



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:49 AM GMT

PDB ID : 3G4K
Title : Crystal structure of human phosphodiesterase 4d with rolipram
Authors : Staker, B.L.
Deposited on : 2009-02-03
Resolution : 1.95 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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

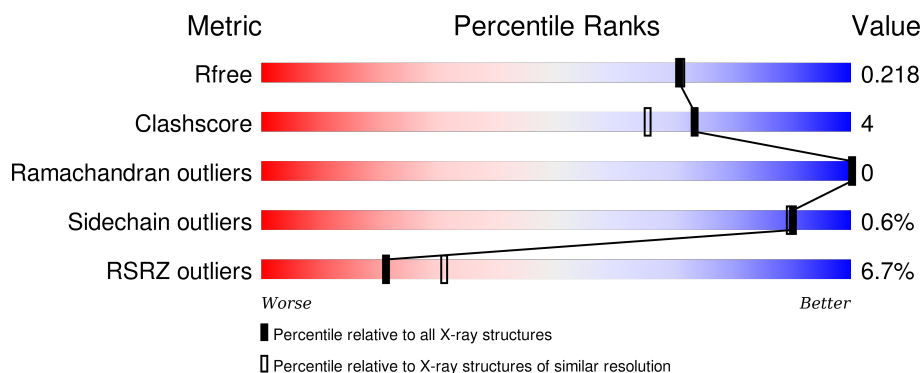
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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 ≥ 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	381	 7% 81% 5% 13%
1	B	381	 4% 76% 9% 14%
1	C	381	 7% 77% 8% 14%
1	D	381	 5% 83% 5% 13%

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	SO4	C	3	-	-	-	X
5	ROL	A	901	-	-	-	X
5	ROL	B	902	-	-	-	X
5	ROL	C	903[A]	X	-	-	-
5	ROL	D	904[A]	X	-	-	X
5	ROL	D	904[B]	-	-	-	X
6	EDO	A	12	-	-	-	X
6	EDO	A	14	-	-	-	X
6	EDO	A	6	-	-	-	X
6	EDO	A	7	-	-	-	X
6	EDO	B	11	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11857 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called cAMP-specific 3',5'-cyclic phosphodiesterase 4D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	S	0	0	0
			2667	1690	455	508	14			
1	B	326	Total	C	N	O	S	0	0	0
			2626	1660	446	506	14			
1	C	327	Total	C	N	O	S	0	0	0
			2643	1671	451	507	14			
1	D	333	Total	C	N	O	S	0	0	0
			2688	1700	460	514	14			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	243	MET	-	expression tag	UNP Q08499
A	579	ALA	SER	engineered	UNP Q08499
A	581	ALA	SER	engineered	UNP Q08499
A	618	HIS	-	expression tag	UNP Q08499
A	619	HIS	-	expression tag	UNP Q08499
A	620	HIS	-	expression tag	UNP Q08499
A	621	HIS	-	expression tag	UNP Q08499
A	622	HIS	-	expression tag	UNP Q08499
A	623	HIS	-	expression tag	UNP Q08499
B	243	MET	-	expression tag	UNP Q08499
B	579	ALA	SER	engineered	UNP Q08499
B	581	ALA	SER	engineered	UNP Q08499
B	618	HIS	-	expression tag	UNP Q08499
B	619	HIS	-	expression tag	UNP Q08499
B	620	HIS	-	expression tag	UNP Q08499
B	621	HIS	-	expression tag	UNP Q08499
B	622	HIS	-	expression tag	UNP Q08499
B	623	HIS	-	expression tag	UNP Q08499
C	243	MET	-	expression tag	UNP Q08499
C	579	ALA	SER	engineered	UNP Q08499
C	581	ALA	SER	engineered	UNP Q08499

