



Full wwPDB X-ray Structure Validation Report

Feb 5, 2024 – 09:32 PM EST

PDB ID : 1ZKN
Title : Structure of PDE4D2-IBMX
Authors : Huai, Q.; Liu, Y.; Francis, S.H.; Corbin, J.D.; Ke, H.
Deposited on : 2005-05-03
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the  symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

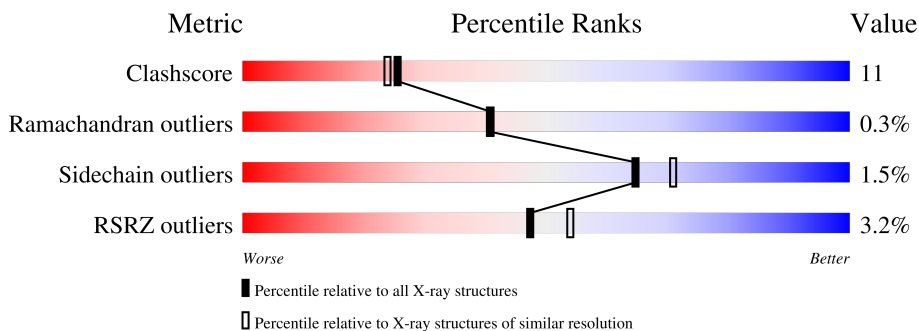
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	334	
1	B	334	
1	C	334	
1	D	334	

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
4	IBM	D	501	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 10987 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
			Total	C	N	O	S			
1	A	334	2705	1712	463	516	14	0	0	0
1	B	327	2648	1673	452	509	14	0	0	0
1	C	330	2668	1686	456	512	14	0	0	0
1	D	334	2705	1712	463	516	14	0	0	0

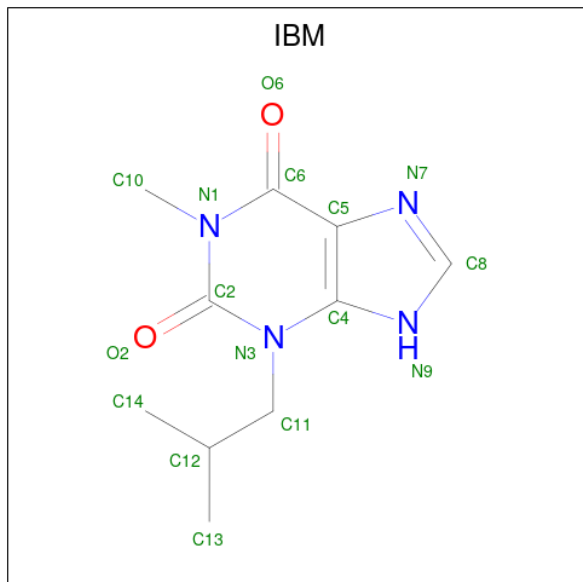
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 4 is 3-ISOBUTYL-1-METHYLXANTHINE (three-letter code: IBM) (formula: $C_{10}H_{14}N_4O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	Total	C	N	O	0	0
			16	10	4	2		
4	B	1	Total	C	N	O	0	0
			16	10	4	2		
4	C	1	Total	C	N	O	0	0
			16	10	4	2		
4	D	1	Total	C	N	O	0	0
			16	10	4	2		

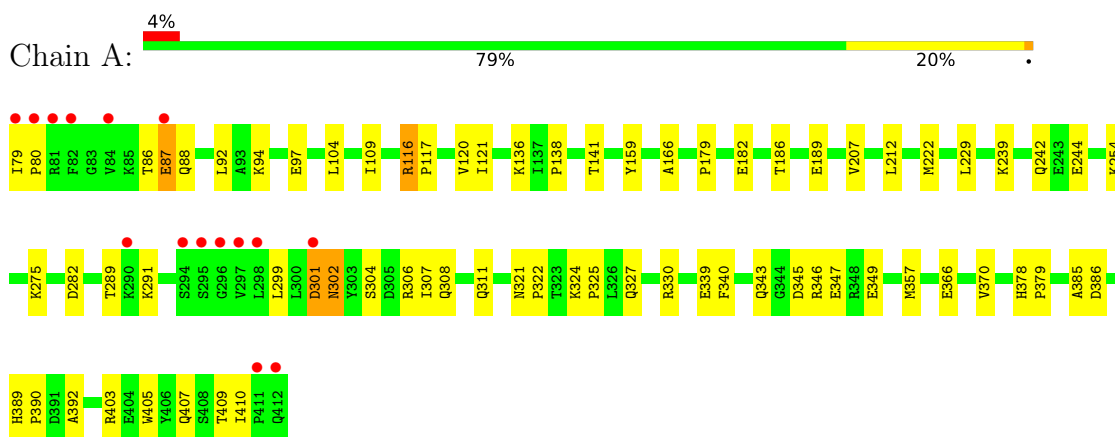
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	53	Total	O	0	0
			53	53		
5	B	43	Total	O	0	0
			43	43		
5	C	34	Total	O	0	0
			34	34		
5	D	59	Total	O	0	0
			59	59		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

