



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:04 am GMT

PDB ID : 3G4I
Title : Crystal structure of human phosphodiesterase 4d with d155871
Authors : Staker, B.L.
Deposited on : 2009-02-03
Resolution : 1.90 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

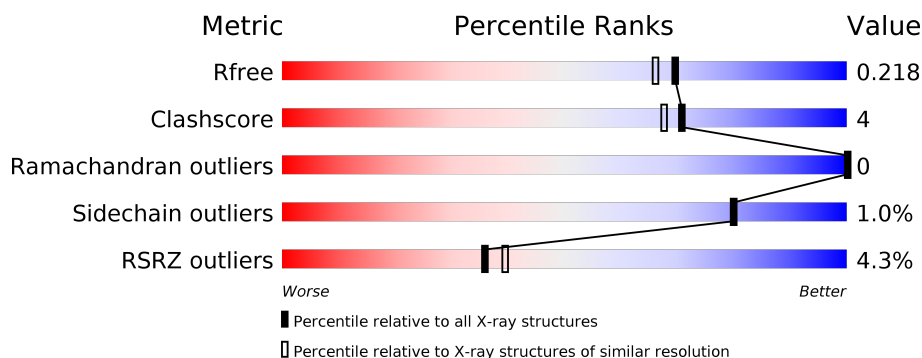
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	5047 (1.90-1.90)
Clashscore	112137	5731 (1.90-1.90)
Ramachandran outliers	110173	5669 (1.90-1.90)
Sidechain outliers	110143	5670 (1.90-1.90)
RSRZ outliers	101464	5100 (1.90-1.90)

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	<div> <div>5%</div> <div> <div></div> <div>80%</div> <div>7%</div> <div>13%</div> </div> </div>
1	B	381	<div> <div>2%</div> <div> <div></div> <div>78%</div> <div>7%</div> <div>14%</div> </div> </div>
1	C	381	<div> <div>5%</div> <div> <div></div> <div>79%</div> <div>7%</div> <div>14%</div> </div> </div>
1	D	381	<div> <div>3%</div> <div> <div></div> <div>82%</div> <div>6%</div> <div>12%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	B	4	-	-	X	X
5	D71	A	901	-	-	-	X
5	D71	B	902	-	-	-	X
5	D71	C	903	-	-	-	X
6	EOH	A	12	-	-	-	X
6	EOH	A	5	-	-	X	X
6	EOH	A	9	-	-	-	X
6	EOH	B	10	-	-	-	X
6	EOH	B	11	-	-	X	X
6	EOH	B	8	-	-	-	X
6	EOH	C	6	-	-	-	X
6	EOH	D	7	-	-	X	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12017 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	331	Total	C	N	O	S	0	0	0
			2678	1695	457	512	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
			2647	1673	452	508	14			
1	D	334	Total	C	N	O	S	0	0	0
			2704	1712	463	515	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

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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).

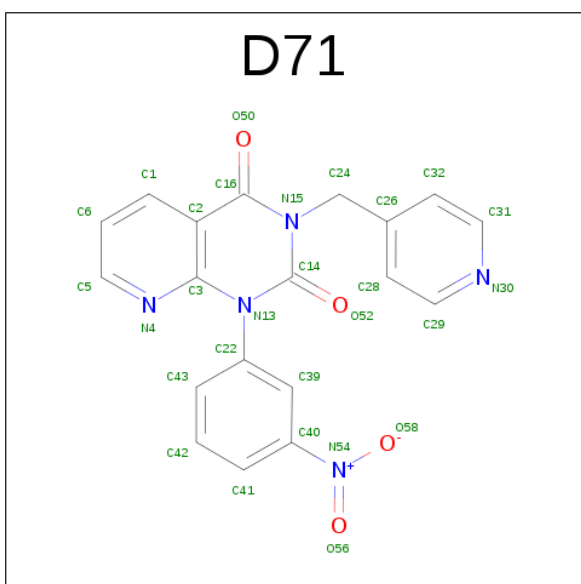
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Mg 1 1	0	0
3	A	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0

