



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:05 PM UTC

PDB ID : 7Q0N / pdb_00007q0n
Title : Arbitrium receptor from Katmira phage
Authors : Gallego del Sol, F.; Marina, A.
Deposited on : 2021-10-15
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

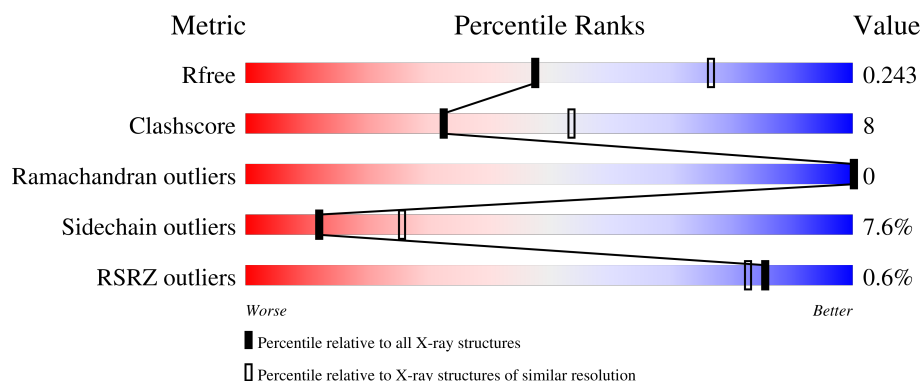
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	386	81% 17% .
1	B	386	83% 14% .
2	C	45	36% 42% 22%
3	D	45	18% 56% 27%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8310 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 Arbitrium receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	386	Total	C	N	O	S	0	1	0
			3186	2041	522	603	20			
1	B	386	Total	C	N	O	S	0	2	0
			3195	2045	521	609	20			

- Molecule 2 is a DNA chain called DNA (45-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	45	Total	C	N	O	P	0	0	0
			923	443	169	266	45			

- Molecule 3 is a DNA chain called DNA (45-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	45	Total	C	N	O	P	0	0	0
			922	444	159	274	45			

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

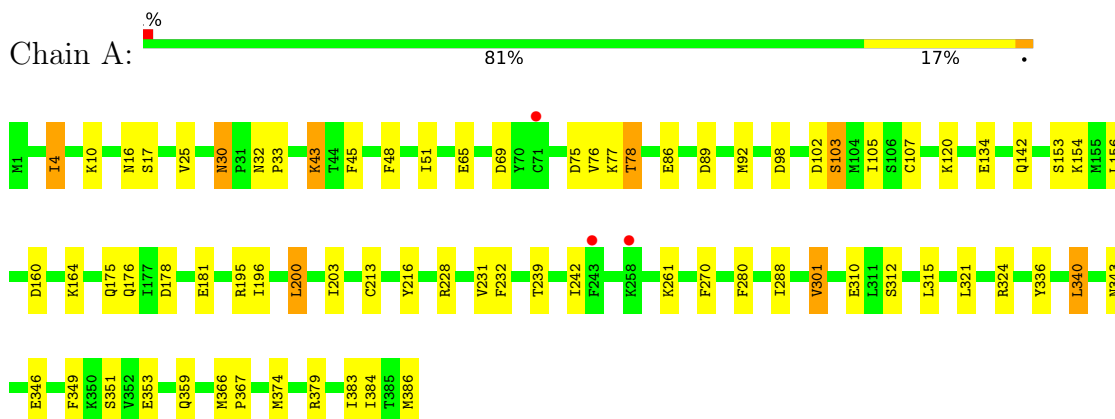
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	30	Total	O	0	0
			30	30		
5	B	18	Total	O	0	0
			18	18		
5	D	1	Total	O	0	0
			1	1		

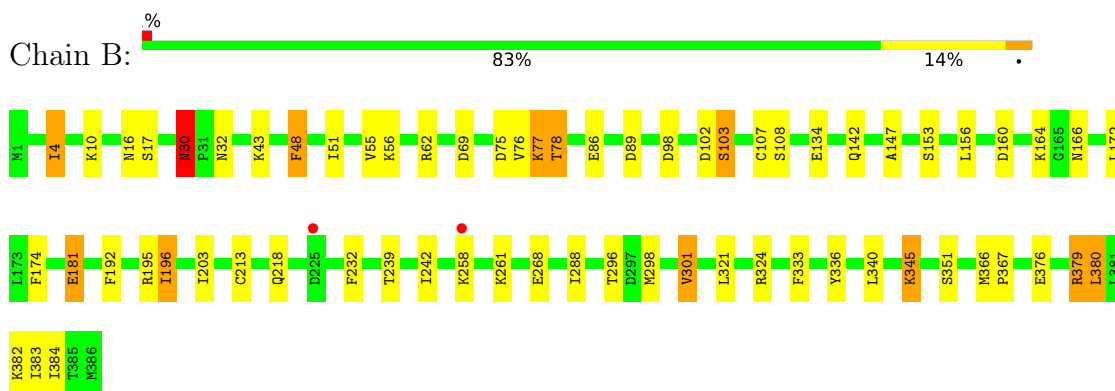
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

