

Full wwPDB X-ray Structure Validation Report (i)

Jan 23, 2021 – 01:06 PM GMT

PDB ID	:	6XTW
Title	:	HumRadA33F in complex with peptidic inhibitor 6
Authors	:	Fischer, G.; Marsh, M.E.; Scott, D.E.; Coyne, A.G.; Skidmore, J.; Abell, C.;
		Hyvonen, M.
Deposited on	:	2020-01-16
$\operatorname{Resolution}$:	2.31 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

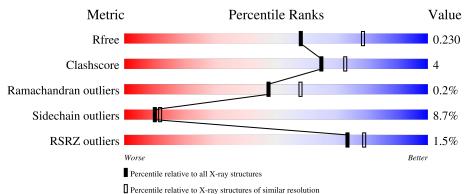
9	:	4.02b-467 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.16
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.16

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 2.31 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$		
R _{free}	130704	5974(2.34-2.30)		
Clashscore	141614	6604(2.34-2.30)		
Ramachandran outliers	138981	6523 (2.34-2.30)		
Sidechain outliers	138945	6523 (2.34-2.30)		
RSRZ outliers	127900	5855(2.34-2.30)		

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 <=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	А	231	83%	13%	••				
1	В	231	2% 8 5%	11%	•••				



$6 \mathrm{XTW}$

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3656 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Λ	225	Total	С	Ν	Ο	S	0	0	0
		220	1737	1089	314	329	5	0		
1	р	228	Total	С	Ν	Ο	S	0	0	0
	220	1757	1102	317	333	5	0	U		

• Molecule 1 is a protein called DNA repair and recombination protein RadA.

Chain	Residue	Modelled	Actual	Comment	Reference
А	107	MET	-	initiating methionine	UNP 074036
А	167	LYS	SER	engineered mutation	UNP 074036
А	168	ALA	VAL	engineered mutation	UNP 074036
А	169	MET	ILE	engineered mutation	UNP 074036
А	170	TYR	TRP	engineered mutation	UNP 074036
А	175	GLY	ASN	engineered mutation	UNP 074036
А	182	LEU	ILE	engineered mutation	UNP 074036
А	183	LEU	ARG	engineered mutation	UNP 074036
А	192	SER	ASP	engineered mutation	UNP 074036
А	193	GLY	PRO	engineered mutation	UNP 074036
А	194	SER	ASP	engineered mutation	UNP 074036
А	195	ASP	GLU	engineered mutation	UNP 074036
А	198	ASP	LYS	engineered mutation	UNP 074036
А	199	ASN	HIS	engineered mutation	UNP 074036
А	200	VAL	ILE	engineered mutation	UNP 074036
А	201	ALA	TYR	engineered mutation	UNP 074036
А	202	TYR	VAL	engineered mutation	UNP 074036
А	219	SER	GLU	engineered mutation	UNP 074036
А	221	MET	LYS	engineered mutation	UNP 074036
А	222	MET	ILE	engineered mutation	UNP 074036
А	223	VAL	LYS	engineered mutation	UNP 074036
А	232	TYR	VAL	engineered mutation	UNP 074036
А	288	ASN	ARG	engineered mutation	UNP 074036
А	?	-	PRO	deletion	UNP 074036
А	?	-	ASP	deletion	UNP 074036

There are 70 discrepancies between the modelled and reference sequences:

