

# Full wwPDB X-ray Structure Validation Report (i)

#### Jan 2, 2024 – 03:58 pm GMT

PDB ID	:	5A3S
Title	:	Crystal structure of the (SR) Calcium ATPase E2-vanadate complex bound to
		thapsigargin and TNP-ATP
Authors	:	Clausen, J.D.; Bublitz, M.; Arnou, B.; Olesen, C.; Andersen, J.P.; Moller,
		J.V.; Nissen, P.
Deposited on	:	2015-06-03
Resolution	:	3.30  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 types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
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)	:	2.36

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

The reported resolution of this entry is 3.30 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.



Motric	Whole archive	Similar resolution
IVIETIC	$(\# { m Entries})$	$(\# { m Entries},  { m resolution}  { m range}({ m \AA}))$
$R_{free}$	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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	995	<u>6%</u> 83%	16%	-			
1	В	995	<u>6%</u> 83%	16%				



## 2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 15554 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 SARCOPLASMIC RETICULUM CALCIUM ATPASE 1 MOLECULE SARCOPLASMIC/ENDOPLASMIC RETICULUM CALCIUM ATPASE 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	А	995	Total 7672	C 4877	N 1287	0 1451	S 57	0	0	0
1	В	995	Total 7674	C 4878	N 1287	0 1452	S 57	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	0	ACE	-	acetylation	UNP PO4191
В	0	ACE	-	acetylation	UNP PO4191

• Molecule 2 is OCTANOIC ACID [3S-[3ALPHA, 3ABETA, 4ALPHA, 6BETA, 6ABETA, 7BETA, 8ALPHA(Z), 9BALPHA]]-6-(ACETYLOXY)-2,3,-3A,4,5,6,6A,7,8,9B-DECAHYD RO-3,3A-DIHYDROXY-3,6,9-TRIMETHYL-8-[(2-METHYL-1-OXO-2-BUTENYL)OX Y ]-2-OXO-4-(1-OXOBUTOXY)-AZULENO[4,5-B]FURAN-7-YL ESTER (three-letter code: TG1) (formula: C<sub>34</sub>H<sub>50</sub>O<sub>12</sub>).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	Total         C         O           46         34         12	0	0
2	В	1	Total         C         O           46         34         12	0	0

• Molecule 3 is oxido<br/>(dioxo)vanadium (three-letter code: VN4) (formula:  ${\rm O}_{3}{\rm V}).$ 



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



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- Molecule 4 is SPIRO(2,4,6-TRINITROBENZENE[1,2A]-2O',3O'-METHYLENE-ADENIN E-TRIPHOSPHATE (three-letter code: 128) (formula:  $C_{16}H_{17}N_8O_{19}P_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
4	Δ	1	Total	С	Ν	Ο	Р	0	0
4 A	A	L	46	16	8	19	3	0	
4	D	1	Total	С	Ν	0	Р	0	0
4 B	D	1	46	16	8	19	3	0	0

• Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	2	Total Mg 2 2	0	0
5	В	2	Total Mg 2 2	0	0

• Molecule 6 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	1	Total K 1 1	0	0
6	В	1	Total K 1 1	0	0

• Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	А	1	Total Cl 1 1	0	0
7	В	1	Total Cl 1 1	0	0

• Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	А	4	Total O 4 4	0	0
8	В	4	Total O 4 4	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.

 $\bullet$  Molecule 1: SARCOPLASMIC RETICULUM CALCIUM ATPASE 1 MOLECULE SARCOPL ASMIC/ENDOPLASMIC RETICULUM CALCIUM ATPASE 1



• Molecule 1: SARCOPLASMIC RETICULUM CALCIUM ATPASE 1 MOLECULE SARCOPL ASMIC/ENDOPLASMIC RETICULUM CALCIUM ATPASE 1





#### I 368 431 1761 3762 A563 L564 G595 V596 R567 D568 A786 L787 F835 R836 Y837 G842 Y843 V844 M897 T898 V865 P86 4 2 V950 D951 P952 L953 P954 P954 F957 K958 K958 K958 K960 L962 D963 D963 D963 D981 E982 G994 M899 A900



## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	130.56Å $93.78$ Å $135.69$ Å	Deperitor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $107.26^{\circ}$ $90.00^{\circ}$	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	78.91 - 3.30	Depositor
Resolution (A)	$78.90 \ - \ 3.30$	EDS
% Data completeness	99.8 (78.91-3.30)	Depositor
(in resolution range)	99.8 (78.90-3.30)	EDS
R <sub>merge</sub>	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.15 (at 3.33Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
P. P.	0.210 , $0.245$	Depositor
$n, n_{free}$	0.210 , $0.245$	DCC
$R_{free}$ test set	783 reflections $(1.65\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	97.1	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.27 , $70.0$	EDS
L-test for twinning <sup>2</sup>	$< L >=0.48, < L^2>=0.31$	Xtriage
Estimated twinning fraction	0.015 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	15554	wwPDB-VP
Average B, all atoms $(Å^2)$	135.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.57% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical 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.



<sup>&</sup>lt;sup>1</sup>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: TG1, MG, ACE, K, CL, 128, VN4

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).

Mal	Chain	Bond lengths		Bond	angles
Moi Chain		RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.26	0/7810	0.43	0/10588
1	В	0.26	0/7813	0.43	0/10594
All	All	0.26	0/15623	0.43	0/21182

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	7672	0	7765	117	0
1	В	7674	0	7767	107	0
2	А	46	0	50	15	0
2	В	46	0	50	13	0
3	А	4	0	0	0	0
3	В	4	0	0	0	0
4	А	46	0	13	1	0
4	В	46	0	13	1	0
5	А	2	0	0	0	0
5	В	2	0	0	0	0
6	А	1	0	0	0	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	В	1	0	0	0	0
7	А	1	0	0	0	0
7	В	1	0	0	0	0
8	А	4	0	0	0	0
8	В	4	0	0	1	0
All	All	15554	0	15658	236	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 (236) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	A + a	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:848:THR:HG23	1:B:900:ALA:HB1	1.58	0.86
1:A:950:VAL:HG12	1:A:952:PRO:HD2	1.60	0.83
1:A:82:GLU:CA	1:A:83:GLU:N	2.43	0.82
1:A:260:LEU:HD13	2:A:1000:TG1:H232	1.61	0.80
2:A:1000:TG1:H313	2:A:1000:TG1:H332	1.63	0.80
1:B:769:VAL:HG21	2:B:1000:TG1:H333	1.62	0.80
1:A:894:PRO:HB3	1:A:959:LEU:H	1.50	0.76
1:B:646:GLU:OE2	1:B:651:ARG:NH1	2.19	0.74
1:B:786:ALA:HA	1:B:897:MET:HA	1.70	0.73
1:A:790:VAL:HB	1:A:957:PHE:HE1	1.54	0.72
1:A:848:THR:HG23	1:A:900:ALA:HB1	1.71	0.72
1:A:947:ILE:HD13	1:A:953:LEU:HD13	1.70	0.71
1:A:829:ILE:HG21	2:A:1000:TG1:H333	1.72	0.70
1:B:811:PRO:HD3	1:B:930:ASN:HD21	1.57	0.69
1:A:23:GLY:HA3	1:A:131:ARG:HA	1.74	0.69
1:A:85:ILE:O	1:A:88:PHE:HB3	1.91	0.69
1:A:829:ILE:HA	1:A:833:LEU:HD23	1.75	0.68
1:A:773:VAL:HG11	1:A:842:GLY:HA2	1.77	0.66
1:A:773:VAL:HG22	2:A:1000:TG1:H202	1.76	0.66
1:A:894:PRO:HA	1:A:958:LYS:HD2	1.75	0.66
1:A:260:LEU:HD11	1:A:306:ALA:HB1	1.77	0.66
1:A:651:ARG:NH2	1:A:674:CYS:SG	2.69	0.66
1:A:769:VAL:HA	2:A:1000:TG1:H251	1.79	0.65
1:A:897:MET:HB2	1:A:958:LYS:HG3	1.81	0.63
1:B:829:ILE:HD12	2:B:1000:TG1:HC91	1.80	0.62
1:B:835:PHE:HA	1:B:838:MET:HB3	1.81	0.62
1:B:125:GLU:HG3	1:B:126:MET:HG2	1.81	0.62
1:A:790:VAL:HB	1:A:957:PHE:CE1	2.34	0.62



