



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 3, 2024 – 02:20 am GMT

PDB ID : 2XUC
Title : Natural product-guided discovery of a fungal chitinase inhibitor
Authors : Rush, C.L.; Schuttelkopf, A.W.; Hurtado-Guerrero, R.; Blair, D.E.; Ibrahim, A.F.M.; Desvergnès, S.; Eggleston, I.M.; van Aalten, D.M.F.
Deposited on : 2010-10-18
Resolution : 2.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

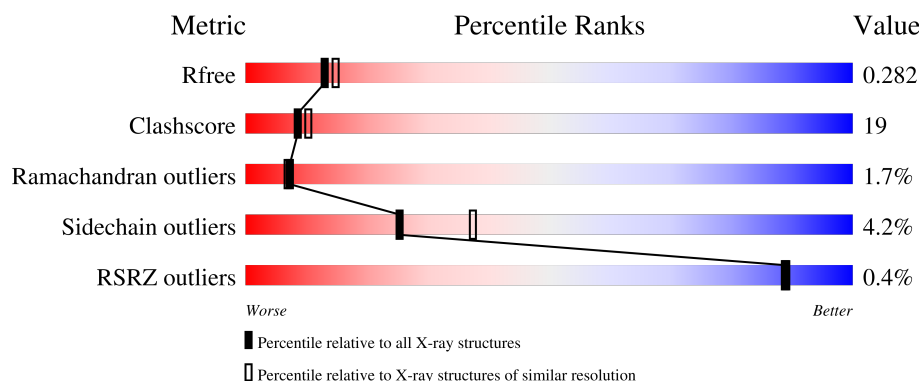
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION




The reported resolution of this entry is 2.30 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}	164625	5963 (2.30-2.30)
Clashscore	180529	6698 (2.30-2.30)
Ramachandran outliers	177936	6640 (2.30-2.30)
Sidechain outliers	177891	6640 (2.30-2.30)
RSRZ outliers	164620	5963 (2.30-2.30)

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	310	 87% 11% •
1	B	310	 88% 11% •
1	C	310	 % 50% 38% 5% • 5%

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	XRG	C	1337	-	-	X	-
3	PO4	B	1340	-	X	-	-
3	PO4	B	1341	-	X	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7338 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.

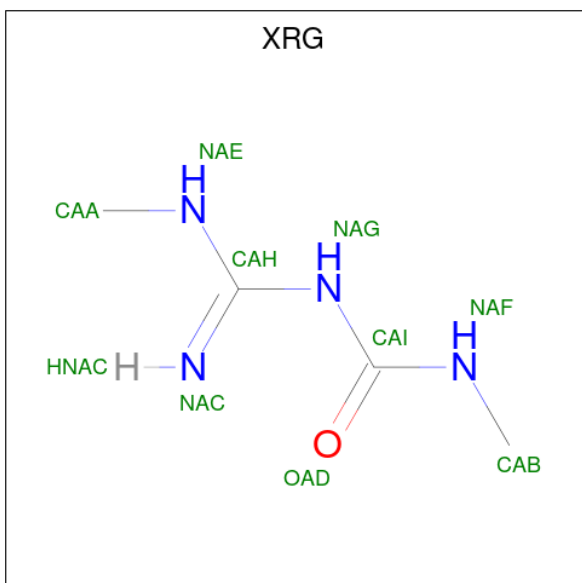
- Molecule 1 is a protein called CHITINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	310	Total	C	N	O	S	0	0	0
			2408	1550	383	463	12			
1	B	310	Total	C	N	O	S	0	0	0
			2408	1550	383	463	12			
1	C	293	Total	C	N	O	S	0	0	0
			2278	1469	361	436	12			

There are 3 discrepancies between the modelled and reference sequences:

