



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:47 AM UTC

PDB ID : 7L27 / pdb_00007L27
Title : Crystal structure of the catalytic domain of human PDE3A
Authors : Horner, S.W.; Garvie, C.
Deposited on : 2020-12-16
Resolution : 1.70 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

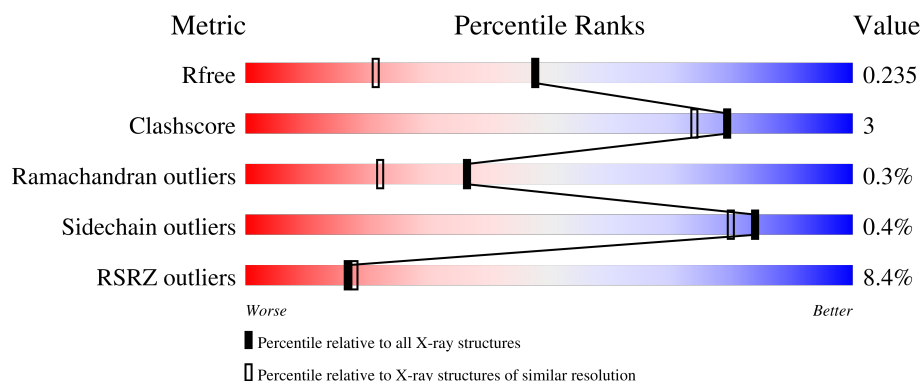
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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}	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	380	7% 90% 5% .
1	B	380	11% 91% 5% 5%
1	C	380	7% 91% 5% .
1	D	380	7% 92% 6% .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12424 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 cGMP-inhibited 3',5'-cyclic phosphodiesterase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	363	Total	C	N	O	S	0	1	0
			2935	1893	492	531	19			
1	B	362	Total	C	N	O	S	0	1	0
			2931	1892	491	529	19			
1	C	366	Total	C	N	O	S	0	0	0
			2949	1899	494	538	18			
1	D	370	Total	C	N	O	S	0	2	0
			2982	1920	500	543	19			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	668	GLY	-	expression tag	UNP Q14432
A	795	GLY	-	linker	UNP Q14432
A	796	GLY	-	linker	UNP Q14432
A	797	SER	-	linker	UNP Q14432
A	798	GLY	-	linker	UNP Q14432
A	799	GLY	-	linker	UNP Q14432
A	800	SER	-	linker	UNP Q14432
A	1062	GLY	-	linker	UNP Q14432
A	1063	GLY	-	linker	UNP Q14432
A	1064	SER	-	linker	UNP Q14432
A	1065	GLY	-	linker	UNP Q14432
A	1066	GLY	-	linker	UNP Q14432
A	1067	SER	-	linker	UNP Q14432
B	668	GLY	-	expression tag	UNP Q14432
B	795	GLY	-	linker	UNP Q14432
B	796	GLY	-	linker	UNP Q14432
B	797	SER	-	linker	UNP Q14432
B	798	GLY	-	linker	UNP Q14432
B	799	GLY	-	linker	UNP Q14432
B	800	SER	-	linker	UNP Q14432
B	1062	GLY	-	linker	UNP Q14432

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1063	GLY	-	linker	UNP Q14432
B	1064	SER	-	linker	UNP Q14432
B	1065	GLY	-	linker	UNP Q14432
B	1066	GLY	-	linker	UNP Q14432
B	1067	SER	-	linker	UNP Q14432
C	668	GLY	-	expression tag	UNP Q14432
C	795	GLY	-	linker	UNP Q14432
C	796	GLY	-	linker	UNP Q14432
C	797	SER	-	linker	UNP Q14432
C	798	GLY	-	linker	UNP Q14432
C	799	GLY	-	linker	UNP Q14432
C	800	SER	-	linker	UNP Q14432
C	1029	GLY	-	linker	UNP Q14432
C	1063	GLY	-	linker	UNP Q14432
C	1064	SER	-	linker	UNP Q14432
C	1065	GLY	-	linker	UNP Q14432
C	1066	GLY	-	linker	UNP Q14432
C	1067	SER	-	linker	UNP Q14432
D	668	GLY	-	expression tag	UNP Q14432
D	795	GLY	-	linker	UNP Q14432
D	796	GLY	-	linker	UNP Q14432
D	797	SER	-	linker	UNP Q14432
D	798	GLY	-	linker	UNP Q14432
D	799	GLY	-	linker	UNP Q14432
D	800	SER	-	linker	UNP Q14432
D	1062	GLY	-	linker	UNP Q14432
D	1063	GLY	-	linker	UNP Q14432
D	1064	SER	-	linker	UNP Q14432
D	1065	GLY	-	linker	UNP Q14432
D	1066	GLY	-	linker	UNP Q14432
D	1067	SER	-	linker	UNP Q14432