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:19:SER:HB3	1:A:22:THR:HG22	1.82	0.62
2:B:1000:TG1:O10	2:B:1000:TG1:HC92	1.99	0.62
1:B:866:THR:CG2	1:B:870:LEU:HB2	2.29	0.61
1:A:76:ALA:HB1	1:A:88:PHE:CD2	2.35	0.61
1:A:786:ALA:HA	1:A:897:MET:HG2	1.83	0.61
1:A:155:VAL:HG12	1:A:216:ALA:HA	1.81	0.61
1:A:665:GLU:O	1:A:669:ALA:HB2	2.01	0.60
1:B:648:VAL:HG13	1:B:651:ARG:HB2	1.83	0.60
1:A:90:GLU:HG3	1:A:91:PRO:HD3	1.83	0.60
1:B:368:ILE:HG21	1:B:409:GLY:HA3	1.83	0.60
1:A:603:PRO:HB3	1:A:639:ILE:HD11	1.84	0.59
1:A:836:ARG:NH1	1:A:981:ASP:OD1	2.35	0.59
1:A:834:PHE:CZ	2:A:1000:TG1:H142	2.38	0.58
1:B:109:GLU:HG2	1:B:110:ARG:H	1.69	0.58
1:A:91:PRO:O	1:A:95:LEU:N	2.34	0.57
1:B:183:GLU:OE2	8:B:2002:HOH:O	2.16	0.57
1:B:155:VAL:HG12	1:B:216:ALA:HA	1.86	0.57
1:A:948:LEU:HD13	1:A:960:LYS:HG3	1.86	0.57
1:B:424:SER:O	1:B:437:VAL:HB	2.05	0.57
1:B:486:GLU:O	1:B:491:ARG:NH2	2.36	0.57
1:B:529:ARG:NH2	1:B:568:ASP:OD1	2.37	0.57
1:A:459:VAL:HA	1:A:462:LEU:HG	1.87	0.56
2:B:1000:TG1:C24	2:B:1000:TG1:H311	2.36	0.56
1:A:757:MET:HA	1:A:760:PHE:CE2	2.41	0.56
1:B:705:VAL:HG22	1:B:726:VAL:HG11	1.88	0.55
1:A:837:TYR:HA	1:A:840:ILE:HG22	1.89	0.55
2:B:1000:TG1:H262	2:B:1000:TG1:H233	1.88	0.55
1:A:529:ARG:NH2	1:A:568:ASP:OD1	2.40	0.55
1:A:758:LYS:HG2	1:A:828:LEU:HD23	1.89	0.55
1:B:491:ARG:NH1	1:B:588:GLU:OE2	2.40	0.55
1:A:512:MET:HB2	1:A:567:ARG:HB3	1.89	0.54
1:B:512:MET:HB2	1:B:567:ARG:HB3	1.88	0.54
1:A:611:ILE:HG13	1:A:639:ILE:HG22	1.90	0.54
1:B:41:LEU:HB3	1:B:236:ARG:HD2	1.90	0.54
1:A:301:ALA:HB2	1:A:789:PRO:HG3	1.88	0.54
1:A:762:ARG:NH2	1:A:828:LEU:O	2.39	0.54
1:A:828:LEU:HD13	2:A:1000:TG1:H303	1.89	0.54
1:A:107:TRP:HA	1:A:110:ARG:HG2	1.89	0.53
1:B:246:LYS:HE2	1:B:251:GLN:HG2	1.88	0.53
1:B:773:VAL:HG11	1:B:842:GLY:HA2	1.89	0.53
1:B:914:ASN:HD21	1:B:978:ILE:HA	1.73	0.53



	i as pagem	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:B:837:TYR:HA	1:B:840:ILE:HG22	1.89	0.53	
1:A:560:ARG:HG3	4:A:1002:128:C2	2.39	0.53	
1:B:357:THR:HA	1:B:603:PRO:HA	1.91	0.53	
1:B:256:PHE:CE1	2:B:1000:TG1:H24	2.45	0.52	
1:B:701:THR:HA	1:B:718:ILE:O	2.09	0.52	
1:A:829:ILE:HG12	2:A:1000:TG1:HC8	1.92	0.52	
1:A:59:ASP:HB3	1:A:62:VAL:HG12	1.92	0.52	
1:A:943:LEU:O	1:A:947:ILE:HG12	2.11	0.51	
1:A:72:SER:HB3	1:A:91:PRO:HB3	1.91	0.51	
1:A:527:TYR:CD1	1:A:534:ARG:HD3	2.46	0.51	
1:A:834:PHE:HZ	2:A:1000:TG1:H142	1.74	0.51	
1:A:179:ILE:HD13	1:A:212:THR:HA	1.91	0.51	
1:A:68:ALA:HB1	1:A:300:VAL:HG23	1.93	0.51	
1:A:120:LYS:O	1:A:123:GLU:HG2	2.10	0.51	
1:B:256:PHE:HE1	2:B:1000:TG1:H24	1.77	0.50	
1:B:656:ARG:NH1	1:B:660:ASP:OD1	2.45	0.50	
1:B:836:ARG:NH1	1:B:981:ASP:OD1	2.45	0.50	
1:B:68:ALA:HB1	1:B:300:VAL:HG23	1.93	0.50	
1:B:844:VAL:HB	1:B:907:ILE:HG21	1.93	0.50	
1:B:950:VAL:HG22	1:B:951:ASP:H	1.76	0.49	
2:B:1000:TG1:H233	2:B:1000:TG1:C4	2.43	0.49	
1:A:604:ARG:HB2	1:A:607:VAL:HG23	1.94	0.49	
1:B:247:THR:O	1:B:250:GLN:HG2	2.13	0.49	
1:B:68:ALA:O	1:B:72:SER:OG	2.24	0.49	
1:B:757:MET:O	1:B:760:PHE:HD1	1.95	0.49	
1:B:431:LYS:HG3	1:B:435:GLU:OE2	2.12	0.49	
2:B:1000:TG1:H332	2:B:1000:TG1:H142	1.93	0.49	
1:B:281:ASP:HB2	1:B:282:PRO:HD3	1.95	0.49	
1:A:795:VAL:HA	1:A:799:THR:HG22	1.95	0.48	
2:A:1000:TG1:H333	2:A:1000:TG1:HC91	1.94	0.48	
1:B:866:THR:HG23	1:B:870:LEU:HB2	1.94	0.48	
1:B:757:MET:O	1:B:758:LYS:C	2.52	0.48	
1:B:950:VAL:HG13	1:B:954:PRO:HD3	1.95	0.48	
1:B:847:ALA:HB2	1:B:973:ILE:HG21	1.95	0.48	
1:B:901:LEU:HD23	1:B:957:PHE:CZ	2.48	0.48	
1:B:539:GLY:O	1:B:543:GLU:HG2	2.13	0.48	
1:B:898:THR:HG21	1:B:960:LYS:HB3	1.96	0.48	
1:A:844:VAL:HB	1:A:907:ILE:HG21	1.95	0.48	
1:A:907:ILE:O	1:A:911:ASN:HB2	2.13	0.48	
1:A:323:THR:HG23	1:A:333:VAL:HB	1.95	0.47	
1:A:436:LYS:HB2	1:A:443:THR:HG21	1.96	0.47	