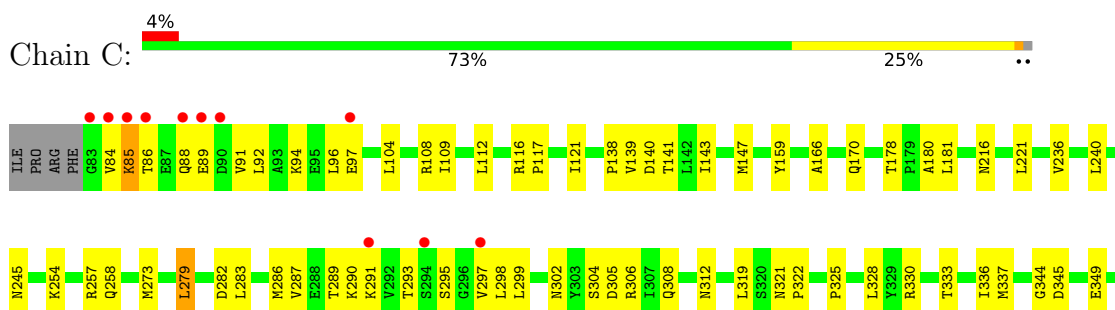
- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D



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

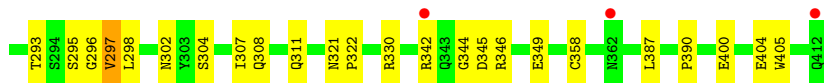
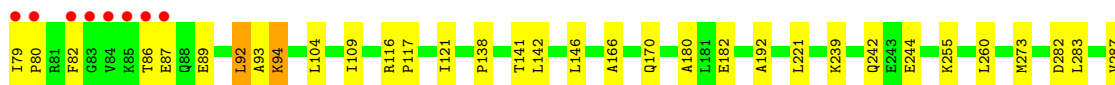
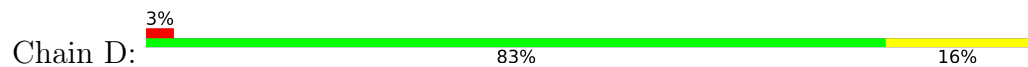


- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D





- 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, α , β , γ	99.70Å 111.70Å 159.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.10 91.48 – 2.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.10) 86.6 (91.48-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.09 (at 2.10Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.226 , 0.260 0.222 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	26.5	Xtrriage
Anisotropy	0.099	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 39.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10987	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: MG, ZN, IBM

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	0.33	0/2761	0.54	0/3749
1	B	0.33	0/2702	0.54	0/3670
1	C	0.31	0/2722	0.52	0/3696
1	D	0.34	0/2761	0.56	0/3749
All	All	0.33	0/10946	0.54	0/14864

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	2705	0	2664	53	0
1	B	2648	0	2599	68	0
1	C	2668	0	2624	69	0
1	D	2705	0	2664	47	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