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



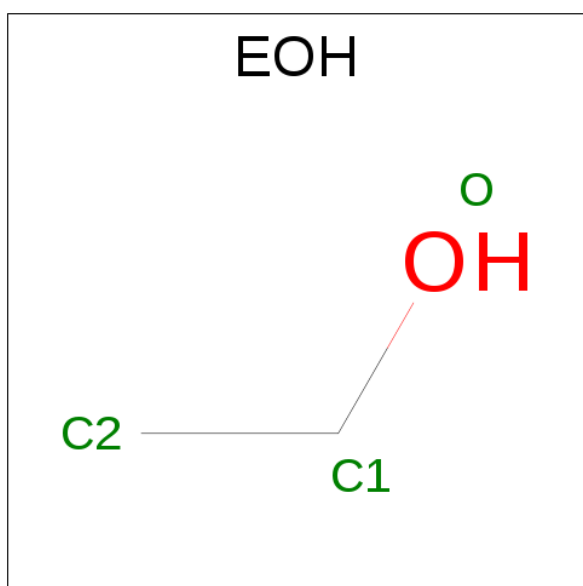
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is 1-(3-NITROPHENYL)-3-(PYRIDIN-4-YLMETHYL)PYRIDO[2,3-D]PYRIMIDINE-2,4(1H,3H)-DIONE (three-letter code: D71) (formula: C₁₉H₁₃N₅O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			28	19	5	4		
5	B	1	Total	C	N	O	0	0
			28	19	5	4		
5	C	1	Total	C	N	O	0	0
			28	19	5	4		
5	D	1	Total	C	N	O	0	0
			28	19	5	4		

- Molecule 6 is ETHANOL (three-letter code: EOH) (formula: C₂H₆O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			3	2	1		
6	A	1	Total	C	O	0	0
			3	2	1		
6	A	1	Total	C	O	0	0
			3	2	1		
6	B	1	Total	C	O	0	0
			3	2	1		
6	B	1	Total	C	O	0	0
			3	2	1		
6	B	1	Total	C	O	0	0
			3	2	1		
6	C	1	Total	C	O	0	0
			3	2	1		
6	D	1	Total	C	O	0	0
			3	2	1		

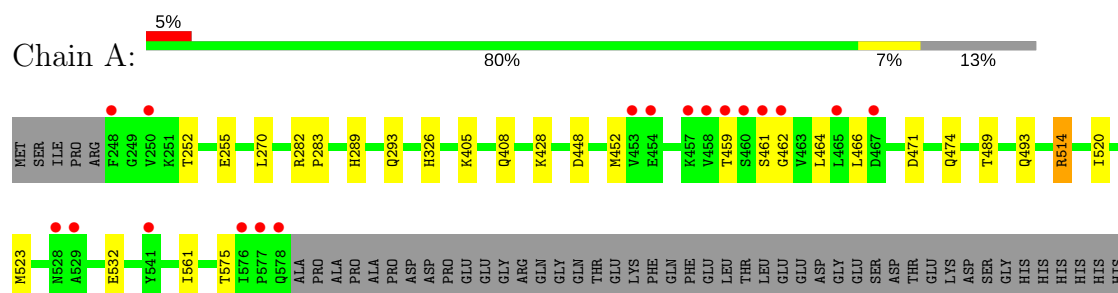
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	302	Total 302	O 302	0	0
7	B	286	Total 286	O 286	0	0
7	C	287	Total 287	O 287	0	0
7	D	328	Total 328	O 328	0	0

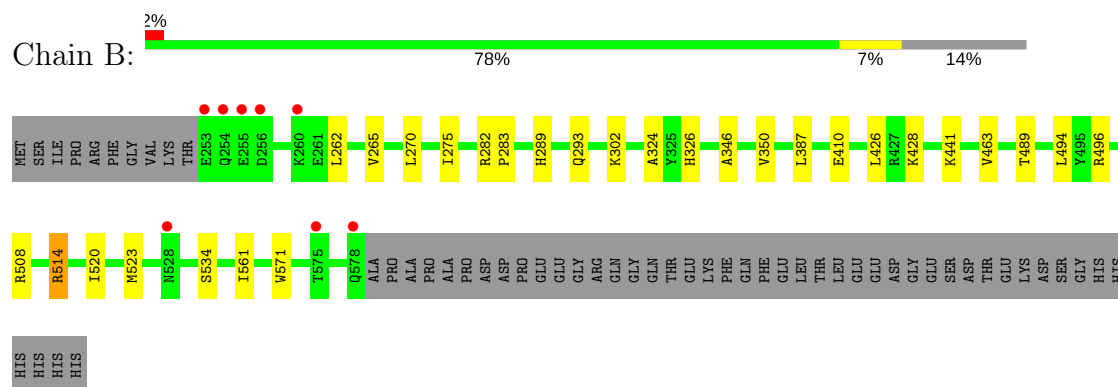
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