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	618	HIS	-	expression tag	UNP Q08499
C	619	HIS	-	expression tag	UNP Q08499
C	620	HIS	-	expression tag	UNP Q08499
C	621	HIS	-	expression tag	UNP Q08499
C	622	HIS	-	expression tag	UNP Q08499
C	623	HIS	-	expression tag	UNP Q08499
D	243	MET	-	expression tag	UNP Q08499
D	579	ALA	SER	engineered	UNP Q08499
D	581	ALA	SER	engineered	UNP Q08499
D	618	HIS	-	expression tag	UNP Q08499
D	619	HIS	-	expression tag	UNP Q08499
D	620	HIS	-	expression tag	UNP Q08499
D	621	HIS	-	expression tag	UNP Q08499
D	622	HIS	-	expression tag	UNP Q08499
D	623	HIS	-	expression tag	UNP Q08499

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

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

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

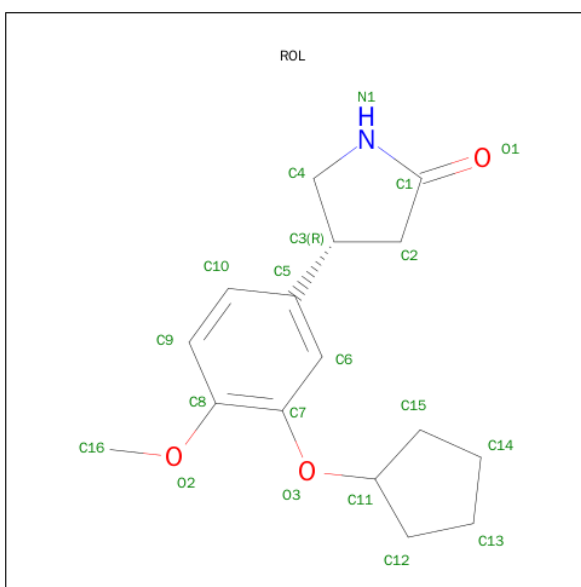
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Mg 1 1	0	0
3	A	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is ROLIPRAM (three-letter code: ROL) (formula: C₁₆H₂₁NO₃).



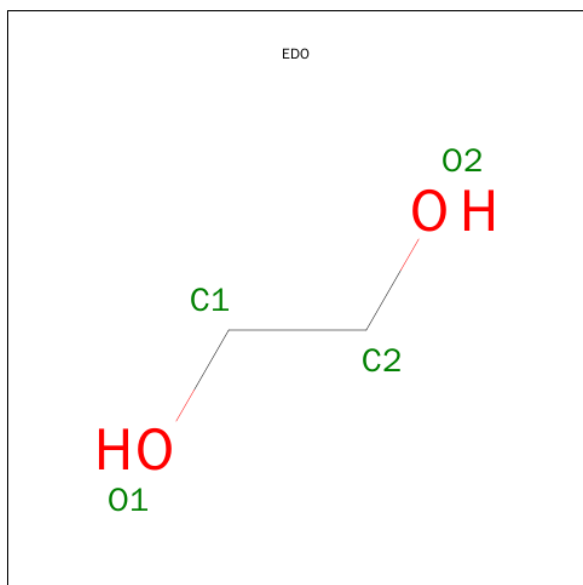
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			20	16	1	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			20	16	1	3		
5	C	1	Total	C	N	O	0	1
			40	32	2	6		
5	D	1	Total	C	N	O	0	1
			40	32	2	6		

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

Continued on next page...

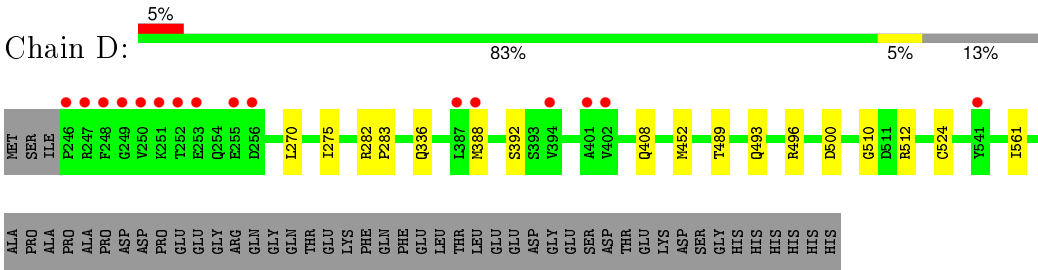
Continued from previous page...

