



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:28 PM GMT

PDB ID : 1XC9
Title : Structure of a high-fidelity polymerase bound to a benzo[a]pyrene adduct that blocks replication
Authors : Hsu, G.W.; Huang, X.; Luneva, N.P.; Geacintov, N.E.; Beese, L.S.
Deposited on : 2004-09-01
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 (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

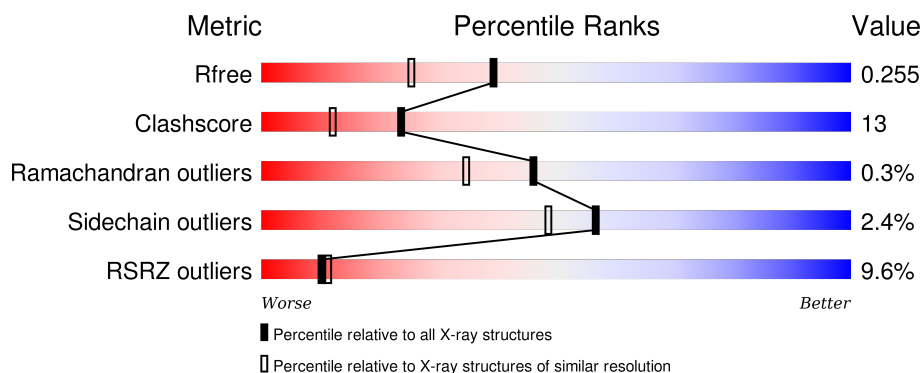
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (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	B	10	<div> <div>40%</div> <div>60%</div> <div>40%</div> </div>
2	C	15	<div> <div>20%</div> <div>7%</div> <div>73%</div> <div>20%</div> </div>
3	A	580	<div> <div>9%</div> <div>75%</div> <div>23%</div> <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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SUC	A	901	-	-	-	X
7	BAP	C	444	-	-	-	X

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 5533 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 DNA chain called DNA primer strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	10	Total	C	N	O	P	0	0	0
			209	99	42	59	9			

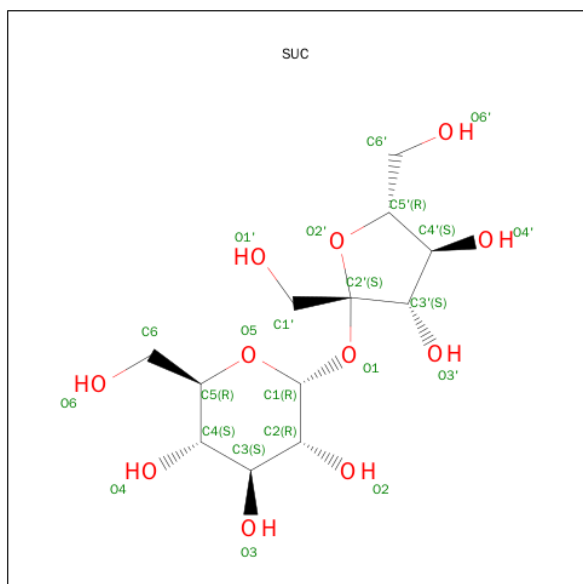
- Molecule 2 is a DNA chain called DNA template strand with benzo[a]pyrene adduct.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	12	Total	C	N	O	P	0	0	0
			234	113	40	70	11			

- Molecule 3 is a protein called DNA polymerase I.

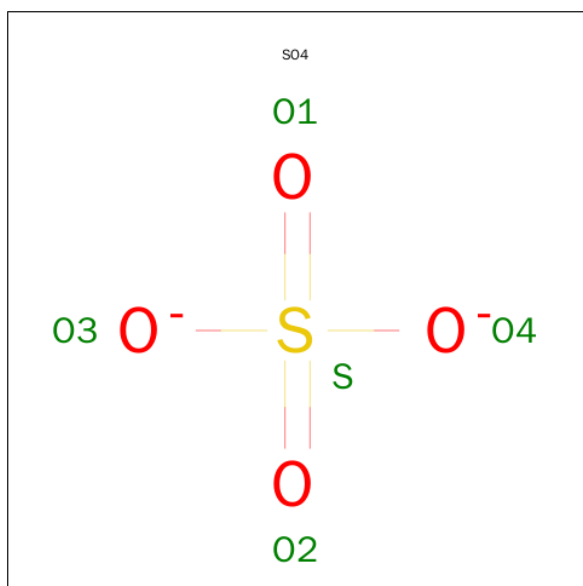
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	580	Total	C	N	O	S	0	0	0
			4650	2956	807	870	17			

- Molecule 4 is SUGAR (SUCROSE) (three-letter code: SUC) (formula: C₁₂H₂₂O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			23	12	11		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).

