET:CE	2.42	0.50
1:D:86:THR:HG21	1:D:92:LEU:HD12	1.94	0.50
1:B:99:VAL:HG21	1:B:124:THR:HG21	1.92	0.50
1:C:254:LYS:HG2	1:C:257:ARG:NH2	2.27	0.50
1:A:343:GLN:O	1:A:347:GLU:HG3	2.12	0.50
1:C:298:LEU:HD11	1:C:387:LEU:HG	1.94	0.49
1:D:79:ILE:HG22	1:D:79:ILE:O	2.11	0.49
1:A:292:VAL:HG12	1:A:298:LEU:HA	1.94	0.49
1:A:116:ARG:N	1:A:117:PRO:CD	2.75	0.49
1:C:389:HIS:CE1	1:C:390:PRO:HB3	2.47	0.49
1:C:293:THR:HG23	1:C:295:SER:N	2.22	0.49
1:A:179:PRO:HA	1:A:182:GLU:HG3	1.93	0.48
1:B:116:ARG:N	1:B:117:PRO:CD	2.77	0.48
1:B:375:TYR:CD1	1:B:375:TYR:N	2.81	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:LEU:HD11	1:A:229:LEU:HD21	1.95	0.48
1:C:291:LYS:HE3	1:C:299:LEU:O	2.13	0.48
1:C:411:PRO:O	1:C:412:GLN:HG3	2.12	0.48
1:A:142:LEU:O	1:A:146:LEU:HG	2.13	0.48
1:B:403:ARG:HG2	1:B:403:ARG:HH11	1.77	0.48
1:C:378:HIS:HB3	1:C:379:PRO:HD3	1.96	0.48
1:A:192:ALA:HB2	1:A:260:LEU:HD12	1.95	0.48
1:A:86:THR:HG22	1:A:87:GLU:N	2.28	0.48
1:A:207:VAL:HG11	1:A:346:ARG:NH2	2.28	0.48
1:B:121:ILE:HD12	1:B:166:ALA:HB1	1.96	0.48
1:C:366:GLU:HG2	1:C:409:THR:HG22	1.96	0.48
1:A:230:GLU:HG2	1:A:272:ASP:HB2	1.95	0.48
1:A:409:THR:HG22	1:A:409:THR:O	2.12	0.48
1:D:116:ARG:N	1:D:117:PRO:CD	2.77	0.48
1:B:411:PRO:O	1:B:412:GLN:CB	2.61	0.48
1:B:104:LEU:HD11	1:B:109:ILE:HD11	1.95	0.47
1:A:378:HIS:HB3	1:A:379:PRO:HD3	1.96	0.47
1:B:283:LEU:HD11	1:B:387:LEU:HD22	1.96	0.47
1:A:340:PHE:CE2	3:A:503:ROL:H151	2.50	0.47
1:B:357:MET:SD	3:B:505:ROL:H131	2.56	0.46
1:C:87:GLU:HG3	1:C:88:GLN:H	1.80	0.46
1:B:244:GLU:HG3	1:C:254:LYS:HZ1	1.78	0.46
1:C:330:ARG:HD3	1:C:405:TRP:CZ3	2.50	0.46
1:D:336:ILE:HD11	1:D:340:PHE:CE1	2.51	0.46
1:A:349:GLU:HB3	1:C:147:MET:HE1	1.99	0.45
1:B:132:LEU:HD12	1:B:132:LEU:H	1.81	0.45
1:A:298:LEU:HD21	1:A:300:LEU:HD21	1.98	0.45
1:B:182:GLU:O	1:B:297:VAL:HG11	2.16	0.45
1:B:330:ARG:HD3	1:B:405:TRP:CZ3	2.51	0.45
1:B:253:THR:OG1	1:B:256:GLN:HG3	2.17	0.45
1:C:154:HIS:HB3	1:C:156:ASP:OD1	2.16	0.45
1:C:344:GLY:HA3	1:C:358:CYS:O	2.17	0.45
1:D:299:LEU:O	1:D:300:LEU:HD23	2.16	0.45
1:A:79:ILE:HG13	1:A:89:GLU:OE2	2.17	0.45
1:B:104:LEU:HD12	1:B:105:HIS:H	1.81	0.45
1:B:298:LEU:HD23	1:B:299:LEU:H	1.82	0.45
1:A:209:ASN:OD1	1:A:229:LEU:HG	2.17	0.45
1:B:345:ASP:OD1	1:B:348:ARG:NH2	2.49	0.45
1:A:104:LEU:HD22	1:A:170:GLN:HG3	1.98	0.45
1:C:406:TYR:O	1:C:409:THR:HB	2.17	0.45
1:D:209:ASN:O	1:D:213:ILE:HG13	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:94:LYS:NZ	1:D:94:LYS:HB2	2.32	0.44
1:B:367:LYS:HE3	1:B:410:ILE:HG23	1.99	0.44
1:C:221:LEU:C	1:C:221:LEU:HD23	2.37	0.44
1:C:116:ARG:N	1:C:117:PRO:CD	2.80	0.44
1:D:330:ARG:HD3	1:D:405:TRP:CH2	2.53	0.44
1:C:91:VAL:HG12	1:C:112:LEU:HD11	2.00	0.44
1:D:302:ASN:H	1:D:302:ASN:HD22	1.61	0.44
3:D:509:ROL:H61	3:D:509:ROL:H21	1.78	0.44
1:B:284:LYS:HA	1:B:287:VAL:HG23	2.00	0.44
1:D:176:LEU:HG	1:D:313:MET:SD	2.58	0.44
1:A:90:ASP:O	1:A:94:LYS:HG3	2.17	0.44
1:C:324:LYS:O	1:C:325:PRO:C	2.56	0.44
1:C:143:ILE:O	1:C:147:MET:HG3	2.19	0.43
1:C:104:LEU:HD22	1:C:170:GLN:HG3	2.00	0.43