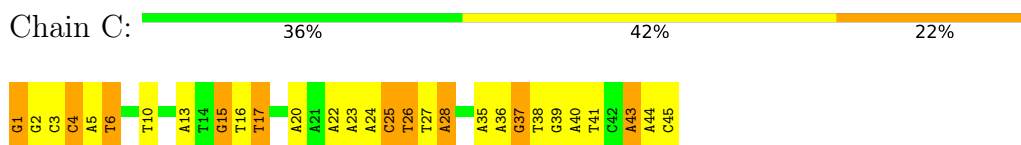
• Molecule 1: Arbitrium receptor



• Molecule 1: Arbitrium receptor



• Molecule 2: DNA (45-MER)



• Molecule 3: DNA (45-MER)



G1	T2	T3	G4	A5	T6	C7	A8	C9	T10	T11		T15	A16	T17	T18	A19	A20	G21		T24	T25	T26	A27	T28	A29	A30	C31	A32	T33	C34	T35	A36	G37	T38	G39	A40	T41	G42	G43	C44	C45
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	132.72Å 39.87Å 143.01Å 90.00° 100.49° 90.00°	Depositor
Resolution (Å)	65.34 – 2.50 65.34 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.4 (65.34-2.50) 96.4 (65.34-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.202 , 0.249 0.205 , 0.243	Depositor DCC
R_{free} test set	2549 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	68.0	Xtriage
Anisotropy	0.551	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 45.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	8310	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.72% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	1.07	2/3248 (0.1%)	1.48	8/4360 (0.2%)
1	B	1.03	0/3254	1.49	6/4369 (0.1%)
2	C	1.05	4/1036 (0.4%)	1.49	24/1596 (1.5%)
3	D	1.02	1/1032 (0.1%)	1.56	19/1591 (1.2%)
All	All	1.05	7/8570 (0.1%)	1.50	57/11916 (0.5%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	4	DC	C4-C5	6.31	1.55	1.43
1	A	340	LEU	C-O	-6.13	1.17	1.24
1	A	280	PHE	C-O	-5.65	1.17	1.24
2	C	3	DC	C4-C5	5.60	1.54	1.43
2	C	3	DC	N1-C2	5.41	1.51	1.40
3	D	44	DC	C4-C5	5.12	1.53	1.43
2	C	45	DC	C4-C5	5.06	1.53	1.43