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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	272	Total 272	O 272	0	0
7	B	249	Total 249	O 249	0	0
7	C	240	Total 240	O 240	0	0
7	D	273	Total 273	O 273	0	0

● 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	98.61Å 112.76Å 160.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.95 48.94 – 1.95	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-1.95) 99.6 (48.94-1.95)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.67 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.183 , 0.215 0.188 , 0.218	Depositor DCC
R_{free} test set	6540 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	27.4	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 52.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 129779 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11857	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, MG, ROL, ZN, 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	A	0.48	0/2722	0.60	2/3698 (0.1%)
1	B	0.44	0/2680	0.59	3/3645 (0.1%)
1	C	0.45	0/2697	0.58	0/3665
1	D	0.48	0/2744	0.58	0/3729
All	All	0.46	0/10843	0.59	5/14737 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	514	ARG	NE-CZ-NH2	-6.72	116.94	120.30
1	B	514	ARG	NE-CZ-NH2	-6.29	117.16	120.30
1	B	514	ARG	NE-CZ-NH1	6.23	123.41	120.30
1	A	514	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	B	512	ARG	NE-CZ-NH2	-5.44	117.58	120.30

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	2667	0	2619	19	0
1	B	2626	0	2559	26	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2643	0	2593	25	0
1	D	2688	0	2632	18	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	5	0	0	0	0
4	C	5	0	0	0	0
4	D	5	0	0	1	0
5	A	20	0	21	0	0
5	B	20	0	21	0	0
5	C	40	0	42	0	0
5	D	40	0	42	1	0
6	A	32	0	48	3	0
6	B	12	0	18	2	0
6	C	4	0	6	0	0
6	D	8	0	12	0	0
7	A	272	0	0	4	0
7	B	249	0	0	3	0
7	C	240	0	0	5	0
7	D	273	0	0	7	0
All	All	11857	0	10613	88	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 4.