1:C:306:ARG:HH11	1:C:306:ARG:CB	2.26	0.43
1:B:89:GLU:HG2	1:B:93:ALA:HB2	1.99	0.43
1:C:300:LEU:HD13	1:C:306:ARG:HA	1.99	0.43
1:A:207:VAL:CG1	1:A:346:ARG:HH21	2.31	0.43
1:D:316:CYS:HB3	1:D:381:TRP:CZ2	2.53	0.43
1:A:239:LYS:NZ	1:D:239:LYS:NZ	2.66	0.43
1:B:96:LEU:HD11	1:B:120:VAL:CG1	2.49	0.43
1:D:154:HIS:N	1:D:154:HIS:CD2	2.86	0.43
1:A:336:ILE:HD11	1:A:340:PHE:CE1	2.54	0.42
1:A:366:GLU:HG2	1:A:409:THR:HG22	2.01	0.42
1:B:255:LYS:N	1:B:255:LYS:HD2	2.11	0.42
1:D:356:PRO:O	1:D:357:MET:HB2	2.19	0.42
1:B:142:LEU:O	1:B:146:LEU:HG	2.19	0.42
1:B:299:LEU:HD13	1:B:299:LEU:C	2.39	0.42
1:D:343:GLN:O	1:D:347:GLU:HG3	2.18	0.42
1:A:270:ALA:HB1	1:A:279:LEU:HD11	2.02	0.42
1:A:286:MET:HE1	1:A:305:ASP:HA	2.01	0.42
1:B:284:LYS:HG2	1:B:383:THR:CG2	2.49	0.42
1:A:140:ASP:N	1:A:140:ASP:OD2	2.49	0.42
1:A:302:ASN:HD21	1:A:304:SER:HB2	1.84	0.42
1:A:86:THR:HG22	1:A:88:GLN:H	1.84	0.42
1:C:138:PRO:HG2	1:C:141:THR:OG1	2.20	0.42
1:A:79:ILE:HG23	1:A:89:GLU:CD	2.40	0.42
1:B:125:ILE:HD13	1:B:173:HIS:HB2	2.02	0.42
1:B:310:LEU:HD23	1:B:310:LEU:HA	1.94	0.42
1:B:396:LEU:HD23	1:B:396:LEU:O	2.20	0.42
1:A:316:CYS:HB3	1:A:381:TRP:CZ2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:389:HIS:ND1	1:B:390:PRO:HB3	2.35	0.42
1:D:378:HIS:HB3	1:D:379:PRO:HD3	2.01	0.42
3:B:505:ROL:H61	3:B:505:ROL:H111	1.69	0.42
1:B:92:LEU:O	1:B:95:GLU:N	2.53	0.42
1:A:287:VAL:O	1:A:287:VAL:HG12	2.19	0.42
1:C:94:LYS:O	1:C:97:GLU:HB2	2.20	0.42
3:A:503:ROL:H61	3:A:503:ROL:H111	1.59	0.41
1:B:323:THR:HB	1:B:395:ILE:HG23	2.01	0.41
1:C:179:PRO:HD2	1:C:391:ASP:OD2	2.20	0.41
1:B:106:VAL:HG13	1:B:107:PHE:N	2.35	0.41
1:D:213:ILE:HD13	1:D:225:ASP:HB3	2.01	0.41
1:D:299:LEU:HD23	1:D:300:LEU:N	2.35	0.41
1:B:409:THR:O	1:B:409:THR:CG2	2.67	0.41
1:C:171:SER:O	1:C:175:LEU:HG	2.21	0.41
1:D:389:HIS:HA	1:D:390:PRO:HA	1.82	0.41
1:C:367:LYS:HE2	1:C:410:ILE:HG23	2.02	0.41
3:B:505:ROL:H21	3:B:505:ROL:H61	1.79	0.41
1:A:207:VAL:CG1	1:A:346:ARG:NH2	2.84	0.41
1:B:367:LYS:HG3	1:B:410:ILE:HG23	2.02	0.41
1:A:218:GLU:HB3	1:C:239:LYS:HE3	2.03	0.41
1:C:323:THR:HG22	1:C:399:LEU:HD13	2.02	0.41
1:A:338:GLU:O	1:A:342:ARG:HG3	2.20	0.41
1:B:209:ASN:O	1:B:213:ILE:HG13	2.20	0.41
1:C:159:TYR:HB3	1:C:339:GLU:OE1	2.20	0.41
1:C:373:ILE:HA	1:C:377:VAL:HB	2.03	0.41
1:B:307:ILE:HA	1:B:307:ILE:HD12	1.96	0.41
1:B:343:GLN:O	1:B:347:GLU:HG3	2.22	0.40
1:B:349:GLU:HB3	1:D:147:MET:CE	2.51	0.40
1:B:92:LEU:CD2	1:B:96:LEU:HG	2.51	0.40
1:C:254:LYS:CG	1:C:257:ARG:NH2	2.84	0.40
1:A:219:LEU:HA	1:A:219:LEU:HD12	1.92	0.40
1:A:345:ASP:O	1:A:349:GLU:HG3	2.20	0.40
1:C:409:THR:HG22	1:C:409:THR:O	2.20	0.40
1:D:190:ILE:O	1:D:194:ILE:HG13	2.22	0.40
1:B:389:HIS:HA	1:B:390:PRO:HA	1.84	0.40
1:D:409:THR:O	1:D:409:THR:HG22	2.21	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	332/360 (92%)	315 (95%)	15 (4%)	2 (1%)	28	34
1	B	325/360 (90%)	302 (93%)	20 (6%)	3 (1%)	20	23
1	C	327/360 (91%)	301 (92%)	21 (6%)	5 (2%)	12	11
1	D	332/360 (92%)	319 (96%)	13 (4%)	0	100	100
All	All	1316/1440 (91%)	1237 (94%)	69 (5%)	10 (1%)	22	26