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	43	DG	P-O3'-C3'	-14.64	98.24	120.20
2	C	40	DA	P-O3'-C3'	-9.22	106.37	120.20
3	D	42	DG	P-O3'-C3'	-8.73	107.10	120.20
3	D	9	DC	P-O3'-C3'	-8.63	107.25	120.20
2	C	10	DT	P-O3'-C3'	-8.26	107.81	120.20
3	D	3	DT	P-O3'-C3'	-7.68	108.68	120.20
3	D	24	DT	P-O3'-C3'	-7.58	108.82	120.20
2	C	6	DT	P-O3'-C3'	-7.12	109.53	120.20
3	D	26	DT	P-O3'-C3'	-7.03	109.66	120.20
2	C	26	DT	P-O3'-C3'	-6.98	109.73	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	36	DA	O3'-P-O5'	-6.92	93.61	104.00
2	C	39	DG	C4-N9-C1'	-6.90	116.65	127.00
3	D	32	DA	C4'-C3'-O3'	6.66	119.99	110.00
2	C	16	DT	C2'-C3'-O3'	6.56	121.33	111.50
2	C	41	DT	P-O3'-C3'	-6.53	110.41	120.20
1	A	30	ASN	CB-CA-C	6.48	119.72	109.55
2	C	1	DG	C8-N9-C1'	6.45	136.68	127.00
2	C	39	DG	C8-N9-C1'	6.28	136.41	127.00
2	C	28	DA	P-O3'-C3'	-6.22	110.87	120.20
2	C	25	DC	P-O3'-C3'	-6.15	110.97	120.20
2	C	1	DG	C4-N9-C1'	-6.12	117.82	127.00
2	C	1	DG	P-O3'-C3'	-6.04	111.14	120.20
2	C	3	DC	P-O3'-C3'	-5.86	111.41	120.20
3	D	1	DG	P-O3'-C3'	-5.86	111.41	120.20
2	C	15	DG	C8-N9-C1'	5.84	135.76	127.00
1	B	30	ASN	CB-CA-C	5.82	118.99	109.97
3	D	36	DA	O3'-P-O5'	-5.78	95.33	104.00
1	A	203	ILE	N-CA-C	-5.78	104.70	111.00
3	D	19	DA	C4-N9-C1'	-5.70	118.51	127.05
1	B	203	ILE	N-CA-C	-5.61	105.05	110.72
2	C	20	DA	P-O3'-C3'	-5.61	111.79	120.20
1	B	351	SER	N-CA-C	-5.58	105.10	111.07
2	C	37	DG	C4'-C3'-O3'	-5.56	101.67	110.00
3	D	15	DT	P-O3'-C3'	-5.55	111.87	120.20
3	D	41	DT	P-O3'-C3'	5.54	128.51	120.20
2	C	15	DG	C4-N9-C1'	-5.52	118.71	127.00
3	D	41	DT	C2'-C3'-O3'	5.50	119.75	111.50
2	C	43	DA	C4'-C3'-O3'	-5.43	101.86	110.00
3	D	2	DT	P-O3'-C3'	-5.42	112.08	120.20
2	C	13	DA	P-O3'-C3'	-5.39	112.12	120.20
3	D	19	DA	C8-N9-C1'	5.38	135.13	127.05
1	B	98	ASP	CA-CB-CG	5.38	117.98	112.60
1	A	232	PHE	CA-C-O	-5.38	114.85	120.55
3	D	1	DG	C8-N9-C1'	5.37	135.06	127.00
2	C	4	DC	P-O3'-C3'	-5.33	112.20	120.20
3	D	8	DA	P-O3'-C3'	-5.33	112.20	120.20
1	A	98	ASP	CA-CB-CG	5.30	117.90	112.60
2	C	22	DA	P-O3'-C3'	-5.28	112.29	120.20
3	D	7	DC	P-O3'-C3'	5.26	128.09	120.20
2	C	17	DT	P-O3'-C3'	5.22	128.03	120.20
1	B	48	PHE	CA-CB-CG	5.17	118.97	113.80
1	B	232	PHE	CA-C-O	-5.10	115.15	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	32	DA	P-O3'-C3'	5.07	127.80	120.20
1	A	45	PHE	CA-C-N	5.05	127.30	120.38
1	A	45	PHE	C-N-CA	5.05	127.30	120.38
1	A	351	SER	N-CA-C	-5.05	105.67	111.07
1	A	301	VAL	N-CA-C	-5.02	105.65	110.72

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	3186	0	3178	40	0
1	B	3195	0	3173	40	0
2	C	923	0	508	25	0
3	D	922	0	514	38	0
4	A	20	0	0	0	0
4	B	15	0	0	0	0
5	A	30	0	0	0	0
5	B	18	0	0	0	0
5	D	1	0	0	0	0
All	All	8310	0	7373	119	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 8.