All (88) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:575:THR:HG21	7:A:104:HOH:O	1.77	0.85
1:B:387:LEU:HG	7:B:717:HOH:O	1.84	0.77
1:A:408:GLN:OE1	1:D:408:GLN:OE1	2.07	0.73
1:A:575:THR:O	1:A:575:THR:HG22	1.92	0.69
1:B:496:ARG:HD3	1:B:571:TRP:CH2	2.29	0.68
1:C:459:THR:HG22	1:C:463:VAL:O	1.93	0.68
1:C:320:HIS:HE1	1:C:369:ASP:OD1	1.78	0.66
1:B:350:VAL:CG2	1:B:463:VAL:CG1	2.75	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:346:ALA:O	1:B:463:VAL:HG13	1.99	0.62
1:C:464:LEU:HD21	1:C:553:LEU:HD11	1.82	0.62
1:C:496:ARG:HD3	1:C:571:TRP:CH2	2.34	0.62
1:B:350:VAL:HG23	1:B:463:VAL:HG11	1.81	0.61
1:D:452:MET:HE3	7:D:162:HOH:O	2.01	0.61
1:D:496:ARG:HD3	1:D:571:TRP:CH2	2.35	0.61
1:C:408:GLN:NE2	7:C:125:HOH:O	2.34	0.60
1:B:420:LYS:HG2	1:B:424:GLN:HE21	1.65	0.60
1:D:500:ASP:OD1	7:D:956:HOH:O	2.16	0.59
1:B:489:THR:HB	1:B:561:ILE:HG23	1.86	0.58
1:B:270:LEU:HD22	1:B:336:GLN:HG3	1.84	0.58
1:A:270:LEU:HD11	1:A:275:ILE:HD11	1.85	0.57
1:B:262:LEU:HD11	1:B:286:VAL:CG1	2.35	0.56
1:C:573:GLN:NE2	1:C:576:ILE:HD12	2.21	0.56
1:A:428:LYS:NZ	7:A:1023:HOH:O	2.38	0.55
1:B:512:ARG:HD2	7:D:69:HOH:O	2.05	0.55
1:A:512:ARG:HD2	7:C:116:HOH:O	2.07	0.55
1:A:489:THR:HB	1:A:561:ILE:HG23	1.89	0.55
1:D:388:MET:HE2	1:D:388:MET:HA	1.89	0.55
1:B:350:VAL:HG23	1:B:463:VAL:CG1	2.36	0.54
1:B:262:LEU:O	1:B:265:VAL:HG23	2.08	0.54
1:A:511:ASP:O	1:A:515:GLU:HG3	2.09	0.52
1:D:452:MET:CE	7:D:162:HOH:O	2.56	0.52
1:B:511:ASP:OD1	1:B:514:ARG:NH2	2.43	0.52
1:C:573:GLN:HE21	1:C:576:ILE:HD12	1.74	0.52
1:A:575:THR:O	1:A:575:THR:CG2	2.58	0.52
1:A:409:GLU:HG3	6:A:624:EDO:H12	1.93	0.51
1:C:320:HIS:HD2	7:C:52:HOH:O	1.93	0.51
1:C:573:GLN:HA	1:C:573:GLN:HE21	1.76	0.50
1:B:411:ASN:ND2	7:B:693:HOH:O	2.39	0.50
7:A:88:HOH:O	1:C:512:ARG:HD2	2.11	0.50
1:A:289:HIS:CE1	1:A:293:GLN:HE21	2.30	0.50
1:D:392:SER:HB2	7:D:738:HOH:O	2.10	0.50
1:D:270:LEU:HD22	1:D:336:GLN:HG3	1.92	0.49
1:C:571:TRP:O	1:C:575:THR:HG23	2.12	0.49
1:C:489:THR:HB	1:C:561:ILE:HG23	1.93	0.49
1:C:455:THR:HG22	1:C:455:THR:O	2.14	0.48
7:B:121:HOH:O	1:D:512:ARG:HD2	2.14	0.48
1:D:270:LEU:HD11	1:D:275:ILE:CD1	2.45	0.47
1:C:348:GLU:O	1:C:463:VAL:HG11	2.14	0.47
1:B:496:ARG:HD3	1:B:571:TRP:CZ3	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:388:MET:HE2	1:D:388:MET:CA	2.43	0.46