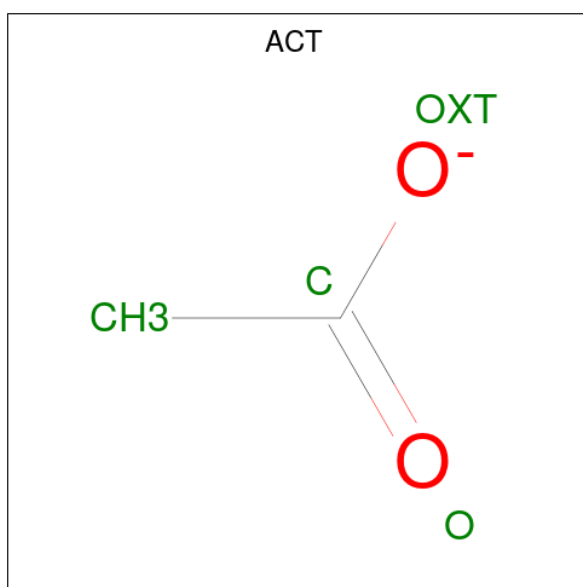
- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

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

- Molecule 3 is MAGNESIUM ION (CCD ID: 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 ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total	Ca	0	0
			1	1		

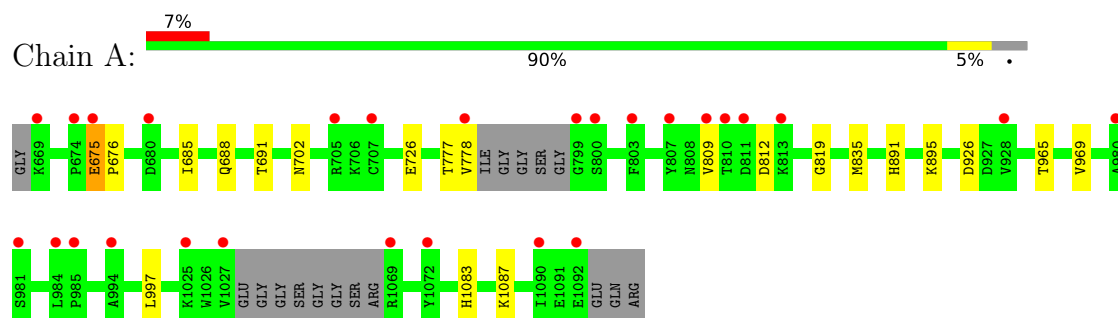
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	139	Total 139	O 139	0	0
6	B	101	Total 101	O 101	0	0
6	C	173	Total 173	O 173	0	0
6	D	189	Total 189	O 189	0	0

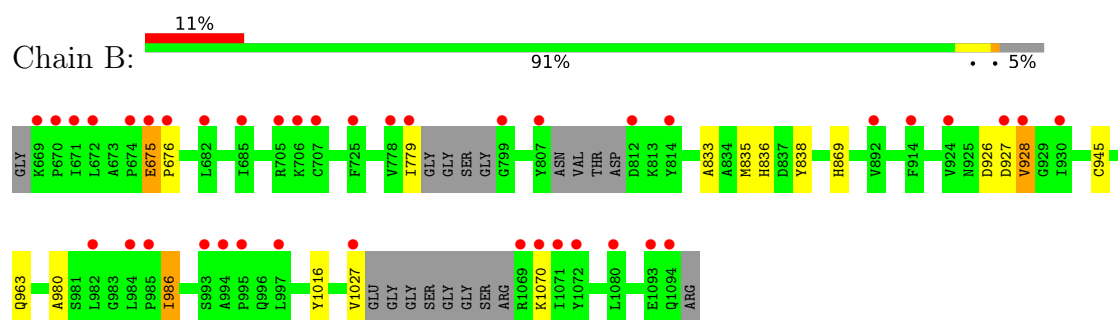
3 Residue-property plots [i](#)

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.