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Chain	Residue	Modelled	Actual	Comment	Reference			
А	?	-	ALA	deletion	UNP 074036			
А	?	-	PHE	deletion	UNP 074036			
А	?	-	PHE	deletion	UNP 074036			
А	?	-	GLY	deletion	UNP 074036			
А	?	-	ASP	deletion	UNP 074036			
А	?	-	PRO	deletion	UNP 074036			
А	?	-	THR	deletion	UNP 074036			
А	?	-	ARG	deletion	UNP 074036			
А	?	-	PRO	deletion	UNP 074036			
А	?	-	ILE	deletion	UNP 074036			
В	107	MET	-	initiating methionine	UNP 074036			
В	167	LYS	SER	engineered mutation	UNP 074036			
В	168	ALA	VAL	engineered mutation	UNP 074036			
В	169	MET	ILE	engineered mutation	UNP 074036			
В	170	TYR	TRP	engineered mutation	UNP 074036			
В	175	GLY	ASN	engineered mutation	UNP 074036			
В	182	LEU	ILE	engineered mutation	UNP 074036			
В	183	LEU	ARG	engineered mutation	UNP 074036			
В	192	SER	ASP	engineered mutation	UNP 074036			
В	193	GLY	PRO	engineered mutation	UNP 074036			
В	194	SER	ASP	engineered mutation	UNP 074036			
В	195	ASP	GLU	engineered mutation	UNP 074036			
В	198	ASP	LYS	engineered mutation	UNP 074036			
В	199	ASN	HIS	engineered mutation	UNP 074036			
В	200	VAL	ILE	engineered mutation	UNP 074036			
В	201	ALA	TYR	engineered mutation	UNP 074036			
В	202	TYR	VAL	engineered mutation	UNP 074036			
В	219	SER	GLU	engineered mutation	UNP 074036			
В	221	MET	LYS	engineered mutation	UNP 074036			
В	222	MET	ILE	engineered mutation	UNP 074036			
В	223	VAL	LYS	engineered mutation	UNP 074036			
В	232	TYR	VAL	engineered mutation	UNP 074036			
В	288	ASN	ARG	engineered mutation	UNP 074036			
В	?	-	PRO	deletion	UNP 074036			
В	?	-	ASP	deletion	UNP 074036			
В	?	-	ALA	deletion	UNP 074036			
В	?	-	PHE	deletion	UNP 074036			
В	?	-	PHE	deletion	UNP 074036			
В	?	-	GLY	deletion	UNP 074036			
В	?	-	ASP	deletion	UNP 074036			
В	?	-	PRO	deletion	UNP 074036			
В	?	-	THR	deletion	UNP 074036			

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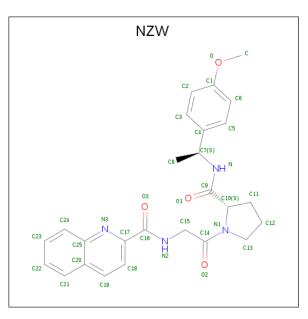
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00111111	Continued from provide page								
Chain	Residue	Residue Modelled		Comment	Reference				
В	?	-	ARG	deletion	UNP 074036				
В	?	-	PRO	deletion	UNP 074036				
В	?	-	ILE	deletion	UNP 074036				

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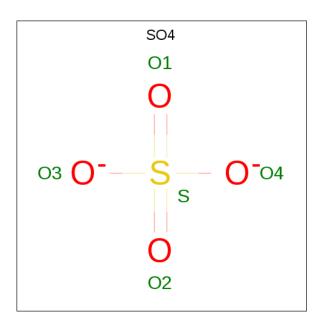
• Molecule 2 is {N}-[2-[(2 {S})-2-[[(1 {S})-1-(4-methoxyphenyl)ethyl]carbamoyl]pyrrolidi n-1-yl]-2-oxidanylidene-ethyl]quinoline-2-carboxamide (three-letter code: NZW) (formula: C₂₆H₂₈N₄O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	А	1	Total 34	С 26	N 4	0 4	0	0

• Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0

• Molecule 4 is water.

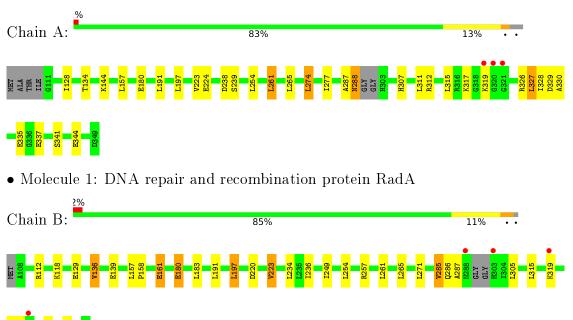
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	62	Total O 62 62	0	0
4	В	56	$\begin{array}{cc} {\rm Total} & {\rm O} \\ 56 & 56 \end{array}$	0	0



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: DNA repair and recombination protein RadA





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants	89.83Å 89.83 Å 100.83 Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.92 - 2.31	Depositor
Resolution (A)	44.92 - 2.31	EDS
% Data completeness	99.3 (44.92-2.31)	Depositor
(in resolution range)	99.3(44.92 - 2.31)	EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.55 \;({\rm at}\; 2.32{\rm \AA})$	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.184 , 0.229	Depositor
It, Itfree	0.184 , 0.230	DCC
R_{free} test set	1036 reflections (4.94%)	wwPDB-VP
Wilson B-factor $(Å^2)$	45.7	Xtriage
Anisotropy	0.114	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.34 , 49.1	EDS
L-test for $twinning^2$	$< L >=0.48, < L^2>=0.31$	Xtriage
Estimated twinning fraction	0.037 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3656	wwPDB-VP
Average B, all atoms $(Å^2)$	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.55% of the height of the origin peak. No significant pseudotranslation is detected.