1:B:494:LEU:HD21	6:B:11:EDO:O1	2.16	0.46
1:C:270:LEU:HD22	1:C:336:GLN:HG3	1.96	0.46
1:C:448:ASP:O	1:C:474:GLN:NE2	2.47	0.46
1:D:493:GLN:NE2	4:D:2:SO4:O3	2.49	0.46
1:D:496:ARG:HD3	1:D:571:TRP:CZ3	2.51	0.46
1:C:448:ASP:C	1:C:474:GLN:NE2	2.70	0.45
1:C:492:LEU:HD21	1:C:571:TRP:CD2	2.52	0.45
1:C:492:LEU:HD21	1:C:571:TRP:CE2	2.52	0.45
6:A:624:EDO:H22	1:C:384:GLU:HB2	1.99	0.45
1:D:282:ARG:N	1:D:283:PRO:CD	2.81	0.44
1:A:388:MET:HB2	1:A:388:MET:HE2	1.75	0.44
1:B:344:THR:HG22	1:B:347:LEU:HD12	2.00	0.44
1:A:511:ASP:OD1	1:A:514:ARG:NH2	2.47	0.44
1:B:262:LEU:HD11	1:B:286:VAL:HG13	2.00	0.44
1:A:512:ARG:CD	7:C:116:HOH:O	2.65	0.44
1:C:253:GLU:O	1:C:257:VAL:HG23	2.18	0.43
1:B:282:ARG:N	1:B:283:PRO:CD	2.81	0.43
1:A:270:LEU:HD11	1:A:275:ILE:CD1	2.47	0.43
1:A:341:LEU:HD23	6:A:14:EDO:H12	2.00	0.43
1:D:270:LEU:HD11	1:D:275:ILE:HD11	2.01	0.43
1:B:362:ALA:O	1:B:366:HIS:HB3	2.19	0.43
1:D:489:THR:HB	1:D:561:ILE:HG23	2.01	0.42
1:B:494:LEU:CD2	6:B:11:EDO:O1	2.67	0.42
1:B:464:LEU:HD21	1:B:553:LEU:HG	2.02	0.42
1:A:487:ASN:HB2	1:A:488:PRO:HD3	2.00	0.42
1:A:493:GLN:NE2	7:A:637:HOH:O	2.52	0.42
1:A:282:ARG:N	1:A:283:PRO:CD	2.82	0.42
1:B:490:LYS:HB3	1:B:491:PRO:HD2	2.02	0.42
1:B:395:LEU:HD23	1:B:395:LEU:HA	1.91	0.41
1:B:326:HIS:ND1	1:B:505:GLU:OE2	2.40	0.41
1:D:452:MET:SD	7:D:162:HOH:O	2.62	0.41
1:C:282:ARG:N	1:C:283:PRO:CD	2.84	0.41
1:C:504:GLU:OE2	1:C:508:ARG:NH2	2.54	0.41
1:D:510:GLY:HA3	1:D:524:CYS:O	2.20	0.41
1:B:264:ASP:HB2	1:B:270:LEU:HD12	2.03	0.40
5:D:904[A]:ROL:H142	7:D:59:HOH:O	2.20	0.40
1:C:350:VAL:HG11	1:C:466:LEU:HD12	2.02	0.40
1:C:443:MET:HE3	7:C:747:HOH:O	2.22	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	328/381 (86%)	321 (98%)	7 (2%)	0	100	100
1	B	324/381 (85%)	317 (98%)	7 (2%)	0	100	100
1	C	325/381 (85%)	319 (98%)	6 (2%)	0	100	100
1	D	331/381 (87%)	327 (99%)	4 (1%)	0	100	100
All	All	1308/1524 (86%)	1284 (98%)	24 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	299/345 (87%)	299 (100%)	0	100	100
1	B	295/345 (86%)	293 (99%)	2 (1%)	88	88
1	C	298/345 (86%)	293 (98%)	5 (2%)	68	63
1	D	302/345 (88%)	302 (100%)	0	100	100
All	All	1194/1380 (86%)	1187 (99%)	7 (1%)	90	89