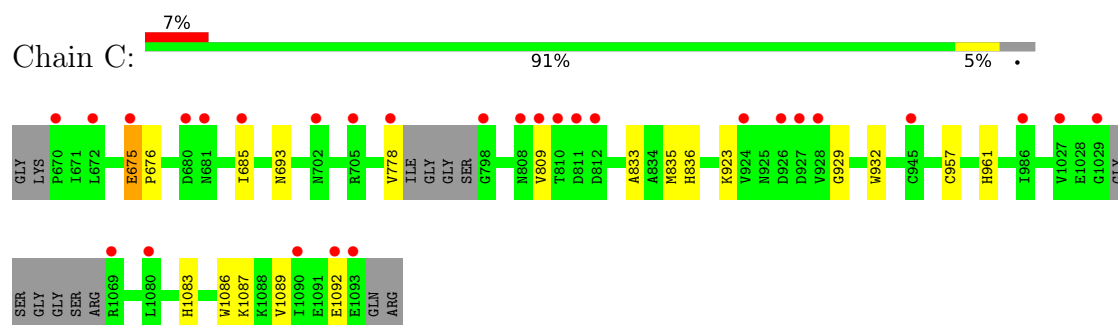
- Molecule 1: cGMP-inhibited 3',5'-cyclic phosphodiesterase A



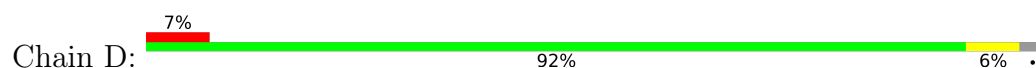
- Molecule 1: cGMP-inhibited 3',5'-cyclic phosphodiesterase A

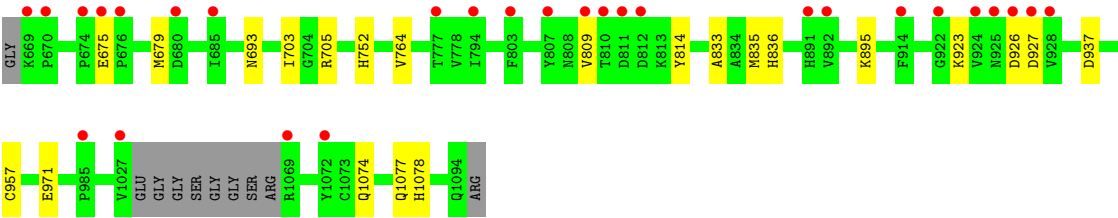


- Molecule 1: cGMP-inhibited 3',5'-cyclic phosphodiesterase A



- Molecule 1: cGMP-inhibited 3',5'-cyclic phosphodiesterase A





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.37Å 58.79Å 157.66Å 90.00° 90.69° 90.00°	Depositor
Resolution (Å)	47.85 – 1.70 47.85 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.2 (47.85-1.70) 99.1 (47.85-1.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.194 , 0.220 (Not available) , 0.235	Depositor DCC
R_{free} test set	8214 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	28.4	Xtriage
Anisotropy	0.355	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 36.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.017 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12424	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% 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: ACT, MN, MG, CA

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	0.67	0/3017	0.85	1/4097 (0.0%)
1	B	0.68	0/3012	0.84	1/4087 (0.0%)
1	C	0.71	0/3028	0.86	1/4111 (0.0%)
1	D	0.71	0/3068	0.86	3/4166 (0.1%)
All	All	0.69	0/12125	0.85	6/16461 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	835	MET	CB-CA-C	-6.41	99.73	110.56
1	A	835	MET	CB-CA-C	-5.88	100.27	110.09
1	D	705	ARG	N-CA-C	5.68	118.25	111.71
1	D	835	MET	CB-CA-C	-5.34	101.17	110.09
1	C	835	MET	CB-CA-C	-5.06	101.64	110.09
1	D	764	VAL	N-CA-CB	5.03	117.38	110.54

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	2935	0	2863	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2931	0	2861	18	0
1	C	2949	0	2864	17	0
1	D	2982	0	2908	12	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	4	0	3	0	0
4	B	4	0	3	0	0
4	C	4	0	3	0	0
4	D	4	0	3	0	0
5	C	1	0	0	0	0
6	A	139	0	0	0	0
6	B	101	0	0	2	0
6	C	173	0	0	1	0
6	D	189	0	0	2	0
All	All	12424	0	11508	64	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 3.