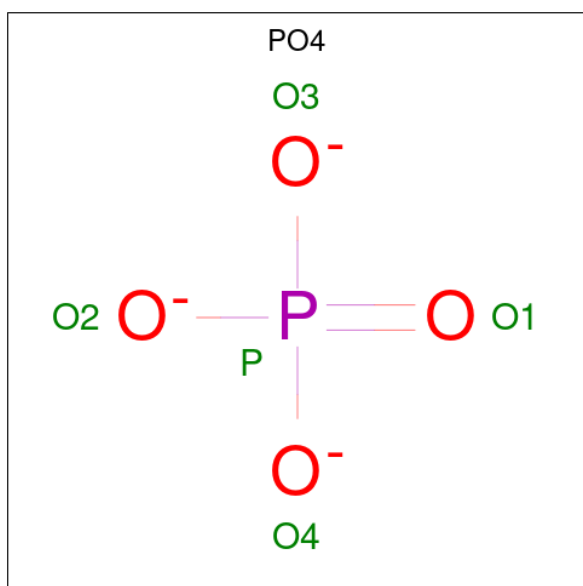
Chain	Residue	Modelled	Actual	Comment	Reference
A	28	PHE	-	expression tag	UNP Q873Y0
B	28	PHE	-	expression tag	UNP Q873Y0
C	28	PHE	-	expression tag	UNP Q873Y0

- Molecule 2 is 1-methyl-3-(N-methylcarbamimidoyl)urea (three-letter code: XRG) (formula: $C_4H_{10}N_4O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			9	4	4	1		
2	A	1	Total	C	N	O	0	0
			9	4	4	1		
2	B	1	Total	C	N	O	0	0
			9	4	4	1		
2	B	1	Total	C	N	O	0	0
			9	4	4	1		
2	C	1	Total	C	N	O	0	0
			9	4	4	1		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total 1	Cl 1	0	0

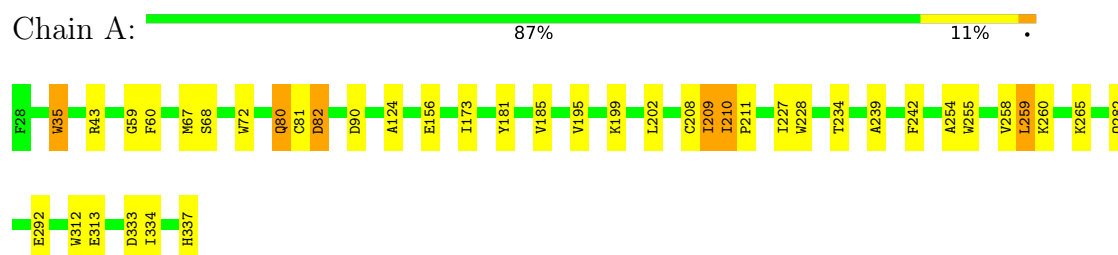
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	67	Total 67	O 67	0	0
5	B	89	Total 89	O 89	0	0
5	C	21	Total 21	O 21	0	0

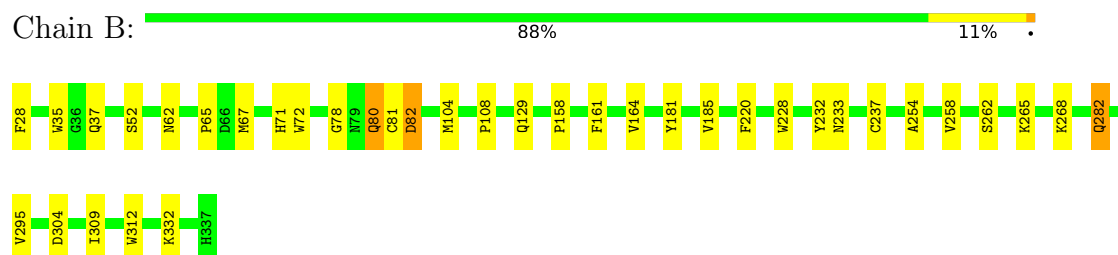
3 Residue-property plots

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.