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
2:B:1000:TG1:H233	2:B:1000:TG1:C26	2.43	0.47
1:A:94:ILE:HG12	1:A:793:LEU:HD21	1.95	0.47
1:B:762:ARG:NH2	1:B:828:LEU:O	2.46	0.47
1:A:357:THR:HA	1:A:603:PRO:HA	1.96	0.47
1:A:829:ILE:HG12	2:A:1000:TG1:C9	2.45	0.47
1:B:72:SER:HB3	1:B:90:GLU:OE1	2.14	0.47
1:B:179:ILE:HD13	1:B:212:THR:HA	1.96	0.47
1:B:282:PRO:HB2	1:B:285:GLY:HA3	1.97	0.47
1:B:795:VAL:HG21	1:B:901:LEU:HD11	1.96	0.47
1:A:950:VAL:HG12	1:A:951:ASP:N	2.29	0.47
1:A:950:VAL:O	1:A:954:PRO:HG2	2.14	0.47
1:A:84:THR:OG1	1:A:87:ALA:HB3	2.14	0.46
1:B:757:MET:O	1:B:760:PHE:CD1	2.69	0.46
1:A:611:ILE:HG13	1:A:639:ILE:CG2	2.46	0.46
1:A:837:TYR:HD2	2:A:1000:TG1:H331	1.81	0.46
1:B:391:PRO:HB3	1:B:450:GLU:HB3	1.96	0.46
1:A:950:VAL:CG1	1:A:952:PRO:HD2	2.39	0.46
1:B:366:MET:HG3	1:B:382:PHE:HB2	1.96	0.46
1:A:424:SER:O	1:A:437:VAL:HB	2.16	0.46
1:B:957:PHE:O	1:B:958:LYS:HB2	2.15	0.46
1:A:609:GLY:O	1:A:613:LEU:HG	2.16	0.46
1:A:951:ASP:HB3	1:A:952:PRO:HD3	1.98	0.46
1:B:61:LEU:HB2	1:B:307:ILE:HD12	1.96	0.46
1:B:459:VAL:HA	1:B:462:LEU:HG	1.97	0.46
1:A:78:PHE:CE2	1:A:293:ILE:HG21	2.50	0.46
1:B:758:LYS:HG2	1:B:828:LEU:HD22	1.97	0.46
1:A:76:ALA:HB1	1:A:88:PHE:HD2	1.78	0.46
1:A:512:MET:O	1:A:566:THR:HA	2.16	0.45
1:A:352:LYS:HD2	1:A:635:ILE:HG13	1.97	0.45
1:A:868:HIS:ND1	1:A:869:GLN:HG3	2.32	0.45
2:A:1000:TG1:HC91	2:A:1000:TG1:C33	2.46	0.45
1:A:129:VAL:HG12	1:A:151:VAL:HG22	1.98	0.45
1:A:312:PRO:HA	1:A:315:ILE:HG12	1.99	0.45
1:B:978:ILE:O	1:B:982:GLU:HB2	2.16	0.45
1:A:379:LEU:HD12	1:A:548:VAL:HG21	1.99	0.45
1:A:985:LYS:HG2	1:A:989:ARG:HH12	1.82	0.45
1:B:368:ILE:HD13	1:B:595:GLY:HA3	1.99	0.45
1:A:78:PHE:CG	1:A:80:GLU:HG3	2.52	0.44
1:A:248:PRO:HD2	1:A:341:THR:HG22	1.99	0.44
1:A:624:ILE:HG22	1:A:684:LYS:HE2	1.98	0.44
1:B:413:LEU:HD12	1:B:564:LEU:HD22	2.00	0.44



	• • • • • •	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:B:635:ILE:O	1:B:639:ILE:HG12	2.17	0.44
1:B:829:ILE:O	2:B:1000:TG1:H343	2.17	0.44
2:B:1000:TG1:H332	2:B:1000:TG1:C14	2.47	0.44
2:B:1000:TG1:H261	2:B:1000:TG1:O5	2.18	0.44
1:A:618:GLY:HA3	1:A:821:PRO:HD3	1.99	0.44
1:A:78:PHE:CZ	1:A:293:ILE:HG13	2.53	0.44
1:A:843:TYR:CE2	1:A:973:ILE:HG23	2.52	0.44
1:B:314:VAL:HG12	1:B:760:PHE:CE2	2.52	0.44
1:B:843:TYR:CE2	1:B:973:ILE:HG23	2.53	0.44
1:A:106:VAL:O	1:A:110:ARG:HG2	2.17	0.44
1:B:560:ARG:HG3	4:B:1002:128:N1	2.33	0.44
1:A:198:ARG:NH2	1:A:660:ASP:OD1	2.51	0.43
1:A:275:ASN:HB2	1:A:278:HIS:HB2	2.00	0.43
1:A:760:PHE:HB2	1:A:804:ALA:HB1	2.00	0.43
1:B:760:PHE:HD1	1:B:761:ILE:N	2.16	0.43
1:A:391:PRO:HB3	1:A:450:GLU:HB3	1.99	0.43
1:B:311:LEU:HD13	1:B:764:LEU:HD12	2.01	0.43
1:B:379:LEU:HD12	1:B:548:VAL:HG21	1.99	0.43
1:B:897:MET:HB2	1:B:958:LYS:HE3	2.00	0.43
1:A:78:PHE:HE2	1:A:293:ILE:HG21	1.84	0.43
1:A:753:ILE:O	1:A:757:MET:HG3	2.18	0.43
1:B:894:PRO:HA	1:B:958:LYS:HD2	2.01	0.43
1:A:502:LYS:HG3	1:A:503:SER:H	1.83	0.43
1:B:417:CYS:HB3	1:B:445:LEU:HB3	1.99	0.43
1:A:648:VAL:HG13	1:A:651:ARG:HB2	2.01	0.43
1:B:759:GLN:OE1	1:B:762:ARG:NH1	2.43	0.43
1:A:90:GLU:O	1:A:94:ILE:HG13	2.18	0.42
1:A:347:VAL:HG11	1:A:691:LEU:HD13	2.01	0.42
1:A:883:PHE:HB3	1:A:886:LEU:HD11	2.01	0.42
1:B:13:LEU:HD21	1:B:166:LEU:HD21	2.01	0.42
1:B:62:VAL:HG23	1:B:98:LEU:HD22	2.01	0.42
1:B:122:TYR:O	1:B:211:GLY:HA2	2.19	0.42
1:B:235:ILE:O	1:B:239:MET:HG3	2.19	0.42
1:B:549:ILE:HD11	1:B:596:VAL:HG21	1.99	0.42
1:A:51:GLU:HA	1:A:54:ILE:HG22	2.02	0.42
1:A:426:ASP:OD1	1:A:427:PHE:N	2.52	0.42
1:A:161:ALA:HA	1:A:210:SER:HB2	2.01	0.42
1:A:278:HIS:CE1	1:A:295:TYR:HH	2.27	0.42
1:A:511:LYS:CD	1:A:568:ASP:HA	2.50	0.42
1:B:310:GLY:O	1:B:314:VAL:HG23	2.20	0.42
1:A:199:ALA:HB1	1:A:203:ASP:HB2	2.01	0.42



