



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:03 AM GMT

PDB ID : 2VP9
Title : STRUCTURAL STUDIES OF NUCLEOSIDE ANALOG AND FEEDBACK
INHIBITOR BINDING TO DROSOPHILA MELANOGASTER MULTISUB-
STRATE DEOXYRIBONUCLEOSIDE KINASE
Authors : Mikkelsen, N.E.; Munch-Petersen, B.; Eklund, H.
Deposited on : 2008-02-27
Resolution : 2.90 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 (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

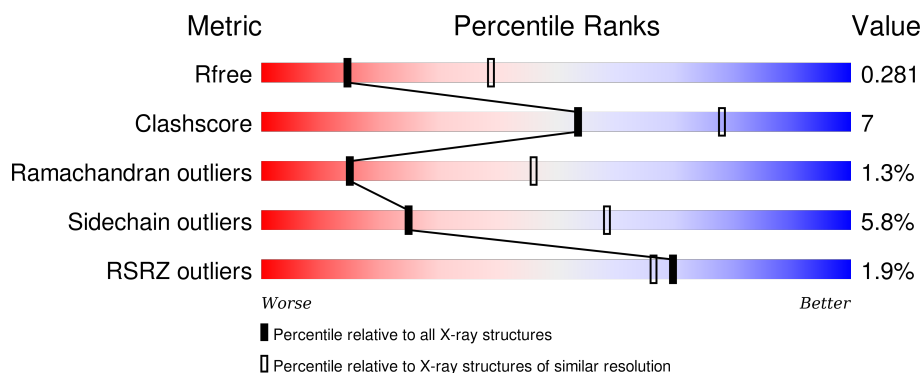
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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	230	<div> <div></div> <div>67% 15% • 14%</div> </div>
1	B	230	<div> <div>2%</div> <div>70% 10% • 17%</div> </div>
1	C	230	<div> <div>2%</div> <div>73% 10% • 14%</div> </div>
1	D	230	<div> <div>2%</div> <div>66% 14% • 17%</div> </div>
1	E	230	<div> <div>%</div> <div>67% 14% • 17%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	230	
1	G	230	
1	H	230	

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
2	SO4	A	1210	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13119 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 DEOXYNUCLEOSIDE KINASE.

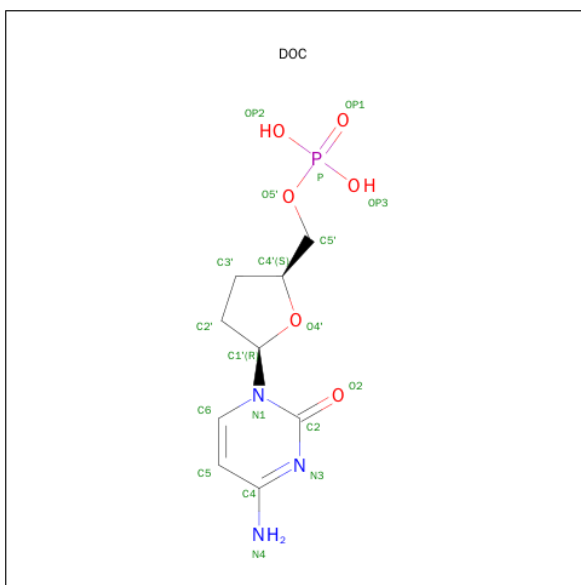
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	197	Total	C	N	O	S	0	0	0
			1640	1046	282	302	10			
1	B	192	Total	C	N	O	S	0	0	0
			1596	1021	270	295	10			
1	C	197	Total	C	N	O	S	0	0	0
			1640	1046	282	302	10			
1	D	191	Total	C	N	O	S	0	0	0
			1587	1016	268	293	10			
1	E	192	Total	C	N	O	S	0	0	0
			1596	1021	270	295	10			
1	F	192	Total	C	N	O	S	0	0	0
			1596	1021	270	295	10			
1	G	192	Total	C	N	O	S	0	0	0
			1596	1021	270	295	10			
1	H	192	Total	C	N	O	S	0	0	0
			1596	1021	270	295	10			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is 2',3'-DIDEOXYCYTIDINE-5'-MONOPHOSPHATE (three-letter code: DOC) (formula: C₉H₁₄N₃O₆P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			15	9	3	3		
3	B	1	Total	C	N	O	0	0
			15	9	3	3		
3	C	1	Total	C	N	O	0	0
			15	9	3	3		
3	D	1	Total	C	N	O	0	0
			15	9	3	3		
3	E	1	Total	C	N	O	0	0
			15	9	3	3		
3	F	1	Total	C	N	O	0	0
			15	9	3	3		
3	G	1	Total	C	N	O	0	0
			15	9	3	3		
3	H	1	Total	C	N	O	0	0
			15	9	3	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	21	Total	O	0	0
			21	21		
4	B	11	Total	O	0	0
			11	11		
4	C	9	Total	O	0	0
			9	9		
4	D	13	Total	O	0	0
			13	13		