All (64) 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:C:961:HIS:HE1	1:C:1086:TRP:HE1	1.12	0.96
1:B:675:GLU:HB3	1:B:676:PRO:CD	1.97	0.95
1:B:675:GLU:HB3	1:B:676:PRO:HD2	1.51	0.93
1:A:675:GLU:HB3	1:A:676:PRO:CD	2.01	0.91
1:A:675:GLU:HB3	1:A:676:PRO:HD2	1.52	0.88
1:C:675:GLU:HB2	1:C:676:PRO:CD	2.09	0.82
1:C:961:HIS:CE1	1:C:1086:TRP:HE1	1.99	0.80
1:C:675:GLU:HB2	1:C:676:PRO:HD2	1.64	0.78
1:D:752:HIS:HD2	1:D:971:GLU:OE2	1.67	0.78
1:B:980:ALA:HB2	1:B:986:ILE:HD11	1.70	0.73
1:A:965:THR:CG2	1:A:997:LEU:HD12	2.19	0.72
1:A:675:GLU:CB	1:A:676:PRO:HD2	2.21	0.68
1:C:675:GLU:CB	1:C:676:PRO:HD2	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:777:THR:HG23	1:A:819:GLY:HA3	1.77	0.67
1:C:778:VAL:HG11	1:C:932:TRP:HB2	1.75	0.67
1:B:675:GLU:CB	1:B:676:PRO:HD2	2.23	0.66
1:C:675:GLU:CB	1:C:676:PRO:CD	2.74	0.65
1:A:675:GLU:CB	1:A:676:PRO:CD	2.73	0.64
1:B:675:GLU:CB	1:B:676:PRO:CD	2.73	0.62
1:A:969:VAL:HG11	1:A:997:LEU:HD13	1.81	0.62
1:D:923:LYS:NZ	1:D:937:ASP:OD1	2.32	0.61
1:B:833:ALA:O	1:B:836:HIS:HD2	1.83	0.60
1:C:675:GLU:CG	1:C:676:PRO:HD2	2.31	0.60
1:C:833:ALA:O	1:C:836:HIS:HD2	1.84	0.60
1:A:778:VAL:HG12	1:A:819:GLY:O	2.02	0.60
1:D:833:ALA:O	1:D:836:HIS:HD2	1.84	0.59
1:B:869:HIS:HE1	6:B:1287:HOH:O	1.85	0.59
1:C:693:ASN:ND2	1:C:957:CYS:H	2.03	0.57
1:D:693:ASN:ND2	1:D:957:CYS:H	2.03	0.57
1:D:895:LYS:HE2	6:D:1302:HOH:O	2.06	0.56
1:D:1074:GLN:HE21	1:D:1078:HIS:HE1	1.54	0.56
1:A:965:THR:HG22	1:A:997:LEU:HD12	1.87	0.55
1:B:963:GLN:NE2	6:B:1203:HOH:O	2.41	0.54
1:B:838:TYR:O	1:B:869:HIS:HD2	1.91	0.53
1:C:693:ASN:HD21	1:C:957:CYS:H	1.57	0.53
1:C:675:GLU:HG3	1:C:676:PRO:HD2	1.91	0.52
1:C:1089:VAL:O	1:C:1092:GLU:HG3	2.09	0.52
1:D:693:ASN:HD21	1:D:957:CYS:H	1.58	0.51
1:A:688:GLN:O	1:A:691:THR:HG22	2.09	0.51
1:B:927:ASP:O	1:B:928:VAL:HB	2.13	0.49
1:D:926:ASP:O	1:D:927:ASP:OD1	2.31	0.48
1:B:779:ILE:HD12	1:B:779:ILE:N	2.29	0.48
1:A:969:VAL:HG11	1:A:997:LEU:CD1	2.45	0.47
1:A:685:ILE:HD12	1:A:702:ASN:ND2	2.30	0.47
1:D:809:VAL:HG11	1:D:814:TYR:HB2	1.97	0.47
1:B:945[B]:CYS:HG	1:B:1016:TYR:HH	1.61	0.46
1:C:923:LYS:O	1:C:929:GLY:HA2	2.16	0.45
1:B:1027:VAL:HG22	1:B:1070:LYS:O	2.15	0.45
1:A:726:GLU:H	1:A:726:GLU:CD	2.25	0.45
1:D:1074:GLN:HE21	1:D:1078:HIS:CE1	2.33	0.44
1:B:779:ILE:N	1:B:779:ILE:CD1	2.81	0.43
1:D:679:MET:HE1	1:D:703:ILE:HG13	1.99	0.43
1:A:777:THR:HG22	1:A:778:VAL:C	2.44	0.43
1:A:1083:HIS:CE1	1:A:1087:LYS:HE3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:675:GLU:HB3	1:B:676:PRO:HD3	1.92	0.42
1:B:980:ALA:HB2	1:B:986:ILE:CD1	2.46	0.42
1:A:891:HIS:CE1	1:A:895:LYS:HE2	2.55	0.42
1:C:961:HIS:HD2	6:C:1353:HOH:O	2.03	0.42
1:D:1077:GLN:NE2	6:D:1206:HOH:O	2.53	0.42
1:A:926:ASP:OD1	1:A:926:ASP:C	2.64	0.41
1:C:675:GLU:HB2	1:C:676:PRO:HD3	1.99	0.40
1:B:1027:VAL:HG21	1:B:1070:LYS:HB2	2.02	0.40
1:B:926:ASP:C	1:B:926:ASP:OD1	2.65	0.40
1:C:1083:HIS:CE1	1:C:1087:LYS:HE3	2.57	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	358/380 (94%)	351 (98%)	5 (1%)	2 (1%)	21	9
1	B	355/380 (93%)	347 (98%)	6 (2%)	2 (1%)	21	9
1	C	360/380 (95%)	353 (98%)	6 (2%)	1 (0%)	36	22
1	D	368/380 (97%)	359 (98%)	9 (2%)	0	100	100
All	All	1441/1520 (95%)	1410 (98%)	26 (2%)	5 (0%)	36	22