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:B:83:GLU:HB2	1:B:86:THR:HB	2.02	0.42
1:A:611:ILE:HD12	1:A:621:VAL:HG11	2.02	0.42
1:B:52:LEU:HD23	1:B:52:LEU:O	2.20	0.42
1:B:760:PHE:CD1	1:B:761:ILE:N	2.88	0.42
1:B:760:PHE:O	1:B:763:TYR:HB3	2.20	0.42
1:B:760:PHE:HD2	1:B:804:ALA:O	2.01	0.42
1:B:865:VAL:O	1:B:866:THR:HB	2.20	0.42
1:A:122:TYR:O	1:A:211:GLY:HA2	2.20	0.42
1:A:950:VAL:HG12	1:A:951:ASP:H	1.85	0.42
2:A:1000:TG1:H203	2:A:1000:TG1:H172	1.77	0.42
1:B:495:SER:HA	1:B:513:PHE:O	2.19	0.42
1:B:950:VAL:CG1	1:B:954:PRO:HD3	2.50	0.42
1:A:93:VAL:HA	1:A:96:LEU:HG	2.02	0.42
1:A:389:TYR:HB3	1:A:425:LEU:HD11	2.01	0.41
1:A:88:PHE:O	1:A:91:PRO:HD2	2.20	0.41
1:B:138:GLN:HB3	1:B:140:ILE:HG23	2.02	0.41
1:A:90:GLU:OE1	1:A:789:PRO:HB2	2.18	0.41
1:B:834:PHE:O	1:B:838:MET:HB2	2.20	0.41
1:A:367:PHE:CD1	1:A:379:LEU:HD13	2.56	0.41
1:B:102:ALA:O	1:B:106:VAL:HG23	2.21	0.41
1:A:713:LYS:HD2	1:A:713:LYS:HA	1.88	0.41
1:A:829:ILE:CG1	2:A:1000:TG1:HC8	2.50	0.41
1:B:491:ARG:NH1	1:B:584:PHE:HB3	2.35	0.41
1:B:158:LYS:HB2	1:B:158:LYS:HE3	1.92	0.41
1:B:314:VAL:HG13	1:B:805:THR:OG1	2.21	0.41
1:A:202:GLN:N	1:A:202:GLN:OE1	2.53	0.41
1:A:321:LEU:HD13	1:A:809:PHE:HZ	1.85	0.41
1:A:420:CYS:HA	1:A:496:VAL:HG21	2.03	0.41
1:B:24:LEU:HG	1:B:149:ASP:HA	2.03	0.41
1:B:120:LYS:O	1:B:123:GLU:HG2	2.21	0.41
1:B:787:LEU:HD21	1:B:848:THR:HG21	2.03	0.41
1:B:907:ILE:HD11	1:B:973:ILE:HG22	2.03	0.41
1:A:443:THR:O	1:A:447:THR:HG22	2.21	0.41
1:B:351:ASP:O	1:B:355:THR:HB	2.21	0.41
1:B:77:TRP:HD1	1:B:78:PHE:CE1	2.38	0.40
1:B:314:VAL:HG12	1:B:760:PHE:HE2	1.85	0.40
1:B:791:GLN:HG2	1:B:957:PHE:CE1	2.56	0.40
1:A:482:GLU:OE2	1:A:573:ARG:NH1	2.54	0.40
1:B:423:SER:HB2	1:B:437:VAL:O	2.20	0.40
1:B:431:LYS:HB3	1:B:433:VAL:HG12	2.03	0.40
1:B:863:PRO:HG2	1:B:890:ILE:HG21	2.02	0.40



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:518:PRO:HA	1:B:563:ALA:HB2	2.03	0.40
1:B:161:ALA:HA	1:B:210:SER:HB2	2.04	0.40
1:B:958:LYS:HB2	1:B:958:LYS:HE2	1.89	0.40

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	Perce	entiles
1	А	991/995~(100%)	925~(93%)	66 (7%)	0	100	100
1	В	993/995~(100%)	931~(94%)	55~(6%)	7 (1%)	22	54
All	All	1984/1990~(100%)	1856 (94%)	121 (6%)	7 (0%)	34	66

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	531	GLY
1	В	831	GLY
1	В	950	VAL
1	В	282	PRO
1	В	458	GLU
1	В	951	ASP
1	В	952	PRO

#### 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



Mol	Chain	Analysed	Rotameric Outliers		Percentiles		
1	А	840/840~(100%)	835~(99%)	5 (1%)	86 91		
1	В	840/840 (100%)	832 (99%)	8 (1%)	76 86		
All	All	1680/1680~(100%)	1667~(99%)	13 (1%)	81 89		

analysed, and the total number of residues.

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	$\mathbf{Res}$	Type
1	А	78	PHE
1	А	79	GLU
1	А	88	PHE
1	А	790	VAL
1	А	882	HIS
1	В	88	PHE
1	В	90	GLU
1	В	421	ASN
1	В	430	THR
1	В	472	ASN
1	В	757	MET
1	В	759	GLN
1	В	760	PHE

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such side chains are listed below:

Mol	Chain	Res	Type
1	В	810	ASN
1	В	930	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 monosaccharides in this entry.



### 5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 8 are 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).

Mal	Turne	Chain	Dec	Tink	Bo	ond leng	ths	B	ond ang	les
	туре	Unam	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
3	VN4	А	1001	1,8,5	0,3,3	-	-	-		
3	VN4	В	1001	1,8,5	0,3,3	-	-	-		
2	TG1	А	1000	-	43,48,48	0.93	1 (2%)	44,72,72	1.24	4 (9%)
4	128	А	1002	5	$33,\!50,\!50$	1.47	6 (18%)	36,80,80	1.18	2(5%)
2	TG1	В	1000	-	43,48,48	0.88	1 (2%)	44,72,72	0.86	1 (2%)
4	128	В	1002	5	33,50,50	1.48	6 (18%)	36,80,80	1.32	6 (16%)

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	128	В	1002	5	-	5/22/80/80	0/5/5/5
2	TG1	В	1000	-	-	9/33/99/99	0/3/3/3
4	128	А	1002	5	-	5/22/80/80	0/5/5/5
2	TG1	А	1000	-	-	18/33/99/99	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$\operatorname{Observed}(\operatorname{\AA})$	$\mathrm{Ideal}(\mathrm{\AA})$
4	В	1002	128	C5F-C6F	4.71	1.51	1.37
4	А	1002	128	C5F-C6F	4.60	1.50	1.37
4	В	1002	128	PG-O1G	3.03	1.60	1.50
4	А	1002	128	PG-O1G	3.00	1.60	1.50
4	А	1002	128	C8-N7	-2.45	1.30	1.34
4	В	1002	128	C8-N7	-2.40	1.30	1.34
4	В	1002	128	PG-O3G	-2.36	1.45	1.54
4	А	1002	128	PG-O3G	-2.30	1.46	1.54



Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
4	А	1002	128	C5F-C4F	-2.28	1.32	1.40
4	В	1002	128	PA-O1A	2.28	1.59	1.50
4	А	1002	128	PA-O1A	2.27	1.59	1.50
4	В	1002	128	C5F-C4F	-2.20	1.32	1.40
2	В	1000	TG1	C1-C5	2.02	1.54	1.51
2	А	1000	TG1	C1-C5	2.01	1.54	1.51

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	А	1000	TG1	C10-O9-C32	4.09	131.25	121.53
4	В	1002	128	O3G-PG-O3B	3.42	116.12	104.64
4	А	1002	128	O3G-PG-O3B	3.27	115.62	104.64
4	В	1002	128	O2'-C1F-C2F	-3.12	106.20	110.47
4	В	1002	128	O2'-C1F-C6F	2.46	113.83	110.47
4	А	1002	128	O3'-C1F-C6F	-2.44	107.13	110.47
2	А	1000	TG1	O7-C8-C9	2.40	110.92	106.63
2	В	1000	TG1	C10-O9-C32	2.36	127.15	121.53
2	А	1000	TG1	O1-C13-C14	2.18	116.21	111.50
2	А	1000	TG1	O1-C13-O2	-2.17	118.47	123.70
4	В	1002	128	O3'-C1F-C6F	-2.15	107.53	110.47
4	В	1002	128	C5'-C4'-C3'	2.13	121.47	114.40
4	В	1002	128	O3'-C3'-C2'	2.03	106.83	103.58