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.



 $^{^1 {\}rm Intensities}$ estimated from amplitudes.

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: NZW, 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	А	0.37	0/1762	0.56	0/2373	
1	В	0.39	0/1782	0.58	0/2401	
All	All	0.38	0/3544	0.57	0/4774	

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 (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	А	1737	0	1755	18	0
1	В	1757	0	1778	13	0
2	А	34	0	0	0	0
3	А	5	0	0	0	0
3	В	5	0	0	0	0
4	А	62	0	0	1	0
4	В	56	0	0	1	0
All	All	3656	0	3533	29	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 4.



A., 1	A.L. 0	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:312:ARG:NH2	1:B:220:ASP:OD1	2.26	0.68
1:B:157:LEU:HD21	1:B:191:LEU:HD11	1.79	0.65
1:A:312:ARG:NH1	1:A:329:ASP:HB2	2.23	0.53
1:A:261:LEU:HD13	1:A:307:HIS:HB3	1.91	0.52
1:A:326:ARG:HG3	1:A:337:GLU:HG2	1.92	0.52
1:B:183:LEU:HD21	1:B:197:LEU:HD22	1.94	0.48
1:A:144:LYS:HG2	1:A:315:LEU:HD12	1.95	0.48
1:A:261:LEU:HD22	1:A:265:LEU:HD23	1.97	0.47
1:B:112:ARG:NH1	1:B:129:GLU:OE2	2.48	0.47
1:A:328:ILE:HD12	1:B:223:VAL:HG11	1.97	0.46
1:A:312:ARG:HH11	1:A:329:ASP:HB2	1.78	0.46
1:A:327:LEU:HG	1:A:330:ALA:HB2	1.99	0.44
1:B:136:VAL:HG22	1:B:315:LEU:HG	2.00	0.44
1:A:312:ARG:HD3	4:A:523:HOH:O	2.17	0.44
1:A:287:ALA:HA	1:A:288:ASN:HA	1.74	0.43
1:A:265:LEU:HA	1:A:265:LEU:HD13	1.91	0.43
1:B:249:ILE:H	1:B:249:ILE:HG13	1.65	0.43
1:B:139:GLU:HA	1:B:285:VAL:O	2.18	0.43
1:B:158:PRO:HG2	1:B:161:GLU:CG	2.48	0.43
1:A:157:LEU:HD21	1:A:191:LEU:HD11	2.01	0.42
1:A:238:ASP:HA	1:A:239:SER:HA	1.71	0.42
1:A:180:GLU:CD	1:A:180:GLU:H	2.23	0.42
1:B:335:GLU:H	1:B:335:GLU:CD	2.23	0.42
1:B:234:LEU:HD21	1:B:236:ILE:HD11	2.02	0.41
1:A:274:LEU:HD12	1:A:274:LEU:HA	1.87	0.41
1:B:180:GLU:HB2	4:B:504:HOH:O	2.19	0.41
1:A:128:ILE:HD12	1:A:134:THR:HG21	2.03	0.41
1:A:288:ASN:N	1:A:288:ASN:OD1	2.54	0.41
1:B:328:ILE:HA	1:B:328:ILE:HD13	1.83	0.40

All (29) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

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.