All (119) 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:345:LYS:HE2	1:B:376:GLU:OE1	1.80	0.82
1:B:77:LYS:NZ	3:D:17:DT:OP1	2.14	0.81
2:C:25:DC:C2'	2:C:26:DT:H71	2.11	0.80
1:B:30:ASN:C	1:B:30:ASN:HD22	1.92	0.78
1:A:346:GLU:OE2	1:B:379:ARG:NH2	2.18	0.77
1:A:346:GLU:CD	1:B:379:ARG:HH21	1.94	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:25:DT:H2'	3:D:26:DT:H71	1.70	0.71
2:C:25:DC:H2''	2:C:26:DT:H71	1.71	0.71
1:A:346:GLU:CD	1:B:379:ARG:NH2	2.50	0.70
2:C:43:DA:H62	3:D:3:DT:H3	1.42	0.68
1:B:43:LYS:NZ	2:C:35:DA:OP2	2.26	0.67
1:B:345:LYS:CE	1:B:376:GLU:OE1	2.43	0.67
1:A:178:ASP:O	1:A:181:GLU:HG2	1.95	0.67
1:A:43:LYS:NZ	3:D:35:DT:OP2	2.25	0.67
1:B:174:PHE:CE1	1:B:196:ILE:HD13	2.30	0.66
1:B:16:ASN:O	3:D:5:DA:H5''	1.97	0.65
3:D:32:DA:H4'	3:D:33:DT:OP1	1.97	0.64
3:D:30:DA:H2''	3:D:31:DC:OP2	1.96	0.64
1:B:147:ALA:HB1	1:B:181:GLU:HB3	1.79	0.64
1:A:346:GLU:OE1	1:B:379:ARG:NH2	2.28	0.64
1:A:379:ARG:HG2	1:A:379:ARG:NH1	2.15	0.61
1:B:192:PHE:O	1:B:196:ILE:HG23	2.00	0.61
1:A:349:PHE:CE1	1:B:380:LEU:HD13	2.36	0.60
2:C:43:DA:H1'	2:C:44:DA:H5'	1.84	0.59
1:A:92:MET:HE2	1:A:228:ARG:HG3	1.83	0.59
2:C:25:DC:H2'	2:C:26:DT:H71	1.82	0.59
2:C:26:DT:H2'	2:C:27:DT:H72	1.83	0.58
2:C:6:DT:H3	3:D:40:DA:H62	1.53	0.57
1:A:77:LYS:HE2	2:C:17:DT:OP1	2.05	0.57
3:D:7:DC:H2''	3:D:8:DA:C8	2.39	0.56
1:B:174:PHE:HE1	1:B:196:ILE:HD13	1.67	0.56
1:A:16:ASN:O	2:C:5:DA:H5''	2.05	0.56
3:D:32:DA:H2''	3:D:33:DT:H5'	1.87	0.56
1:A:379:ARG:HG2	1:A:379:ARG:HH11	1.69	0.56
3:D:10:DT:H4'	3:D:11:DT:OP1	2.05	0.56
1:A:383:ILE:O	1:A:386:MET:HG2	2.06	0.55
2:C:25:DC:H2''	2:C:26:DT:C6	2.41	0.55
3:D:29:DA:H2''	3:D:30:DA:OP2	2.06	0.55
1:A:154:LYS:NZ	1:A:176:GLN:OE1	2.39	0.54
3:D:9:DC:C2'	3:D:10:DT:O5'	2.56	0.54
1:B:156:LEU:C	1:B:156:LEU:HD12	2.33	0.54
1:A:156:LEU:C	1:A:156:LEU:HD12	2.33	0.53
3:D:20:DA:H2'	3:D:20:DA:OP2	2.10	0.52
2:C:23:DA:H2''	2:C:24:DA:O5'	2.10	0.51
1:B:86:GLU:OE1	1:B:195:ARG:NH1	2.44	0.51
2:C:2:DG:H1	3:D:44:DC:H42	1.59	0.50
1:A:379:ARG:HH11	1:A:379:ARG:CG	2.22	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:366:MET:HB2	1:B:367:PRO:CD	2.41	0.50
1:A:343:ASN:O	1:A:374:MET:HE1	2.12	0.50
1:B:89:ASP:OD2	1:B:195:ARG:NH2	2.34	0.50
3:D:10:DT:H2'	3:D:11:DT:C6	2.47	0.50
3:D:28:DT:H2''	3:D:29:DA:OP2	2.12	0.49
2:C:44:DA:H62	3:D:2:DT:H3	1.61	0.49
1:A:86:GLU:OE1	1:A:195:ARG:NH1	2.46	0.49
2:C:26:DT:H2'	2:C:27:DT:C7	2.43	0.49
1:A:77:LYS:CE	2:C:17:DT:OP1	2.60	0.48
2:C:4:DC:N3	3:D:42:DG:N2	2.50	0.48
1:B:32:ASN:HD21	3:D:7:DC:H41	1.60	0.48
1:A:239:THR:HA	1:A:242:ILE:HG13	1.96	0.48
3:D:7:DC:C2'	3:D:8:DA:C8	2.97	0.48
1:B:160:ASP:OD1	1:B:164:LYS:NZ	2.46	0.48
3:D:8:DA:H2''	3:D:9:DC:H6	1.78	0.48
2:C:37:DG:C2'	2:C:38:DT:O5'	2.63	0.47
