



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:39 AM UTC

PDB ID : 2A3A / pdb_00002a3a
Title : Crystal structure of Aspergillus fumigatus chitinase B1 in complex with theophylline
Authors : Rao, F.V.; Andersen, O.A.; Vora, K.A.; DeMartino, J.A.; van Aalten, D.M.F.
Deposited on : 2005-06-24
Resolution : 2.10 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

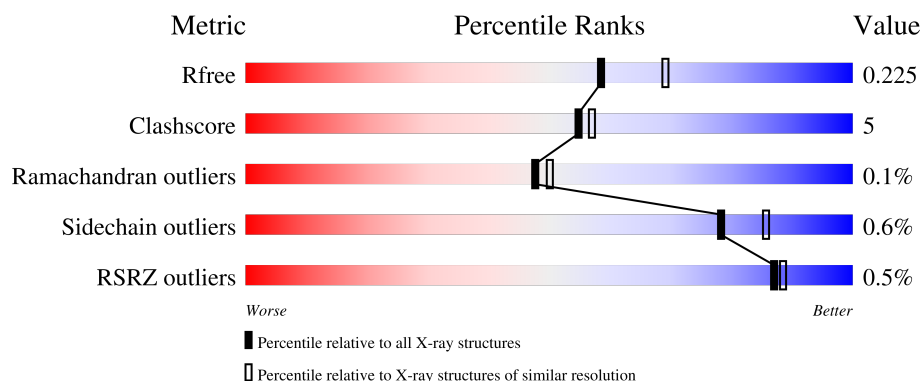
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	433	 83% 8% 9%
1	B	433	 77% 13% 9%

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
3	TEP	B	2435	-	-	X	-

2 Entry composition [i](#)

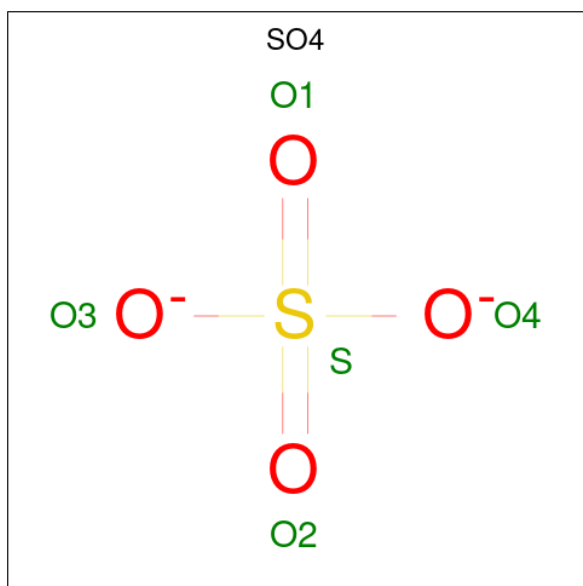
There are 4 unique types of molecules in this entry. The entry contains 7034 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 chitinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	394	Total	C	N	O	S	0	5	0
			3075	1947	514	606	8			
1	B	394	Total	C	N	O	S	0	3	0
			3071	1946	514	603	8			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



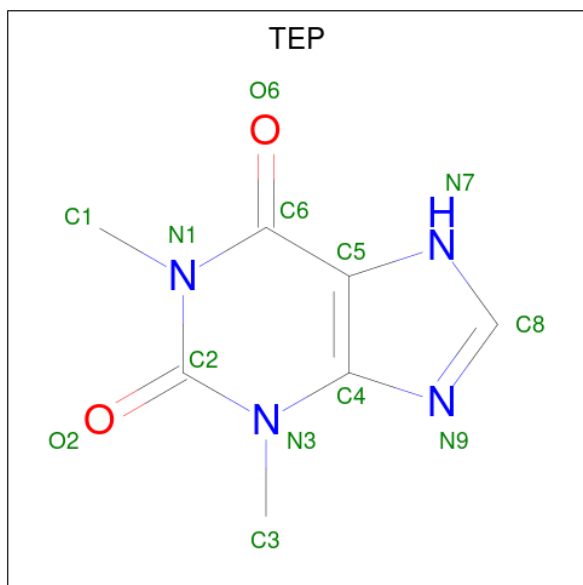
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 3 is THEOPHYLLINE (CCD ID: TEP) (formula: $C_7H_8N_4O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			13	7	4	2		
3	A	1	Total	C	N	O	0	0
			13	7	4	2		
3	A	1	Total	C	N	O	0	0
			13	7	4	2		
3	A	1	Total	C	N	O	0	0
			13	7	4	2		
3	B	1	Total	C	N	O	0	0
			13	7	4	2		
3	B	1	Total	C	N	O	0	0
			13	7	4	2		
3	B	1	Total	C	N	O	0	0
			13	7	4	2		
3	B	1	Total	C	N	O	0	0
			13	7	4	2		

- Molecule 4 is water.