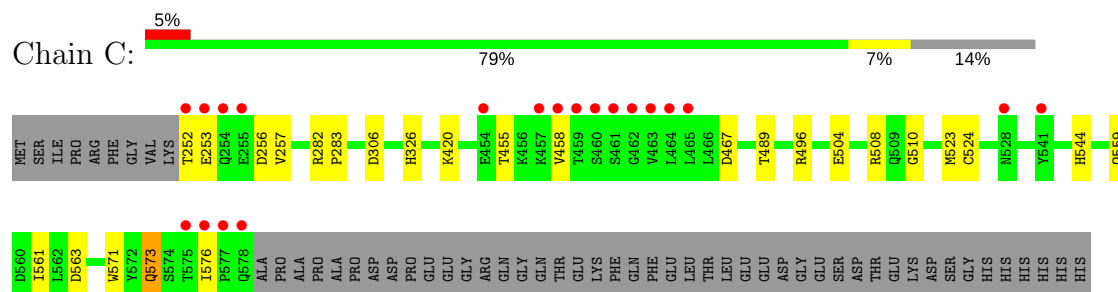
- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D



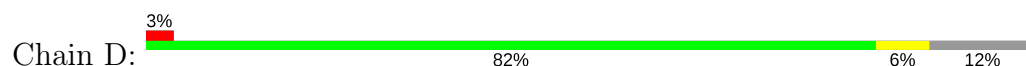
- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D

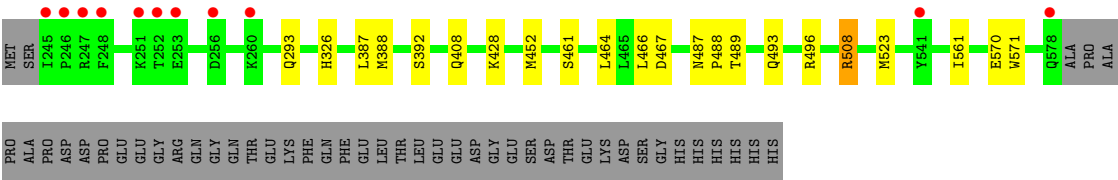


- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D



- 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	98.86Å 113.24Å 161.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.90 49.13 – 1.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-1.90) 92.9 (49.13-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.181 , 0.215 0.186 , 0.218	Depositor DCC
R_{free} test set	6596 reflections (5.24%)	DCC
Wilson B-factor (Å ²)	24.0	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 55.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12017	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EOH, MG, D71, ZN, SO4

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	0.53	0/2733	0.60	2/3712 (0.1%)
1	B	0.48	0/2680	0.59	2/3645 (0.1%)
1	C	0.52	0/2701	0.58	0/3670
1	D	0.55	0/2760	0.60	0/3749
All	All	0.52	0/10874	0.59	4/14776 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	514	ARG	NE-CZ-NH2	-7.31	116.64	120.30
1	B	514	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	A	514	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	A	514	ARG	NE-CZ-NH1	5.44	123.02	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	461	SER	Peptide