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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	16	0	14	2	0
4	B	16	0	14	4	0
4	C	16	0	14	2	0
4	D	16	0	14	7	0
5	A	53	0	0	1	0
5	B	43	0	0	1	0
5	C	34	0	0	0	0
5	D	59	0	0	2	0
All	All	10987	0	10607	227	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 (227) 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:364:SER:HB3	1:B:367:LYS:HD3	1.27	1.13
1:B:255:LYS:H	1:B:255:LYS:HD2	1.11	1.05
1:B:403:ARG:HH12	1:B:407:GLN:HG3	1.38	0.86
1:C:84:VAL:HG22	1:C:85:LYS:H	1.40	0.86
1:B:255:LYS:HD2	1:B:255:LYS:N	1.92	0.83
1:D:273:MET:HG3	4:D:501:IBM:C13	2.09	0.83
1:B:403:ARG:HH12	1:B:407:GLN:CG	1.93	0.81
1:C:364:SER:HB3	1:C:367:LYS:HD2	1.62	0.81
1:D:79:ILE:N	1:D:80:PRO:HD2	1.99	0.78
1:B:302:ASN:O	1:B:306:ARG:HG3	1.90	0.72
1:B:364:SER:CB	1:B:367:LYS:HD3	2.15	0.72
1:C:293:THR:HG23	1:C:295:SER:H	1.57	0.70
1:A:302:ASN:HD22	1:A:304:SER:HB2	1.56	0.70
1:D:273:MET:HG3	4:D:501:IBM:H133	1.73	0.70
1:C:254:LYS:HG2	1:C:257:ARG:NH2	2.07	0.68
1:A:87:GLU:HG3	1:A:88:GLN:N	2.09	0.68
1:A:104:LEU:HD11	1:A:109:ILE:HD11	1.77	0.67
1:A:403:ARG:NH1	1:A:407:GLN:HG3	2.09	0.67
1:C:279:LEU:HD22	1:C:312:ASN:OD1	1.95	0.67
1:B:244:GLU:HB3	5:B:604:HOH:O	1.95	0.66
1:D:273:MET:HG3	4:D:501:IBM:H131	1.76	0.66
1:C:94:LYS:HD2	1:C:97:GLU:OE2	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:ILE:N	1:A:80:PRO:HD2	2.11	0.65
1:C:84:VAL:HG22	1:C:85:LYS:N	2.10	0.64
1:A:389:HIS:CE1	1:A:390:PRO:HB3	2.32	0.64
1:D:321:ASN:HB2	1:D:322:PRO:HD3	1.78	0.64
1:B:338:GLU:OE2	1:B:342:ARG:NH2	2.31	0.64
1:C:254:LYS:HG2	1:C:257:ARG:HH22	1.63	0.63
1:B:298:LEU:HD11	1:B:387:LEU:HD11	1.79	0.62
1:C:221:LEU:O	1:C:221:LEU:HD23	1.98	0.62
1:B:273:MET:HG3	4:B:603:IBM:H131	1.82	0.62
1:B:96:LEU:O	1:B:99:VAL:HG23	1.99	0.61
1:B:273:MET:HG3	4:B:603:IBM:C13	2.29	0.61
1:D:344:GLY:HA3	1:D:358:CYS:O	2.00	0.61
1:B:270:ALA:HB1	1:B:279:LEU:HD11	1.82	0.61
1:D:79:ILE:N	1:D:79:ILE:HD12	2.15	0.61
1:D:82:PHE:HZ	1:D:93:ALA:HB2	1.65	0.61
1:A:136:LYS:HD2	1:A:136:LYS:N	2.17	0.60
1:A:282:ASP:HB3	1:A:308:GLN:NE2	2.16	0.60
1:B:300:LEU:HB3	1:B:306:ARG:HG2	1.84	0.60
1:C:180:ALA:O	1:C:297:VAL:HG13	2.00	0.60
1:D:79:ILE:N	1:D:80:PRO:CD	2.65	0.60
1:D:86:THR:O	1:D:89:GLU:HB2	2.00	0.60
1:B:86:THR:HA	1:B:89:GLU:HB3	1.83	0.59
1:C:344:GLY:HA3	1:C:358:CYS:O	2.03	0.58
1:A:302:ASN:O	1:A:306:ARG:HG3	2.03	0.58
1:A:343:GLN:O	1:A:347:GLU:HG3	2.04	0.58
1:C:321:ASN:HB2	1:C:322:PRO:HD3	1.85	0.58
1:A:321:ASN:HB2	1:A:322:PRO:HD3	1.85	0.58
1:B:87:GLU:HG3	1:B:88:GLN:HG3	1.85	0.58
1:B:132:LEU:H	1:B:132:LEU:HD12	1.69	0.58
1:D:400:GLU:O	1:D:404:GLU:HG2	2.05	0.57