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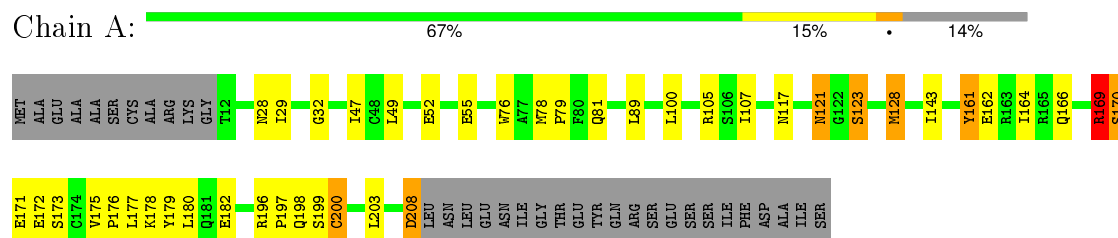
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	16	Total 16	O 16	0	0
4	F	11	Total 11	O 11	0	0
4	G	9	Total 9	O 9	0	0
4	H	17	Total 17	O 17	0	0

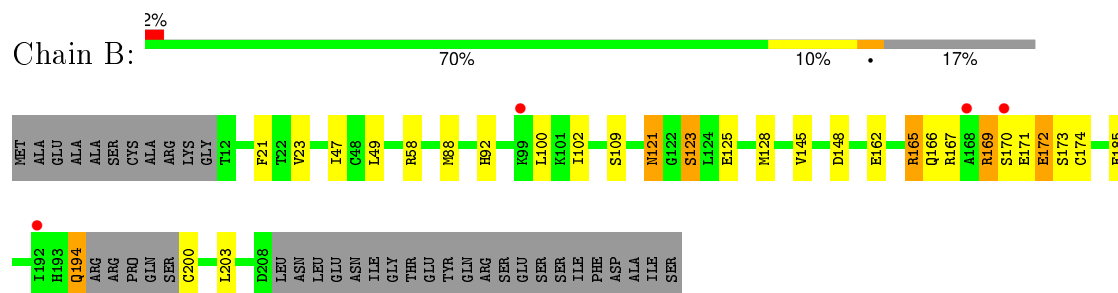
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

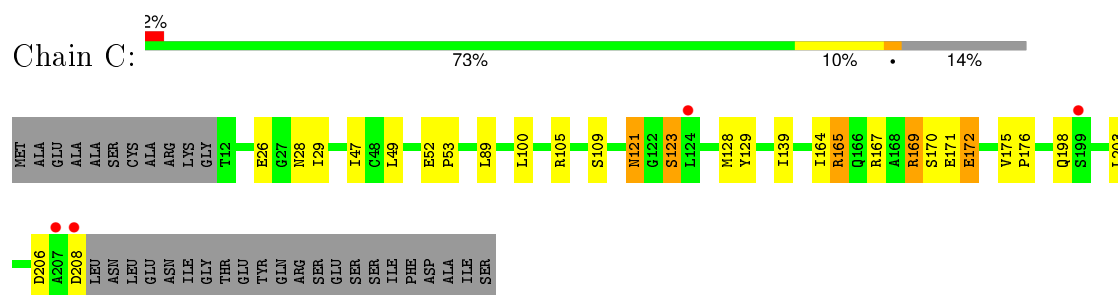
• Molecule 1: DEOXYNUCLEOSIDE KINASE



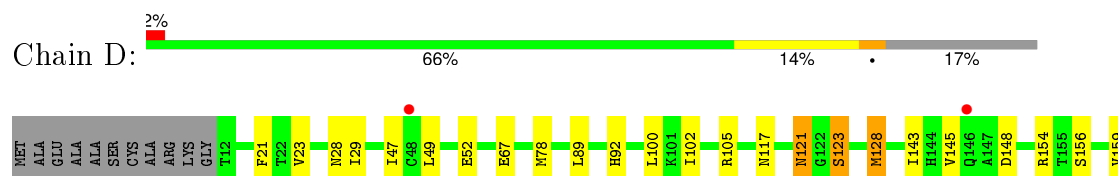
• Molecule 1: DEOXYNUCLEOSIDE KINASE

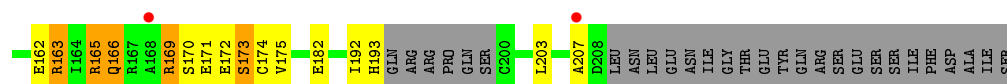


• Molecule 1: DEOXYNUCLEOSIDE KINASE



• Molecule 1: DEOXYNUCLEOSIDE KINASE

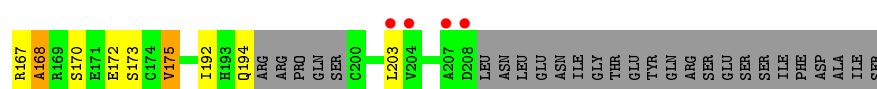




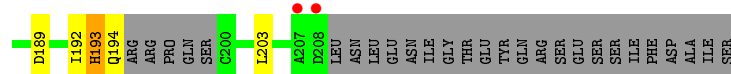
• Molecule 1: DEOXYNUCLEOSIDE KINASE



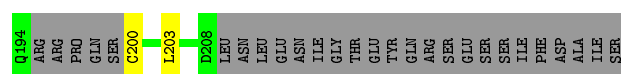
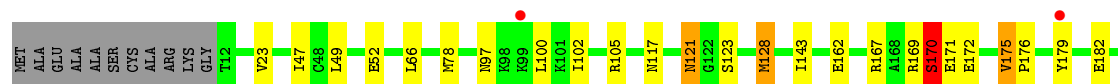
• Molecule 1: DEOXYNUCLEOSIDE KINASE



