

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

#### Jan 23, 2021 - 05:27 PM EST

PDB ID	:	2HY3
Title	:	Crystal structure of the human tyrosine receptor phosphate gamma in complex
		with vanadate
Authors	:	Jin, X.; Min, T.; Bera, A.; Mu, H.; Sauder, J.M.; Freeman, J.C.; Reyes,
		C.; Smith, D.; Wasserman, S.R.; Burley, S.K.; Shapiro, L.; New York SGX
		Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2006-08-04
Resolution	:	2.60 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:

er 25th 2019)

## 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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	313	58%	24%	6%	12%
1	В	313	% <b>4</b> 6%	33%	8% •	12%

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	VO4	В	159	-	-	Х	-



## 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4561 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	А	276	Total 2251	C 1428	N 397	0 416	$\frac{S}{4}$	${ m Se} { m 6}$	0	0	0
1	В	276	Total 2250	C 1426	N 399	O 415	$\frac{S}{4}$	${f Se}{6}$	0	0	0

• Molecule 1 is a protein called Receptor-type tyrosine-protein phosphatase gamma.

Chain	Residue	Modelled	Actual	Comment	Reference
А	818	SER	-	cloning artifact	UNP P23470
А	819	LEU	-	cloning artifact	UNP P23470
А	825	MSE	MET	modified residue	UNP P23470
А	862	MSE	MET	modified residue	UNP P23470
А	938	MSE	MET	modified residue	UNP P23470
А	949	MSE	MET	modified residue	UNP P23470
А	1029	MSE	MET	modified residue	UNP P23470
А	1050	MSE	MET	modified residue	UNP P23470
А	1076	MSE	MET	modified residue	UNP P23470
В	818	SER	-	cloning artifact	UNP P23470
В	819	LEU	-	cloning artifact	UNP P23470
В	825	MSE	MET	modified residue	UNP P23470
В	862	MSE	MET	modified residue	UNP P23470
В	938	MSE	MET	modified residue	UNP P23470
В	949	MSE	MET	modified residue	UNP P23470
В	1029	MSE	MET	modified residue	UNP P23470
В	1050	MSE	MET	modified residue	UNP P23470
В	1076	MSE	MET	modified residue	UNP P23470

There are 18 discrepancies between the modelled and reference sequences:

• Molecule 2 is VANADATE ION (three-letter code: VO4) (formula:  $O_4V$ ).





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

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	31	Total         O           31         31	0	0
3	В	19	Total         O           19         19	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: Receptor-type tyrosine-protein phosphatase gamma



## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	58.17Å 74.79Å 82.07Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $99.58^{\circ}$ $90.00^{\circ}$	Depositor
Bosolution (Å)	17.00 - 2.60	Depositor
Resolution (A)	16.99 - 2.48	EDS
% Data completeness	81.9 (17.00-2.60)	Depositor
(in resolution range)	81.6 (16.99-2.48)	EDS
$R_{merge}$	(Not available)	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.15 (at 2.49 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
B B.	0.202 , $0.288$	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.198 , $0.275$	DCC
$R_{free}$ test set	1021 reflections $(5.09%)$	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	49.3	Xtriage
Anisotropy	0.254	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.37, $48.0$	EDS
L-test for $twinning^2$	$ < L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4561	wwPDB-VP
Average B, all atoms $(Å^2)$	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 9.73% 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:  $\mathrm{VO4}$ 

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	Bo	nd lengths	Bond angles		
	Unain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	1.05	1/2296~(0.0%)	1.04	8/3100~(0.3%)	
1	В	0.92	2/2294~(0.1%)	0.98	8/3097~(0.3%)	
All	All	0.99	3/4590~(0.1%)	1.01	16/6197~(0.3%)	

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	В	0	3

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
1	В	1107	GLU	CG-CD	5.38	1.60	1.51
1	А	1026	TRP	CB-CG	5.17	1.59	1.50
1	В	961	CYS	CB-SG	-5.13	1.73	1.81

All (3) bond length outliers are listed below:

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$\mathbf{Ideal}(^{o})$
1	В	917	LYS	CB-CA-C	9.89	130.18	110.40
1	А	1086	VAL	CB-CA-C	-7.27	97.58	111.40
1	А	1057	LEU	CB-CG-CD1	6.79	122.55	111.00
1	А	1057	LEU	CA-CB-CG	6.60	130.48	115.30
1	В	1080	ILE	CG1-CB-CG2	-6.36	97.40	111.40
1	В	918	ALA	N-CA-CB	5.81	118.24	110.10
1	В	1016	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	А	905	ASP	CB-CG-OD1	5.63	123.36	118.30



Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
1	В	918	ALA	N-CA-C	-5.61	95.86	111.00
1	В	895	PRO	N-CA-CB	5.59	110.01	103.30
1	А	843	ASN	N-CA-C	5.41	125.59	111.00
1	А	1049	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	В	915	TYR	CB-CA-C	-5.16	100.09	110.40
1	А	844	ASN	N-CA-CB	5.10	119.77	110.60
1	В	958	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	А	1049	ARG	NE-CZ-NH1	5.04	122.82	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	В	905	ASP	Peptide
1	В	914	GLY	Peptide
1	В	915	TYR	Peptide

### 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	2251	0	2209	58	0
1	В	2250	0	2200	110	0
2	А	5	0	0	1	0
2	В	5	0	0	3	0
3	А	31	0	0	0	0
3	В	19	0	0	2	0
All	All	4561	0	4409	168	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.

All (168) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} \text{Interatomic} \\ \text{distance} \ (\text{\AA}) \end{array}$	Clash overlap (Å)
1:B:915:TYR:OH	1:B:1082:ASP:OD2	1.59	1.19



	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:B:891:VAL:HB	1:B:938:MSE:CE	1.77	1.14
1:B:907:ILE:CG2	1:B:938:MSE:HE3	1.86	1.05
1:B:891:VAL:CB	1:B:938:MSE:HE2	1.87	1.04
1:B:891:VAL:HB	1:B:938:MSE:HE2	1.07	1.03
1:B:993:ARG:HG3	1:B:993:ARG:HH11	1.25	1.02
1:B:907:ILE:HG21	1:B:938:MSE:HE3	1.44	0.98
1:B:920:ALA:O	1:B:1049:ARG:NH2	2.02	0.92
1:B:1094:HIS:O	1:B:1097:THR:HB	1.69	0.92
1:B:909:ALA:HB3	1:B:938:MSE:HE1	1.50	0.92
1:A:992:ARG:HH12	1:A:1022:HIS:HD2	1.21	0.86
1:B:992:ARG:HH12	1:B:1022:HIS:HD2	1.25	0.83
1:A:992:ARG:HH12	1:A:1022:HIS:CD2	1.96	0.83
1:B:1060:CYS:SG	2:B:159:VO4:O2	2.36	0.82
1:B:915:TYR:OH	1:B:1082:ASP:CG	2.19	0.81
1:B:907:ILE:HG23	1:B:938:MSE:HE3	1.63	0.78
1:B:977:ILE:HD11	1:B:997:ARG:HB3	1.65	0.78
1:B:937:ARG:NH1	1:B:941:GLU:OE2	2.17	0.77
1:A:845:GLN:HG2	1:A:1110:ILE:HD13	1.65	0.77
1:B:1073:ILE:HG13	1:B:1074:ASP:N	2.00	0.74
1:A:833:PHE:O	1:A:837:ILE:HG12	1.87	0.74
1:A:875:LYS:NZ	1:A:875:LYS:HB3	2.05	0.71
1:B:1082:ASP:C	1:B:1082:ASP:OD1	2.28	0.71
1:B:993:ARG:HG3	1:B:993:ARG:NH1	2.04	0.71
1:B:1069:THR:O	1:B:1073:ILE:HG23	1.94	0.68
1:A:920:ALA:O	1:A:1049:ARG:NH2	2.26	0.68
1:B:992:ARG:HH12	1:B:1022:HIS:CD2	2.10	0.68
1:B:909:ALA:CB	1:B:938:MSE:HE1	2.23	0.66
1:A:1087:ASN:ND2	1:A:1090:GLY:H	1.94	0.66
1:B:1064:VAL:N	2:B:159:VO4:O1	2.24	0.65
1:B:843:ASN:O	1:B:844:ASN:HB2	1.97	0.65
1:B:993:ARG:CG	1:B:993:ARG:HH11	2.06	0.65
1:B:1069:THR:HG21	1:B:1108:GLN:HB3	1.78	0.64
1:A:844:ASN:O	1:A:845:GLN:HB2	1.98	0.64
1:A:1060:CYS:SG	2:A:158:VO4:O4	2.57	0.63
1:B:891:VAL:CG1	1:B:938:MSE:HE2	2.29	0.62
1:B:977:ILE:CD1	1:B:997:ARG:HB3	2.30	0.62
1:B:946:ILE:HG13	1:B:946:ILE:O	2.00	0.61
1:B:935:PHE:O	1:B:939:ILE:HG23	2.00	0.60
1:B:1095:ILE:C	1:B:1097:THR:H	2.04	0.60
1:A:944:THR:HB	1:A:1055:PRO:O	2.01	0.59
1:B:854:GLU:OE2	3:B:28:HOH:O	2.17	0.59



