



Full wwPDB X-ray Structure Validation Report ⓘ

May 31, 2022 – 06:33 pm BST

PDB ID : 7QJK
Title : Crystal structure of PDE6D in complex with Compound-2
Authors : Yelland, T.; Ismail, S.
Deposited on : 2021-12-16
Resolution : 3.10 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.28.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0267
CCP4 : 7.1.010 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.28.1

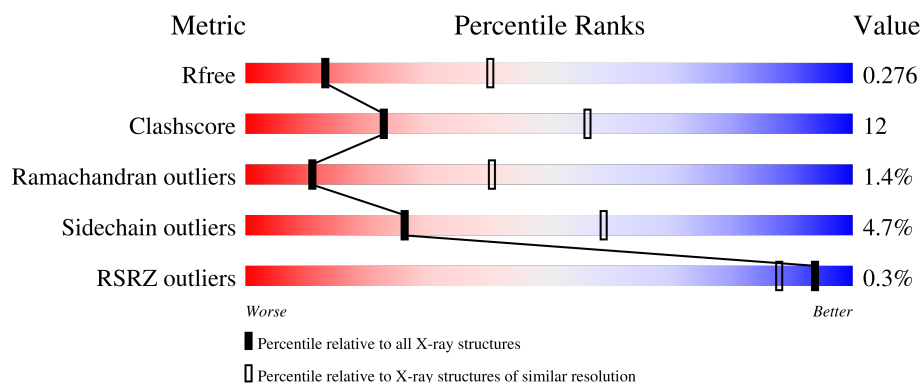
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION





The reported resolution of this entry is 3.10 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))
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	AAA	151	 76% 19% . .
1	BBB	151	 81% 14% . .
1	CCC	151	 77% 17% . .
1	DDD	151	 62% 26% 5% 7%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4799 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 Retinal rod rhodopsin-sensitive cGMP 3',5'-cyclic phosphodiesterase subunit delta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	BBB	145	Total	C	N	O	S	0	0	0
			1178	756	198	218	6			
1	AAA	148	Total	C	N	O	S	0	0	0
			1202	772	201	222	7			
1	CCC	146	Total	C	N	O	S	0	1	0
			1180	757	194	222	7			
1	DDD	141	Total	C	N	O	S	0	1	0
			1134	730	186	212	6			

There are 4 discrepancies between the modelled and reference sequences:

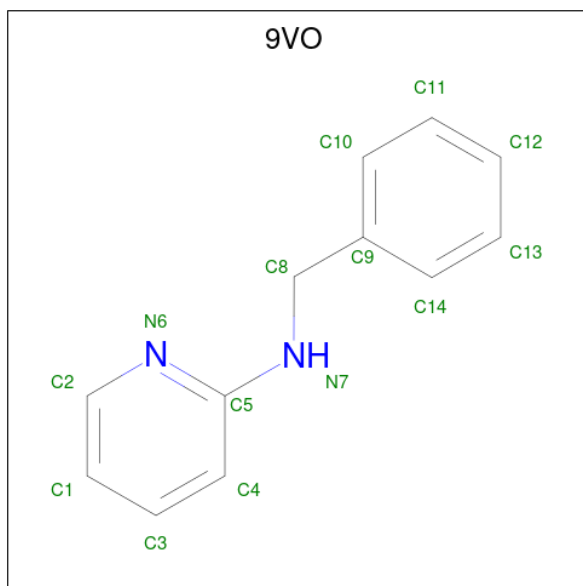
Chain	Residue	Modelled	Actual	Comment	Reference
BBB	0	ALA	-	expression tag	UNP O43924
AAA	0	ALA	-	expression tag	UNP O43924
CCC	0	ALA	-	expression tag	UNP O43924
DDD	0	ALA	-	expression tag	UNP O43924

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	BBB	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is N-(phenylmethyl)pyridin-2-amine (three-letter code: 9VO) (formula: $C_{12}H_{12}N_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	BBB	1	Total	C	N	0	0
			14	12	2		
3	AAA	1	Total	C	N	0	0
			14	12	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	AAA	1	Total	C	N	0	0
			14	12	2		
3	CCC	1	Total	C	N	0	0
			14	12	2		
3	DDD	1	Total	C	N	0	0
			14	12	2		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	BBB	1	Total	O	S	0	0
			5	4	1		


- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	BBB	7	Total	O	0	0
			7	7		
5	AAA	5	Total	O	0	0
			5	5		
5	CCC	10	Total	O	0	0
			10	10		
5	DDD	4	Total	O	0	0
			4	4		

3 Residue-property plots


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.