1:B:154:HIS:HB3	1:B:156:ASP:OD1	2.05	0.57
1:C:286:MET:HE1	1:C:308:GLN:HB3	1.86	0.56
1:A:405:TRP:O	1:A:409:THR:HG23	2.05	0.56
1:C:289:THR:O	1:C:291:LYS:HG3	2.05	0.56
1:B:396:LEU:O	1:B:396:LEU:HD23	2.06	0.55
1:D:282:ASP:HB3	1:D:308:GLN:NE2	2.21	0.55
1:A:121:ILE:HD12	1:A:166:ALA:HB1	1.87	0.55
1:B:130:ASP:OD1	1:B:133:LYS:HD2	2.07	0.55
1:D:298:LEU:HD11	1:D:387:LEU:HG	1.89	0.55
1:B:321:ASN:HB2	1:B:322:PRO:HD3	1.90	0.54
1:C:84:VAL:O	1:C:86:THR:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:88:GLN:HE22	1:C:89:GLU:HB2	1.73	0.54
1:D:307:ILE:O	1:D:311:GLN:HG3	2.07	0.54
1:B:123:HIS:O	1:B:127:GLN:HG3	2.08	0.54
1:A:79:ILE:N	1:A:80:PRO:CD	2.71	0.54
1:B:367:LYS:NZ	1:B:411:PRO:HG2	2.23	0.54
1:D:104:LEU:HD22	1:D:170:GLN:HG3	1.90	0.54
1:B:367:LYS:HG3	1:B:410:ILE:HG23	1.90	0.53
1:A:385:ALA:HA	1:A:392:ALA:HB3	1.89	0.53
1:B:286:MET:HE2	1:B:387:LEU:HD11	1.90	0.53
1:C:366:GLU:CD	1:C:366:GLU:H	2.13	0.52
1:C:254:LYS:HZ3	1:C:257:ARG:HH22	1.58	0.52
1:D:345:ASP:O	1:D:349:GLU:HG3	2.08	0.52
1:C:378:HIS:HA	1:C:399:LEU:HD21	1.92	0.52
1:A:357:MET:SD	4:A:603:IBM:H103	2.50	0.52
1:B:91:VAL:O	1:B:95:GLU:HG2	2.09	0.51
1:A:275:LYS:HE3	5:A:643:HOH:O	2.11	0.51
1:C:330:ARG:HD3	1:C:405:TRP:CH2	2.45	0.51
1:B:249:PHE:HA	1:B:252:LEU:HD13	1.92	0.51
1:B:255:LYS:H	1:B:255:LYS:CD	1.98	0.51
1:D:293:THR:O	1:D:295:SER:O	2.28	0.51
1:A:239:LYS:HE3	1:D:239:LYS:NZ	2.26	0.51
1:A:86:THR:HG22	1:A:87:GLU:N	2.25	0.51
1:A:242:GLN:NE2	1:D:242:GLN:OE1	2.43	0.51
1:C:138:PRO:HG2	1:C:141:THR:OG1	2.11	0.51
1:C:143:ILE:O	1:C:147:MET:HG3	2.11	0.51
1:A:302:ASN:ND2	1:A:304:SER:HB2	2.24	0.50
1:B:125:ILE:HD13	1:B:173:HIS:HB2	1.94	0.50
1:A:207:VAL:CG1	1:A:346:ARG:HH21	2.24	0.50
1:B:403:ARG:NH1	1:B:407:GLN:HG3	2.17	0.50
1:B:87:GLU:HG3	1:B:88:GLN:N	2.26	0.50
1:C:279:LEU:HD22	1:C:312:ASN:CG	2.32	0.50
1:C:405:TRP:O	1:C:409:THR:HG23	2.11	0.50
1:A:370:VAL:HG21	1:A:410:ILE:HD11	1.93	0.50
1:B:159:TYR:OH	1:B:321:ASN:ND2	2.43	0.49
1:A:282:ASP:HB3	1:A:308:GLN:CD	2.32	0.49
1:C:282:ASP:HB3	1:C:308:GLN:NE2	2.27	0.49
1:D:104:LEU:HD11	1:D:109:ILE:HD11	1.95	0.49
1:C:104:LEU:HD22	1:C:170:GLN:HG3	1.95	0.49
1:A:94:LYS:O	1:A:97:GLU:HB2	2.12	0.49
1:B:138:PRO:HG2	1:B:141:THR:OG1	2.13	0.49
1:C:283:LEU:O	1:C:287:VAL:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:ILE:HG22	1:B:332:TRP:HH2	1.78	0.49
1:B:330:ARG:HH11	1:B:405:TRP:HH2	1.60	0.49
1:D:180:ALA:O	1:D:297:VAL:HG22	2.12	0.49
1:C:333:THR:O	1:C:336:ILE:HG22	2.13	0.48
1:D:302:ASN:OD1	1:D:304:SER:HB3	2.13	0.48
1:A:138:PRO:HG2	1:A:141:THR:OG1	2.12	0.48
1:B:116:ARG:N	1:B:117:PRO:CD	2.77	0.48
1:B:373:ILE:HA	1:B:377:VAL:HB	1.94	0.48