1:B:75:ASP:O	1:B:78:THR:HG22	2.15	0.47
1:B:321:LEU:O	1:B:324:ARG:HB3	2.14	0.47
1:B:366:MET:HB2	1:B:367:PRO:HD3	1.96	0.47
1:A:76:VAL:HG11	1:A:103:SER:HB2	1.97	0.46
3:D:1:DG:H2'	3:D:1:DG:OP1	2.16	0.46
1:B:239:THR:HA	1:B:242:ILE:HG13	1.97	0.46
2:C:1:DG:H8	2:C:1:DG:P	2.39	0.46
3:D:3:DT:H2''	3:D:4:DG:C8	2.50	0.46
1:A:366:MET:HB2	1:A:367:PRO:CD	2.45	0.46
1:B:76:VAL:HG11	1:B:103:SER:HB2	1.97	0.46
2:C:24:DA:H2''	2:C:25:DC:OP2	2.16	0.46
1:A:75:ASP:O	1:A:78:THR:HG22	2.16	0.45
1:A:353:GLU:CD	1:B:379:ARG:NH1	2.74	0.45
2:C:4:DC:N4	3:D:42:DG:H1	2.15	0.45
2:C:25:DC:H2''	2:C:26:DT:H6	1.82	0.44
1:A:160:ASP:OD1	1:A:164:LYS:NZ	2.41	0.44
1:A:153:SER:O	1:A:156:LEU:HG	2.17	0.44
1:A:366:MET:HB2	1:A:367:PRO:HD3	2.00	0.43
1:B:153:SER:O	1:B:156:LEU:HG	2.19	0.43
3:D:1:DG:H8	3:D:1:DG:OP2	2.01	0.43
1:A:32:ASN:N	1:A:33:PRO:HD2	2.33	0.43
1:B:4:ILE:HG12	1:B:51:ILE:HD11	2.01	0.43
2:C:15:DG:C2	3:D:32:DA:C2	3.07	0.43
3:D:24:DT:C6	3:D:25:DT:H72	2.53	0.43
1:A:48:PHE:O	1:A:51:ILE:HG22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:ILE:HG22	1:B:384:ILE:HG12	2.00	0.43
1:B:333:PHE:CD1	1:B:366:MET:HE1	2.54	0.43
3:D:8:DA:H2''	3:D:9:DC:C6	2.54	0.42
3:D:6:DT:H2''	3:D:7:DC:O4'	2.19	0.42
1:A:336:TYR:CE2	1:A:340:LEU:HD11	2.55	0.42
1:B:48:PHE:O	1:B:51:ILE:HG22	2.18	0.42
3:D:24:DT:H2''	3:D:25:DT:C7	2.49	0.42
1:B:336:TYR:CE2	1:B:340:LEU:HD11	2.54	0.42
1:A:231:VAL:HG13	1:A:270:PHE:HE2	1.85	0.42
1:A:315:LEU:HD12	1:A:315:LEU:HA	1.87	0.42
3:D:34:DC:H2''	3:D:35:DT:H5'	2.01	0.42
3:D:16:DA:H1'	3:D:17:DT:H5'	2.01	0.41
3:D:42:DG:H2''	3:D:43:DG:C8	2.55	0.41
1:B:166:ASN:N	1:B:166:ASN:HD22	2.17	0.41
3:D:37:DG:H2''	3:D:38:DT:H5'	2.02	0.41
3:D:26:DT:H2''	3:D:27:DA:C8	2.55	0.41
1:A:353:GLU:OE2	1:B:379:ARG:NH1	2.53	0.41
1:A:321:LEU:O	1:A:324:ARG:HB3	2.21	0.41
1:B:4:ILE:HD13	1:B:55:VAL:HG22	2.02	0.41
1:B:174:PHE:CE1	1:B:196:ILE:CD1	3.02	0.41
1:B:380:LEU:HD12	1:B:380:LEU:HA	1.82	0.41
1:B:298:MET:HA	1:B:301:VAL:HG13	2.02	0.41
2:C:37:DG:H2''	2:C:38:DT:H5'	2.03	0.41
1:A:105:ILE:HD11	1:A:120:LYS:CD	2.51	0.41
1:A:384:ILE:HG12	1:B:383:ILE:HG22	2.01	0.40
1:A:4:ILE:HG12	1:A:51:ILE:HD11	2.04	0.40
1:A:200:LEU:HD23	1:A:216:TYR:CE1	2.56	0.40
3:D:20:DA:H1'	3:D:21:DG:C8	2.57	0.40
1:A:89:ASP:OD2	1:A:195:ARG:NH2	2.37	0.40
2:C:27:DT:H1'	2:C:28:DA:C8	2.57	0.40
3:D:43:DG:H8	3:D:43:DG:H5''	1.85	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	385/386 (100%)	373 (97%)	12 (3%)	0	100	100
1	B	386/386 (100%)	374 (97%)	12 (3%)	0	100	100
All	All	771/772 (100%)	747 (97%)	24 (3%)	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	354/353 (100%)	330 (93%)	24 (7%)	14	31
1	B	355/353 (101%)	325 (92%)	30 (8%)	10	22
All	All	709/706 (100%)	655 (92%)	54 (8%)	12	26