• Molecule 1: DEOXYNUCLEOSIDE KINASE



• Molecule 1: DEOXYNUCLEOSIDE KINASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.50Å 70.82Å 226.03Å 90.00° 90.10° 90.00°	Depositor
Resolution (Å)	30.00 – 2.90 29.88 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.0 (30.00-2.90) 96.6 (29.88-2.90)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.45 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.248 , 0.287 0.244 , 0.281	Depositor DCC
R_{free} test set	2468 reflections (5.37%)	DCC
Wilson B-factor (Å ²)	56.4	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 12.4	EDS
Estimated twinning fraction	0.034 for -k,-h,-l 0.048 for k,h,-l 0.126 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	1 of 48406 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	13119	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.47% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DOC, 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	0.71	0/1678	0.72	0/2268
1	B	0.71	2/1632 (0.1%)	0.69	0/2205
1	C	0.67	0/1678	0.68	0/2268
1	D	0.71	0/1623	0.72	1/2193 (0.0%)
1	E	0.66	0/1632	0.68	0/2205
1	F	0.68	0/1632	0.70	0/2205
1	G	0.69	0/1632	0.70	0/2205
1	H	0.67	0/1632	0.70	0/2205
All	All	0.69	2/13139 (0.0%)	0.70	1/17754 (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
1	H	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	174	CYS	CB-SG	-6.29	1.71	1.82
1	B	185	GLU	CG-CD	5.14	1.59	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	154	ARG	NE-CZ-NH2	-5.07	117.77	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	169	ARG	Peptide
1	H	170	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	1640	0	1629	28	0
1	B	1596	0	1582	25	0
1	C	1640	0	1629	20	0
1	D	1587	0	1574	19	0
1	E	1596	0	1582	34	0
1	F	1596	0	1582	20	0
1	G	1596	0	1582	14	0
1	H	1596	0	1582	14	0
2	A	10	0	0	3	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	1	0
2	G	5	0	0	1	0
2	H	5	0	0	0	0
3	A	15	0	12	1	0
3	B	15	0	12	1	0
3	C	15	0	12	1	0
3	D	15	0	12	0	0
3	E	15	0	12	0	0
3	F	15	0	12	1	0
3	G	15	0	12	0	0
3	H	15	0	12	0	0
4	A	21	0	0	4	0
4	B	11	0	0	3	0
4	C	9	0	0	2	0
4	D	13	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	16	0	0	6	0
4	F	11	0	0	3	0
4	G	9	0	0	1	0
4	H	17	0	0	3	0
All	All	13119	0	12838	169	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 7.