1:A:222:MET:HE1	1:B:239:LYS:NZ	2.29	0.48
1:C:376:ILE:C	1:C:379:PRO:HD2	2.34	0.48
1:C:302:ASN:O	1:C:306:ARG:HG3	2.13	0.48
1:B:244:GLU:HG3	1:C:254:LYS:NZ	2.29	0.48
1:B:344:GLY:HA3	1:B:358:CYS:O	2.14	0.48
1:C:221:LEU:HD23	1:C:221:LEU:C	2.35	0.48
1:B:298:LEU:HD23	1:B:299:LEU:N	2.29	0.47
1:D:82:PHE:CD2	1:D:92:LEU:HD13	2.49	0.47
1:A:186:THR:OG1	1:A:189:GLU:HG3	2.14	0.47
1:B:120:VAL:HG23	1:B:121:ILE:N	2.30	0.47
1:B:147:MET:CE	1:D:349:GLU:HB3	2.44	0.47
1:D:192:ALA:HB2	1:D:260:LEU:HD12	1.97	0.47
1:D:346:ARG:HD2	5:D:632:HOH:O	2.15	0.47
1:C:116:ARG:N	1:C:117:PRO:CD	2.78	0.47
1:C:236:VAL:O	1:C:240:LEU:HG	2.15	0.46
1:C:373:ILE:HA	1:C:377:VAL:HB	1.96	0.46
1:C:364:SER:HB3	1:C:367:LYS:CD	2.41	0.46
1:C:364:SER:CB	1:C:367:LYS:HB2	2.46	0.46
1:D:273:MET:CE	4:D:501:IBM:H131	2.45	0.46
1:C:181:LEU:HD21	1:C:298:LEU:HD12	1.98	0.46
1:C:325:PRO:HD2	1:C:328:LEU:HD12	1.97	0.46
1:A:207:VAL:HG11	1:A:346:ARG:NH2	2.30	0.46
1:A:403:ARG:HD3	1:A:403:ARG:C	2.36	0.46
1:B:403:ARG:HH12	1:B:407:GLN:HG2	1.75	0.46
1:C:139:VAL:HG13	1:C:140:ASP:N	2.30	0.46
1:B:336:ILE:HD11	1:B:340:PHE:CE1	2.51	0.46
1:C:121:ILE:HD12	1:C:166:ALA:HB1	1.98	0.46
1:A:378:HIS:HB3	1:A:379:PRO:HD3	1.98	0.46
1:C:84:VAL:HG13	1:C:86:THR:HG23	1.96	0.45
1:B:164:HIS:O	1:B:168:VAL:HG23	2.16	0.45
1:C:84:VAL:CG2	1:C:85:LYS:H	2.20	0.45
1:A:159:TYR:HB3	1:A:339:GLU:OE1	2.17	0.45
1:B:244:GLU:CG	1:C:254:LYS:HE3	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:82:PHE:CZ	1:D:93:ALA:HB2	2.49	0.45
1:B:244:GLU:HG3	1:C:254:LYS:HZ1	1.82	0.45
1:B:370:VAL:HG21	1:B:410:ILE:HD11	1.98	0.45
1:C:336:ILE:HG23	1:C:337:MET:N	2.33	0.44
1:C:293:THR:HG22	1:C:297:VAL:O	2.17	0.44
1:A:116:ARG:N	1:A:117:PRO:CD	2.80	0.44
1:A:242:GLN:CD	1:D:242:GLN:OE1	2.55	0.44
1:D:255:LYS:HA	1:D:255:LYS:HD2	1.78	0.44
1:D:330:ARG:HD3	1:D:405:TRP:CH2	2.52	0.44
1:B:86:THR:HA	1:B:89:GLU:CB	2.47	0.44
1:D:273:MET:CG	4:D:501:IBM:H131	2.45	0.44
1:A:389:HIS:HA	1:A:390:PRO:HA	1.75	0.44
1:B:201:ASP:O	1:B:204:HIS:HB2	2.18	0.44
1:A:179:PRO:O	1:A:182:GLU:HB2	2.18	0.43
1:B:244:GLU:CG	1:C:254:LYS:HZ1	2.31	0.43
1:B:286:MET:CE	1:B:387:LEU:HD11	2.49	0.43
1:D:94:LYS:HB2	1:D:94:LYS:NZ	2.33	0.43
1:A:299:LEU:C	1:A:299:LEU:HD23	2.38	0.43
1:A:299:LEU:HD21	1:A:301:ASP:OD2	2.18	0.43
1:A:366:GLU:O	1:A:370:VAL:HG23	2.18	0.43
1:D:221:LEU:HD23	1:D:221:LEU:O	2.18	0.43
1:C:291:LYS:O	1:C:299:LEU:HB3	2.18	0.43
1:D:116:ARG:N	1:D:117:PRO:CD	2.81	0.43
1:C:319:LEU:HD22	1:C:372:PHE:HZ	1.83	0.43
1:D:283:LEU:O	1:D:287:VAL:HG23	2.18	0.43
1:A:242:GLN:OE1	1:D:242:GLN:OE1	2.37	0.43
1:A:340:PHE:HZ	4:A:603:IBM:H143	1.84	0.43
1:B:273:MET:HG3	4:B:603:IBM:H132	1.99	0.43