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	$\mathbf{Res}$	Type	Atoms
2	А	1000	TG1	O3-C21-C22-C23
2	А	1000	TG1	O3-C21-C22-C24
2	А	1000	TG1	O10-C32-O9-C10
2	А	1000	TG1	C33-C32-O9-C10
2	А	1000	TG1	O8-C27-O7-C8
2	А	1000	TG1	C28-C27-O7-C8
2	В	1000	TG1	C9-C10-O9-C32
2	В	1000	TG1	C1-C10-O9-C32
2	В	1000	TG1	C14-C13-O1-C2
2	В	1000	TG1	C2-C3-O3-C21
2	В	1000	TG1	C22-C21-O3-C3
4	А	1002	128	C5'-O5'-PA-O2A
4	А	1002	128	O4'-C4'-C5'-O5'
4	В	1002	128	C5'-O5'-PA-O1A



Mol	Chain	Res	Type	Atoms
4	В	1002	128	C5'-O5'-PA-O2A
2	В	1000	TG1	O2-C13-O1-C2
4	А	1002	128	C3'-C4'-C5'-O5'
2	А	1000	TG1	C13-C14-C15-C16
2	В	1000	TG1	O4-C21-O3-C3
4	В	1002	128	O4'-C4'-C5'-O5'
4	В	1002	128	C3'-C4'-C5'-O5'
2	А	1000	TG1	O4-C21-C22-C23
2	В	1000	TG1	C14-C15-C16-C17
2	А	1000	TG1	C16-C17-C18-C19
2	А	1000	TG1	C17-C18-C19-C20
2	А	1000	TG1	O4-C21-C22-C24
2	А	1000	TG1	C14-C13-O1-C2
2	В	1000	TG1	C15-C16-C17-C18
2	А	1000	TG1	O2-C13-O1-C2
4	А	1002	128	C5'-O5'-PA-O3A
4	В	1002	128	C5'-O5'-PA-O3A
4	А	1002	128	C5'-O5'-PA-O1A
2	А	1000	TG1	C21-C22-C24-C25
2	А	1000	TG1	C14-C15-C16-C17
2	А	1000	TG1	O7-C27-C28-C29
2	А	1000	TG1	O8-C27-C28-C29
2	А	1000	TG1	C27-C28-C29-C30

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There are no ring outliers.

4 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	А	1000	TG1	15	0
4	А	1002	128	1	0
2	В	1000	TG1	13	0
4	В	1002	128	1	0

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	$OWAB(Å^2)$	Q<0.9
1	А	994/995~(99%)	0.25	58 (5%) 23 22	51, 110, 250, 425	0
1	В	994/995~(99%)	0.20	55 (5%) 25 23	50, 126, 250, 377	0
All	All	1988/1990~(99%)	0.23	113 (5%) 23 23	50, 119, 250, 425	0

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	961	ALA	12.9
1	А	284	HIS	10.1
1	А	878	GLU	9.7
1	В	281	ASP	8.8
1	А	283	VAL	8.8
1	А	994	GLY	8.3
1	В	282	PRO	8.3
1	В	283	VAL	8.0
1	А	505	ARG	7.5
1	А	993	GLU	7.0
1	А	285	GLY	6.9
1	А	965	THR	6.6
1	В	47	LYS	6.6
1	В	962	LEU	6.6
1	В	46	GLY	6.4
1	В	278	HIS	5.5
1	В	280	ASN	5.4
1	А	286	GLY	5.2
1	В	957	PHE	5.0
1	А	287	SER	5.0
1	А	992	LEU	4.9
1	А	282	PRO	4.8
1	В	110	ARG	4.6
1	А	281	ASP	4.5



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 Mol
 Chain
 Res
 Type
 RSRZ