A 4 1	A + 0	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:A:871:HIS:HD2	1:A:873:GLU:H	1.50	0.59
1:A:875:LYS:HZ3	1:A:875:LYS:HB3	1.67	0.59
1:B:1076:MSE:HA	1:B:1076:MSE:HE3	1.84	0.59
1:B:977:ILE:HD11	1:B:997:ARG:CB	2.30	0.59
1:A:837:ILE:HD13	1:A:1117:LEU:HD13	1.86	0.58
1:B:1065:GLY:O	1:B:1069:THR:HG23	2.03	0.58
1:B:1026:TRP:C	1:B:1026:TRP:CD1	2.76	0.57
1:B:893:LEU:HD11	1:B:934:ASP:HB3	1.86	0.57
1:B:1100:ASN:N	1:B:1100:ASN:HD22	2.01	0.57
1:B:871:HIS:ND1	1:B:872:PRO:HD2	2.19	0.57
1:B:1022:HIS:CE1	1:B:1024:THR:HG22	2.39	0.57
1:B:1079:GLN:HG2	1:B:1085:THR:O	2.05	0.57
1:A:992:ARG:NH1	1:A:1022:HIS:HD2	1.98	0.56
1:A:917:LYS:HB3	1:A:920:ALA:HB2	1.87	0.56
1:B:1116:LEU:O	1:B:1120:ILE:HG23	2.06	0.56
1:B:852:PHE:CE1	1:B:1106:GLU:N	2.73	0.55
1:B:1032:PRO:HG2	1:B:1111:PHE:CZ	2.42	0.55
1:B:977:ILE:CG1	1:B:997:ARG:HB3	2.37	0.55
1:B:920:ALA:HB1	1:B:1049:ARG:NH2	2.21	0.54
1:B:1036:LEU:HD23	1:B:1040:THR:CG2	2.38	0.54
1:A:852:PHE:O	1:A:855:VAL:HB	2.08	0.54
1:A:913:ASP:CG	1:A:1098:GLN:HE22	2.11	0.53
1:B:1076:MSE:HE1	1:B:1086:VAL:HA	1.90	0.53
1:B:855:VAL:HG22	1:B:856:GLN:N	2.24	0.53
1:A:1039:LEU:HD21	1:A:1119:ALA:HB2	1.91	0.53
1:B:888:HIS:HE1	1:B:1097:THR:O	1.91	0.52
1:B:891:VAL:HG21	1:B:922:ILE:HD13	1.92	0.52
1:B:1076:MSE:CE	1:B:1086:VAL:HA	2.40	0.52
1:A:873:GLU:CG	1:A:873:GLU:O	2.58	0.52
1:A:1031:VAL:HB	1:A:1032:PRO:HD2	1.92	0.52
1:B:1023:TYR:OH	1:B:1037:PRO:HB2	2.10	0.52
1:B:855:VAL:CG2	1:B:856:GLN:N	2.73	0.51
1:A:1087:ASN:C	1:A:1087:ASN:HD22	2.14	0.51
1:A:890:ARG:NH1	1:A:892:LYS:HE2	2.25	0.51
1:B:1099:ARG:HG2	1:B:1100:ASN:HD22	1.75	0.51
1:B:907:ILE:HG23	1:B:938:MSE:CE	2.38	0.51
1:B:960:LYS:HB3	1:B:1061:SER:HB2	1.92	0.51
1:B:1061:SER:N	2:B:159:VO4:O2	2.44	0.51
1:A:963:GLN:HE22	1:A:967:THR:HB	1.77	0.50
1:B:928:LEU:O	1:B:932:PHE:CD1	2.63	0.50
1:B:1036:LEU:O	1:B:1039:LEU:HB2	2.13	0.49