All (169) 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:E:121:ASN:HB3	4:E:2013:HOH:O	1.46	1.15
1:D:165:ARG:HD2	4:D:2010:HOH:O	1.52	1.08
1:E:169:ARG:HD3	1:E:170:SER:H	1.22	1.01
1:G:169:ARG:HD3	1:G:170:SER:H	1.25	1.00
1:A:208:ASP:HA	4:A:2020:HOH:O	1.63	0.98
1:B:169:ARG:HH11	1:B:169:ARG:HG2	1.31	0.95
1:A:198:GLN:NE2	1:A:199:SER:O	2.07	0.88
1:E:169:ARG:HD3	1:E:170:SER:N	1.90	0.85
1:D:174:CYS:HB3	4:D:2011:HOH:O	1.77	0.82
1:B:169:ARG:HH11	1:B:169:ARG:CG	1.94	0.79
1:B:169:ARG:NH1	1:B:169:ARG:HG2	1.96	0.76
1:E:42:LYS:HG2	4:E:2005:HOH:O	1.87	0.74
1:B:169:ARG:NH2	1:B:171:GLU:H	1.88	0.71
1:A:169:ARG:NH1	2:A:1210:SO4:O3	2.24	0.70
1:B:194:GLN:HE21	1:B:194:GLN:HA	1.55	0.70
1:G:169:ARG:HD2	1:G:172:GLU:H	1.56	0.69
1:D:169:ARG:HD3	1:D:170:SER:H	1.56	0.69
1:H:175:VAL:HB	1:H:179:TYR:CD2	2.30	0.67
1:D:67:GLU:HG3	4:D:2005:HOH:O	1.93	0.66
1:E:16:GLU:HG3	4:E:2001:HOH:O	1.97	0.65
1:G:169:ARG:HD3	1:G:170:SER:N	2.07	0.63
1:D:172:GLU:O	1:D:174:CYS:N	2.31	0.63
1:G:32:GLY:N	2:G:1209:SO4:O1	2.31	0.62
1:B:47:ILE:HG12	1:B:100:LEU:HD23	1.82	0.62
1:E:58:ARG:NH2	1:E:169:ARG:HH21	1.96	0.62
1:B:121:ASN:ND2	1:B:123:SER:OG	2.33	0.62
1:B:88:MET:HE3	4:B:2003:HOH:O	2.00	0.62
1:H:97:ASN:HB2	4:H:2009:HOH:O	2.00	0.61
1:B:125:GLU:HG2	4:B:2006:HOH:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:163:ARG:NH2	1:D:207:ALA:O	2.29	0.61
1:A:161:TYR:C	1:A:161:TYR:CD2	2.74	0.60
1:B:88:MET:CE	4:B:2003:HOH:O	2.49	0.60
1:A:47:ILE:HG12	1:A:100:LEU:HD23	1.83	0.60
1:E:159:VAL:HG21	1:E:208:ASP:OD2	2.02	0.59
1:F:47:ILE:HG12	1:F:100:LEU:HD23	1.85	0.59
1:D:28:ASN:OD1	1:D:29:ILE:N	2.36	0.59
1:A:169:ARG:O	1:A:173:SER:OG	2.21	0.58
1:A:164:ILE:HD12	1:A:180:LEU:HD11	1.86	0.58
1:E:172:GLU:O	1:E:175:VAL:HG22	2.04	0.58
1:B:169:ARG:HH21	1:B:171:GLU:H	1.50	0.57
1:C:121:ASN:ND2	1:C:123:SER:OG	2.38	0.57
1:E:121:ASN:ND2	1:E:123:SER:OG	2.38	0.57
1:G:47:ILE:HG12	1:G:100:LEU:HD23	1.88	0.56
1:F:94:ALA:HB3	4:F:2004:HOH:O	2.06	0.56
1:B:169:ARG:CD	1:B:170:SER:H	2.19	0.55
1:C:47:ILE:HG12	1:C:100:LEU:HD23	1.87	0.55
1:G:16:GLU:HA	1:G:144:HIS:CD2	2.41	0.55
1:G:44:LYS:HD3	4:G:2001:HOH:O	2.06	0.55
1:A:178:LYS:HE3	4:A:2016:HOH:O	2.06	0.55
1:C:165:ARG:HH11	1:E:165:ARG:HH11	1.54	0.54
1:B:171:GLU:C	1:B:173:SER:H	2.11	0.54
1:A:121:ASN:ND2	1:A:123:SER:OG	2.41	0.53
1:D:121:ASN:ND2	1:D:123:SER:OG	2.41	0.53
1:H:162:GLU:HG2	4:H:2012:HOH:O	2.09	0.53
1:F:56:LYS:HE2	4:F:2001:HOH:O	2.08	0.53
1:F:92:HIS:CG	1:F:145:VAL:HG13	2.44	0.53
1:G:52:GLU:OE2	1:G:105:ARG:HD2	2.09	0.52
1:E:172:GLU:O	1:E:173:SER:C	2.48	0.52
1:A:161:TYR:HD2	1:A:161:TYR:C	2.12	0.52
1:D:47:ILE:HG12	1:D:100:LEU:HD23	1.89	0.52
1:F:21:PHE:HA	1:F:148:ASP:OD2	2.10	0.52
1:F:172:GLU:O	1:F:175:VAL:HG13	2.10	0.52
1:F:52:GLU:OE2	1:F:105:ARG:HD2	2.10	0.52
1:H:47:ILE:HG12	1:H:100:LEU:HD23	1.91	0.51
1:H:121:ASN:HD22	1:H:121:ASN:C	2.14	0.51
1:C:165:ARG:NH1	1:E:165:ARG:HD3	2.26	0.51
1:H:172:GLU:O	1:H:175:VAL:HG13	2.11	0.51
1:D:89:LEU:HD22	1:D:143:ILE:HG21	1.92	0.51
1:E:206:ASP:OD2	1:E:208:ASP:HB2	2.11	0.51
1:F:121:ASN:ND2	1:F:123:SER:OG	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:121:ASN:HD22	1:C:121:ASN:C	2.15	0.50
1:A:52:GLU:OE2	1:A:105:ARG:HD2	2.10	0.50
1:D:162:GLU:O	1:D:166:GLN:HG2	2.11	0.50
1:E:58:ARG:HE	1:E:171:GLU:CD	2.15	0.50
1:A:162:GLU:O	1:A:166:GLN:HG2	2.11	0.50
1:D:92:HIS:CG	1:D:145:VAL:HG13	2.46	0.50
1:D:52:GLU:OE2	1:D:105:ARG:HD2	2.12	0.50
1:E:47:ILE:HG12	1:E:100:LEU:HD23	1.93	0.50
1:A:32:GLY:N	2:A:1209:SO4:O2	2.37	0.50
1:C:52:GLU:OE2	1:C:105:ARG:HD2	2.12	0.50
1:F:121:ASN:HD22	1:F:121:ASN:C	2.15	0.49
1:A:169:ARG:HD2	2:A:1210:SO4:O3	2.12	0.49
1:F:192:ILE:O	1:F:194:GLN:N	2.45	0.49
1:E:170:SER:O	1:E:173:SER:OG	2.24	0.49
1:E:86:LEU:HD11	1:F:138:PHE:CB	2.43	0.49
1:A:117:ASN:HD21	1:A:182:GLU:HB3	1.77	0.48
1:A:161:TYR:CD2	1:A:161:TYR:O	2.66	0.48
1:H:167:ARG:NH2	1:H:172:GLU:OE1	2.46	0.48