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	А	221/231~(96%)	219~(99%)	2(1%)	0	100 100
1	В	224/231~(97%)	219~(98%)	4 (2%)	1 (0%)	34 41
All	All	445/462~(96%)	438 (98%)	6 (1%)	1 (0%)	47 58

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

All (1) Ramachandran outliers are listed below:

Mol	Chain	\mathbf{Res}	Type
1	В	287	ALA

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	А	183/186~(98%)	168~(92%)	15 (8%)	11 14
1	В	185/186~(100%)	168~(91%)	17 (9%)	9 10
All	All	368/372~(99%)	336~(91%)	32 (9%)	10 12

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	197	LEU
1	А	223	VAL
1	А	224	GLU
1	А	254	LEU
1	А	261	LEU
1	А	274	LEU
1	А	277	ILE
1	А	288	ASN
1	А	311	LEU
1	А	317	LYS
1	А	319	LYS
1	A	327	LEU

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\mathbf{Mol}	Chain	Res	Type
1	А	335	GLU
1	А	341	SER
1	А	344	GLU
1	В	118	LYS
1	В	136	VAL
1	В	161	GLU
1	В	180	GLU
1	В	197	LEU
1	В	223	VAL
1	В	254	LEU
1	В	257	ARG
1	В	261	LEU
1	В	265	LEU
1	В	271	LEU
1	В	285	VAL
1	В	286	GLN
1	В	305	LEU
1	В	319	LYS
1	В	327	LEU
1	В	344	GLU

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Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

3 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	Bo	ond leng	\mathbf{ths}	В	ond ang	les
	Type	Unam	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	А	402	-	4,4,4	0.17	0	$6,\!6,\!6$	0.43	0
3	SO4	В	401	-	4,4,4	0.39	0	$6,\!6,\!6$	0.28	0
2	NZW	А	401	-	37,37,37	0.18	0	$51,\!51,\!51$	0.32	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	NZW	А	401	-	-	0/27/37/37	0/4/4/4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

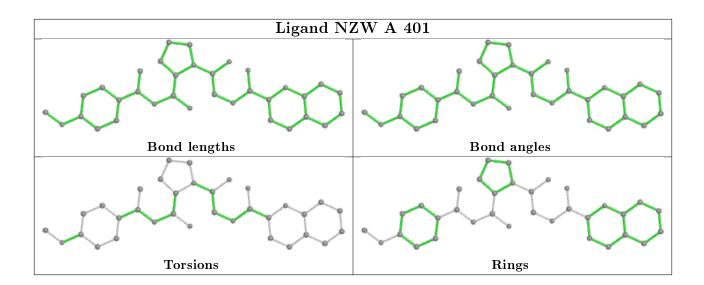
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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, 95^{th} 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 $>$	$\# RSRZ {>}2$	$\mathbf{OWAB}(\mathbf{\AA}^2)$	$Q{<}0.9$
1	А	225/231~(97%)	-0.02	3 (1%) 77 81	33, 48, 72, 99	0
1	В	228/231 (98%)	-0.17	4 (1%) 68 75	31, 46, 64, 89	0
All	All	453/462~(98%)	-0.10	7 (1%) 73 79	31, 47, 71, 99	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ	
1	А	320	GLY	7.4	
1	А	321	GLY	5.4	
1	А	319	LYS	4.6	
1	В	288	ASN	3.3	
1	В	319	LYS	2.3	
1	В	329	ASP	2.1	
1	В	303	HIS	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 monosaccharides in this entry.

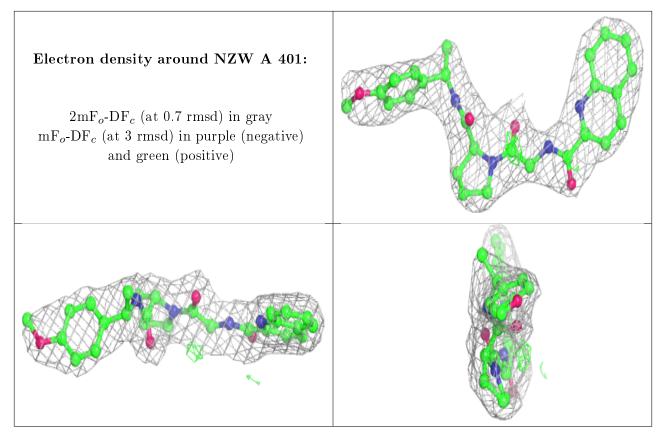
6.4 Ligands (i)

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, 95^{th} 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	$\mathbf{B} ext{-factors}(\mathbf{\AA}^2)$	$Q{<}0.9$
2	NZW	А	401	34/34	0.94	0.12	$39,\!51,\!61,\!64$	0
3	SO4	А	402	5/5	0.98	0.10	$53,\!53,\!54,\!55$	0
3	SO4	В	401	5/5	0.99	0.12	43,43,44,46	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers (i)

There are no such residues in this entry.