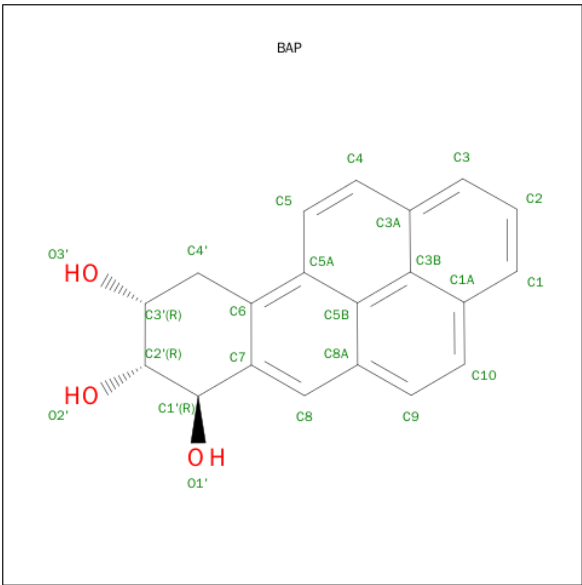


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mg	0	0
			1	1		

- Molecule 7 is 1,2,3-TRIHYDROXY-1,2,3,4-TETRAHYDROBENZO[A]PYRENE (three-letter code: BAP) (formula: C₂₀H₁₆O₃).



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	88.75Å 93.73Å 104.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.76 – 1.90 42.76 – 1.85	Depositor EDS
% Data completeness (in resolution range)	96.8 (42.76-1.90) 95.8 (42.76-1.85)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 1.86Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.221 , 0.255 0.222 , 0.255	Depositor DCC
R_{free} test set	3413 reflections (5.09%)	DCC
Wilson B-factor (Å ²)	25.0	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 49.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 71883 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5533	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.00% 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: MG, SUC, SO4, BAP

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	B	0.29	0/235	0.68	0/363
2	C	0.33	0/260	0.77	0/397
3	A	0.32	0/4734	0.56	0/6398
All	All	0.32	0/5229	0.58	0/7158

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	B	209	0	114	3	0
2	C	234	0	135	12	0
3	A	4650	0	4698	123	0
4	A	23	0	22	1	0
5	A	20	0	0	0	0
6	A	1	0	0	0	0
7	C	23	0	15	0	0
8	A	361	0	0	10	0
8	B	4	0	0	0	0
8	C	8	0	0	0	0
All	All	5533	0	4984	134	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 13.