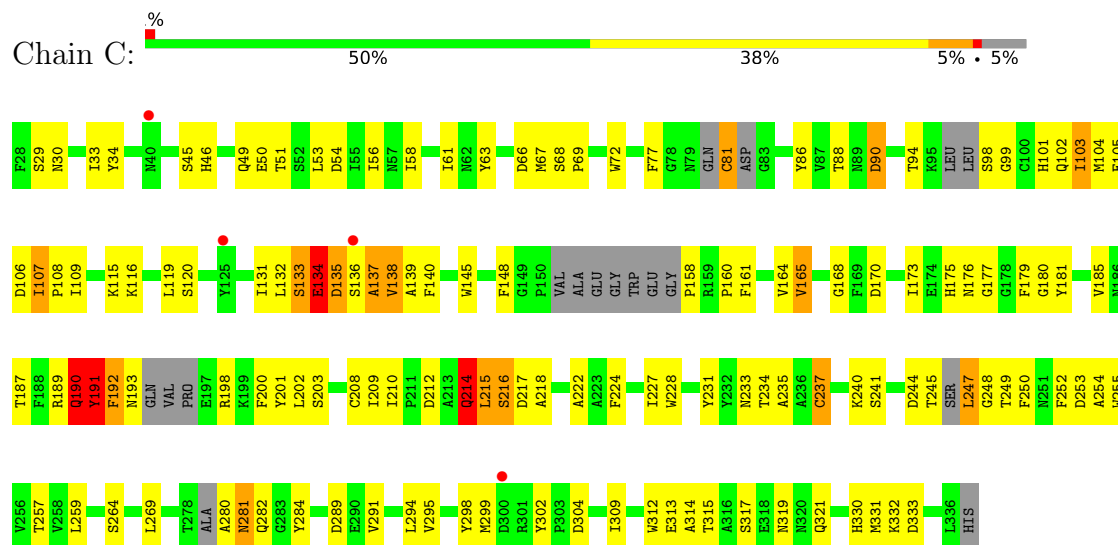
• Molecule 1: CHITINASE



• Molecule 1: CHITINASE



• Molecule 1: CHITINASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	100.04Å 100.04Å 111.16Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	86.64 – 2.30 86.64 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (86.64-2.30) 97.5 (86.64-2.30)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.60 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.233 , 0.277 0.245 , 0.282	Depositor DCC
R_{free} test set	527 reflections (0.96%)	wwPDB-VP
Wilson B-factor (Å ²)	25.9	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 16.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.025 for -h,-k,l 0.469 for h,-h-k,-l 0.027 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7338	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.34% 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: XRG, CL, PO4

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	0.94	1/2481 (0.0%)	0.85	4/3384 (0.1%)
1	B	0.97	0/2481	0.88	4/3384 (0.1%)
1	C	1.08	2/2340 (0.1%)	1.04	12/3179 (0.4%)
All	All	1.00	3/7302 (0.0%)	0.92	20/9947 (0.2%)

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	C	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	214	GLN	C-N	-9.26	1.12	1.34
1	C	165	VAL	CB-CG2	5.11	1.63	1.52
1	A	35	TRP	CB-CG	5.10	1.59	1.50

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	103	ILE	N-CA-CB	14.80	144.83	110.80
1	A	82	ASP	N-CA-CB	12.67	133.41	110.60
1	C	102	GLN	N-CA-C	-10.38	82.98	111.00
1	C	81	CYS	N-CA-C	10.26	138.69	111.00
1	B	82	ASP	N-CA-CB	10.01	128.62	110.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	214	GLN	Mainchain
1	C	29	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	2408	0	2245	44	0
1	B	2408	0	2245	22	0
1	C	2278	0	2118	187	0
2	A	18	0	18	4	0
2	B	18	0	18	2	0
2	C	9	0	9	8	0
3	A	5	0	0	0	0
3	B	10	0	0	5	0
3	C	5	0	0	1	0
4	A	1	0	0	1	0
4	B	1	0	0	1	0
5	A	67	0	0	1	0
5	B	89	0	0	0	0
5	C	21	0	0	0	0
All	All	7338	0	6653	254	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 19.

The worst 5 of 254 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:C:138:VAL:HG13	1:C:187:THR:CG2	1.47	1.44
1:C:131:ILE:HD11	1:C:181:TYR:CE1	1.55	1.41
1:A:210:ILE:HD11	1:A:255:TRP:NE1	1.34	1.39
1:C:138:VAL:CG1	1:C:187:THR:HG21	1.55	1.35
1:C:312:TRP:NE1	2:C:1337:XRG:NAC	1.76	1.29

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	308/310 (99%)	293 (95%)	13 (4%)	2 (1%)	22	27
1	B	308/310 (99%)	299 (97%)	8 (3%)	1 (0%)	37	47
1	C	278/310 (90%)	243 (87%)	23 (8%)	12 (4%)	2	1
All	All	894/930 (96%)	835 (93%)	44 (5%)	15 (2%)	7	7

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	209	ILE
1	C	103	ILE
1	C	133	SER
1	C	135	ASP
1	C	192	PHE

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	253/253 (100%)	244 (96%)	9 (4%)	30	44
1	B	253/253 (100%)	247 (98%)	6 (2%)	44	61
1	C	240/253 (95%)	224 (93%)	16 (7%)	13	19
All	All	746/759 (98%)	715 (96%)	31 (4%)	25	37