1       A $853$ ALA $4.5$ 1       B $878$ GLU $4.4$ 1       B $960$ LYS $4.4$ 1       A $877$ THR $4.3$ 1       A $277$ GLY $4.1$ 1       B $284$ HIS $4.1$ 1       A $276$ ILE $4.0$ 1       B $284$ HIS $4.1$ 1       A $276$ ILE $4.0$ 1       B $286$ GLU $3.9$ 1       A $961$ ALA $3.9$ 1       B $289$ ILE $3.8$ 1       B $286$ GLV $3.6$ 1       A $972$ LYS $3.7$ 1       B $286$ GLY $3.6$ 1       A $974$ SER $3.4$ 1       A $949$ TYR $3.4$ 1       B $854$ TRP $3$				01	
1       A       289       ILE       4.5         1       B       878       GLU       4.4         1       A       877       THR       4.3         1       A       277       GLY       4.1         1       B       284       HIS       4.1         1       B       284       HIS       4.1         1       A       276       ILE       4.0         1       B       860       GLU       3.9         1       A       961       ALA       3.9         1       B       289       ILE       3.8         1       B       287       GLN       3.7         1       A       972       LYS       3.7         1       B       286       GLY       3.6         1       A       974       SER       3.4         1       A       964       LEU       3.5         1       B       974       SER       3.4         1       A       949       TYR       3.4         1       B       86       THR       3.3         1       A       9	1	А	853	ALA	4.5
1         B $878$ GLU $4.4$ 1         B $960$ LYS $4.4$ 1         A $277$ GLY $4.1$ 1         B $284$ HIS $4.1$ 1         B $284$ HIS $4.1$ 1         A $276$ ILE $4.0$ 1         B $860$ GLU $3.9$ 1         A $961$ ALA $3.9$ 1         B $289$ ILE $3.8$ 1         B $286$ GLY $3.6$ 1         A $972$ LYS $3.7$ 1         B $286$ GLY $3.6$ 1         A $974$ SER $3.4$ 1         A $949$ TYR $3.4$ 1         B $854$ TRP $3.3$ 1         A $922$ GLU $3.3$ 1         B	1	А	289	ILE	4.5
1       B       960       LYS       4.4         1       A       877       THR       4.3         1       A       277       GLY       4.1         1       B       284       HIS       4.1         1       A       276       ILE       4.0         1       B       860       GLU       3.9         1       A       961       ALA       3.9         1       B       289       ILE       3.8         1       B       289       ILE       3.8         1       B       286       GLY       3.6         1       A       972       LYS       3.7         1       B       286       GLY       3.6         1       A       974       HIS       3.6         1       B       949       TYR       3.5         1       B       974       SER       3.4         1       A       949       TYR       3.3         1       A       82       GLU       3.3         1       A       820       ALA       3.3         1       A       9	1	В	878	GLU	4.4
1       A $877$ THR $4.3$ 1       A $277$ GLY $4.1$ 1       B $284$ HIS $4.1$ 1       A $276$ ILE $4.0$ 1       B $860$ GLU $3.9$ 1       A $961$ ALA $3.9$ 1       B $289$ ILE $3.8$ 1       B $289$ ILE $3.8$ 1       B $276$ GLY $3.7$ 1       A $972$ LYS $3.7$ 1       A $972$ LYS $3.7$ 1       A $974$ SER $3.6$ 1       A $964$ LEU $3.5$ 1       B $949$ TYR $3.4$ 1       A $949$ TYR $3.4$ 1       A $949$ TYR $3.3$ 1       A $82$ GLU $3.3$ 1       A $920$ TRP $3.$	1	В	960	LYS	4.4
1       A       277       GLY       4.1         1       B       284       HIS       4.1         1       A       276       ILE       4.0         1       B       860       GLU       3.9         1       B       289       ILE       3.8         1       B       289       ILE       3.8         1       B       289       ILE       3.8         1       A       972       LYS       3.7         1       A       278       HIS       3.6         1       A       278       HIS       3.6         1       A       964       LEU       3.5         1       B       949       TYR       3.5         1       B       507       ALA       3.5         1       B       974       SER       3.4         1       A       949       TYR       3.4         1       B       854       TRP       3.3         1       A       82       GLU       3.3         1       A       932       TRP       3.2         1       A       9	1	А	877	THR	4.3
1       B       284       HIS       4.1         1       A       276       ILE       4.0         1       B       860       GLU $3.9$ 1       A       961       ALA $3.9$ 1       B       289       ILE $3.8$ 1       B       875       GLN $3.7$ 1       A       972       LYS $3.7$ 1       A       974       SER $3.6$ 1       A       964       LEU $3.5$ 1       B       949       TYR $3.5$ 1       B       974       SER $3.4$ 1       A       949       TYR $3.3$ 1       A       82       GLU $3.3$ 1       A       82       GLU $3.3$ 1       A       949       TYR $3.4$ 1 <td>1</td> <td>А</td> <td>277</td> <td>GLY</td> <td>4.1</td>	1	А	277	GLY	4.1
1       A       276       ILE       4.0         1       B       860       GLU $3.9$ 1       A       961       ALA $3.9$ 1       B       289       ILE $3.8$ 1       B       875       GLN $3.7$ 1       A       972       LYS $3.7$ 1       A       972       LYS $3.7$ 1       A       974       ST $3.6$ 1       A       964       LEU $3.5$ 1       B       949       TYR $3.5$ 1       B       974       SER $3.4$ 1       A       949       TYR $3.3$ 1       B       854       TRP $3.3$ 1       A       82       GLU $3.3$ 1       B       86       THR $3.3$ 1       A       924       TRP $3.2$ 1       A       915       SER $3.2$ 1       A       960       LYS $3.0$ 1 </td <td>1</td> <td>В</td> <td>284</td> <td>HIS</td> <td>4.1</td>	1	В	284	HIS	4.1
1       B       860       GLU $3.9$ 1       B       289       ILE $3.8$ 1       B       875       GLN $3.7$ 1       A       972       LYS $3.7$ 1       B       286       GLY $3.6$ 1       A       972       LYS $3.7$ 1       B       286       GLY $3.6$ 1       A       974       HIS $3.6$ 1       B       949       TYR $3.5$ 1       B       974       SER $3.4$ 1       A       949       TYR $3.3$ 1       B       854       TRP $3.3$ 1       A       82       GLU $3.3$ 1       B       86       THR $3.3$ 1       A       924       GLU $3.3$ 1       A       932       TRP $3.2$ 1       A       915       SER $3.2$ 1       A       915       SER $3.2$	1	А	276	ILE	4.0
1       A       961       ALA $3.9$ 1       B       289       ILE $3.8$ 1       B       875       GLN $3.7$ 1       A       972       LYS $3.7$ 1       B       286       GLY $3.6$ 1       A       278       HIS $3.6$ 1       A       964       LEU $3.5$ 1       B       949       TYR $3.5$ 1       B       974       SER $3.4$ 1       B       974       SER $3.4$ 1       A       949       TYR $3.3$ 1       B       854       TRP $3.3$ 1       A       82       GLU $3.3$ 1       B       861       THR $3.3$ 1       B       431       LYS $3.3$ 1       A       902       TRP $3.2$ 1       A       915       SER $3.2$ 1       A       979       ASP $3.2$ <td< td=""><td>1</td><td>В</td><td>860</td><td>GLU</td><td>3.9</td></td<>	1	В	860	GLU	3.9
1       B       289       ILE       3.8         1       B       875       GLN       3.7         1       A       972       LYS       3.7         1       B       286       GLY       3.6         1       A       278       HIS       3.6         1       A       964       LEU       3.5         1       B       949       TYR       3.5         1       B       507       ALA       3.5         1       B       974       SER       3.4         1       A       949       TYR       3.4         1       B       854       TRP       3.3         1       A       82       GLU       3.3         1       A       949       TRP       3.2         1       A       932       TRP       3.2         1       A       915       SER       3.2         1       A       960 </td <td>1</td> <td>А</td> <td>961</td> <td>ALA</td> <td>3.9</td>	1	А	961	ALA	3.9
1       B       875       GLN       3.7         1       A       972       LYS       3.7         1       B       286       GLY       3.6         1       A       278       HIS       3.6         1       A       964       LEU       3.5         1       B       949       TYR       3.5         1       B       507       ALA       3.5         1       B       974       SER       3.4         1       A       949       TYR       3.3         1       B       854       TRP       3.3         1       A       82       GLU       3.3         1       A       932       TRP       3.2         1       A       932       TRP       3.2         1       A       979       ASP       3.1         1       B       87 <td>1</td> <td>В</td> <td>289</td> <td>ILE</td> <td>3.8</td>	1	В	289	ILE	3.8
1       A       972       LYS $3.7$ 1       B       286       GLY $3.6$ 1       A       278       HIS $3.6$ 1       A       964       LEU $3.5$ 1       B       949       TYR $3.5$ 1       B       974       SER $3.4$ 1       A       949       TYR $3.3$ 1       B       854       TRP $3.3$ 1       A       82       GLU $3.3$ 1       B       86       THR $3.3$ 1       A       932       TRP $3.2$ 1       A       915       SER $3.2$ 1       A       879       ASP $3.2$ 1       A       960       LYS $3.0$ 1       B       924       ARG $3.0$ 1 </td <td>1</td> <td>В</td> <td>875</td> <td>GLN</td> <td>3.7</td>	1	В	875	GLN	3.7
1       B       286       GLY $3.6$ 1       A       278       HIS $3.6$ 1       A       964       LEU $3.5$ 1       B       949       TYR $3.5$ 1       B       974       SER $3.4$ 1       A       949       TYR $3.3$ 1       A       949       TYR $3.3$ 1       A       949       TYR $3.4$ 1       A       949       TYR $3.4$ 1       B       854       TRP $3.3$ 1       A       82       GLU $3.3$ 1       B       86       THR $3.3$ 1       B       86       THR $3.3$ 1       A       906       ALA $3.3$ 1       A       915       SER $3.2$ 1       A       879       ASP $3.2$ 1       B       861       ASP $3.1$ 1       B       960       LYS $3.0$ 1	1	А	972	LYS	3.7
1       A       278       HIS       3.6         1       A       964       LEU       3.5         1       B       949       TYR       3.5         1       B       507       ALA       3.5         1       B       974       SER       3.4         1       A       949       TYR       3.4         1       B       854       TRP       3.3         1       A       82       GLU       3.3         1       B       86       THR       3.3         1       B       431       LYS       3.3         1       A       932       TRP       3.2         1       A       915       SER       3.2         1       A       915       SER       3.2         1       B       861       ASP       3.1         1       B       87       ALA       3.1         1       B       924<	1	В	286	GLY	3.6
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	А	278	HIS	3.6
1       B       949       TYR       3.5         1       B       507       ALA       3.5         1       B       974       SER       3.4         1       A       949       TYR       3.4         1       B       854       TRP       3.3         1       B       854       TRP       3.3         1       A       82       GLU       3.3         1       B       86       THR       3.3         1       B       431       LYS       3.3         1       A       506       ALA       3.3         1       A       932       TRP       3.2         1       A       915       SER       3.2         1       A       915       SER       3.2         1       A       915       SER       3.2         1       B       861       ASP       3.1         1       B       861       ASP       3.1         1       B       960       LYS       3.0         1       B       924       ARG       3.0         1       B       981	1	А	964	LEU	3.5
1       B       507       ALA       3.5         1       B       974       SER       3.4         1       A       949       TYR       3.4         1       B       854       TRP       3.3         1       A       82       GLU       3.3         1       B       86       THR       3.3         1       B       431       LYS       3.3         1       B       431       LYS       3.3         1       A       506       ALA       3.3         1       A       932       TRP       3.2         1       A       915       SER       3.2         1       A       915       SER       3.2         1       A       879       ASP       3.2         1       B       861       ASP       3.1         1       B       87       ALA       3.1         1       B       87       ALA       3.1         1       B       924       ARG       3.0         1       B       924       ARG       3.0         1       B       901 </td <td>1</td> <td>В</td> <td>949</td> <td>TYR</td> <td>3.5</td>	1	В	949	TYR	3.5
1       B       974       SER       3.4         1       A       949       TYR       3.4         1       B       854       TRP       3.3         1       A       82       GLU       3.3         1       B       86       THR       3.3         1       B       86       THR       3.3         1       B       431       LYS       3.3         1       A       506       ALA       3.3         1       A       932       TRP       3.2         1       A       915       SER       3.2         1       A       915       SER       3.2         1       A       879       ASP       3.2         1       A       879       ASP       3.2         1       B       861       ASP       3.1         1       B       861       ASP       3.1         1       B       924       ARG       3.0         1       A       981       ASP       2.9         1       A       981       ASP       2.9         1       A       272<	1	В	507	ALA	3.5
1       A       949       TYR       3.4         1       B       854       TRP       3.3         1       A       82       GLU       3.3         1       B       86       THR       3.3         1       B       431       LYS       3.3         1       B       431       LYS       3.3         1       A       506       ALA       3.3         1       A       932       TRP       3.2         1       A       915       SER       3.2         1       A       915       SER       3.2         1       A       960       LYS       3.0         1       B       861       ASP       3.1         1       B       924       ARG       3.0         1       A       960       LYS       3.0         1       A       981       ASP       2.9         1       A       981       ASP       2.9         1       A       974       SER       3.0         1       A       786       ALA       2.8         1       A       776	1	В	974	SER	3.4