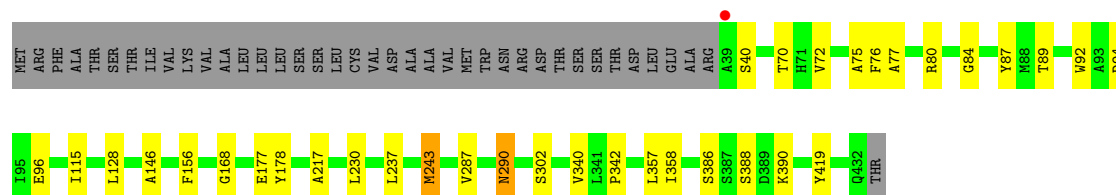
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	397	Total 397	O 397	0	0
4	B	352	Total 352	O 352	0	0

3 Residue-property plots [i](#)

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.

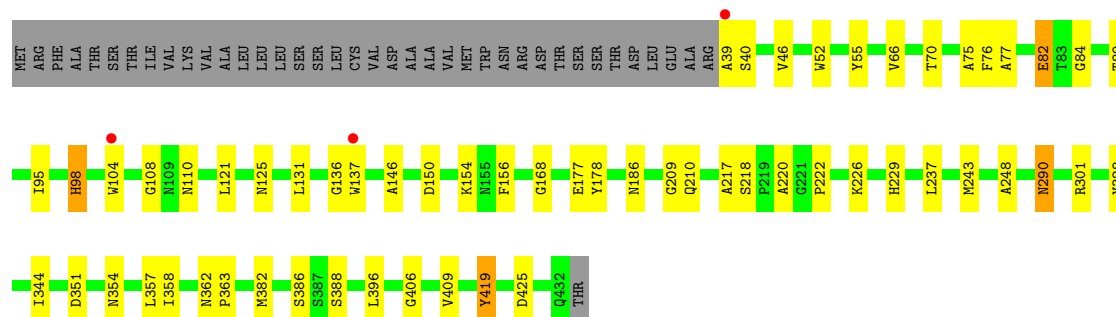
- Molecule 1: chitinase

Chain A: 



- Molecule 1: chitinase

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	117.23Å 117.23Å 100.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10 20.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.10) 99.4 (20.00-2.10)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 2.09Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.187 , 0.226 0.187 , 0.225	Depositor DCC
R_{free} test set	780 reflections (0.99%)	wwPDB-VP
Wilson B-factor (Å ²)	28.2	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 48.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.023 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7034	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% 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: SO4, TEP

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	0.59	1/3182 (0.0%)	0.99	12/4337 (0.3%)
1	B	0.54	0/3168	0.97	16/4318 (0.4%)
All	All	0.56	1/6350 (0.0%)	0.98	28/8655 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	243	MET	SD-CE	5.84	1.94	1.79

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	237	LEU	N-CA-C	6.92	120.95	109.95
1	A	388	SER	N-CA-C	6.83	120.92	112.59
1	A	89	THR	N-CA-C	6.81	121.75	113.17
1	B	89	THR	N-CA-C	6.80	122.41	113.30
1	B	344	ILE	N-CA-C	-6.69	106.28	112.43
1	B	386	SER	N-CA-C	6.57	120.39	112.38
1	B	77	ALA	N-CA-C	-6.54	99.64	110.17
1	B	110	ASN	N-CA-C	6.46	120.06	109.85
1	A	237	LEU	N-CA-C	6.38	120.43	110.17
1	B	388	SER	N-CA-C	6.26	120.96	112.88
1	A	390	LYS	N-CA-C	-6.17	102.57	110.53
1	A	386	SER	N-CA-C	6.17	119.64	111.75
1	A	40	SER	N-CA-C	6.06	118.28	109.07
1	A	217	ALA	N-CA-C	-5.93	100.83	110.20
1	B	70	THR	N-CA-C	-5.86	106.77	114.04
1	B	217	ALA	N-CA-C	-5.67	100.04	109.46
1	B	95	ILE	N-CA-C	5.63	121.05	109.34
1	A	77	ALA	N-CA-C	-5.58	101.46	110.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	419	TYR	CA-C-N	5.49	125.32	119.28
1	B	419	TYR	C-N-CA	5.49	125.32	119.28
1	A	287	VAL	CA-C-N	-5.36	114.40	119.76
1	A	287	VAL	C-N-CA	-5.36	114.40	119.76
1	B	136	GLY	N-CA-C	-5.31	105.91	112.33
1	B	218	SER	CA-C-N	5.17	125.07	119.85
1	B	218	SER	C-N-CA	5.17	125.07	119.85
1	A	230	LEU	N-CA-C	5.11	117.24	111.11
1	A	70	THR	N-CA-C	-5.10	107.60	113.88
1	B	220	ALA	N-CA-C	-5.03	107.17	113.72