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	282	GLN
1	C	240	LYS
1	C	90	ASP
1	C	264	SER
1	C	216	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	102	GLN
1	C	214	GLN
1	C	321	GLN
1	C	319	ASN
1	B	207	GLN

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](#)

Of 11 ligands modelled in this entry, 2 are monoatomic - leaving 9 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
2	XRG	A	1339	-	7,8,8	1.11	0	7,9,9	1.24	1 (14%)
2	XRG	C	1337	-	7,8,8	1.26	0	7,9,9	0.95	0
3	PO4	C	1338	-	4,4,4	0.97	0	6,6,6	0.47	0
2	XRG	A	1338	-	7,8,8	1.65	1 (14%)	7,9,9	1.91	2 (28%)
3	PO4	A	1340	-	4,4,4	0.82	0	6,6,6	0.86	0
3	PO4	B	1340	-	4,4,4	2.96	4 (100%)	6,6,6	0.43	0
2	XRG	B	1339	-	7,8,8	1.39	1 (14%)	7,9,9	0.59	0
2	XRG	B	1338	-	7,8,8	1.15	1 (14%)	7,9,9	0.98	0
3	PO4	B	1341	-	4,4,4	2.96	4 (100%)	6,6,6	0.43	0

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	XRG	A	1339	-	-	1/7/8/8	-
2	XRG	C	1337	-	-	1/7/8/8	-
2	XRG	A	1338	-	-	0/7/8/8	-
2	XRG	B	1339	-	-	1/7/8/8	-
2	XRG	B	1338	-	-	0/7/8/8	-

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1340	PO4	P-O1	4.51	1.61	1.50
3	B	1341	PO4	P-O1	4.51	1.61	1.50
2	A	1338	XRG	CAA-NAE	3.64	1.52	1.45
2	B	1338	XRG	CAA-NAE	2.78	1.50	1.45
2	B	1339	XRG	CAB-NAF	2.73	1.50	1.45

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1338	XRG	CAB-NAF-CAI	-4.38	113.69	121.61
2	A	1338	XRG	CAA-NAE-CAH	-2.27	118.84	123.86
2	A	1339	XRG	CAH-NAG-CAI	2.09	129.00	125.42

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1339	XRG	NAC-CAH-NAG-CAI
2	B	1339	XRG	NAC-CAH-NAG-CAI
2	C	1337	XRG	NAC-CAH-NAG-CAI

There are no ring outliers.

7 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1339	XRG	3	0
2	C	1337	XRG	8	0
3	C	1338	PO4	1	0
2	A	1338	XRG	1	0
3	B	1340	PO4	1	0
2	B	1339	XRG	2	0
3	B	1341	PO4	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	214:GLN	C	215:LEU	N	1.12

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	310/310 (100%)	-1.53	0 100 100	10, 19, 33, 52	1 (0%)
1	B	310/310 (100%)	-1.59	0 100 100	9, 18, 32, 50	1 (0%)
1	C	293/310 (94%)	-1.05	4 (1%) 73 74	0, 37, 49, 58	14 (4%)
All	All	913/930 (98%)	-1.40	4 (0%) 89 89	0, 22, 45, 58	16 (1%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	136	SER	6.2
1	C	125	TYR	5.7
1	C	40	ASN	3.2
1	C	300	ASP	2.3

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 monosaccharides 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(\AA^2)	Q<0.9
2	XRG	A	1339	9/9	0.98	0.04	26,33,35,37	0
2	XRG	B	1339	9/9	0.98	0.05	27,36,38,38	0
3	PO4	B	1340	5/5	0.98	0.09	30,30,30,30	0
3	PO4	B	1341	5/5	0.98	0.09	30,30,30,30	0
3	PO4	A	1340	5/5	0.99	0.03	50,51,53,53	0
2	XRG	A	1338	9/9	0.99	0.03	9,13,15,22	0
2	XRG	C	1337	9/9	0.99	0.04	28,36,46,50	0
3	PO4	C	1338	5/5	0.99	0.10	57,58,59,60	0
4	CL	A	1341	1/1	0.99	0.04	30,30,30,30	0
4	CL	B	1342	1/1	0.99	0.06	30,30,30,30	0
2	XRG	B	1338	9/9	1.00	0.02	9,13,16,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.