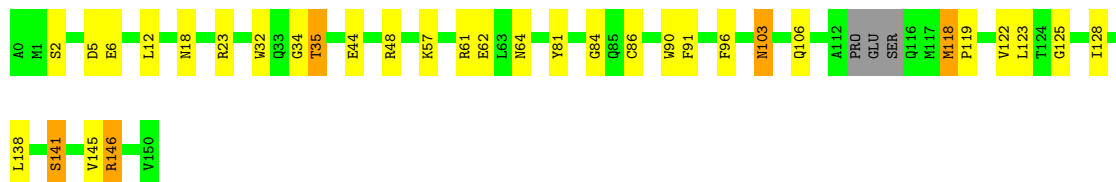
- Molecule 1: Retinal rod rhodopsin-sensitive cGMP 3',5'-cyclic phosphodiesterase subunit delta

Chain BBB: 




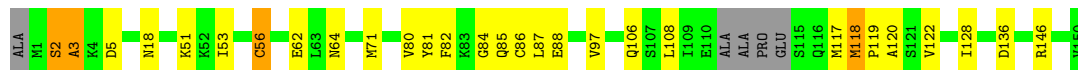
- Molecule 1: Retinal rod rhodopsin-sensitive cGMP 3',5'-cyclic phosphodiesterase subunit delta

Chain AAA: 



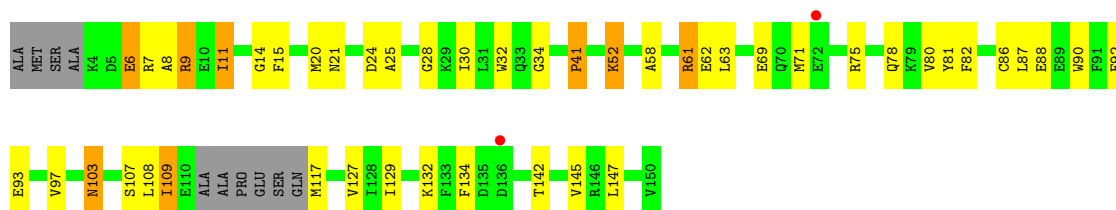
- Molecule 1: Retinal rod rhodopsin-sensitive cGMP 3',5'-cyclic phosphodiesterase subunit delta

Chain CCC: 



- Molecule 1: Retinal rod rhodopsin-sensitive cGMP 3',5'-cyclic phosphodiesterase subunit delta

Chain DDD: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	76.55Å 76.55Å 238.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	64.46 – 3.10 64.38 – 3.10	Depositor EDS
% Data completeness (in resolution range)	88.8 (64.46-3.10) 88.8 (64.38-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 3.13Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.246 , 0.283 0.245 , 0.276	Depositor DCC
R_{free} test set	625 reflections (5.17%)	wwPDB-VP
Wilson B-factor (Å ²)	69.3	Xtriage
Anisotropy	0.168	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	4799	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.89% 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: SO4, 9VO, EDO

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	AAA	0.64	0/1226	0.68	0/1650
1	BBB	0.63	0/1202	0.67	0/1620
1	CCC	0.64	0/1204	0.67	0/1625
1	DDD	0.65	0/1157	0.67	0/1563
All	All	0.64	0/4789	0.67	0/6458

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	AAA	1202	0	1197	31	0
1	BBB	1178	0	1161	14	0
1	CCC	1180	0	1144	23	0
1	DDD	1134	0	1098	45	0
2	BBB	4	0	6	0	0
3	AAA	28	0	0	0	0
3	BBB	14	0	0	0	0
3	CCC	14	0	0	0	0
3	DDD	14	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	BBB	5	0	0	0	0
5	AAA	5	0	0	1	0
5	BBB	7	0	0	0	0
5	CCC	10	0	0	0	0
5	DDD	4	0	0	0	0
All	All	4799	0	4606	108	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 12.