1       B       854       TRP       3.3         1       A       82       GLU       3.3         1       B       86       THR       3.3         1       B       431       LYS       3.3         1       A       506       ALA       3.3         1       A       932       TRP       3.2         1       A       932       TRP       3.2         1       A       915       SER       3.2         1       A       879       ASP       3.2         1       A       879       ASP       3.2         1       B       861       ASP       3.1         1       B       87       ALA       3.1         1       A       960       LYS       3.0         1       B       924       ARG       3.0         1       A       111       ASN       3.0         1       B       927       SER       3.0         1       A       981       ASP       2.9         1       A       972       TRP       2.8         1       B       277<	1	А	949	TYR	3.4
1       A       82       GLU       3.3         1       B       86       THR       3.3         1       B       431       LYS       3.3         1       A       506       ALA       3.3         1       A       932       TRP       3.2         1       A       915       SER       3.2         1       A       915       SER       3.2         1       A       915       SER       3.2         1       A       879       ASP       3.2         1       B       861       ASP       3.1         1       B       87       ALA       3.1         1       B       924       ARG       3.0         1       A       960       LYS       3.0         1       A       911       ASN       3.0         1       A       981       ASP       2.9         1       A       981       ASP       2.9         1       A       272       TRP       2.8         1       B       277       GLY       2.8         1       A       786<	1	В	854	TRP	3.3
1       B       86       THR       3.3         1       B       431       LYS       3.3         1       A       506       ALA       3.3         1       A       932       TRP       3.2         1       A       915       SER       3.2         1       A       915       SER       3.2         1       A       915       SER       3.2         1       A       879       ASP       3.2         1       A       879       ASP       3.2         1       B       861       ASP       3.1         1       B       87       ALA       3.1         1       A       960       LYS       3.0         1       B       924       ARG       3.0         1       A       111       ASN       3.0         1       B       287       SER       3.0         1       A       981       ASP       2.9         1       A       981       ASP       2.9         1       A       272       TRP       2.8         1       B       277	1	А	82	GLU	3.3
1       B       431       LYS       3.3         1       A       506       ALA       3.3         1       A       932       TRP       3.2         1       A       915       SER       3.2         1       A       915       SER       3.2         1       A       915       SER       3.2         1       A       879       ASP       3.2         1       B       861       ASP       3.1         1       B       87       ALA       3.1         1       A       960       LYS       3.0         1       B       924       ARG       3.0         1       B       924       ARG       3.0         1       A       111       ASN       3.0         1       B       287       SER       3.0         1       A       981       ASP       2.9         1       A       981       ASP       2.9         1       A       272       TRP       2.8         1       B       277       GLY       2.8         1       A       78	1	В	86	THR	3.3
1       A       506       ALA       3.3         1       A       932       TRP       3.2         1       A       915       SER       3.2         1       A       915       SER       3.2         1       A       879       ASP       3.2         1       B       861       ASP       3.1         1       B       87       ALA       3.1         1       B       87       ALA       3.1         1       B       960       LYS       3.0         1       A       960       LYS       3.0         1       B       924       ARG       3.0         1       A       111       ASN       3.0         1       A       111       ASN       3.0         1       B       287       SER       3.0         1       A       981       ASP       2.9         1       B       901       LEU       2.9         1       A       272       TRP       2.8         1       B       277       GLY       2.8         1       A       974	1	В	431	LYS	3.3
1       A       932       TRP       3.2         1       A       915       SER       3.2         1       A       879       ASP       3.2         1       B       861       ASP       3.1         1       B       87       ALA       3.1         1       B       87       ALA       3.1         1       B       960       LYS       3.0         1       B       924       ARG       3.0         1       B       924       ARG       3.0         1       A       111       ASN       3.0         1       B       287       SER       3.0         1       A       111       ASN       3.0         1       B       287       SER       3.0         1       B       981       ASP       2.9         1       B       901       LEU       2.9         1       A       272       TRP       2.8         1       B       277       GLY       2.8         1       A       786       ALA       2.8         1       A       974	1	А	506	ALA	3.3
1       A       915       SER       3.2         1       A       879       ASP       3.2         1       B       861       ASP       3.1         1       B       87       ALA       3.1         1       B       87       ALA       3.1         1       A       960       LYS       3.0         1       B       924       ARG       3.0         1       A       111       ASN       3.0         1       A       111       ASN       3.0         1       A       981       ASP       2.9         1       A       981       ASP       2.9         1       A       981       ASP       2.9         1       B       901       LEU       2.9         1       A       272       TRP       2.8         1       B       277       GLY       2.8         1       A       786       ALA       2.8         1       A       974       SER       2.8         1       B       785       GLU       2.8         1       B       950	1	А	932	TRP	3.2
1       A       879       ASP       3.2         1       B       861       ASP       3.1         1       B       87       ALA       3.1         1       B       87       ALA       3.1         1       A       960       LYS       3.0         1       B       924       ARG       3.0         1       A       111       ASN       3.0         1       A       111       ASN       3.0         1       A       111       ASN       3.0         1       A       981       ASP       2.9         1       A       981       ASP       2.9         1       B       901       LEU       2.9         1       A       272       TRP       2.8         1       B       277       GLY       2.8         1       A       786       ALA       2.8         1       A       974       SER       2.8         1       B       785       GLU       2.8         1       B       950       VAL       2.8	1	А	915	SER	3.2
1       B       861       ASP       3.1         1       B       87       ALA       3.1         1       A       960       LYS       3.0         1       B       924       ARG       3.0         1       B       924       ARG       3.0         1       A       111       ASN       3.0         1       A       111       ASN       3.0         1       A       111       ASN       3.0         1       B       287       SER       3.0         1       A       111       ASN       3.0         1       B       287       SER       3.0         1       A       981       ASP       2.9         1       A       981       ASP       2.9         1       A       272       TRP       2.8         1       B       277       GLY       2.8         1       A       786       ALA       2.8         1       A       974       SER       2.8         1       B       785       GLU       2.8         1       B       95	1	А	879	ASP	3.2
1       B       87       ALA       3.1         1       A       960       LYS       3.0         1       B       924       ARG       3.0         1       B       924       ARG       3.0         1       A       111       ASN       3.0         1       A       111       ASN       3.0         1       A       111       ASN       3.0         1       B       287       SER       3.0         1       A       111       ASN       3.0         1       B       287       SER       3.0         1       A       981       ASP       2.9         1       B       901       LEU       2.9         1       A       272       TRP       2.8         1       B       277       GLY       2.8         1       A       786       ALA       2.8         1       A       974       SER       2.8         1       B       785       GLU       2.8         1       B       950       VAL       2.8	1	В	861	ASP	3.1
1       A       960       LYS       3.0         1       B       924       ARG       3.0         1       A       111       ASN       3.0         1       A       111       ASN       3.0         1       A       111       ASN       3.0         1       B       287       SER       3.0         1       B       287       SER       3.0         1       A       981       ASP       2.9         1       A       981       ASP       2.9         1       A       272       TRP       2.8         1       B       277       GLY       2.8         1       A       786       ALA       2.8         1       A       974       SER       2.8         1       B       785       GLU       2.8         1       B       950       VAL       2.8	1	В	87	ALA	3.1
1       B       924       ARG       3.0         1       A       111       ASN       3.0         1       B       287       SER       3.0         1       B       287       SER       3.0         1       B       287       SER       3.0         1       A       981       ASP       2.9         1       B       901       LEU       2.9         1       A       272       TRP       2.8         1       B       277       GLY       2.8         1       A       786       ALA       2.8         1       A       974       SER       2.8         1       B       785       GLU       2.8         1       B       785       GLU       2.8         1       B       950       VAL       2.8	1	А	960	LYS	3.0
1       A       111       ASN       3.0         1       B       287       SER       3.0         1       A       981       ASP       2.9         1       A       981       ASP       2.9         1       B       901       LEU       2.9         1       A       272       TRP       2.8         1       B       277       GLY       2.8         1       A       786       ALA       2.8         1       A       974       SER       2.8         1       B       785       GLU       2.8         1       B       785       GLU       2.8         1       B       785       GLU       2.8	1	В	924	ARG	3.0
1         B         287         SER         3.0           1         A         981         ASP         2.9           1         B         901         LEU         2.9           1         A         272         TRP         2.8           1         B         277         GLY         2.8           1         A         786         ALA         2.8           1         A         974         SER         2.8           1         B         785         GLU         2.8           1         B         785         SER         2.8           1         B         785         GLU         2.8           1         B         785         GLU         2.8	1	А	111	ASN	3.0
1         A         981         ASP         2.9           1         B         901         LEU         2.9           1         A         272         TRP         2.8           1         B         277         GLY         2.8           1         A         786         ALA         2.8           1         A         974         SER         2.8           1         B         785         GLU         2.8           1         B         950         VAL         2.8	1	В	287	SER	3.0
1         B         901         LEU         2.9           1         A         272         TRP         2.8           1         B         277         GLY         2.8           1         A         786         ALA         2.8           1         A         974         SER         2.8           1         B         785         GLU         2.8           1         B         950         VAL         2.8	1	А	981	ASP	2.9
1         A         272         TRP         2.8           1         B         277         GLY         2.8           1         A         786         ALA         2.8           1         A         974         SER         2.8           1         B         785         GLU         2.8           1         B         785         SER         2.8           1         B         285         2.8	1	В	901	LEU	2.9
1         B         277         GLY         2.8           1         A         786         ALA         2.8           1         A         974         SER         2.8           1         B         785         GLU         2.8           1         B         785         GLU         2.8           1         B         950         VAL         2.8	1	А	272	TRP	2.8
1         A         786         ALA         2.8           1         A         974         SER         2.8           1         B         785         GLU         2.8           1         B         950         VAL         2.8	1	В	277	GLY	2.8
1         A         974         SER         2.8           1         B         785         GLU         2.8           1         B         950         VAL         2.8	1	А	786	ALA	2.8
1         B         785         GLU         2.8           1         B         950         VAL         2.8	1	А	974	SER	2.8
1 B 950 VAL 2.8	1	В	785	GLU	2.8
	1	В	950	VAL	2.8