All (134) 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)
3:A:712:ILE:H	3:A:712:ILE:HD13	1.36	0.86
3:A:364:GLU:HG2	3:A:388:CYS:HB3	1.58	0.85
3:A:590:GLY:HA2	3:A:593:LYS:HE2	1.59	0.84
3:A:527:ASN:H	3:A:533:GLN:NE2	1.78	0.81
3:A:729:ARG:H	3:A:729:ARG:NE	1.79	0.80
3:A:534:LEU:HD11	3:A:574:ILE:HD13	1.65	0.78
3:A:328:HIS:HD2	3:A:382:TRP:HE1	1.34	0.74
3:A:456:GLU:HG2	8:A:2809:HOH:O	1.89	0.71
2:C:8:DC:H2'	2:C:9:DA:C8	2.26	0.71
3:A:691:GLN:HG3	3:A:738:ARG:HH22	1.57	0.69
3:A:729:ARG:HE	3:A:729:ARG:H	1.39	0.69
3:A:431:LYS:HD2	3:A:431:LYS:N	2.08	0.68
3:A:675:PHE:CZ	3:A:681:ILE:HG21	2.29	0.68
3:A:804:ILE:HD11	8:A:2772:HOH:O	1.94	0.66
2:C:13:DC:H2''	2:C:14:DT:H72	1.78	0.66
3:A:339:ASN:HD22	3:A:339:ASN:C	1.97	0.65
3:A:779:ARG:NH1	3:A:779:ARG:HB2	2.11	0.65
3:A:718:ASP:HB2	3:A:733:ALA:HB2	1.79	0.65
3:A:737:GLU:O	3:A:741:GLU:HG3	1.97	0.64
1:B:22:DG:H2''	1:B:23:DA:H5'	1.77	0.64
3:A:712:ILE:HB	3:A:750:MET:HE1	1.78	0.64
3:A:624:GLN:HG2	3:A:828:VAL:HG12	1.80	0.63
3:A:728:SER:OG	3:A:731:GLU:HG3	1.99	0.62
3:A:677:ARG:HB2	3:A:679:LEU:HD13	1.80	0.62
3:A:589:GLU:O	3:A:593:LYS:HG3	1.99	0.61
3:A:707:ALA:HB3	3:A:725:LEU:HD21	1.82	0.61
3:A:681:ILE:HD12	3:A:682:HIS:N	2.16	0.61
3:A:754:VAL:HG12	3:A:758:LYS:HE2	1.83	0.60
3:A:657:ILE:HG21	8:A:2772:HOH:O	2.02	0.59
3:A:690:PHE:CD2	3:A:701:MET:HE2	2.37	0.59
3:A:459:ARG:HB3	3:A:460:PRO:HD3	1.84	0.59
3:A:813:ALA:O	3:A:817:GLU:HG3	2.02	0.59
3:A:505:LYS:NZ	3:A:505:LYS:HB3	2.18	0.59
2:C:6:DA:H2''	2:C:7:DC:H5'	1.84	0.58
3:A:547:LEU:C	3:A:548:LYS:HD2	2.24	0.58
3:A:339:ASN:ND2	3:A:341:HIS:H	2.02	0.57
3:A:729:ARG:H	3:A:729:ARG:CD	2.18	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:692:VAL:HB	3:A:696:GLU:HB2	1.87	0.56
3:A:675:PHE:CE1	3:A:681:ILE:HG21	2.41	0.55
3:A:733:ALA:O	3:A:736:ILE:HG12	2.06	0.55
3:A:550:THR:HG23	3:A:553:GLY:H	1.71	0.55
1:B:24:DT:OP1	3:A:552:THR:HG22	2.07	0.54
2:C:3:DC:H1'	3:A:716:ILE:HG21	1.90	0.54
3:A:498:LYS:O	3:A:502:GLN:HG3	2.08	0.54
2:C:9:DA:H2''	2:C:10:DT:H5'	1.90	0.53
3:A:519:TYR:CD1	3:A:525:GLU:HA	2.43	0.53
3:A:621:PRO:HG2	3:A:623:LEU:CD2	2.39	0.53
3:A:547:LEU:HB2	3:A:548:LYS:HD2	1.90	0.52
3:A:607:ASN:ND2	4:A:901:SUC:H4'	2.24	0.52
3:A:725:LEU:O	3:A:727:ILE:HG23	2.10	0.52
3:A:517:ARG:O	3:A:520:GLU:HG2	2.09	0.52
3:A:685:THR:O	3:A:689:ILE:HG12	2.10	0.52
2:C:6:DA:H2''	2:C:7:DC:C5'	2.40	0.51
3:A:550:THR:HG22	3:A:553:GLY:O	2.10	0.51
3:A:779:ARG:HH11	3:A:779:ARG:HB2	1.74	0.51
3:A:677:ARG:CB	3:A:679:LEU:HD13	2.39	0.51
3:A:784:ARG:O	3:A:788:GLU:HG3	2.10	0.51
3:A:754:VAL:CG1	3:A:758:LYS:HE2	2.41	0.50
3:A:505:LYS:HZ3	3:A:505:LYS:HB3	1.75	0.50
3:A:630:LEU:HD12	3:A:630:LEU:N	2.27	0.50
1:B:28:DG:H2''	3:A:829:HIS:CE1	2.46	0.50
3:A:713:VAL:HG13	3:A:797:GLN:HE21	1.77	0.50
2:C:4:DG:H2''	2:C:5:DC:O5'	2.12	0.50
3:A:527:ASN:H	3:A:533:GLN:HE22	1.54	0.49
3:A:392:PHE:HA	3:A:479:GLN:HE22	1.76	0.49
2:C:13:DC:C2'	2:C:14:DT:H72	2.42	0.49
3:A:510:GLN:O	3:A:514:VAL:HG23	2.11	0.49
2:C:13:DC:H2''	2:C:14:DT:C7	2.43	0.49