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	258	LEU
1	B	508	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	289	HIS
1	C	320	HIS
1	C	408	GLN
1	C	523	MET
1	C	573	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	254	GLN
1	A	289	HIS
1	A	411	ASN
1	A	424	GLN
1	A	474	GLN
1	B	289	HIS
1	B	411	ASN
1	B	424	GLN
1	B	474	GLN
1	B	573	GLN
1	C	320	HIS
1	C	408	GLN
1	C	411	ASN
1	C	424	GLN
1	C	559	GLN
1	C	573	GLN
1	D	289	HIS
1	D	293	GLN
1	D	411	ASN
1	D	474	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 31 ligands modelled in this entry, 8 are monoatomic - leaving 23 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	SO4	A	1	-	4,4,4	0.45	0	6,6,6	0.37	0
6	EDO	A	12	-	3,3,3	0.44	0	2,2,2	0.49	0
6	EDO	A	13	-	3,3,3	0.44	0	2,2,2	0.48	0
6	EDO	A	14	-	3,3,3	0.42	0	2,2,2	0.31	0
6	EDO	A	4	-	3,3,3	0.54	0	2,2,2	0.16	0
6	EDO	A	6	-	3,3,3	0.41	0	2,2,2	0.57	0
6	EDO	A	624	-	3,3,3	0.47	0	2,2,2	0.56	0
6	EDO	A	7	-	3,3,3	0.45	0	2,2,2	0.51	0
6	EDO	A	9	-	3,3,3	0.46	0	2,2,2	0.46	0
5	ROL	A	901	-	21,22,22	0.94	1 (4%)	27,30,30	1.15	2 (7%)
6	EDO	B	11	-	3,3,3	0.27	0	2,2,2	0.81	0
6	EDO	B	3	-	3,3,3	0.43	0	2,2,2	0.51	0
6	EDO	B	8	-	3,3,3	0.46	0	2,2,2	0.29	0
5	ROL	B	902	-	21,22,22	0.88	1 (4%)	27,30,30	1.31	2 (7%)
4	SO4	C	3	-	4,4,4	0.36	0	6,6,6	0.42	0
6	EDO	C	5	-	3,3,3	0.45	0	2,2,2	0.39	0
5	ROL	C	903[A]	-	21,22,22	0.99	1 (4%)	27,30,30	1.29	3 (11%)
5	ROL	C	903[B]	-	21,22,22	0.97	1 (4%)	27,30,30	1.20	3 (11%)
6	EDO	D	10	-	3,3,3	0.46	0	2,2,2	0.35	0
4	SO4	D	2	-	4,4,4	0.42	0	6,6,6	0.52	0
6	EDO	D	624	-	3,3,3	0.49	0	2,2,2	0.04	0
5	ROL	D	904[A]	-	21,22,22	0.97	1 (4%)	27,30,30	1.21	3 (11%)
5	ROL	D	904[B]	-	21,22,22	0.92	1 (4%)	27,30,30	1.32	3 (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
4	SO4	A	1	-	-	0/0/0/0	0/0/0/0
6	EDO	A	12	-	-	0/1/1/1	0/0/0/0
6	EDO	A	13	-	-	0/1/1/1	0/0/0/0
6	EDO	A	14	-	-	0/1/1/1	0/0/0/0
6	EDO	A	4	-	-	0/1/1/1	0/0/0/0
6	EDO	A	6	-	-	0/1/1/1	0/0/0/0
6	EDO	A	624	-	-	0/1/1/1	0/0/0/0
6	EDO	A	7	-	-	0/1/1/1	0/0/0/0
6	EDO	A	9	-	-	0/1/1/1	0/0/0/0
5	ROL	A	901	-	-	0/10/26/26	0/3/3/3
6	EDO	B	11	-	-	0/1/1/1	0/0/0/0
6	EDO	B	3	-	-	0/1/1/1	0/0/0/0
6	EDO	B	8	-	-	0/1/1/1	0/0/0/0
5	ROL	B	902	-	-	0/10/26/26	0/3/3/3
4	SO4	C	3	-	-	0/0/0/0	0/0/0/0
6	EDO	C	5	-	-	0/1/1/1	0/0/0/0
5	ROL	C	903[A]	-	1/1/3/4	0/10/26/26	0/3/3/3
5	ROL	C	903[B]	-	-	0/10/26/26	0/3/3/3
6	EDO	D	10	-	-	0/1/1/1	0/0/0/0
4	SO4	D	2	-	-	0/0/0/0	0/0/0/0
6	EDO	D	624	-	-	0/1/1/1	0/0/0/0
5	ROL	D	904[A]	-	1/1/3/4	0/10/26/26	0/3/3/3
5	ROL	D	904[B]	-	-	0/10/26/26	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	902	ROL	C8-C7	3.15	1.47	1.40
5	A	901	ROL	C8-C7	3.33	1.47	1.40
5	D	904[B]	ROL	C8-C7	3.52	1.48	1.40
5	C	903[B]	ROL	C8-C7	3.82	1.48	1.40
5	D	904[A]	ROL	C8-C7	3.92	1.49	1.40
5	C	903[A]	ROL	C8-C7	3.99	1.49	1.40