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	675	GLU
1	B	675	GLU
1	B	928	VAL
1	C	675	GLU
1	A	812	ASP

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	319/327 (98%)	318 (100%)	1 (0%)	86	83
1	B	318/327 (97%)	317 (100%)	1 (0%)	86	83
1	C	319/327 (98%)	317 (99%)	2 (1%)	78	72
1	D	324/327 (99%)	323 (100%)	1 (0%)	86	83
All	All	1280/1308 (98%)	1275 (100%)	5 (0%)	84	80

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	809	VAL
1	B	986	ILE
1	C	685	ILE
1	C	809	VAL
1	D	675	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	855	GLN
1	A	867	ASN
1	A	891	HIS
1	A	952	ASN
1	A	999	ASN
1	A	1001	GLN
1	A	1074	GLN
1	B	836	HIS
1	B	869	HIS
1	B	888	ASN
1	B	891	HIS
1	B	963	GLN
1	B	996	GLN
1	B	999	ASN

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Mol	Chain	Res	Type
1	C	770	GLN
1	C	836	HIS
1	C	855	GLN
1	C	867	ASN
1	C	888	ASN
1	C	961	HIS
1	C	963	GLN
1	C	999	ASN
1	D	693	ASN
1	D	752	HIS
1	D	770	GLN
1	D	836	HIS
1	D	867	ASN
1	D	888	ASN
1	D	963	GLN
1	D	999	ASN
1	D	1078	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 9 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	ACT	D	1103	-	3,3,3	1.05	0	3,3,3	0.84	0
4	ACT	C	1104	-	3,3,3	0.95	0	3,3,3	0.97	0
4	ACT	B	1103	-	3,3,3	1.04	0	3,3,3	0.83	0
4	ACT	A	1103	-	3,3,3	1.03	0	3,3,3	0.85	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	363/380 (95%)	0.57	27 (7%)	20	22	18, 38, 65, 97	1 (0%)
1	B	362/380 (95%)	0.78	40 (11%)	10	10	19, 41, 73, 109	1 (0%)
1	C	366/380 (96%)	0.51	28 (7%)	19	21	19, 34, 64, 88	0
1	D	370/380 (97%)	0.44	28 (7%)	20	21	16, 32, 63, 122	2 (0%)
All	All	1461/1520 (96%)	0.58	123 (8%)	17	18	16, 36, 68, 122	4 (0%)