1:B:403:ARG:NH1	1:B:407:GLN:CG	2.73	0.43
1:A:327:GLN:H	1:A:327:GLN:HG3	1.59	0.43
1:B:234:LEU:HD21	1:B:268:VAL:HB	2.00	0.43
1:C:91:VAL:HG12	1:C:112:LEU:HD11	2.00	0.43
1:C:94:LYS:O	1:C:97:GLU:HB2	2.19	0.43
1:B:389:HIS:HA	1:B:390:PRO:HA	1.81	0.43
1:C:254:LYS:O	1:C:258:GLN:HG3	2.18	0.43
1:C:389:HIS:CE1	1:C:390:PRO:HB3	2.53	0.43
1:D:182:GLU:O	1:D:297:VAL:HG21	2.19	0.43
1:C:88:GLN:NE2	1:C:89:GLU:HB2	2.34	0.42
1:A:289:THR:O	1:A:291:LYS:HG3	2.19	0.42
1:D:104:LEU:HD11	1:D:109:ILE:CD1	2.49	0.42
1:C:345:ASP:O	1:C:349:GLU:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:378:HIS:HB3	1:C:379:PRO:HD3	2.02	0.42
1:A:212:LEU:HD11	1:A:229:LEU:HD21	2.01	0.42
1:A:244:GLU:OE1	1:C:216:ASN:ND2	2.53	0.42
1:B:298:LEU:HD23	1:B:299:LEU:H	1.85	0.42
1:C:96:LEU:HD23	1:C:109:ILE:HD13	2.01	0.42
1:C:178:THR:HG22	1:C:181:LEU:HD12	2.01	0.42
4:B:603:IBM:O2	4:B:603:IBM:H143	2.20	0.42
1:D:138:PRO:HG2	1:D:141:THR:OG1	2.19	0.42
1:A:324:LYS:O	1:A:325:PRO:C	2.57	0.41
1:C:302:ASN:ND2	1:C:305:ASP:OD2	2.52	0.41
1:A:330:ARG:HD3	1:A:405:TRP:CH2	2.55	0.41
1:B:367:LYS:HE3	1:B:410:ILE:HG23	2.02	0.41
1:C:304:SER:O	1:C:308:GLN:HB2	2.20	0.41
1:A:345:ASP:O	1:A:349:GLU:HG3	2.20	0.41
1:C:287:VAL:HG11	1:C:386:ASP:HB3	2.00	0.41
1:D:296:GLY:HA3	5:D:661:HOH:O	2.19	0.41
1:A:254:LYS:HE2	1:D:244:GLU:CD	2.40	0.41
1:B:192:ALA:HB2	1:B:260:LEU:HD12	2.03	0.41
4:C:603:IBM:O2	4:C:603:IBM:H142	2.20	0.41
1:D:121:ILE:HD12	1:D:166:ALA:HB1	2.02	0.41
1:A:307:ILE:O	1:A:311:GLN:HG3	2.21	0.41
1:C:88:GLN:NE2	1:C:89:GLU:N	2.68	0.41
1:D:273:MET:SD	4:D:501:IBM:H131	2.60	0.41
1:A:207:VAL:HG13	1:A:346:ARG:HH21	1.85	0.41
1:C:178:THR:OG1	1:C:391:ASP:HB3	2.21	0.41
1:C:181:LEU:CD2	1:C:298:LEU:HD12	2.51	0.41
1:C:273:MET:HG3	4:C:603:IBM:C13	2.51	0.41
1:C:364:SER:HB2	1:C:367:LYS:HB2	2.03	0.41
1:B:283:LEU:HG	1:B:383:THR:HG22	2.04	0.40
1:D:273:MET:HE2	4:D:501:IBM:H131	2.02	0.40
1:A:366:GLU:HG2	1:A:409:THR:OG1	2.21	0.40
1:B:189:GLU:OE1	1:B:306:ARG:NH2	2.54	0.40
1:D:87:GLU:H	1:D:87:GLU:HG2	1.61	0.40
1:A:116:ARG:O	1:A:120:VAL:HG22	2.21	0.40
1:B:132:LEU:HD12	1:B:132:LEU:N	2.36	0.40
1:B:179:PRO:HD2	1:B:391:ASP:CG	2.42	0.40
1:B:324:LYS:HB3	1:B:325:PRO:HD2	2.02	0.40
1:B:136:LYS:HE2	1:B:136:LYS:HB2	1.94	0.40
1:B:163:ILE:HG22	1:B:332:TRP:CH2	2.56	0.40
1:C:159:TYR:OH	1:C:321:ASN:ND2	2.53	0.40
1:D:142:LEU:O	1:D:146:LEU:HG	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	332/334 (99%)	322 (97%)	8 (2%)	2 (1%)	25	21
1	B	325/334 (97%)	312 (96%)	13 (4%)	0	100	100
1	C	328/334 (98%)	307 (94%)	19 (6%)	2 (1%)	25	21
1	D	332/334 (99%)	323 (97%)	9 (3%)	0	100	100
All	All	1317/1336 (99%)	1264 (96%)	49 (4%)	4 (0%)	41	41