1:B:194:GLN:NE2	1:B:194:GLN:HA	2.27	0.47
1:B:169:ARG:NH1	1:B:169:ARG:CG	2.63	0.47
1:H:23:VAL:HB	1:H:102:ILE:HG12	1.97	0.47
1:D:117:ASN:HD21	1:D:182:GLU:HB3	1.79	0.47
1:C:164:ILE:HG23	1:C:167:ARG:HH21	1.79	0.47
1:A:161:TYR:CD1	1:A:177:LEU:HB2	2.50	0.47
1:A:89:LEU:HD22	1:A:143:ILE:HG21	1.96	0.47
1:C:172:GLU:O	1:C:175:VAL:HG13	2.15	0.47
1:D:21:PHE:HA	1:D:148:ASP:OD2	2.15	0.47
1:H:170:SER:C	4:H:2013:HOH:O	2.53	0.47
1:A:178:LYS:CE	4:A:2016:HOH:O	2.63	0.47
1:E:58:ARG:CZ	1:E:169:ARG:HH21	2.27	0.46
1:G:121:ASN:C	1:G:121:ASN:HD22	2.18	0.46
1:F:23:VAL:HB	1:F:102:ILE:HG12	1.97	0.46
1:H:175:VAL:HA	1:H:176:PRO:HD3	1.46	0.46
1:E:156:SER:OG	1:E:159:VAL:HG23	2.15	0.46
1:B:169:ARG:NE	1:B:170:SER:H	2.14	0.46
1:G:28:ASN:OD1	1:G:29:ILE:N	2.46	0.46
1:G:192:ILE:HG22	1:G:193:HIS:ND1	2.31	0.46
1:E:172:GLU:H	1:E:172:GLU:CD	2.19	0.46
1:B:58:ARG:HE	1:B:171:GLU:CD	2.18	0.46
1:F:140:GLU:HA	4:F:2008:HOH:O	2.16	0.45
1:C:129:TYR:HE1	4:C:2005:HOH:O	2.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:167:ARG:O	1:F:168:ALA:C	2.54	0.45
1:D:172:GLU:C	1:D:174:CYS:H	2.17	0.45
1:E:193:HIS:HE1	4:E:2014:HOH:O	1.99	0.45
1:A:81:GLN:HE22	3:A:1211:DOC:HN41	1.64	0.45
1:G:189:ASP:HA	1:G:193:HIS:HB2	1.98	0.45
1:C:206:ASP:OD2	1:C:208:ASP:HB2	2.17	0.45
1:B:92:HIS:CG	1:B:145:VAL:HG13	2.51	0.45
1:B:121:ASN:HD22	1:B:121:ASN:C	2.20	0.44
1:B:23:VAL:HB	1:B:102:ILE:HG12	2.00	0.44
1:B:172:GLU:HB3	3:B:1210:DOC:H3'2	2.00	0.44
1:A:78:MET:HB2	1:A:128:MET:HG2	2.00	0.44
1:H:66:LEU:HG	1:H:171:GLU:HG2	2.00	0.44
1:E:52:GLU:HA	1:E:53:PRO:HD3	1.85	0.44
1:A:55:GLU:HB2	4:A:2002:HOH:O	2.18	0.44
1:E:52:GLU:HB3	4:E:2007:HOH:O	2.18	0.44
1:C:26:GLU:OE2	1:C:109:SER:HB3	2.18	0.43
1:A:175:VAL:HB	1:A:179:TYR:CD2	2.53	0.43
1:D:156:SER:OG	1:D:159:VAL:HG23	2.17	0.43
1:B:58:ARG:HH21	1:B:169:ARG:HH22	1.66	0.43
1:F:156:SER:OG	1:F:159:VAL:HG23	2.18	0.43
1:B:21:PHE:HA	1:B:148:ASP:OD2	2.18	0.43
1:D:78:MET:HB2	1:D:128:MET:HG2	2.00	0.43
1:E:121:ASN:HD22	1:E:121:ASN:C	2.21	0.43
1:G:121:ASN:ND2	1:G:123:SER:OG	2.51	0.43
1:F:167:ARG:NH2	2:F:1209:SO4:O1	2.42	0.43
1:C:175:VAL:HA	1:C:176:PRO:HD3	1.81	0.43
1:E:21:PHE:HA	1:E:148:ASP:OD2	2.18	0.43
1:H:78:MET:HB2	1:H:128:MET:HG2	2.01	0.43
1:C:52:GLU:OE1	3:C:1210:DOC:O5'	2.36	0.43
1:E:25:ILE:HG13	1:E:37:LEU:HD21	2.01	0.43
1:F:70:TYR:OH	3:F:1210:DOC:H2''	2.18	0.43
1:E:52:GLU:OE2	1:E:105:ARG:HD2	2.19	0.43
1:C:89:LEU:HD11	1:C:139:ILE:HG12	2.01	0.43
1:D:23:VAL:HB	1:D:102:ILE:HG12	2.01	0.42
1:E:80:PHE:O	1:E:84:VAL:HG23	2.20	0.42
1:A:121:ASN:HD22	1:A:121:ASN:C	2.22	0.42
1:H:52:GLU:OE2	1:H:105:ARG:HD2	2.19	0.42
1:C:28:ASN:OD1	1:C:29:ILE:N	2.51	0.42
1:E:175:VAL:HA	1:E:176:PRO:HD3	1.87	0.42
1:B:165:ARG:NH2	1:B:173:SER:O	2.52	0.42
1:A:28:ASN:OD1	1:A:29:ILE:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:GLU:C	1:B:173:SER:N	2.73	0.42
1:C:53:PRO:HG3	4:C:2003:HOH:O	2.19	0.42
1:G:78:MET:HB2	1:G:128:MET:HG2	2.01	0.41
1:E:86:LEU:HD11	1:F:138:PHE:HB2	2.01	0.41
1:A:175:VAL:HA	1:A:176:PRO:HD3	1.63	0.41
1:E:172:GLU:O	1:E:175:VAL:N	2.52	0.41
1:C:165:ARG:NH1	1:E:165:ARG:HH11	2.17	0.41
1:C:172:GLU:O	1:C:175:VAL:HG22	2.19	0.41
1:F:162:GLU:HG3	1:F:166:GLN:HE21	1.86	0.41
1:A:89:LEU:HG	1:A:107:ILE:HD12	2.02	0.41
1:C:89:LEU:HA	1:C:89:LEU:HD23	1.98	0.41
1:C:52:GLU:HA	1:C:53:PRO:HD3	1.89	0.41
1:E:58:ARG:NH2	1:E:169:ARG:HE	2.19	0.40
1:E:67:GLU:HG3	4:E:2010:HOH:O	2.21	0.40
1:F:52:GLU:HA	1:F:53:PRO:HD3	1.90	0.40
1:H:117:ASN:HD21	1:H:182:GLU:HB3	1.87	0.40
1:A:76:TRP:HA	1:A:79:PRO:HG2	2.02	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	195/230 (85%)	180 (92%)	10 (5%)	5 (3%)	7	26
1	B	188/230 (82%)	169 (90%)	17 (9%)	2 (1%)	17	51
1	C	195/230 (85%)	176 (90%)	16 (8%)	3 (2%)	13	42
1	D	187/230 (81%)	174 (93%)	11 (6%)	2 (1%)	17	51
1	E	188/230 (82%)	174 (93%)	11 (6%)	3 (2%)	12	40
1	F	188/230 (82%)	172 (92%)	14 (7%)	2 (1%)	17	51
1	G	188/230 (82%)	176 (94%)	11 (6%)	1 (0%)	34	71