3:A:681:ILE:HG13	8:A:2123:HOH:O	2.12	0.49
3:A:621:PRO:HG2	3:A:623:LEU:HD21	1.93	0.49
3:A:393:ASP:H	3:A:479:GLN:NE2	2.10	0.49
3:A:617:SER:HA	3:A:624:GLN:HE22	1.77	0.49
3:A:328:HIS:CD2	3:A:382:TRP:HE1	2.23	0.49
3:A:550:THR:CG2	3:A:553:GLY:H	2.25	0.49
2:C:7:DC:H2''	2:C:8:DC:O5'	2.13	0.48
3:A:607:ASN:HD22	3:A:609:ALA:H	1.61	0.48
3:A:729:ARG:N	3:A:729:ARG:CD	2.76	0.48
3:A:583:LEU:HD13	8:A:2802:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:736:ILE:HG13	3:A:737:GLU:N	2.29	0.48
3:A:629:ARG:HH11	3:A:629:ARG:HG2	1.79	0.48
3:A:550:THR:HG22	3:A:553:GLY:C	2.33	0.48
3:A:823:HIS:HD2	8:A:2159:HOH:O	1.97	0.47
3:A:822:ALA:CB	3:A:836:ALA:HB2	2.44	0.47
3:A:748:ARG:HD2	8:A:2960:HOH:O	2.13	0.47
3:A:456:GLU:HB3	8:A:3025:HOH:O	2.14	0.47
3:A:653:ASP:HB3	3:A:831:GLU:HB3	1.97	0.47
3:A:847:LEU:C	3:A:847:LEU:HD23	2.34	0.47
3:A:466:ARG:HG3	3:A:466:ARG:HH11	1.80	0.47
3:A:530:SER:OG	3:A:533:GLN:HG3	2.15	0.47
2:C:12:DC:H2"	2:C:13:DC:C5	2.50	0.47
3:A:663:ALA:HB2	3:A:671:LEU:HG	1.97	0.47
3:A:548:LYS:HD2	3:A:548:LYS:N	2.30	0.46
3:A:607:ASN:C	3:A:607:ASN:HD22	2.18	0.46
3:A:548:LYS:HD3	3:A:560:VAL:HG22	1.97	0.46
3:A:515:GLU:HG3	3:A:516:GLN:N	2.30	0.46
3:A:654:TYR:HB3	3:A:657:ILE:HB	1.98	0.45
3:A:716:ILE:HD12	3:A:721:LEU:N	2.32	0.45
3:A:536:VAL:O	3:A:540:GLU:HB2	2.18	0.44
3:A:693:SER:OG	3:A:696:GLU:HG3	2.17	0.44
3:A:700:ASN:O	3:A:704:GLN:HG2	2.17	0.44
3:A:431:LYS:N	3:A:431:LYS:CD	2.79	0.44
3:A:717:SER:N	3:A:789:ARG:HH11	2.16	0.44
3:A:719:TYR:O	3:A:722:ALA:HB3	2.18	0.43
3:A:819:ARG:HG2	8:A:2827:HOH:O	2.17	0.43
3:A:524:GLN:HE21	3:A:541:LYS:NZ	2.15	0.43
3:A:565:ALA:HB3	3:A:566:PRO:HD3	2.00	0.43
3:A:823:HIS:HE1	3:A:835:GLU:OE2	2.01	0.43
3:A:750:MET:SD	3:A:792:MET:HB3	2.59	0.43
3:A:305:ASP:HB2	3:A:306:ARG:HD2	2.00	0.43
3:A:725:LEU:HB2	3:A:727:ILE:HG12	2.00	0.43
3:A:557:SER:HB3	3:A:560:VAL:HG23	2.01	0.43
3:A:499:ARG:HG3	3:A:503:MET:HE3	2.01	0.43
3:A:584:GLN:O	3:A:589:GLU:HG3	2.19	0.42
3:A:607:ASN:ND2	3:A:609:ALA:H	2.17	0.42
3:A:848:VAL:HB	3:A:849:PRO:HD3	2.00	0.42
3:A:547:LEU:CB	3:A:548:LYS:HD2	2.49	0.42
3:A:715:GLY:O	3:A:789:ARG:HD2	2.19	0.42
3:A:710:PHE:HB3	3:A:714:TYR:CD2	2.54	0.42
3:A:827:GLN:HG2	3:A:832:LEU:HD23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:624:GLN:CG	3:A:828:VAL:HG12	2.49	0.42
3:A:561:LEU:O	3:A:571:VAL:HG11	2.20	0.42
3:A:715:GLY:HA2	8:A:2798:HOH:O	2.20	0.41
3:A:356:GLN:H	3:A:356:GLN:NE2	2.19	0.41
3:A:746:VAL:O	3:A:750:MET:HG2	2.21	0.41
3:A:517:ARG:HG2	3:A:517:ARG:HH11	1.85	0.41
2:C:3:DC:O3'	3:A:716:ILE:HG22	2.20	0.41
3:A:653:ASP:CB	3:A:831:GLU:HB3	2.51	0.41
3:A:794:THR:HB	3:A:795:PRO:HD3	2.03	0.41
3:A:499:ARG:HG3	3:A:503:MET:CE	2.51	0.40
3:A:740:PHE:CD1	3:A:747:LYS:HB2	2.56	0.40
3:A:339:ASN:ND2	3:A:339:ASN:C	2.70	0.40
3:A:440:GLU:HB3	3:A:441:PRO:HD3	2.04	0.40
3:A:517:ARG:NE	3:A:521:LEU:HD11	2.36	0.40
3:A:681:ILE:CD1	3:A:682:HIS:CE1	3.05	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
3	A	578/580 (100%)	562 (97%)	14 (2%)	2 (0%)	46 35