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	301	ASP
1	C	86	THR
1	C	87	GLU
1	C	289	THR
1	C	290	LYS
1	A	290	LYS
1	A	301	ASP
1	B	103	GLY
1	C	292	VAL
1	B	99	VAL

### 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	305/328 (93%)	300 (98%)	5 (2%)	68	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	299/328 (91%)	294 (98%)	5 (2%)	66	81
1	C	301/328 (92%)	296 (98%)	5 (2%)	66	81
1	D	305/328 (93%)	301 (99%)	4 (1%)	73	86
All	All	1210/1312 (92%)	1191 (98%)	19 (2%)	68	82

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	87	GLU
1	A	116	ARG
1	A	279	LEU
1	A	391	ASP
1	A	407	GLN
1	B	219	LEU
1	B	255	LYS
1	B	298	LEU
1	B	391	ASP
1	B	407	GLN
1	C	86	THR
1	C	92	LEU
1	C	279	LEU
1	C	306	ARG
1	C	390	PRO
1	D	92	LEU
1	D	94	LYS
1	D	298	LEU
1	D	342	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	245	ASN
1	A	308	GLN
1	A	407	GLN
1	B	170	GLN
1	B	245	ASN
1	B	250	GLN
1	B	378	HIS
1	C	242	GLN
1	C	245	ASN

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Mol	Chain	Res	Type
1	D	127	GLN
1	D	210	GLN
1	D	245	ASN
1	D	361	HIS
1	D	407	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	$\# Z  > 2$
3	ROL	A	503	-	21,22,22	0.68	0	26,30,30	1.41	4 (15%)
3	ROL	B	505	-	21,22,22	0.56	0	26,30,30	1.38	3 (11%)
3	ROL	C	507	-	21,22,22	0.56	0	26,30,30	1.30	3 (11%)
3	ROL	D	509	-	21,22,22	0.62	0	26,30,30	1.36	2 (7%)

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
3	ROL	A	503	-	-	0/10/26/26	0/3/3/3
3	ROL	B	505	-	-	0/10/26/26	0/3/3/3
3	ROL	C	507	-	-	0/10/26/26	0/3/3/3
3	ROL	D	509	-	-	0/10/26/26	0/3/3/3