5A	3S

Mol	Chain	Res	Type	RSRZ
1	А	928	TRP	2.7
1	А	991	TYR	2.7
1	А	959	LEU	2.7
1	В	968	LEU	2.7
1	А	866	THR	2.7
1	В	273	LEU	2.7
1	В	784	PRO	2.7
1	А	290	ARG	2.6
1	В	994	GLY	2.6
1	В	865	VAL	2.6
1	В	853	ALA	2.6
1	В	506	ALA	2.5
1	В	290	ARG	2.5
1	В	965	THR	2.5
1	А	784	PRO	2.4
1	В	503	SER	2.4
1	А	916	LEU	2.4
1	В	82	GLU	2.4
1	В	781	LEU	2.4
1	А	787	LEU	2.4
1	А	851	ALA	2.4
1	А	860	GLU	2.4
1	А	848	THR	2.3
1	А	919	ASN	2.3
1	В	787	LEU	2.3
1	А	896	PRO	2.3
1	А	968	LEU	2.3
1	А	983	ILE	2.2
1	В	953	LEU	2.2
1	А	403	ARG	2.2
1	A	75	LEU	2.1
1	A	83	GLU	2.1
1	A	920	GLN	2.1
1	B	857	MET	2.1
1	A	273	LEU	2.1
1	A	891	PHE	2.1
1	A	785	GLU	2.1
1	В	786	ALA	2.1
1	B	848	THR	2.0
1	B	934	LEU	2.0
1	B	964	LEU	2.0
1	В	899	MET	2.0



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Mol	Chain	Res	Type	RSRZ
1	В	951	ASP	2.0
1	В	927	PRO	2.0
1	А	288	TRP	2.0
1	В	504	SER	2.0
1	А	869	GLN	2.0

#### 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	$B-factors(Å^2)$	Q<0.9
4	128	В	1002	46/46	0.84	0.23	153,187,205,208	0
2	TG1	В	1000	46/46	0.85	0.41	157,200,218,226	0
5	MG	А	1004	1/1	0.87	0.15	142,142,142,142	0
7	CL	В	1009	1/1	0.89	0.10	74,74,74,74	0
6	K	В	1008	1/1	0.90	0.08	106,106,106,106	0
4	128	А	1002	46/46	0.90	0.20	107,144,157,169	0
2	TG1	А	1000	46/46	0.91	0.47	122,165,182,193	0
5	MG	В	1004	1/1	0.92	0.11	195,195,195,195	0
7	CL	А	1009	1/1	0.96	0.14	74,74,74,74	0
5	MG	А	1003	1/1	0.96	0.28	92,92,92,92	0
6	K	А	1008	1/1	0.97	0.12	94,94,94,94	0
5	MG	В	1003	1/1	0.98	0.12	102,102,102,102	0
3	VN4	A	1001	4/4	0.99	0.26	85,95,118,119	0
3	VN4	В	1001	4/4	0.99	0.23	88,92,121,134	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.