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	188/230 (82%)	174 (93%)	12 (6%)	2 (1%)	17	51
All	All	1517/1840 (82%)	1395 (92%)	102 (7%)	20 (1%)	15	46

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	171	GLU
1	C	198	GLN
1	D	173	SER
1	E	174	CYS
1	F	173	SER
1	A	170	SER
1	A	200	CYS
1	C	169	ARG
1	F	168	ALA
1	G	92	HIS
1	A	169	ARG
1	E	173	SER
1	H	169	ARG
1	B	166	GLN
1	B	167	ARG
1	C	170	SER
1	D	171	GLU
1	E	170	SER
1	H	170	SER
1	A	197	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	A	182/208 (88%)	171 (94%)	11 (6%)	24	57
1	B	177/208 (85%)	165 (93%)	12 (7%)	20	49
1	C	182/208 (88%)	173 (95%)	9 (5%)	31	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	176/208 (85%)	163 (93%)	13 (7%)	17	44
1	E	177/208 (85%)	169 (96%)	8 (4%)	34	70
1	F	177/208 (85%)	170 (96%)	7 (4%)	38	74
1	G	177/208 (85%)	163 (92%)	14 (8%)	15	41
1	H	177/208 (85%)	169 (96%)	8 (4%)	34	70
All	All	1425/1664 (86%)	1343 (94%)	82 (6%)	25	58

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	LEU
1	A	121	ASN
1	A	123	SER
1	A	128	MET
1	A	161	TYR
1	A	170	SER
1	A	172	GLU
1	A	196	ARG
1	A	200	CYS
1	A	203	LEU
1	A	208	ASP
1	B	49	LEU
1	B	109	SER
1	B	121	ASN
1	B	123	SER
1	B	128	MET
1	B	162	GLU
1	B	165	ARG
1	B	169	ARG
1	B	172	GLU
1	B	194	GLN
1	B	200	CYS
1	B	203	LEU
1	C	49	LEU
1	C	121	ASN
1	C	123	SER
1	C	128	MET
1	C	165	ARG
1	C	169	ARG
1	C	171	GLU

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Mol	Chain	Res	Type
1	C	172	GLU
1	C	203	LEU
1	D	49	LEU
1	D	121	ASN
1	D	123	SER
1	D	128	MET
1	D	163	ARG
1	D	165	ARG
1	D	166	GLN
1	D	169	ARG
1	D	173	SER
1	D	175	VAL
1	D	192	ILE
1	D	193	HIS
1	D	203	LEU
1	E	49	LEU
1	E	121	ASN
1	E	123	SER
1	E	128	MET
1	E	167	ARG
1	E	169	ARG
1	E	194	GLN
1	E	203	LEU
1	F	49	LEU
1	F	121	ASN
1	F	123	SER
1	F	128	MET
1	F	170	SER
1	F	175	VAL
1	F	203	LEU
1	G	49	LEU
1	G	109	SER
1	G	121	ASN
1	G	123	SER
1	G	128	MET
1	G	145	VAL
1	G	165	ARG
1	G	169	ARG
1	G	170	SER
1	G	171	GLU
1	G	172	GLU
1	G	193	HIS

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Mol	Chain	Res	Type
1	G	194	GLN
1	G	203	LEU
1	H	49	LEU
1	H	121	ASN
1	H	123	SER
1	H	128	MET
1	H	143	ILE
1	H	175	VAL
1	H	200	CYS
1	H	203	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	GLN
1	A	117	ASN
1	A	121	ASN
1	A	166	GLN
1	B	81	GLN
1	B	117	ASN
1	B	121	ASN
1	B	194	GLN
1	C	81	GLN
1	C	117	ASN
1	C	121	ASN
1	C	198	GLN
1	D	81	GLN
1	D	117	ASN
1	D	121	ASN
1	E	81	GLN
1	E	117	ASN
1	E	121	ASN
1	E	193	HIS
1	F	81	GLN
1	F	117	ASN
1	F	121	ASN
1	G	81	GLN
1	G	117	ASN
1	G	121	ASN
1	G	130	ASN
1	G	194	GLN
1	H	81	GLN