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	505	ROL	C16-O2-C8	-3.19	112.95	117.54
3	A	503	ROL	C16-O2-C8	-3.17	112.97	117.54
3	D	509	ROL	C16-O2-C8	-3.03	113.18	117.54
3	C	507	ROL	C16-O2-C8	-2.87	113.40	117.54
3	A	503	ROL	C4-C3-C5	-2.60	109.14	114.25
3	B	505	ROL	C4-C3-C5	-2.36	109.60	114.25
3	C	507	ROL	C4-C3-C5	-2.06	110.19	114.25
3	A	503	ROL	C2-C3-C5	-2.02	110.33	114.68
3	C	507	ROL	C3-C2-C1	3.88	109.72	104.84
3	A	503	ROL	C3-C2-C1	3.93	109.79	104.84
3	B	505	ROL	C3-C2-C1	3.94	109.80	104.84
3	D	509	ROL	C3-C2-C1	4.21	110.13	104.84

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	503	ROL	2	0
3	B	505	ROL	3	0
3	C	507	ROL	1	0
3	D	509	ROL	1	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	334/360 (92%)	0.20	15 (4%) 34 41	16, 30, 71, 97	0
1	B	327/360 (90%)	0.49	22 (6%) 19 25	18, 42, 76, 100	0
1	C	329/360 (91%)	0.28	13 (3%) 39 46	17, 39, 79, 92	0
1	D	334/360 (92%)	0.06	6 (1%) 69 74	16, 30, 53, 76	0
All	All	1324/1440 (91%)	0.26	56 (4%) 37 44	16, 35, 73, 100	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	79	ILE	10.6
1	A	82	PHE	8.2
1	A	81	ARG	8.2
1	A	80	PRO	7.8
1	B	297	VAL	4.9
1	B	296	GLY	4.6
1	A	295	SER	4.6
1	B	395	ILE	4.3
1	C	84	VAL	4.3
1	B	86	THR	4.2
1	B	292	VAL	4.0
1	B	88	GLN	3.9
1	A	83	GLY	3.7
1	C	295	SER	3.5
1	B	244	GLU	3.5
1	C	298	LEU	3.4
1	A	294	SER	3.4
1	C	294	SER	3.4
1	A	299	LEU	3.3
1	A	412	GLN	3.1
1	A	298	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	294	SER	3.0
1	B	387	LEU	3.0
1	B	394	ASP	2.8
1	C	296	GLY	2.8
1	C	287	VAL	2.8
1	C	292	VAL	2.8
1	D	87	GLU	2.8
1	A	301	ASP	2.7
1	C	86	THR	2.7
1	D	86	THR	2.7
1	C	85	LYS	2.7
1	B	92	LEU	2.7
1	A	411	PRO	2.5
1	D	296	GLY	2.5
1	D	412	GLN	2.5
1	B	181	LEU	2.5
1	B	87	GLU	2.4
1	B	291	LYS	2.4
1	C	89	GLU	2.3
1	D	221	LEU	2.3
1	B	89	GLU	2.3
1	D	342	ARG	2.3
1	A	342	ARG	2.2
1	B	299	LEU	2.2
1	C	326	LEU	2.2
1	A	409	THR	2.1
1	A	291	LYS	2.1
1	C	94	LYS	2.1
1	B	405	TRP	2.1
1	B	239	LYS	2.1
1	B	221	LEU	2.1
1	C	301	ASP	2.1
1	B	404	GLU	2.1
1	B	140	ASP	2.1
1	B	99	VAL	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 [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
3	ROL	A	503	20/20	0.91	0.21	3.12	34,36,37,40	0
3	ROL	D	509	20/20	0.92	0.19	3.07	32,37,41,44	0
3	ROL	C	507	20/20	0.91	0.18	3.00	38,39,46,48	0
3	ROL	B	505	20/20	0.94	0.17	1.44	34,37,41,43	0
2	ZN	D	507	1/1	0.98	0.14	0.09	31,31,31,31	0
2	ZN	A	502	1/1	0.93	0.13	-0.10	61,61,61,61	0
2	ZN	A	501	1/1	0.98	0.12	-1.03	30,30,30,30	0
2	ZN	B	504	1/1	0.94	0.11	-1.87	64,64,64,64	0
2	ZN	C	505	1/1	0.98	0.10	-2.51	32,32,32,32	0
2	ZN	B	503	1/1	0.97	0.09	-2.93	34,34,34,34	0
2	ZN	C	506	1/1	0.96	0.07	-4.44	59,59,59,59	0
2	ZN	D	508	1/1	0.94	0.05	-7.36	61,61,61,61	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.