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	A	3075	0	2914	18	0
1	B	3071	0	2913	40	0
2	A	15	0	0	0	0
2	B	20	0	0	0	0
3	A	52	0	32	0	0
3	B	52	0	32	10	0
4	A	397	0	0	1	0
4	B	352	0	0	1	0
All	All	7034	0	5891	58	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 5.

All (58) 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:137:TRP:HD1	1:B:177:GLU:OE2	1.73	0.71
1:A:290:ASN:HD22	1:A:290:ASN:C	1.99	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:290:ASN:C	1:B:290:ASN:HD22	2.02	0.68
1:B:150:ASP:OD1	1:B:154:LYS:HE3	1.93	0.68
1:B:137:TRP:CD2	3:B:2435:TEP:N9	2.63	0.67
1:B:222:PRO:O	1:B:226:LYS:HG2	1.95	0.65
1:A:92:TRP:HA	1:A:96:GLU:HB2	1.77	0.65
1:B:82:GLU:H	1:B:82:GLU:CD	2.05	0.64
1:A:72:VAL:HG23	1:A:128:LEU:HD11	1.82	0.61
1:B:357:LEU:HD23	1:B:358:ILE:N	2.19	0.57
1:A:357:LEU:C	1:A:357:LEU:HD23	2.30	0.57
1:B:137:TRP:CE3	3:B:2435:TEP:H33	2.40	0.56
1:A:357:LEU:HD23	1:A:358:ILE:N	2.22	0.54
1:B:137:TRP:CD1	1:B:177:GLU:OE2	2.59	0.54
1:A:243:MET:HE3	4:A:1612:HOH:O	2.06	0.54
1:B:137:TRP:CE2	3:B:2435:TEP:N9	2.76	0.53
1:B:243:MET:SD	3:B:2433:TEP:C8	2.98	0.52
1:B:108:GLY:HA3	1:B:425:ASP:OD2	2.11	0.51
1:B:84:GLY:O	1:B:156:PHE:HA	2.10	0.51
1:A:168:GLY:HA2	1:A:419:TYR:CE2	2.46	0.51
1:B:46:VAL:O	1:B:382:MET:HA	2.10	0.51
1:B:248:ALA:O	1:B:301:ARG:HD2	2.11	0.50
1:A:94:ASP:O	1:A:115:ILE:HG12	2.12	0.49
1:B:406:GLY:O	1:B:409:VAL:HG22	2.13	0.48
1:B:52:TRP:HB3	3:B:2434:TEP:C8	2.43	0.48
1:B:290:ASN:C	1:B:290:ASN:ND2	2.71	0.47
1:B:168:GLY:HA2	1:B:419:TYR:CE2	2.50	0.47
1:B:75:ALA:HA	1:B:76:PHE:HA	1.75	0.47
1:A:177:GLU:HA	1:A:178:TYR:CG	2.51	0.46
1:B:137:TRP:CZ3	3:B:2435:TEP:H33	2.51	0.46
1:B:357:LEU:HD23	1:B:357:LEU:C	2.40	0.46
1:A:80:ARG:HH11	1:A:80:ARG:HG3	1.82	0.45
1:A:340:VAL:O	1:A:342:PRO:HD3	2.17	0.45
1:B:177:GLU:HA	1:B:178:TYR:CG	2.52	0.45
1:A:75:ALA:HB1	1:A:76:PHE:CG	2.52	0.44
1:A:84:GLY:HA2	1:A:146:ALA:HB1	1.98	0.44
1:B:243:MET:SD	3:B:2433:TEP:H8	2.58	0.44
1:B:137:TRP:CE2	3:B:2435:TEP:C8	3.01	0.43
1:A:75:ALA:HA	1:A:76:PHE:HA	1.74	0.43
1:B:137:TRP:CE3	3:B:2433:TEP:H13	2.54	0.43
1:B:137:TRP:CE3	3:B:2435:TEP:C3	3.01	0.43
1:B:351:ASP:HB3	1:B:354:ASN:OD1	2.18	0.43
1:B:66:VAL:HG11	1:B:121:LEU:HD22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:362:ASN:HB2	1:B:363:PRO:CD	2.49	0.43
1:B:328:TYR:CE2	1:B:396:LEU:HG	2.54	0.42
1:A:290:ASN:C	1:A:290:ASN:ND2	2.69	0.42
1:B:98:HIS:CE1	1:B:104:TRP:CH2	3.08	0.42
1:B:150:ASP:O	1:B:154:LYS:HG3	2.19	0.41
1:B:84:GLY:HA2	1:B:146:ALA:HB1	2.02	0.41
1:B:125:ASN:HB3	4:B:2529:HOH:O	2.19	0.41
1:B:186:ASN:OD1	1:B:229:HIS:CE1	2.74	0.41
1:A:80:ARG:HG2	1:A:87:TYR:CE1	2.56	0.41
1:A:84:GLY:O	1:A:156:PHE:HA	2.21	0.40
1:A:302:SER:HB3	1:A:358:ILE:HG12	2.02	0.40
1:B:131:LEU:HD12	1:B:131:LEU:N	2.36	0.40
1:B:156:PHE:CD1	1:B:156:PHE:C	2.99	0.40
1:B:39:ALA:O	1:B:40:SER:HB3	2.21	0.40
1:B:209:GLY:O	1:B:210:GLN:C	2.65	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	397/433 (92%)	387 (98%)	10 (2%)	0	100	100
1	B	395/433 (91%)	384 (97%)	10 (2%)	1 (0%)	36	36
All	All	792/866 (92%)	771 (97%)	20 (2%)	1 (0%)	48	50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	55	TYR