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	301	ASP
1	A	302	ASN
1	C	85	LYS
1	C	290	LYS

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	305/305 (100%)	301 (99%)	4 (1%)	69	75
1	B	299/305 (98%)	294 (98%)	5 (2%)	60	67
1	C	301/305 (99%)	297 (99%)	4 (1%)	69	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	305/305 (100%)	300 (98%)	5 (2%)	62	69
All	All	1210/1220 (99%)	1192 (98%)	18 (2%)	65	71

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	87	GLU
1	A	92	LEU
1	A	116	ARG
1	A	386	ASP
1	B	92	LEU
1	B	298	LEU
1	B	308	GLN
1	B	390	PRO
1	B	407	GLN
1	C	92	LEU
1	C	108	ARG
1	C	245	ASN
1	C	279	LEU
1	D	92	LEU
1	D	94	LYS
1	D	297	VAL
1	D	342	ARG
1	D	390	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	HIS
1	A	245	ASN
1	A	302	ASN
1	A	308	GLN
1	A	321	ASN
1	A	407	GLN
1	B	245	ASN
1	B	250	GLN
1	B	258	GLN
1	B	321	ASN
1	B	407	GLN
1	C	245	ASN
1	C	321	ASN

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Mol	Chain	Res	Type
1	D	127	GLN
1	D	245	ASN
1	D	250	GLN
1	D	308	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 monosaccharides 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$
4	IBM	D	501	-	8,17,17	1.31	1 (12%)	10,25,25	2.54	3 (30%)
4	IBM	B	603	-	8,17,17	0.75	0	10,25,25	2.48	3 (30%)
4	IBM	C	603	-	8,17,17	0.68	0	10,25,25	2.66	3 (30%)
4	IBM	A	603	-	8,17,17	0.89	0	10,25,25	2.56	3 (30%)

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
4	IBM	D	501	-	-	2/4/4/4	0/2/2/2
4	IBM	B	603	-	-	2/4/4/4	0/2/2/2
4	IBM	C	603	-	-	2/4/4/4	0/2/2/2
4	IBM	A	603	-	-	0/4/4/4	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	501	IBM	C11-N3	-3.17	1.45	1.48