5.2 Too-close contacts ⓘ

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	2678	0	2633	26	0
1	B	2626	0	2559	27	0
1	C	2647	0	2599	18	0
1	D	2704	0	2664	15	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	B	5	0	0	2	0
4	C	5	0	0	0	0
5	A	28	0	13	3	0
5	B	28	0	13	6	0
5	C	28	0	13	2	0
5	D	28	0	13	1	0
6	A	9	0	18	2	0
6	B	9	0	18	3	0
6	C	3	0	6	0	0
6	D	3	0	6	2	0
7	A	302	0	0	4	0
7	B	286	0	0	7	0
7	C	287	0	0	7	0
7	D	328	0	0	4	0
All	All	12017	0	10555	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:B:523:MET:SD	5:B:902:D71:C41	2.57	0.92
1:B:387:LEU:HG	7:B:1212:HOH:O	1.74	0.87
6:B:10:EOH:H23	7:B:111:HOH:O	1.81	0.79
1:B:494:LEU:HD21	4:B:4:SO4:O4	1.84	0.77
1:A:405:LYS:NZ	1:A:408:GLN:OE1	2.21	0.74
1:C:252:THR:N	7:C:641:HOH:O	2.24	0.70
7:C:1068:HOH:O	1:D:387:LEU:HG	1.91	0.70
1:D:508:ARG:NH1	7:D:925:HOH:O	2.26	0.68
1:B:508:ARG:HG3	7:B:729:HOH:O	1.94	0.66
1:D:392:SER:HB2	7:D:702:HOH:O	1.96	0.65
1:B:534:SER:HB3	5:B:902:D71:H41	1.78	0.64
1:A:428:LYS:HG3	6:A:5:EOH:H23	1.81	0.63
1:D:523:MET:HG2	7:D:933:HOH:O	2.01	0.61
1:A:408:GLN:OE1	1:D:408:GLN:OE1	2.18	0.61
1:C:496:ARG:HD3	1:C:571:TRP:CH2	2.35	0.60
1:C:504:GLU:OE2	1:C:508:ARG:NH2	2.34	0.60
1:C:573:GLN:HE21	1:C:576:ILE:HD12	1.67	0.60
1:A:523:MET:SD	5:A:901:D71:C41	2.91	0.59
1:B:346:ALA:O	1:B:463:VAL:HG13	2.03	0.59
1:C:523:MET:HG2	7:C:717:HOH:O	2.02	0.58
1:C:326:HIS:CE1	5:C:903:D71:H29	2.39	0.57
1:B:523:MET:SD	5:B:902:D71:C40	2.93	0.57
1:A:252:THR:CG2	1:A:255:GLU:H	2.17	0.57
1:D:452:MET:HE3	7:D:1060:HOH:O	2.05	0.57
1:A:532:GLU:HG2	1:A:575:THR:HG22	1.86	0.56
1:A:252:THR:HG22	1:A:255:GLU:CG	2.37	0.55
6:A:5:EOH:H22	7:B:704:HOH:O	2.06	0.55
1:A:252:THR:HG23	1:A:255:GLU:H	1.71	0.55
1:B:350:VAL:CG2	1:B:463:VAL:CG1	2.85	0.54
1:D:496:ARG:HD3	1:D:571:TRP:CH2	2.42	0.54
1:A:514:ARG:HD3	1:A:520:ILE:HD11	1.91	0.53
1:D:428:LYS:HG3	6:D:7:EOH:H23	1.90	0.53
1:C:489:THR:HB	1:C:561:ILE:HG23	1.91	0.52
1:B:428:LYS:HG3	6:B:11:EOH:H23	1.92	0.52
1:D:508:ARG:HB2	1:D:508:ARG:HH11	1.74	0.52
1:B:489:THR:HB	1:B:561:ILE:HG23	1.92	0.52
1:B:350:VAL:HG23	1:B:463:VAL:HG11	1.92	0.51
1:A:448:ASP:HB3	1:A:474:GLN:NE2	2.25	0.51
1:C:306:ASP:HB3	7:C:729:HOH:O	2.11	0.51
1:A:575:THR:HG22	1:A:575:THR:O	2.11	0.50
1:C:326:HIS:NE2	5:C:903:D71:H29	2.26	0.50
7:C:137:HOH:O	6:D:7:EOH:H22	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:HIS:CE1	5:A:901:D71:H29	2.47	0.49
1:B:326:HIS:CE1	5:B:902:D71:H29	2.47	0.49
1:B:494:LEU:CD2	4:B:4:SO4:O4	2.58	0.49
1:B:514:ARG:HD3	1:B:520:ILE:HD11	1.95	0.49
1:B:270:LEU:HD11	1:B:275:ILE:HD11	1.95	0.49
1:A:464:LEU:HD21	1:A:466:LEU:HD21	1.95	0.49
1:B:262:LEU:O	1:B:265:VAL:HG23	2.13	0.49
1:A:489:THR:HB	1:A:561:ILE:HG23	1.95	0.48
1:B:289:HIS:CE1	1:B:293:GLN:HE21	2.32	0.48
1:D:326:HIS:CE1	5:D:904:D71:H29	2.50	0.47
1:A:523:MET:SD	5:A:901:D71:C40	3.03	0.47
1:B:326:HIS:NE2	5:B:902:D71:H29	2.29	0.47
1:B:350:VAL:HG23	1:B:463:VAL:CG1	2.44	0.46
1:A:289:HIS:CE1	1:A:293:GLN:HE21	2.34	0.46
1:D:489:THR:HB	1:D:561:ILE:HG23	1.97	0.46
1:A:448:ASP:C	1:A:474:GLN:NE2	2.69	0.46
1:C:573:GLN:NE2	1:C:576:ILE:HD12	2.29	0.46
7:A:633:HOH:O	6:B:11:EOH:H22	2.15	0.46
1:B:496:ARG:HD3	1:B:571:TRP:CH2	2.50	0.45
1:C:253:GLU:O	1:C:257:VAL:HG23	2.16	0.45
1:B:387:LEU:HD12	7:B:1194:HOH:O	2.15	0.45
1:A:575:THR:HG21	7:A:642:HOH:O	2.16	0.45
1:D:388:MET:HE3	1:D:388:MET:HB2	1.74	0.44
1:C:282:ARG:N	1:C:283:PRO:CD	2.81	0.44
1:B:324:ALA:H	1:B:508:ARG:HH22	1.65	0.43
1:D:464:LEU:HD21	1:D:466:LEU:HD21	1.99	0.43
1:C:420:LYS:HB2	1:C:420:LYS:HE2	1.68	0.42
1:B:523:MET:SD	5:B:902:D71:H41	2.55	0.42
1:A:493:GLN:NE2	7:A:942:HOH:O	2.48	0.41
1:A:282:ARG:N	1:A:283:PRO:CD	2.83	0.41
1:B:282:ARG:N	1:B:283:PRO:CD	2.83	0.41
1:C:508:ARG:NH1	7:C:692:HOH:O	2.53	0.41
1:D:487:ASN:HB2	1:D:488:PRO:HD3	2.02	0.41
1:A:252:THR:HG22	1:A:255:GLU:CB	2.50	0.41
1:B:302:LYS:NZ	7:B:634:HOH:O	2.52	0.41
1:D:496:ARG:HD3	1:D:571:TRP:CZ3	2.55	0.41
1:A:448:ASP:CB	1:A:474:GLN:NE2	2.83	0.41
1:A:575:THR:CG2	1:A:575:THR:O	2.69	0.41
1:A:459:THR:O	1:A:462:GLY:HA2	2.20	0.41
1:B:441:LYS:NZ	7:B:875:HOH:O	2.43	0.41
1:C:510:GLY:HA3	1:C:524:CYS:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:544:HIS:ND1	7:C:672:HOH:O	2.37	0.40
1:A:452:MET:HE1	1:A:471:ASP:HA	2.02	0.40
1:C:559:GLN:NE2	1:C:563:ASP:OD1	2.51	0.40
1:A:270:LEU:HD12	7:A:710:HOH:O	2.21	0.40
1:B:410:GLU:OE2	1:C:420:LYS:NZ	2.45	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	329/381 (86%)	321 (98%)	8 (2%)	0	100	100
1	B	324/381 (85%)	319 (98%)	5 (2%)	0	100	100
1	C	325/381 (85%)	317 (98%)	8 (2%)	0	100	100
1	D	332/381 (87%)	325 (98%)	7 (2%)	0	100	100
All	All	1310/1524 (86%)	1282 (98%)	28 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	302/345 (88%)	302 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	295/345 (86%)	294 (100%)	1 (0%)	94	94
1	C	299/345 (87%)	294 (98%)	5 (2%)	66	62
1	D	305/345 (88%)	299 (98%)	6 (2%)	60	55
All	All	1201/1380 (87%)	1189 (99%)	12 (1%)	80	80