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	330/359 (92%)	329 (100%)	1 (0%)	86	91
1	B	328/359 (91%)	325 (99%)	3 (1%)	70	78
All	All	658/718 (92%)	654 (99%)	4 (1%)	78	86

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	290	ASN
1	B	82	GLU
1	B	98	HIS
1	B	290	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	GLN
1	A	142	ASN
1	A	186	ASN
1	A	236	GLN
1	A	290	ASN
1	B	60	ASN
1	B	98	HIS
1	B	290	ASN
1	B	429	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](#)

15 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
3	TEP	B	2436	-	14,14,14	1.27	1 (7%)	21,21,21	3.38	10 (47%)
2	SO4	A	1004	-	4,4,4	0.30	0	6,6,6	0.09	0
3	TEP	A	1434	-	14,14,14	1.28	1 (7%)	21,21,21	3.39	9 (42%)
2	SO4	B	1005	-	4,4,4	0.39	0	6,6,6	0.07	0
3	TEP	A	1433	-	14,14,14	1.26	1 (7%)	21,21,21	3.33	10 (47%)
2	SO4	B	1003	-	4,4,4	0.34	0	6,6,6	0.07	0
3	TEP	B	2434	-	14,14,14	1.28	1 (7%)	21,21,21	3.28	10 (47%)
3	TEP	B	2433	-	14,14,14	1.26	1 (7%)	21,21,21	3.34	10 (47%)
2	SO4	A	1002	-	4,4,4	0.35	0	6,6,6	0.12	0
2	SO4	B	1001	-	4,4,4	0.36	0	6,6,6	0.15	0
3	TEP	A	1435	-	14,14,14	1.29	1 (7%)	21,21,21	3.37	10 (47%)
3	TEP	B	2435	-	14,14,14	1.28	1 (7%)	21,21,21	3.43	10 (47%)
2	SO4	B	1007	-	4,4,4	0.44	0	6,6,6	0.17	0
2	SO4	A	1006	-	4,4,4	0.43	0	6,6,6	0.30	0
3	TEP	A	1436	-	14,14,14	1.28	1 (7%)	21,21,21	3.43	10 (47%)