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Mol	Chain	Res	Type
1	H	117	ASN
1	H	121	ASN

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 ⓘ

17 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	$\# Z > 2$
2	SO4	A	1209	-	4,4,4	0.25	0	6,6,6	0.82	0
2	SO4	A	1210	-	4,4,4	0.34	0	6,6,6	0.27	0
3	DOC	A	1211	-	12,16,20	0.48	0	15,22,29	1.85	5 (33%)
2	SO4	B	1209	-	4,4,4	0.40	0	6,6,6	0.74	0
3	DOC	B	1210	-	12,16,20	0.68	0	15,22,29	2.47	6 (40%)
2	SO4	C	1209	-	4,4,4	0.28	0	6,6,6	0.75	0
3	DOC	C	1210	-	12,16,20	0.67	0	15,22,29	2.50	5 (33%)
2	SO4	D	1209	-	4,4,4	0.18	0	6,6,6	0.92	1 (16%)
3	DOC	D	1210	-	12,16,20	0.57	0	15,22,29	2.50	7 (46%)
2	SO4	E	1209	-	4,4,4	0.25	0	6,6,6	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	DOC	E	1210	-	12,16,20	0.43	0	15,22,29	2.72	7 (46%)
2	SO4	F	1209	-	4,4,4	0.31	0	6,6,6	0.79	0
3	DOC	F	1210	-	12,16,20	0.76	0	15,22,29	2.49	5 (33%)
2	SO4	G	1209	-	4,4,4	0.32	0	6,6,6	0.55	0
3	DOC	G	1210	-	12,16,20	0.59	0	15,22,29	1.83	3 (20%)
2	SO4	H	1209	-	4,4,4	0.38	0	6,6,6	0.77	0
3	DOC	H	1210	-	12,16,20	0.86	0	15,22,29	1.58	4 (26%)

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
2	SO4	A	1209	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1210	-	-	0/0/0/0	0/0/0/0
3	DOC	A	1211	-	-	0/2/15/19	0/2/2/2
2	SO4	B	1209	-	-	0/0/0/0	0/0/0/0
3	DOC	B	1210	-	-	0/2/15/19	0/2/2/2
2	SO4	C	1209	-	-	0/0/0/0	0/0/0/0
3	DOC	C	1210	-	-	0/2/15/19	0/2/2/2
2	SO4	D	1209	-	-	0/0/0/0	0/0/0/0
3	DOC	D	1210	-	-	0/2/15/19	0/2/2/2
2	SO4	E	1209	-	-	0/0/0/0	0/0/0/0
3	DOC	E	1210	-	-	0/2/15/19	0/2/2/2
2	SO4	F	1209	-	-	0/0/0/0	0/0/0/0
3	DOC	F	1210	-	-	0/2/15/19	0/2/2/2
2	SO4	G	1209	-	-	0/0/0/0	0/0/0/0
3	DOC	G	1210	-	-	0/2/15/19	0/2/2/2
2	SO4	H	1209	-	-	0/0/0/0	0/0/0/0
3	DOC	H	1210	-	-	0/2/15/19	0/2/2/2

There are no bond length outliers.