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	432	GLY
3	A	628	ILE

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
3	A	495/496 (100%)	483 (98%)	12 (2%)	57 49

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

Mol	Chain	Res	Type
3	A	306	ARG
3	A	339	ASN
3	A	443	LEU
3	A	499	ARG
3	A	517	ARG
3	A	527	ASN
3	A	607	ASN
3	A	712	ILE
3	A	723	GLN
3	A	729	ARG
3	A	793	ASN
3	A	827	GLN

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

Mol	Chain	Res	Type
3	A	328	HIS
3	A	339	ASN
3	A	356	GLN
3	A	479	GLN
3	A	502	GLN
3	A	510	GLN
3	A	524	GLN
3	A	527	ASN
3	A	533	GLN
3	A	543	GLN
3	A	579	GLN
3	A	607	ASN
3	A	608	GLN

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Mol	Chain	Res	Type
3	A	624	GLN
3	A	656	GLN
3	A	723	GLN
3	A	724	ASN
3	A	797	GLN
3	A	823	HIS
3	A	827	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 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 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	SUC	A	901	-	24,24,24	1.59	3 (12%)	36,36,36	0.97	2 (5%)
5	SO4	A	910	-	4,4,4	0.23	0	6,6,6	0.06	0
5	SO4	A	911	-	4,4,4	0.23	0	6,6,6	0.11	0
5	SO4	A	912	-	4,4,4	0.18	0	6,6,6	0.09	0
5	SO4	A	913	-	4,4,4	0.24	0	6,6,6	0.10	0
7	BAP	C	444	2	26,27,27	2.83	12 (46%)	36,42,42	1.42	3 (8%)

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	SUC	A	901	-	-	0/12/51/51	0/2/2/2
5	SO4	A	910	-	-	0/0/0/0	0/0/0/0
5	SO4	A	911	-	-	0/0/0/0	0/0/0/0
5	SO4	A	912	-	-	0/0/0/0	0/0/0/0
5	SO4	A	913	-	-	0/0/0/0	0/0/0/0
7	BAP	C	444	2	-	0/0/16/16	0/5/5/5