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	10	LYS
1	A	17	SER
1	A	25	VAL
1	A	30	ASN
1	A	43	LYS
1	A	65	GLU
1	A	69	ASP
1	A	78	THR
1	A	102	ASP
1	A	103	SER
1	A	107	CYS
1	A	134	GLU
1	A	142	GLN
1	A	175	GLN

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Mol	Chain	Res	Type
1	A	196	ILE
1	A	200	LEU
1	A	213	CYS
1	A	261	LYS
1	A	288	ILE
1	A	301	VAL
1	A	310	GLU
1	A	312	SER
1	A	359	GLN
1	B	4	ILE
1	B	10	LYS
1	B	17	SER
1	B	30	ASN
1	B	56	LYS
1	B	62	ARG
1	B	69	ASP
1	B	77	LYS
1	B	78	THR
1	B	102	ASP
1	B	103	SER
1	B	107	CYS
1	B	108	SER
1	B	134	GLU
1	B	142	GLN
1	B	172	LEU
1	B	181	GLU
1	B	196	ILE
1	B	213	CYS
1	B	218	GLN
1	B	258	LYS
1	B	261	LYS
1	B	268	GLU
1	B	288	ILE
1	B	296	THR
1	B	301	VAL
1	B	345	LYS
1	B	379	ARG
1	B	380	LEU
1	B	382	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	122	HIS
1	A	190	ASN
1	A	227	GLN
1	A	252	ASN
1	A	273	ASN
1	A	282	ASN
1	A	307	ASN
1	A	329	ASN
1	A	343	ASN
1	B	30	ASN
1	B	32	ASN
1	B	122	HIS
1	B	166	ASN
1	B	190	ASN
1	B	197	ASN
1	B	227	GLN
1	B	252	ASN
1	B	273	ASN
1	B	282	ASN
1	B	307	ASN
1	B	329	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

7 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	SO4	B	402	-	4,4,4	0.31	0	6,6,6	0.08	0
4	SO4	A	402	-	4,4,4	0.28	0	6,6,6	0.07	0
4	SO4	A	401	-	4,4,4	0.28	0	6,6,6	0.17	0
4	SO4	B	401	-	4,4,4	0.28	0	6,6,6	0.15	0
4	SO4	B	403	-	4,4,4	0.30	0	6,6,6	0.08	0
4	SO4	A	403	-	4,4,4	0.29	0	6,6,6	0.09	0
4	SO4	A	404	-	4,4,4	0.30	0	6,6,6	0.07	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	386/386 (100%)	-0.05	3 (0%) 82 80	44, 77, 109, 138	2 (0%)
1	B	386/386 (100%)	0.00	2 (0%) 87 85	41, 81, 114, 133	3 (0%)
2	C	45/45 (100%)	-0.07	0 100 100	93, 118, 161, 163	0
3	D	45/45 (100%)	-0.07	0 100 100	90, 121, 165, 176	0
All	All	862/862 (100%)	-0.03	5 (0%) 85 83	41, 83, 124, 176	5 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	258	LYS	5.0
1	B	258	LYS	3.5
1	B	225[A]	ASP	2.3
1	A	243	PHE	2.3
1	A	71	CYS	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SO4	B	403	5/5	0.71	0.16	132,132,146,153	0
4	SO4	A	404	5/5	0.72	0.09	135,146,161,165	0
4	SO4	A	403	5/5	0.79	0.16	135,142,160,161	0
4	SO4	B	401	5/5	0.83	0.14	126,130,148,149	0
4	SO4	A	401	5/5	0.84	0.16	124,127,151,158	0
4	SO4	A	402	5/5	0.84	0.12	121,122,135,135	0
4	SO4	B	402	5/5	0.91	0.09	133,137,140,141	0

6.5 Other polymers [i](#)

There are no such residues in this entry.