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1210	DOC	C3'-C4'-C5'	-5.85	104.62	115.31
3	B	1210	DOC	C3'-C4'-C5'	-5.49	105.27	115.31
3	E	1210	DOC	C3'-C4'-C5'	-5.47	105.31	115.31
3	D	1210	DOC	C3'-C4'-C5'	-4.73	106.66	115.31
3	E	1210	DOC	C2'-C1'-N1	-4.48	103.41	112.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1210	DOC	C3'-C4'-C5'	-4.26	107.51	115.31
3	G	1210	DOC	C3'-C4'-C5'	-3.77	108.41	115.31
3	H	1210	DOC	C3'-C4'-C5'	-3.42	109.05	115.31
3	D	1210	DOC	C2'-C1'-N1	-3.17	106.06	112.49
3	A	1211	DOC	C3'-C4'-C5'	-2.83	110.13	115.31
3	B	1210	DOC	C2'-C1'-N1	-2.42	107.58	112.49
3	C	1210	DOC	O5'-C5'-C4'	-2.40	104.65	111.66
3	A	1211	DOC	C2'-C1'-N1	-2.25	107.92	112.49
3	F	1210	DOC	C5-C4-N3	-2.06	119.20	121.80
3	D	1210	DOC	C5-C4-N3	-2.04	119.23	121.80
2	D	1209	SO4	O2-S-O1	-2.00	103.16	109.50
3	A	1211	DOC	O4'-C4'-C3'	2.06	108.14	104.69
3	B	1210	DOC	C2'-C3'-C4'	2.06	106.60	102.59
3	E	1210	DOC	C2'-C3'-C4'	2.12	106.73	102.59
3	G	1210	DOC	C2'-C3'-C4'	2.19	106.85	102.59
3	D	1210	DOC	C3'-C2'-C1'	2.20	105.17	102.71
3	H	1210	DOC	O4'-C1'-C2'	2.24	109.09	106.67
3	E	1210	DOC	C3'-C2'-C1'	2.31	105.29	102.71
3	B	1210	DOC	N4-C4-N3	2.32	120.73	116.50
3	C	1210	DOC	C3'-C2'-C1'	2.53	105.53	102.71
3	H	1210	DOC	C2'-C3'-C4'	2.55	107.55	102.59
3	E	1210	DOC	O4'-C4'-C5'	2.58	113.39	109.42
3	D	1210	DOC	N4-C4-N3	2.63	121.30	116.50
3	B	1210	DOC	O4'-C1'-N1	2.82	112.59	107.72
3	H	1210	DOC	C2-N3-C4	2.85	119.63	115.61
3	E	1210	DOC	C2-N3-C4	2.91	119.71	115.61
3	F	1210	DOC	C2'-C3'-C4'	2.97	108.38	102.59
3	C	1210	DOC	O4'-C4'-C3'	3.04	109.79	104.69
3	A	1211	DOC	O4'-C1'-N1	3.26	113.36	107.72
3	G	1210	DOC	C2-N3-C4	3.48	120.53	115.61
3	A	1211	DOC	C2-N3-C4	3.59	120.67	115.61
3	D	1210	DOC	O4'-C1'-N1	3.64	114.01	107.72
3	D	1210	DOC	C2-N3-C4	3.96	121.20	115.61
3	B	1210	DOC	C2-N3-C4	4.46	121.90	115.61
3	F	1210	DOC	C2-N3-C4	4.80	122.39	115.61
3	F	1210	DOC	O4'-C1'-N1	5.03	116.43	107.72
3	C	1210	DOC	O4'-C1'-N1	5.36	116.99	107.72
3	E	1210	DOC	O4'-C1'-N1	5.46	117.17	107.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1209	SO4	1	0
2	A	1210	SO4	2	0
3	A	1211	DOC	1	0
3	B	1210	DOC	1	0
3	C	1210	DOC	1	0
2	F	1209	SO4	1	0
3	F	1210	DOC	1	0
2	G	1209	SO4	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	197/230 (85%)	0.25	0 100 100	30, 44, 59, 70	0
1	B	192/230 (83%)	0.18	4 (2%) 67 62	30, 45, 62, 72	0
1	C	197/230 (85%)	0.21	4 (2%) 68 64	30, 45, 70, 80	0
1	D	191/230 (83%)	0.20	4 (2%) 67 62	30, 45, 67, 78	0
1	E	192/230 (83%)	0.17	2 (1%) 84 82	30, 45, 66, 75	0
1	F	192/230 (83%)	0.23	5 (2%) 59 54	30, 45, 68, 79	0
1	G	192/230 (83%)	0.20	8 (4%) 40 33	30, 45, 67, 79	0
1	H	192/230 (83%)	0.30	2 (1%) 84 82	30, 43, 59, 70	0
All	All	1545/1840 (83%)	0.22	29 (1%) 70 66	30, 45, 66, 80	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	208	ASP	4.7
1	G	207	ALA	4.5
1	D	168	ALA	4.2
1	F	207	ALA	4.2
1	B	168	ALA	3.9
1	C	207	ALA	3.9
1	F	99	LYS	3.4
1	G	170	SER	3.3
1	E	168	ALA	3.1
1	B	99	LYS	2.9
1	C	208	ASP	2.9
1	D	207	ALA	2.8
1	G	30	GLY	2.8
1	C	199	SER	2.7
1	B	170	SER	2.6
1	D	48	CYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	203	LEU	2.5
1	G	124	LEU	2.5
1	H	179	TYR	2.4
1	H	99	LYS	2.3
1	E	208	ASP	2.2
1	C	124	LEU	2.2
1	G	39	HIS	2.2
1	B	192	ILE	2.1
1	F	204	VAL	2.1
1	G	97	ASN	2.1
1	G	99	LYS	2.1
1	F	208	ASP	2.1
1	D	146	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no 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
3	DOC	A	1211	15/19	0.95	0.23	0.14	22,27,30,31	0
3	DOC	B	1210	15/19	0.96	0.21	0.07	34,37,39,40	0
3	DOC	D	1210	15/19	0.96	0.20	-0.26	36,39,40,42	0
2	SO4	B	1209	5/5	0.99	0.17	-0.57	29,33,35,35	0
3	DOC	G	1210	15/19	0.96	0.19	-0.57	38,40,42,44	0
3	DOC	C	1210	15/19	0.95	0.18	-0.76	27,29,32,33	0
2	SO4	G	1209	5/5	0.96	0.16	-0.86	45,45,48,50	0
2	SO4	D	1209	5/5	0.98	0.13	-1.05	39,39,44,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	DOC	H	1210	15/19	0.97	0.19	-1.07	22,24,25,25	0
2	SO4	C	1209	5/5	0.97	0.14	-1.12	37,40,43,43	0
3	DOC	E	1210	15/19	0.96	0.17	-1.27	31,32,34,34	0
2	SO4	E	1209	5/5	0.99	0.16	-1.30	39,39,41,42	0
2	SO4	F	1209	5/5	0.98	0.13	-1.37	40,41,42,42	0
2	SO4	A	1209	5/5	0.98	0.13	-1.44	22,24,26,27	0
3	DOC	F	1210	15/19	0.95	0.14	-1.45	33,35,38,38	0
2	SO4	H	1209	5/5	0.98	0.16	-1.52	19,21,23,26	0
2	SO4	A	1210	5/5	0.96	0.13	-	46,46,47,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.