All (108) 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:AAA:118:MET:HB2	1:AAA:119:PRO:HD2	1.45	0.96
1:AAA:119:PRO:HG2	1:AAA:122:VAL:HG23	1.55	0.86
1:DDD:75:ARG:HB2	1:DDD:92:PHE:O	1.83	0.79
1:DDD:11:ILE:HD12	1:DDD:69:GLU:HG3	1.65	0.76
1:CCC:62:GLU:HG2	1:CCC:106:GLN:HG3	1.68	0.76
1:AAA:119:PRO:CG	1:AAA:122:VAL:HG23	2.17	0.74
1:AAA:118:MET:HB2	1:AAA:119:PRO:CD	2.18	0.74
1:DDD:127:VAL:HG13	1:DDD:147:LEU:HB2	1.68	0.74
1:DDD:20:MET:HE3	1:DDD:32:TRP:HZ3	1.56	0.71
1:DDD:11:ILE:O	1:DDD:15:PHE:N	2.25	0.69
1:DDD:61[B]:ARG:NH2	1:DDD:107:SER:HB2	2.06	0.69
1:AAA:119:PRO:HG2	1:AAA:122:VAL:CG2	2.23	0.69
1:DDD:11:ILE:CD1	1:DDD:69:GLU:HG3	2.23	0.68
1:DDD:92:PHE:HZ	1:DDD:109:ILE:HG22	1.58	0.68
1:DDD:25:ALA:HB3	1:DDD:58:ALA:HB1	1.76	0.67
1:DDD:11:ILE:HD12	1:DDD:69:GLU:CG	2.26	0.65
1:DDD:11:ILE:HD12	1:DDD:69:GLU:CB	2.26	0.65
1:AAA:118:MET:HG3	1:AAA:123:LEU:HD21	1.80	0.64
1:DDD:7:ARG:O	1:DDD:9:ARG:N	2.31	0.63
1:CCC:2:SER:HA	1:CCC:5:ASP:HB2	1.79	0.63
1:DDD:61[B]:ARG:HG2	1:DDD:61[B]:ARG:O	1.98	0.63
1:AAA:34:GLY:O	1:AAA:35:THR:OG1	2.16	0.61
1:DDD:20:MET:HE3	1:DDD:32:TRP:CZ3	2.35	0.61
1:CCC:85:GLN:O	1:CCC:87:LEU:HD12	2.01	0.60
1:BBB:45:HIS:HB2	1:BBB:145:VAL:HG22	1.83	0.60
1:AAA:118:MET:CG	1:AAA:123:LEU:HD21	2.32	0.59
1:DDD:11:ILE:N	1:DDD:11:ILE:HD13	2.17	0.59
1:BBB:1:MET:CB	1:BBB:6:GLU:OE2	2.52	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:127:VAL:HG13	1:BBB:147:LEU:HB2	1.84	0.58
1:DDD:11:ILE:O	1:DDD:14:GLY:N	2.37	0.58
1:AAA:119:PRO:CG	1:AAA:122:VAL:CG2	2.82	0.56
1:DDD:92:PHE:HZ	1:DDD:109:ILE:CG2	2.18	0.56
1:CCC:2:SER:O	1:CCC:3:ALA:HB3	2.06	0.56
1:CCC:53:ILE:O	1:CCC:56:CYS:SG	2.65	0.55
1:DDD:71:MET:HB2	1:DDD:97:VAL:HG22	1.88	0.54
1:DDD:61[A]:ARG:HD2	1:DDD:63:LEU:HD11	1.89	0.54
1:DDD:92:PHE:CZ	1:DDD:109:ILE:CG2	2.91	0.54
1:BBB:82:PHE:HB3	1:BBB:87:LEU:HD11	1.90	0.53
1:AAA:57:LYS:N	1:AAA:57:LYS:HD3	2.24	0.52
1:CCC:82:PHE:HB3	1:CCC:87:LEU:CD1	2.40	0.51
1:DDD:61[B]:ARG:NE	1:DDD:63:LEU:HD11	2.26	0.51
1:CCC:119:PRO:O	1:CCC:122:VAL:HG12	2.10	0.51
1:CCC:82:PHE:HB3	1:CCC:87:LEU:HD11	1.93	0.51
1:DDD:21:ASN:HB2	1:DDD:62:GLU:HB2	1.92	0.50
1:AAA:91:PHE:CE1	1:CCC:84:GLY:HA2	2.47	0.50
1:DDD:82:PHE:HB3	1:DDD:87:LEU:HD23	1.94	0.50
1:CCC:128:ILE:HD11	1:CCC:146:ARG:CZ	2.41	0.50
1:BBB:40:VAL:HG22	1:BBB:45:HIS:NE2	2.28	0.49
1:AAA:61:ARG:NH1	5:AAA:301:HOH:O	2.45	0.49
1:DDD:80:VAL:HB	1:DDD:88:GLU:HB2	1.93	0.49
1:DDD:25:ALA:HB3	1:DDD:58:ALA:CB	2.41	0.49
1:DDD:92:PHE:CZ	1:DDD:109:ILE:HG22	2.45	0.48
1:DDD:61[B]:ARG:CZ	1:DDD:63:LEU:HD11	2.44	0.47
1:DDD:30:ILE:HG13	1:DDD:30:ILE:O	2.14	0.47
1:DDD:90:TRP:HB3	1:DDD:92:PHE:CE2	2.49	0.47
1:DDD:132:LYS:HB3	1:DDD:134:PHE:CE2	2.50	0.47