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	426	LEU
1	C	256	ASP
1	C	455	THR
1	C	458	VAL
1	C	467	ASP
1	C	573	GLN
1	D	293	GLN
1	D	461	SER
1	D	467	ASP
1	D	493	GLN
1	D	508	ARG
1	D	570	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	254	GLN
1	A	289	HIS
1	B	289	HIS
1	B	573	GLN
1	C	474	GLN
1	C	573	GLN
1	C	578	GLN
1	D	289	HIS
1	D	293	GLN
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 [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 23 ligands modelled in this entry, 8 are monoatomic - leaving 15 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	$\# Z > 2$
6	EOH	A	12	-	2,2,2	0.49	0	1,1,1	0.08	0
4	SO4	A	3	-	4,4,4	0.24	0	6,6,6	0.54	0
6	EOH	A	5	-	2,2,2	0.60	0	1,1,1	0.12	0
6	EOH	A	9	-	2,2,2	0.50	0	1,1,1	0.13	0
5	D71	A	901	-	26,31,31	4.04	14 (53%)	30,44,44	1.99	10 (33%)
6	EOH	B	10	-	2,2,2	0.51	0	1,1,1	0.10	0
6	EOH	B	11	-	2,2,2	0.54	0	1,1,1	0.14	0
4	SO4	B	4	-	4,4,4	0.18	0	6,6,6	0.30	0
6	EOH	B	8	-	2,2,2	0.50	0	1,1,1	0.11	0
5	D71	B	902	-	26,31,31	3.96	14 (53%)	30,44,44	2.34	10 (33%)
4	SO4	C	2	-	4,4,4	0.17	0	6,6,6	0.40	0
6	EOH	C	6	-	2,2,2	0.59	0	1,1,1	0.09	0
5	D71	C	903	-	26,31,31	3.89	14 (53%)	30,44,44	1.99	11 (36%)
6	EOH	D	7	-	2,2,2	0.62	0	1,1,1	0.18	0
5	D71	D	904	-	26,31,31	3.87	13 (50%)	30,44,44	2.21	13 (43%)