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	444	BAP	C9-C8A	2.00	1.46	1.41
7	C	444	BAP	C5A-C5B	2.01	1.46	1.42
7	C	444	BAP	C10-C1A	2.11	1.47	1.41
7	C	444	BAP	C3B-C3A	2.21	1.47	1.42
4	A	901	SUC	C4-C5	2.29	1.57	1.53
7	C	444	BAP	C5-C4	2.33	1.42	1.34
4	A	901	SUC	O5-C1	2.63	1.48	1.41
7	C	444	BAP	C5-C5A	2.65	1.47	1.42
7	C	444	BAP	C6-C5A	2.99	1.48	1.43
7	C	444	BAP	C10-C9	3.76	1.46	1.34
7	C	444	BAP	C2-C1	3.82	1.45	1.36
7	C	444	BAP	C2-C3	3.89	1.45	1.36
7	C	444	BAP	C4'-C6	4.47	1.58	1.51
4	A	901	SUC	C3-C2	5.60	1.67	1.52
7	C	444	BAP	C8-C7	9.02	1.48	1.36

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	444	BAP	O1'-C1'-C7	-6.27	97.36	110.42
7	C	444	BAP	C8-C7-C6	-2.25	115.92	119.70
4	A	901	SUC	C1-C2-C3	-2.13	105.78	109.97
4	A	901	SUC	C1-O5-C5	2.07	117.77	113.75
7	C	444	BAP	O1'-C1'-C2'	2.83	114.52	108.63

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	901	SUC	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	B	10/10 (100%)	1.26	4 (40%) 0 0	38, 47, 82, 85	0
2	C	12/15 (80%)	1.38	3 (25%) 1 1	42, 59, 85, 92	0
3	A	580/580 (100%)	0.53	51 (8%) 12 14	16, 28, 57, 72	0
All	All	602/605 (99%)	0.56	58 (9%) 10 11	16, 29, 61, 92	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	719	TYR	8.0
3	A	297	ALA	7.6
3	A	729	ARG	6.1
3	A	552	THR	6.0
3	A	431	LYS	5.6
3	A	551	LYS	5.3
3	A	433	ALA	5.1
3	A	550	THR	5.0
3	A	434	LYS	5.0
2	C	14	DT	4.9
3	A	732	ALA	4.9
3	A	725	LEU	4.4
3	A	723	GLN	4.3
2	C	13	DC	4.1
3	A	548	LYS	3.8
3	A	553	GLY	3.8
3	A	531	PRO	3.5
3	A	629	ARG	3.5
3	A	736	ILE	3.4
3	A	532	LYS	3.4
1	B	22	DG	3.3
3	A	712	ILE	3.3
3	A	513	THR	3.2

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Mol	Chain	Res	Type	RSRZ
3	A	520	GLU	3.2
3	A	306	ARG	3.1
3	A	779	ARG	3.1
3	A	304	ALA	3.1
3	A	516	GLN	3.0
3	A	876	LYS	3.0
3	A	509	GLU	3.0
3	A	303	LEU	3.0
3	A	549	LYS	2.9
3	A	441	PRO	2.8
3	A	579	GLN	2.7
3	A	305	ASP	2.7
3	A	727	ILE	2.7
3	A	726	ASN	2.7
3	A	505	LYS	2.7
3	A	722	ALA	2.7
3	A	738	ARG	2.7
1	B	20	DG	2.6
3	A	733	ALA	2.6
3	A	710	PHE	2.5
3	A	512	GLY	2.5
1	B	21	DG	2.5
2	C	12	DC	2.5
1	B	23	DA	2.4
3	A	432	GLY	2.4
3	A	724	ASN	2.4
3	A	730	LYS	2.3
3	A	681	ILE	2.3
3	A	728	SER	2.2
3	A	439	ASP	2.1
3	A	689	ILE	2.1
3	A	721	LEU	2.1
3	A	731	GLU	2.1
3	A	734	GLU	2.0
3	A	718	ASP	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 [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(\AA^2)	Q<0.9
7	BAP	C	444	23/23	0.56	0.28	3.78	57,57,60,61	0
4	SUC	A	901	23/23	0.74	0.24	3.57	48,50,52,54	0
5	SO4	A	912	5/5	0.95	0.12	0.14	51,51,52,52	0
5	SO4	A	911	5/5	0.89	0.17	0.07	75,75,76,76	0
6	MG	A	920	1/1	0.96	0.06	-3.40	49,49,49,49	0
5	SO4	A	910	5/5	0.96	0.09	-	62,62,62,62	0
5	SO4	A	913	5/5	0.87	0.18	-	75,75,76,76	0

6.5 Other polymers [i](#)

There are no such residues in this entry.