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
3	TEP	B	2436	-	-	-	0/2/2/2
3	TEP	A	1434	-	-	-	0/2/2/2
3	TEP	A	1433	-	-	-	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TEP	B	2434	-	-	-	0/2/2/2
3	TEP	B	2433	-	-	-	0/2/2/2
3	TEP	A	1435	-	-	-	0/2/2/2
3	TEP	B	2435	-	-	-	0/2/2/2
3	TEP	A	1436	-	-	-	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1435	TEP	C5-N7	-3.25	1.33	1.38
3	B	2436	TEP	C5-N7	-3.23	1.33	1.38
3	B	2434	TEP	C5-N7	-3.22	1.33	1.38
3	A	1436	TEP	C5-N7	-3.22	1.33	1.38
3	A	1434	TEP	C5-N7	-3.18	1.33	1.38
3	B	2433	TEP	C5-N7	-3.18	1.33	1.38
3	B	2435	TEP	C5-N7	-3.17	1.33	1.38
3	A	1433	TEP	C5-N7	-3.11	1.33	1.38

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2435	TEP	C8-N9-C4	7.63	108.56	103.45
3	A	1436	TEP	C8-N9-C4	7.45	108.44	103.45
3	A	1434	TEP	C8-N9-C4	7.35	108.37	103.45
3	B	2436	TEP	C8-N9-C4	7.34	108.36	103.45
3	A	1435	TEP	C8-N9-C4	7.27	108.32	103.45
3	B	2433	TEP	C8-N9-C4	7.16	108.24	103.45
3	A	1433	TEP	C8-N9-C4	7.14	108.23	103.45
3	B	2435	TEP	C5-C4-N9	-7.02	106.71	111.63
3	A	1436	TEP	C5-C4-N9	-6.97	106.74	111.63
3	A	1434	TEP	C5-C4-N9	-6.91	106.78	111.63
3	B	2434	TEP	C8-N9-C4	6.89	108.06	103.45
3	A	1435	TEP	C5-C4-N9	-6.81	106.86	111.63
3	B	2436	TEP	C5-C4-N9	-6.74	106.91	111.63
3	B	2433	TEP	C5-C4-N9	-6.67	106.95	111.63
3	A	1433	TEP	C5-C4-N9	-6.63	106.98	111.63
3	B	2434	TEP	C5-C4-N9	-6.56	107.03	111.63
3	A	1433	TEP	C5-C6-N1	6.11	120.27	112.07
3	B	2433	TEP	C5-C6-N1	6.09	120.25	112.07
3	A	1436	TEP	C5-C6-N1	6.07	120.21	112.07
3	B	2436	TEP	C5-C6-N1	5.99	120.12	112.07
3	B	2435	TEP	C5-C6-N1	5.98	120.10	112.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1434	TEP	C5-C6-N1	5.98	120.09	112.07
3	A	1435	TEP	C5-C6-N1	5.95	120.06	112.07
3	B	2434	TEP	C5-C6-N1	5.90	119.99	112.07
3	A	1436	TEP	C4-C5-N7	4.49	107.50	105.29
3	A	1434	TEP	C4-C5-N7	4.47	107.49	105.29
3	B	2435	TEP	C4-C5-N7	4.36	107.43	105.29
3	B	2434	TEP	C4-C5-N7	4.32	107.41	105.29
3	A	1435	TEP	C4-C5-N7	4.25	107.38	105.29
3	B	2433	TEP	C6-C5-C4	-4.18	119.83	123.13
3	A	1436	TEP	C6-C5-C4	-4.17	119.84	123.13
3	A	1434	TEP	C6-C5-C4	-4.17	119.84	123.13
3	B	2433	TEP	C4-C5-N7	4.15	107.33	105.29
3	A	1433	TEP	C6-C5-C4	-4.13	119.87	123.13
3	B	2436	TEP	C4-C5-N7	4.09	107.30	105.29
3	B	2435	TEP	C6-C5-C4	-4.08	119.91	123.13
3	B	2435	TEP	N3-C4-N9	4.08	132.67	126.27
3	A	1436	TEP	N3-C4-N9	4.06	132.65	126.27
3	B	2436	TEP	C6-C5-C4	-4.04	119.94	123.13
3	A	1433	TEP	C4-C5-N7	4.03	107.27	105.29
3	A	1434	TEP	N3-C4-N9	4.03	132.60	126.27
3	A	1435	TEP	C6-C5-C4	-4.03	119.95	123.13
3	A	1435	TEP	N3-C4-N9	4.02	132.59	126.27
3	A	1433	TEP	N3-C4-N9	4.00	132.55	126.27
3	B	2436	TEP	N3-C4-N9	3.99	132.54	126.27
3	B	2434	TEP	C6-C5-C4	-3.98	119.99	123.13
3	B	2433	TEP	N3-C4-N9	3.96	132.50	126.27