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
6	EOH	A	12	-	-	0/0/0/0	0/0/0/0
4	SO4	A	3	-	-	0/0/0/0	0/0/0/0
6	EOH	A	5	-	-	0/0/0/0	0/0/0/0
6	EOH	A	9	-	-	0/0/0/0	0/0/0/0
5	D71	A	901	-	-	0/10/12/12	0/4/4/4
6	EOH	B	10	-	-	0/0/0/0	0/0/0/0
6	EOH	B	11	-	-	0/0/0/0	0/0/0/0
4	SO4	B	4	-	-	0/0/0/0	0/0/0/0
6	EOH	B	8	-	-	0/0/0/0	0/0/0/0
5	D71	B	902	-	-	0/10/12/12	0/4/4/4
4	SO4	C	2	-	-	0/0/0/0	0/0/0/0
6	EOH	C	6	-	-	0/0/0/0	0/0/0/0
5	D71	C	903	-	-	0/10/12/12	0/4/4/4
6	EOH	D	7	-	-	0/0/0/0	0/0/0/0
5	D71	D	904	-	-	0/10/12/12	0/4/4/4

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	901	D71	C3-N4	-2.59	1.31	1.35
5	C	903	D71	C3-N4	-2.57	1.31	1.35
5	C	903	D71	C1-C2	-2.48	1.36	1.41
5	D	904	D71	C1-C2	-2.48	1.36	1.41
5	B	902	D71	C1-C2	-2.27	1.36	1.41
5	B	902	D71	C28-C29	-2.23	1.33	1.38
5	C	903	D71	C28-C29	-2.23	1.33	1.38
5	B	902	D71	C3-N4	-2.21	1.32	1.35
5	A	901	D71	C1-C2	-2.19	1.36	1.41
5	A	901	D71	C28-C29	-2.13	1.34	1.38
5	D	904	D71	C28-C29	-2.04	1.34	1.38
5	D	904	D71	C16-N15	2.24	1.41	1.38
5	C	903	D71	C16-N15	2.95	1.42	1.38
5	C	903	D71	C29-N30	3.16	1.43	1.33
5	B	902	D71	C29-N30	3.25	1.43	1.33
5	A	901	D71	C29-N30	3.28	1.43	1.33
5	D	904	D71	C29-N30	3.51	1.44	1.33
5	A	901	D71	C16-N15	3.65	1.43	1.38
5	B	902	D71	C16-N15	3.84	1.44	1.38
5	C	903	D71	C28-C26	4.03	1.47	1.38
5	C	903	D71	C16-C2	4.57	1.49	1.41
5	B	902	D71	C28-C26	4.61	1.48	1.38
5	A	901	D71	C28-C26	4.63	1.48	1.38
5	B	902	D71	C16-C2	4.68	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	903	D71	C6-C1	4.71	1.47	1.36
5	A	901	D71	C16-C2	4.76	1.49	1.41
5	D	904	D71	C32-C31	4.77	1.48	1.38
5	D	904	D71	C28-C26	4.84	1.48	1.38
5	A	901	D71	C32-C31	4.87	1.48	1.38
5	A	901	D71	C6-C1	4.90	1.48	1.36
5	D	904	D71	C16-C2	4.90	1.49	1.41
5	D	904	D71	C6-C1	4.92	1.48	1.36
5	C	903	D71	C32-C31	4.95	1.48	1.38
5	B	902	D71	C32-C31	4.99	1.49	1.38
5	D	904	D71	C5-N4	5.01	1.42	1.32
5	B	902	D71	C6-C1	5.03	1.48	1.36
5	C	903	D71	C5-N4	5.16	1.42	1.32
5	B	902	D71	C5-N4	5.29	1.42	1.32
5	A	901	D71	C5-N4	5.41	1.43	1.32
5	D	904	D71	C42-C43	5.55	1.49	1.38
5	B	902	D71	C42-C43	5.66	1.49	1.38
5	C	903	D71	C42-C43	5.81	1.50	1.38
5	C	903	D71	C41-C40	5.81	1.50	1.38
5	D	904	D71	C41-C40	5.86	1.50	1.38
5	A	901	D71	C42-C43	5.89	1.50	1.38
5	A	901	D71	C41-C40	5.95	1.50	1.38
5	B	902	D71	C41-C40	6.07	1.51	1.38
5	C	903	D71	C39-C22	7.59	1.48	1.38
5	B	902	D71	C39-C22	7.77	1.48	1.38
5	D	904	D71	C39-C22	7.78	1.48	1.38
5	A	901	D71	C39-C22	8.17	1.49	1.38
5	D	904	D71	C2-C3	10.04	1.50	1.40
5	B	902	D71	C2-C3	10.26	1.51	1.40
5	C	903	D71	C2-C3	10.42	1.51	1.40
5	A	901	D71	C2-C3	10.73	1.51	1.40