1:DDD:61[B]:ARG:HH22	1:DDD:107:SER:CB	2.28	0.47
1:AAA:18:ASN:ND2	1:AAA:64:ASN:OD1	2.44	0.47
1:CCC:51:LYS:HG3	1:CCC:120:ALA:CB	2.45	0.47
1:DDD:61[B]:ARG:HH22	1:DDD:107:SER:HB2	1.77	0.47
1:AAA:118:MET:HG3	1:AAA:123:LEU:CD2	2.45	0.46
1:CCC:108:LEU:HD12	1:CCC:108:LEU:HA	1.81	0.46
1:BBB:19:TRP:CE2	1:BBB:64:ASN:HB2	2.52	0.45
1:CCC:2:SER:O	1:CCC:3:ALA:CB	2.64	0.45
1:CCC:108:LEU:N	1:DDD:93:GLU:OE1	2.43	0.45
1:BBB:40:VAL:HG22	1:BBB:45:HIS:CE1	2.51	0.45
1:AAA:125:GLY:O	1:AAA:146:ARG:NH2	2.50	0.45
1:BBB:91:PHE:CE2	1:AAA:84:GLY:HA2	2.52	0.45
1:DDD:52:LYS:HA	1:DDD:52:LYS:HD2	1.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:23:ARG:NE	1:AAA:62:GLU:OE1	2.50	0.44
1:CCC:18:ASN:ND2	1:CCC:64:ASN:OD1	2.47	0.44
1:DDD:81:TYR:CE1	1:DDD:86:CYS:HB2	2.53	0.44
1:AAA:2:SER:O	1:AAA:6:GLU:HG2	2.17	0.44
1:CCC:71:MET:HE3	1:CCC:97:VAL:HG21	1.98	0.44
1:DDD:129:ILE:HB	1:DDD:145:VAL:HG12	1.98	0.44
1:DDD:11:ILE:HG23	1:DDD:69:GLU:HB2	2.00	0.44
1:AAA:57:LYS:HD3	1:AAA:57:LYS:H	1.82	0.44
1:AAA:128:ILE:HA	1:AAA:145:VAL:O	2.18	0.43
1:AAA:57:LYS:H	1:AAA:57:LYS:CD	2.32	0.43
1:DDD:103:ASN:N	1:DDD:103:ASN:OD1	2.51	0.43
1:CCC:71:MET:HB2	1:CCC:97:VAL:HB	1.99	0.43
1:BBB:82:PHE:CB	1:BBB:87:LEU:HD11	2.47	0.43
1:AAA:2:SER:HB3	1:AAA:5:ASP:CG	2.39	0.43
1:CCC:81:TYR:CE1	1:CCC:86:CYS:HB2	2.53	0.43
1:AAA:103:ASN:N	1:AAA:103:ASN:OD1	2.52	0.43
1:BBB:91:PHE:CD2	1:AAA:84:GLY:HA2	2.54	0.42
1:DDD:20:MET:HE3	1:DDD:20:MET:HB3	1.90	0.42
1:BBB:71:MET:HB2	1:BBB:97:VAL:HB	2.01	0.42
1:AAA:32:TRP:CH2	1:AAA:34:GLY:HA2	2.55	0.42
1:AAA:106:GLN:O	1:AAA:106:GLN:HG3	2.19	0.42
1:CCC:118:MET:CB	1:CCC:119:PRO:HD2	2.50	0.42
1:CCC:80:VAL:O	1:CCC:80:VAL:CG2	2.68	0.42
1:DDD:41:PRO:HB3	1:DDD:142:THR:O	2.18	0.42
1:BBB:21:ASN:HD22	1:BBB:21:ASN:C	2.23	0.42
1:DDD:32:TRP:CH2	1:DDD:34:GLY:HA3	2.55	0.42
1:BBB:20:MET:HG2	1:BBB:21:ASN:N	2.34	0.41
1:AAA:119:PRO:HG3	1:AAA:122:VAL:HG23	2.00	0.41
1:AAA:44:GLU:OE1	1:AAA:146:ARG:HG3	2.19	0.41
1:CCC:80:VAL:HG22	1:CCC:88:GLU:HB2	2.03	0.41
1:CCC:117:MET:HA	1:CCC:117:MET:CE	2.51	0.41
1:BBB:26:GLU:H	1:BBB:26:GLU:HG2	1.74	0.41
1:AAA:81:TYR:CE1	1:AAA:86:CYS:HB2	2.56	0.40
1:DDD:61[A]:ARG:HH12	1:DDD:78:GLN:HE22	1.68	0.40
1:DDD:11:ILE:HD13	1:DDD:11:ILE:H	1.84	0.40
1:AAA:12:LEU:HD13	1:AAA:141:SER:HB3	2.03	0.40
1:DDD:24:ASP:O	1:DDD:28:GLY:N	2.52	0.40
1:AAA:90:TRP:CZ3	1:CCC:85:GLN:HB2	2.57	0.40
1:DDD:108:LEU:N	1:DDD:108:LEU:HD23	2.35	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	AAA	144/151 (95%)	135 (94%)	8 (6%)	1 (1%)	22	57
1	BBB	141/151 (93%)	136 (96%)	5 (4%)	0	100	100
1	CCC	143/151 (95%)	136 (95%)	4 (3%)	3 (2%)	7	30
1	DDD	138/151 (91%)	128 (93%)	6 (4%)	4 (3%)	4	24
All	All	566/604 (94%)	535 (94%)	23 (4%)	8 (1%)	11	40