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	902	ROL	C6-C5-C3	-4.03	114.98	120.89
5	D	904[B]	ROL	C6-C5-C3	-3.79	115.32	120.89
5	C	903[A]	ROL	C4-C3-C5	-3.09	110.35	115.88

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	903[B]	ROL	C6-C5-C3	-2.60	117.08	120.89
5	A	901	ROL	C6-C5-C3	-2.59	117.09	120.89
5	D	904[A]	ROL	C2-C3-C5	-2.19	110.09	114.95
5	D	904[B]	ROL	O1-C1-C2	-2.08	123.51	126.43
5	D	904[A]	ROL	C16-O2-C8	2.08	120.70	117.54
5	C	903[B]	ROL	O2-C8-C7	2.53	119.00	115.40
5	D	904[B]	ROL	O2-C8-C7	2.88	119.51	115.40
5	C	903[A]	ROL	C16-O2-C8	3.02	122.12	117.54
5	B	902	ROL	C16-O2-C8	3.11	122.26	117.54
5	C	903[A]	ROL	O2-C8-C7	3.30	120.10	115.40
5	C	903[B]	ROL	C16-O2-C8	3.55	122.93	117.54
5	D	904[A]	ROL	O2-C8-C7	3.61	120.54	115.40
5	A	901	ROL	C16-O2-C8	3.79	123.28	117.54

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	D	904[A]	ROL	C3
5	C	903[A]	ROL	C3