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	904	D71	C24-C26-C28	-3.52	113.84	120.42
5	A	901	D71	C24-C26-C28	-3.39	114.07	120.42
5	B	902	D71	C24-C26-C28	-3.37	114.11	120.42
5	B	902	D71	C2-C3-N4	-3.23	119.49	124.76
5	C	903	D71	C24-C26-C28	-3.21	114.42	120.42
5	C	903	D71	C2-C3-N4	-3.01	119.86	124.76
5	D	904	D71	C2-C3-N4	-2.98	119.91	124.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	901	D71	C2-C3-N4	-2.79	120.22	124.76
5	B	902	D71	C6-C5-N4	-2.61	119.93	123.93
5	C	903	D71	C32-C31-N30	-2.59	119.11	123.63
5	D	904	D71	C26-C24-N15	-2.56	108.56	112.62
5	D	904	D71	C6-C5-N4	-2.48	120.12	123.93
5	C	903	D71	C43-C22-C39	-2.38	119.19	121.55
5	B	902	D71	C41-C40-C39	-2.35	117.05	120.08
5	A	901	D71	C6-C5-N4	-2.31	120.39	123.93
5	B	902	D71	C32-C31-N30	-2.28	119.65	123.63
5	D	904	D71	C32-C31-N30	-2.27	119.67	123.63
5	A	901	D71	C32-C31-N30	-2.26	119.68	123.63
5	D	904	D71	C28-C29-N30	-2.20	119.80	123.63
5	C	903	D71	C6-C5-N4	-2.10	120.70	123.93
5	D	904	D71	C28-C26-C32	2.11	121.50	118.16
5	C	903	D71	C24-C26-C32	2.11	124.36	120.42
5	D	904	D71	O56-N54-C40	2.15	122.22	118.80
5	A	901	D71	C39-C40-N54	2.19	120.69	118.81
5	C	903	D71	O56-N54-C40	2.20	122.31	118.80
5	D	904	D71	C24-C26-C32	2.24	124.60	120.42
5	A	901	D71	C29-N30-C31	2.28	122.33	116.83
5	C	903	D71	C29-N30-C31	2.30	122.36	116.83
5	B	902	D71	C24-C26-C32	2.34	124.79	120.42
5	B	902	D71	C29-N30-C31	2.47	122.79	116.83
5	A	901	D71	C24-C26-C32	2.50	125.08	120.42
5	D	904	D71	C29-N30-C31	2.59	123.06	116.83
5	A	901	D71	C41-C40-N54	2.79	121.54	119.41
5	C	903	D71	C41-C40-N54	3.23	121.87	119.41
5	D	904	D71	C41-C40-N54	3.41	122.01	119.41
5	C	903	D71	C5-N4-C3	3.70	121.83	116.80
5	A	901	D71	C5-N4-C3	3.71	121.84	116.80
5	D	904	D71	C5-N4-C3	4.08	122.34	116.80
5	B	902	D71	C5-N4-C3	4.33	122.69	116.80
5	B	902	D71	C41-C40-N54	4.50	122.84	119.41
5	A	901	D71	C2-C16-N15	4.73	119.38	116.15
5	C	903	D71	C2-C16-N15	4.76	119.40	116.15
5	D	904	D71	C2-C16-N15	5.43	119.86	116.15
5	B	902	D71	C2-C16-N15	5.99	120.24	116.15