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	CCC	3	ALA
1	DDD	8	ALA
1	CCC	2	SER
1	AAA	35	THR
1	DDD	6	GLU
1	DDD	9	ARG
1	CCC	136	ASP
1	DDD	41	PRO

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	AAA	131/135 (97%)	124 (95%)	7 (5%)	22	54
1	BBB	128/135 (95%)	120 (94%)	8 (6%)	18	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	CCC	128/135 (95%)	126 (98%)	2 (2%)	62	84
1	DDD	122/135 (90%)	114 (93%)	8 (7%)	16	47
All	All	509/540 (94%)	484 (95%)	25 (5%)	26	57

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	BBB	21	ASN
1	BBB	38	LEU
1	BBB	49	VAL
1	BBB	75	ARG
1	BBB	91	PHE
1	BBB	103	ASN
1	BBB	104	THR
1	BBB	141	SER
1	AAA	48	ARG
1	AAA	96	PHE
1	AAA	103	ASN
1	AAA	118	MET
1	AAA	138	LEU
1	AAA	141	SER
1	AAA	146	ARG
1	CCC	56	CYS
1	CCC	118	MET
1	DDD	6	GLU
1	DDD	11	ILE
1	DDD	52	LYS
1	DDD	61[A]	ARG
1	DDD	61[B]	ARG
1	DDD	103	ASN
1	DDD	109	ILE
1	DDD	117	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

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](#)

7 ligands are modelled in this entry.