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	14	EDO	1	0
6	A	624	EDO	2	0
6	B	11	EDO	2	0
4	D	2	SO4	1	0
5	D	904[A]	ROL	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	330/381 (86%)	0.55	28 (8%)	13 21	16, 27, 48, 56	0
1	B	326/381 (85%)	0.38	14 (4%)	39 50	17, 29, 49, 69	0
1	C	327/381 (85%)	0.53	28 (8%)	13 21	16, 29, 50, 65	0
1	D	333/381 (87%)	0.31	18 (5%)	29 41	15, 27, 52, 68	0
All	All	1316/1524 (86%)	0.44	88 (6%)	21 31	15, 28, 50, 69	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	460	SER	9.4
1	A	460	SER	7.8
1	C	459	THR	7.3
1	A	459	THR	6.8
1	A	461	SER	6.5
1	C	462	GLY	6.2
1	C	461	SER	5.9
1	C	458	VAL	5.6
1	C	541	TYR	5.6
1	B	253	GLU	5.4
1	C	577	PRO	5.3
1	D	248	PHE	5.1
1	C	463	VAL	5.0
1	C	465	LEU	5.0
1	D	246	PRO	4.9
1	A	458	VAL	4.8
1	D	253	GLU	4.8
1	B	254	GLN	4.7
1	A	577	PRO	4.7
1	C	578	GLN	4.7
1	A	465	LEU	4.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	252	THR	4.6
1	D	247	ARG	4.4
1	C	252	THR	4.2
1	C	575	THR	3.9
1	A	467	ASP	3.9
1	D	578	GLN	3.8
1	D	250	VAL	3.7
1	A	541	TYR	3.5
1	C	464	LEU	3.5
1	A	462	GLY	3.4
1	B	541	TYR	3.4
1	B	260	LYS	3.4
1	A	457	LYS	3.2
1	C	467	ASP	3.2
1	D	541	TYR	3.2
1	B	256	ASP	3.1
1	C	555	HIS	3.0
1	A	463	VAL	3.0
1	B	255	GLU	2.9
1	C	529	ALA	2.9
1	A	576	ILE	2.8
1	C	457	LYS	2.8
1	C	253	GLU	2.8
1	A	528	ASN	2.8
1	C	576	ILE	2.7
1	C	453	VAL	2.7
1	C	528	ASN	2.7
1	A	464	LEU	2.7
1	B	387	LEU	2.6
1	A	454	GLU	2.6
1	C	256	ASP	2.6
1	A	575	THR	2.6
1	C	447	ALA	2.5
1	A	248	PHE	2.5
1	A	455	THR	2.5
1	D	251	LYS	2.4
1	D	402	VAL	2.4
1	A	400	LEU	2.3
1	D	387	LEU	2.3
1	C	454	GLU	2.3
1	A	456	LYS	2.3
1	A	553	LEU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	443	MET	2.3
1	A	250	VAL	2.3
1	D	255	GLU	2.3
1	B	560	ASP	2.2
1	A	519	GLU	2.2
1	D	570	GLU	2.2
1	B	385	LEU	2.2
1	C	387	LEU	2.2
1	D	256	ASP	2.2
1	A	529	ALA	2.2
1	A	389	TYR	2.2
1	D	249	GLY	2.1
1	D	394	VAL	2.1
1	D	388	MET	2.1
1	B	455	THR	2.1
1	B	389	TYR	2.1
1	B	578	GLN	2.1
1	B	570	GLU	2.1
1	A	552	ASP	2.1
1	A	365	ILE	2.0
1	D	401	ALA	2.0
1	A	385	LEU	2.0
1	B	465	LEU	2.0
1	C	452	MET	2.0
1	C	255	GLU	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 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, 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	LLDF	B-factors(Å ²)	Q<0.9
6	EDO	A	6	4/4	0.78	0.33	14.23	43,43,44,47	0
6	EDO	A	12	4/4	0.88	0.24	8.65	42,43,44,46	0
6	EDO	A	14	4/4	0.90	0.18	5.26	46,46,46,47	0
4	SO4	C	3	5/5	0.92	0.31	4.91	58,61,62,63	0
5	ROL	B	902	20/20	0.90	0.15	4.29	29,37,42,42	0
5	ROL	D	904[A]	20/20	0.93	0.17	4.09	37,38,41,41	20
5	ROL	D	904[B]	20/20	0.93	0.17	4.02	17,21,25,26	20
6	EDO	A	7	4/4	0.92	0.23	3.40	41,43,43,44	0
6	EDO	B	11	4/4	0.82	0.25	2.92	44,45,47,49	0
5	ROL	A	901	20/20	0.93	0.13	2.06	29,33,38,39	0
5	ROL	C	903[B]	20/20	0.93	0.15	1.94	21,25,28,28	20
6	EDO	D	10	4/4	0.93	0.18	1.91	32,34,34,35	0
5	ROL	C	903[A]	20/20	0.93	0.15	1.83	37,39,41,41	20
6	EDO	B	3	4/4	0.90	0.19	1.81	39,39,40,40	0
6	EDO	A	624	4/4	0.92	0.22	1.61	21,27,28,30	0
6	EDO	A	9	4/4	0.86	0.13	1.06	49,50,51,51	0
4	SO4	D	2	5/5	0.95	0.14	0.46	41,46,48,48	0
4	SO4	A	1	5/5	0.96	0.13	0.31	39,44,46,47	0
3	MG	C	806	1/1	0.93	0.12	0.29	41,41,41,41	0
2	ZN	C	805	1/1	1.00	0.11	0.24	23,23,23,23	0
6	EDO	C	5	4/4	0.96	0.15	0.19	31,31,32,32	0
2	ZN	A	801	1/1	0.99	0.11	-0.10	21,21,21,21	0
2	ZN	B	803	1/1	0.99	0.09	-0.60	25,25,25,25	0
6	EDO	D	624	4/4	0.96	0.12	-0.62	26,27,27,27	0
6	EDO	A	13	4/4	0.95	0.09	-1.13	34,34,35,35	0
2	ZN	D	807	1/1	1.00	0.11	-1.19	21,21,21,21	0
3	MG	B	804	1/1	0.96	0.08	-1.22	47,47,47,47	0
6	EDO	B	8	4/4	0.98	0.09	-1.42	31,32,32,32	0
6	EDO	A	4	4/4	0.95	0.12	-1.47	28,30,30,32	0
3	MG	A	802	1/1	0.82	0.09	-1.90	47,47,47,47	0
3	MG	D	808	1/1	0.95	0.07	-4.73	43,43,43,43	0

6.5 Other polymers ⓘ

There are no such residues in this entry.