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	5	EOH	2	0
5	A	901	D71	3	0
6	B	10	EOH	1	0
6	B	11	EOH	2	0
4	B	4	SO4	2	0
5	B	902	D71	6	0
5	C	903	D71	2	0
6	D	7	EOH	2	0
5	D	904	D71	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	331/381 (86%)	0.22	18 (5%) 26 30	13, 22, 48, 61	0
1	B	326/381 (85%)	0.03	8 (2%) 58 62	14, 26, 41, 65	0
1	C	327/381 (85%)	0.19	20 (6%) 22 25	13, 24, 53, 67	0
1	D	334/381 (87%)	0.04	11 (3%) 47 50	13, 22, 41, 65	0
All	All	1318/1524 (86%)	0.12	57 (4%) 36 39	13, 23, 46, 67	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	245	ILE	7.6
1	C	460	SER	7.3
1	A	460	SER	6.3
1	C	461	SER	6.1
1	A	578	GLN	5.9
1	B	254	GLN	5.2
1	D	253	GLU	5.2
1	A	577	PRO	5.2
1	C	462	GLY	5.0
1	D	248	PHE	4.9
1	A	461	SER	4.9
1	C	459	THR	4.8
1	A	459	THR	4.7
1	C	254	GLN	4.6
1	A	465	LEU	4.2
1	B	253	GLU	4.0
1	C	458	VAL	4.0
1	A	576	ILE	3.9
1	A	458	VAL	3.7
1	C	465	LEU	3.6
1	C	541	TYR	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	462	GLY	3.5
1	C	463	VAL	3.4
1	C	577	PRO	3.4
1	C	578	GLN	3.3
1	C	457	LYS	3.3
1	B	256	ASP	3.3
1	C	252	THR	3.2
1	A	467	ASP	3.2
1	B	255	GLU	3.2
1	C	576	ILE	3.1
1	C	253	GLU	3.1
1	D	578	GLN	3.1
1	A	529	ALA	3.1
1	D	251	LYS	3.1
1	D	541	TYR	3.1
1	A	248	PHE	3.0
1	D	256	ASP	3.0
1	D	260	LYS	2.8
1	A	454	GLU	2.7
1	D	252	THR	2.7
1	D	246	PRO	2.7
1	B	528	ASN	2.6
1	A	457	LYS	2.5
1	C	464	LEU	2.4
1	C	255	GLU	2.4
1	B	260	LYS	2.4
1	A	541	TYR	2.4
1	C	528	ASN	2.3
1	C	575	THR	2.3
1	A	250	VAL	2.2
1	D	247	ARG	2.2
1	B	575	THR	2.1
1	C	454	GLU	2.1
1	B	578	GLN	2.0
1	A	453	VAL	2.0
1	A	528	ASN	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	EOH	A	5	3/3	0.81	0.27	10.39	19,19,23,23	0
6	EOH	A	12	3/3	0.91	0.28	7.19	31,31,31,32	0
6	EOH	A	9	3/3	0.93	0.18	6.29	24,24,25,25	0
6	EOH	B	11	3/3	0.83	0.22	6.20	24,24,26,26	0
6	EOH	D	7	3/3	0.89	0.25	5.22	19,19,21,21	0
5	D71	B	902	28/28	0.85	0.20	4.87	41,42,45,47	0
6	EOH	B	8	3/3	0.90	0.17	4.52	30,30,31,31	0
5	D71	A	901	28/28	0.84	0.18	3.84	35,37,40,44	0
6	EOH	B	10	3/3	0.90	0.19	3.44	24,24,26,27	0
4	SO4	B	4	5/5	0.93	0.26	3.32	56,56,59,59	0
5	D71	C	903	28/28	0.90	0.17	3.10	30,31,34,40	0
6	EOH	C	6	3/3	0.89	0.22	3.06	25,25,26,26	0
4	SO4	C	2	5/5	0.88	0.21	1.95	46,52,54,54	0
5	D71	D	904	28/28	0.91	0.13	1.34	27,28,32,36	0
4	SO4	A	3	5/5	0.96	0.13	0.55	34,39,42,42	0
3	MG	B	804	1/1	0.98	0.06	-2.04	25,25,25,25	0
3	MG	D	808	1/1	0.99	0.08	-2.24	22,22,22,22	0
3	MG	C	806	1/1	0.99	0.07	-2.43	23,23,23,23	0
3	MG	A	802	1/1	0.98	0.06	-2.52	25,25,25,25	0
2	ZN	A	801	1/1	1.00	0.05	-2.77	24,24,24,24	0
2	ZN	C	805	1/1	1.00	0.04	-3.61	24,24,24,24	0
2	ZN	B	803	1/1	1.00	0.03	-4.35	26,26,26,26	0
2	ZN	D	807	1/1	1.00	0.05	-6.30	23,23,23,23	0

6.5 Other polymers ⓘ

There are no such residues in this entry.