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	603	IBM	C4-C5-C6	-5.76	116.27	119.96
4	D	501	IBM	C4-C5-C6	-5.60	116.36	119.96
4	C	603	IBM	C4-C5-C6	-5.50	116.43	119.96
4	B	603	IBM	C4-C5-C6	-5.41	116.49	119.96
4	C	603	IBM	C11-N3-C4	5.32	123.17	118.41
4	D	501	IBM	C11-N3-C4	4.81	122.72	118.41
4	B	603	IBM	C11-N3-C4	4.67	122.59	118.41
4	A	603	IBM	C11-N3-C4	4.55	122.48	118.41
4	A	603	IBM	C5-C4-N9	-2.53	105.67	110.87
4	B	603	IBM	C5-C4-N9	-2.51	105.70	110.87
4	C	603	IBM	C5-C4-N9	-2.50	105.73	110.87
4	D	501	IBM	C5-C4-N9	-2.48	105.78	110.87

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	603	IBM	N3-C11-C12-C13
4	B	603	IBM	N3-C11-C12-C14
4	C	603	IBM	N3-C11-C12-C13
4	C	603	IBM	N3-C11-C12-C14
4	D	501	IBM	N3-C11-C12-C13
4	D	501	IBM	N3-C11-C12-C14

There are no ring outliers.

4 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	501	IBM	7	0
4	B	603	IBM	4	0
4	C	603	IBM	2	0
4	A	603	IBM	2	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, 95th 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 ²)	Q<0.9
1	A	334/334 (100%)	0.13	15 (4%) 33 38	15, 28, 63, 90	0
1	B	327/334 (97%)	0.03	4 (1%) 79 82	18, 31, 46, 97	0
1	C	330/334 (98%)	0.13	13 (3%) 39 45	17, 33, 73, 93	0
1	D	334/334 (100%)	0.02	11 (3%) 46 53	14, 27, 50, 84	0
All	All	1325/1336 (99%)	0.08	43 (3%) 47 54	14, 30, 60, 97	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	84	VAL	10.6
1	A	79	ILE	10.2
1	D	79	ILE	8.3
1	A	81	ARG	8.0
1	A	80	PRO	7.9
1	C	83	GLY	7.2
1	A	82	PHE	6.7
1	B	87	GLU	6.4
1	D	87	GLU	5.6
1	D	84	VAL	5.5
1	B	86	THR	5.1
1	B	88	GLN	4.9
1	C	85	LYS	4.8
1	D	86	THR	4.8
1	A	295	SER	4.6
1	C	412	GLN	4.5
1	A	84	VAL	4.4
1	A	294	SER	4.3
1	C	88	GLN	4.1
1	C	89	GLU	3.8
1	C	294	SER	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	412	GLN	3.5
1	D	85	LYS	3.4
1	A	411	PRO	3.3
1	D	80	PRO	3.1
1	C	86	THR	3.0
1	C	297	VAL	2.8
1	D	82	PHE	2.8
1	A	298	LEU	2.8
1	A	297	VAL	2.8
1	C	90	ASP	2.7
1	A	87	GLU	2.6
1	C	411	PRO	2.6
1	A	290	LYS	2.5
1	B	412	GLN	2.5
1	D	83	GLY	2.5
1	D	342	ARG	2.5
1	A	296	GLY	2.5
1	A	301	ASP	2.4
1	C	97	GLU	2.3
1	D	362	ASN	2.3
1	C	291	LYS	2.2
1	D	412	GLN	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 monosaccharides 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. The B-factors column lists the minimum, median, 95th 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	B-factors(Å ²)	Q<0.9
4	IBM	C	603	16/16	0.71	0.27	66,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	IBM	B	603	16/16	0.74	0.25	63,64,66,66	0
4	IBM	A	603	16/16	0.78	0.28	64,65,65,65	0
4	IBM	D	501	16/16	0.81	0.22	59,60,61,61	0
3	MG	B	602	1/1	0.82	0.20	44,44,44,44	0
3	MG	D	602	1/1	0.82	0.11	29,29,29,29	0
3	MG	C	602	1/1	0.93	0.12	35,35,35,35	0
3	MG	A	602	1/1	0.97	0.17	30,30,30,30	0
2	ZN	A	601	1/1	0.99	0.12	24,24,24,24	0
2	ZN	B	601	1/1	0.99	0.10	27,27,27,27	0
2	ZN	C	601	1/1	0.99	0.11	28,28,28,28	0
2	ZN	D	601	1/1	0.99	0.11	25,25,25,25	0

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

There are no such residues in this entry.