3	B	2434	TEP	N3-C4-N9	3.90	132.39	126.27
3	B	2436	TEP	O6-C6-C5	-3.73	119.03	126.64
3	A	1435	TEP	O6-C6-C5	-3.67	119.14	126.64
3	A	1436	TEP	O6-C6-C5	-3.63	119.24	126.64
3	B	2435	TEP	O6-C6-C5	-3.51	119.47	126.64
3	B	2434	TEP	O6-C6-C5	-3.49	119.53	126.64
3	A	1434	TEP	O6-C6-C5	-3.46	119.58	126.64
3	A	1433	TEP	C6-N1-C2	-3.45	120.05	125.66
3	B	2436	TEP	C6-N1-C2	-3.42	120.10	125.66
3	A	1436	TEP	C6-N1-C2	-3.41	120.12	125.66
3	B	2433	TEP	C6-N1-C2	-3.40	120.13	125.66
3	B	2435	TEP	C6-N1-C2	-3.37	120.18	125.66
3	B	2434	TEP	C6-N1-C2	-3.36	120.19	125.66
3	A	1435	TEP	C6-N1-C2	-3.35	120.21	125.66
3	B	2433	TEP	O6-C6-C5	-3.34	119.84	126.64
3	A	1434	TEP	C6-N1-C2	-3.31	120.28	125.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1433	TEP	O6-C6-C5	-3.31	119.89	126.64
3	B	2435	TEP	N7-C8-N9	-3.24	109.22	112.98
3	B	2436	TEP	N7-C8-N9	-3.18	109.29	112.98
3	A	1436	TEP	N7-C8-N9	-3.12	109.36	112.98
3	A	1434	TEP	N7-C8-N9	-3.08	109.40	112.98
3	A	1435	TEP	N7-C8-N9	-3.07	109.41	112.98
3	B	2433	TEP	N7-C8-N9	-3.07	109.42	112.98
3	A	1433	TEP	N7-C8-N9	-3.04	109.45	112.98
3	B	2434	TEP	N7-C8-N9	-2.86	109.66	112.98
3	B	2433	TEP	C5-C4-N3	-2.28	120.44	121.73
3	A	1433	TEP	C5-C4-N3	-2.27	120.45	121.73
3	A	1435	TEP	C5-C4-N3	-2.10	120.55	121.73
3	B	2436	TEP	C5-C4-N3	-2.09	120.55	121.73
3	B	2434	TEP	C5-C4-N3	-2.06	120.57	121.73
3	A	1436	TEP	C5-C4-N3	-2.02	120.59	121.73
3	B	2435	TEP	C5-C4-N3	-2.01	120.59	121.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2434	TEP	1	0
3	B	2433	TEP	3	0
3	B	2435	TEP	6	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 [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	394/433 (90%)	-0.47	1 (0%)	90 91	17, 25, 38, 52	5 (1%)
1	B	394/433 (90%)	-0.27	3 (0%)	82 84	19, 29, 42, 52	3 (0%)
All	All	788/866 (90%)	-0.37	4 (0%)	87 88	17, 27, 40, 52	8 (1%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	39	ALA	4.9
1	B	39	ALA	3.8
1	B	137	TRP	2.9
1	B	104	TRP	2.4

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
3	TEP	B	2435	13/13	0.65	0.20	52,56,58,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	TEP	B	2436	13/13	0.72	0.29	26,31,34,34	13
3	TEP	A	1434	13/13	0.76	0.16	43,50,53,54	0
3	TEP	A	1435	13/13	0.79	0.15	50,53,55,57	0
3	TEP	A	1436	13/13	0.82	0.16	52,55,58,58	0
2	SO4	A	1002	5/5	0.83	0.14	63,63,65,65	5
3	TEP	B	2433	13/13	0.89	0.12	34,39,43,43	0
3	TEP	B	2434	13/13	0.89	0.11	38,39,41,43	0
2	SO4	A	1004	5/5	0.91	0.16	35,35,36,37	5
2	SO4	B	1003	5/5	0.92	0.10	57,57,57,57	5
2	SO4	B	1007	5/5	0.93	0.10	41,42,45,48	0
2	SO4	B	1001	5/5	0.94	0.10	49,50,50,51	5
2	SO4	B	1005	5/5	0.94	0.08	51,52,52,53	5
3	TEP	A	1433	13/13	0.95	0.07	32,35,38,40	0
2	SO4	A	1006	5/5	0.97	0.09	36,40,42,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.