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	676	PRO	7.3
1	B	928	VAL	6.9
1	C	778	VAL	5.9
1	D	809	VAL	5.7
1	C	809	VAL	5.5
1	D	675	GLU	5.2
1	B	779	ILE	4.8
1	A	1027	VAL	4.7
1	C	670	PRO	4.5
1	D	928	VAL	4.4
1	C	798	GLY	4.4
1	B	812	ASP	4.2
1	A	809	VAL	4.1
1	D	927	ASP	4.1
1	C	810	THR	4.1
1	A	778	VAL	4.1
1	B	1027	VAL	4.0
1	C	675	GLU	3.8
1	A	807	TYR	3.8
1	D	810	THR	3.8
1	A	803	PHE	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	1094	GLN	3.7
1	B	994	ALA	3.5
1	A	810	THR	3.5
1	B	707	CYS	3.4
1	C	812	ASP	3.4
1	B	930	ILE	3.3
1	B	997	LEU	3.3
1	D	922	GLY	3.3
1	B	669	LYS	3.3
1	C	945	CYS	3.3
1	B	670	PRO	3.2
1	A	705	ARG	3.2
1	A	799	GLY	3.2
1	D	794	ILE	3.1
1	A	675	GLU	3.1
1	B	778	VAL	3.1
1	C	1029	GLY	3.1
1	A	707	CYS	3.1
1	D	803	PHE	3.1
1	D	1072	TYR	3.0
1	C	1093	GLU	3.0
1	B	676	PRO	3.0
1	B	993	SER	2.9
1	A	669	LYS	2.9
1	D	924	VAL	2.9
1	B	807	TYR	2.9
1	B	984	LEU	2.9
1	B	685	ILE	2.9
1	C	811	ASP	2.8
1	C	1090	ILE	2.8
1	A	985	PRO	2.8
1	A	1092	GLU	2.8
1	C	1080	LEU	2.8
1	D	669	LYS	2.8
1	D	807	TYR	2.7
1	C	986	ILE	2.7
1	B	1072	TYR	2.7
1	A	980	ALA	2.7
1	B	671	ILE	2.7
1	C	927	ASP	2.7
1	B	674	PRO	2.6
1	D	925	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	1069	ARG	2.6
1	A	800	SER	2.6
1	C	1092	GLU	2.6
1	D	674	PRO	2.6
1	A	1069	ARG	2.6
1	B	927	ASP	2.5
1	C	1027	VAL	2.5
1	D	680	ASP	2.5
1	B	675	GLU	2.5
1	D	1027	VAL	2.5
1	B	672	LEU	2.4
1	C	926	ASP	2.4
1	C	1069	ARG	2.4
1	D	914	PHE	2.4
1	C	808	ASN	2.4
1	D	685	ILE	2.4
1	D	811	ASP	2.4
1	A	928	VAL	2.4
1	C	702	ASN	2.3
1	B	1080	LEU	2.3
1	D	891	HIS	2.3
1	B	995	PRO	2.3
1	B	682	LEU	2.3
1	B	706	LYS	2.3
1	D	812	ASP	2.3
1	A	994	ALA	2.3
1	A	984	LEU	2.3
1	C	705	ARG	2.3
1	B	799	GLY	2.3
1	C	685	ILE	2.3
1	B	892	VAL	2.2
1	B	924	VAL	2.2
1	A	674	PRO	2.2
1	D	670	PRO	2.2
1	A	813	LYS	2.2
1	A	811	ASP	2.2
1	C	680	ASP	2.2
1	D	926	ASP	2.2
1	B	1071	ILE	2.2
1	C	924	VAL	2.2
1	B	1093	GLU	2.2
1	B	982	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	672	LEU	2.2
1	A	1025	LYS	2.2
1	B	814	TYR	2.2
1	B	705	ARG	2.1
1	B	1070	LYS	2.1
1	B	725	PHE	2.1
1	D	1069	ARG	2.1
1	A	981	SER	2.1
1	D	777	THR	2.1
1	B	914	PHE	2.1
1	A	1072	TYR	2.1
1	A	1090	ILE	2.1
1	C	681	ASN	2.1
1	B	985	PRO	2.1
1	D	985	PRO	2.0
1	A	680	ASP	2.0
1	C	928	VAL	2.0
1	D	892	VAL	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
4	ACT	B	1103	4/4	0.83	0.20	46,59,69,70	0
4	ACT	C	1104	4/4	0.90	0.10	36,38,42,44	0
4	ACT	A	1103	4/4	0.92	0.10	38,39,42,43	0
4	ACT	D	1103	4/4	0.94	0.10	23,25,26,30	0
2	MN	B	1101	1/1	0.96	0.05	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	B	1102	1/1	0.97	0.05	20,20,20,20	0
3	MG	D	1102	1/1	0.97	0.05	15,15,15,15	0
5	CA	C	1103	1/1	0.97	0.07	46,46,46,46	0
2	MN	C	1101	1/1	0.98	0.05	26,26,26,26	0
3	MG	C	1102	1/1	0.98	0.04	19,19,19,19	0
2	MN	D	1101	1/1	0.98	0.03	21,21,21,21	0
3	MG	A	1102	1/1	0.98	0.07	18,18,18,18	0
2	MN	A	1101	1/1	0.99	0.04	24,24,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.