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	9VO	CCC	201	-	15,15,15	1.83	3 (20%)	18,18,18	1.12	1 (5%)
3	9VO	AAA	202	-	15,15,15	1.80	3 (20%)	18,18,18	1.16	3 (16%)
2	EDO	BBB	201	-	3,3,3	0.06	0	2,2,2	0.17	0
3	9VO	BBB	202	-	15,15,15	1.67	2 (13%)	18,18,18	1.10	2 (11%)
3	9VO	AAA	201	-	15,15,15	1.73	3 (20%)	18,18,18	1.15	2 (11%)
4	SO4	BBB	203	-	4,4,4	0.40	0	6,6,6	0.05	0
3	9VO	DDD	201	-	15,15,15	1.69	2 (13%)	18,18,18	1.11	2 (11%)

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	9VO	CCC	201	-	-	2/5/5/5	0/2/2/2
3	9VO	AAA	202	-	-	0/5/5/5	0/2/2/2
2	EDO	BBB	201	-	-	0/1/1/1	-
3	9VO	BBB	202	-	-	3/5/5/5	0/2/2/2
3	9VO	AAA	201	-	-	2/5/5/5	0/2/2/2
3	9VO	DDD	201	-	-	0/5/5/5	0/2/2/2

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	CCC	201	9VO	C8-C9	-5.99	1.38	1.51
3	AAA	202	9VO	C8-C9	-5.73	1.39	1.51
3	DDD	201	9VO	C8-C9	-5.63	1.39	1.51
3	AAA	201	9VO	C8-C9	-5.61	1.39	1.51
3	BBB	202	9VO	C8-C9	-5.31	1.39	1.51
3	BBB	202	9VO	C2-N6	2.84	1.40	1.34
3	AAA	202	9VO	C2-N6	2.77	1.40	1.34
3	DDD	201	9VO	C2-N6	2.59	1.40	1.34
3	AAA	201	9VO	C2-N6	2.55	1.40	1.34
3	CCC	201	9VO	C2-N6	2.54	1.40	1.34
3	AAA	202	9VO	C5-N7	-2.42	1.32	1.36
3	CCC	201	9VO	C5-N7	-2.40	1.32	1.36
3	AAA	201	9VO	C5-N7	-2.18	1.33	1.36

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	DDD	201	9VO	C2-N6-C5	2.58	120.87	117.22
3	AAA	201	9VO	N7-C5-N6	2.37	120.53	116.95
3	AAA	202	9VO	N7-C5-N6	2.27	120.38	116.95
3	DDD	201	9VO	C1-C2-N6	-2.25	119.75	123.43
3	AAA	202	9VO	C2-N6-C5	2.18	120.32	117.22
3	AAA	202	9VO	C1-C2-N6	-2.15	119.91	123.43
3	CCC	201	9VO	C1-C2-N6	-2.13	119.94	123.43
3	BBB	202	9VO	C1-C2-N6	-2.12	119.97	123.43
3	AAA	201	9VO	C1-C2-N6	-2.07	120.05	123.43
3	BBB	202	9VO	C2-N6-C5	2.06	120.14	117.22

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	BBB	202	9VO	C4-C5-N7-C8
3	BBB	202	9VO	N6-C5-N7-C8
3	AAA	201	9VO	C4-C5-N7-C8
3	AAA	201	9VO	N6-C5-N7-C8
3	CCC	201	9VO	C4-C5-N7-C8
3	CCC	201	9VO	N6-C5-N7-C8
3	BBB	202	9VO	C9-C8-N7-C5

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	AAA	148/151 (98%)	-0.09	0 100 100	54, 81, 109, 133	0
1	BBB	145/151 (96%)	-0.24	0 100 100	44, 67, 100, 120	0
1	CCC	146/151 (96%)	-0.10	0 100 100	48, 81, 126, 152	0
1	DDD	141/151 (93%)	0.17	2 (1%) 75 56	49, 98, 147, 166	0
All	All	580/604 (96%)	-0.07	2 (0%) 94 88	44, 80, 128, 166	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	DDD	72	GLU	2.4
1	DDD	136	ASP	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(\AA^2)	Q<0.9
2	EDO	BBB	201	4/4	0.76	0.24	83,88,89,89	0
3	9VO	AAA	202	14/14	0.89	0.39	81,88,103,105	0
3	9VO	BBB	202	14/14	0.91	0.56	67,72,75,75	0
3	9VO	AAA	201	14/14	0.92	0.38	66,72,81,82	0
3	9VO	CCC	201	14/14	0.92	0.43	60,72,82,83	0
3	9VO	DDD	201	14/14	0.94	0.64	74,78,80,81	0
4	SO4	BBB	203	5/5	0.96	0.17	76,79,86,88	0

6.5 Other polymers [i](#)

There are no such residues in this entry.