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:B:915:TYR:CG	15:TYR:CG 1:B:916:ASN:N		0.49
1:A:830:VAL:O	1:A:834:VAL:HG22	2.12	0.49
1:A:875:LYS:HE2	1:A:881:ILE:HG22	1.95	0.48
1:A:1109:TYR:HA	1:A:1112:ILE:HD12	1.94	0.48
1:A:881:ILE:H	1:A:881:ILE:HD13	1.77	0.48
1:B:891:VAL:CB	1:B:938:MSE:CE	2.64	0.48
1:B:874:ASN:OD1	1:B:877:LYS:HD2	2.14	0.48
1:A:888:HIS:CE1	1:A:1097:THR:O	2.67	0.47
1:B:888:HIS:CE1	1:B:1097:THR:O	2.67	0.47
1:A:1066:ARG:HA	1:A:1069:THR:HG23	1.96	0.47
1:B:959:ARG:HH21	1:B:962:ASP:HA	1.80	0.47
1:B:1064:VAL:HG23	1:B:1065:GLY:N	2.30	0.47
1:B:1095:ILE:C	1:B:1097:THR:N	2.68	0.47
1:B:1076:MSE:HE2	1:B:1086:VAL:HG13	1.97	0.47
1:B:1080:ILE:HG21	1:B:1080:ILE:HD12	1.59	0.47
1:B:915:TYR:HA	3:B:7:HOH:O	2.15	0.47
1:A:922:ILE:CD1	1:A:1055:PRO:HG2	2.44	0.47
1:B:1026:TRP:O	1:B:1026:TRP:CD1	2.67	0.46
1:B:920:ALA:C	1:B:1049:ARG:HH22	2.08	0.46
1:B:862:MSE:O	1:B:863:ASN:C	2.53	0.46
1:B:907:ILE:HG21	1:B:938:MSE:CE	2.32	0.46
1:B:873:GLU:H	1:B:873:GLU:HG2	1.58	0.46
1:B:936:TRP:CE2	1:B:978:VAL:HG21	2.51	0.45
1:B:1036:LEU:HB3	1:B:1037:PRO:CD	2.46	0.45
1:B:830:VAL:O	1:B:834:VAL:HG23	2.17	0.45
1:B:1052:GLU:O	1:B:1052:GLU:HG3	2.16	0.45
1:B:907:ILE:CG2	1:B:938:MSE:CE	2.77	0.45
1:B:891:VAL:HB	1:B:938:MSE:HE1	1.84	0.45
1:A:1045:SER:HG	1:A:1070:TYR:HH	1.65	0.45
1:B:1080:ILE:HG22	1:B:1085:THR:O	2.17	0.45
1:B:841:TYR:OH	1:B:1114:ASP:OD1	2.27	0.45
1:A:846:HIS:HA	1:A:849:SER:HB3	1.99	0.44
1:B:955:GLU:O	1:B:956:LYS:C	2.55	0.44
1:B:881:ILE:HG13	1:B:881:ILE:H	1.35	0.44
1:A:1050:MSE:HA	1:A:1051:PRO:HD3	1.62	0.44
1:B:880:TYR:CE2	1:B:1062:ALA:HB2	2.52	0.44
1:A:862:MSE:O	1:A:863:ASN:C	2.56	0.44
1:A:871:HIS:CD2	1:A:873:GLU:H	2.34	0.44
1:B:964:TYR:OH	1:B:1020:GLN:NE2	2.51	0.44
1:A:959:ARG:HH11	1:A:959:ARG:CG	2.30	0.43
1:B:936:TRP:HB3	1:B:976:ILE:HG21	1.99	0.43



A 4 1		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:A:888:HIS:HE1	1:A:1097:THR:O	2.01	0.43
1:B:1082:ASP:OD1	1:B:1083:LYS:N	2.50	0.43
1:B:944:THR:HB	1:B:1055:PRO:O	2.18	0.43
1:B:1089:LEU:HD12	1:B:1093:LYS:HD2	2.00	0.43
1:B:883:ILE:HD11	1:B:1062:ALA:O	2.19	0.43
1:B:985:ILE:O	1:B:985:ILE:HG13	2.18	0.43
1:A:945:GLY:O	1:A:946:ILE:HD13	2.19	0.43
1:A:946:ILE:HG22	1:A:947:ILE:N	2.32	0.43
1:B:888:HIS:CE1	1:B:889:SER:HB3	2.54	0.43
1:B:890:ARG:HH22	1:B:905:ASP:HB3	1.84	0.43
1:A:883:ILE:CD1	1:A:1062:ALA:O	2.68	0.42
1:B:1100:ASN:N	1:B:1100:ASN:ND2	2.64	0.42
1:A:1101:TYR:O	1:A:1102:LEU:C	2.56	0.42
1:B:993:ARG:HG2	1:B:1019:ILE:HG13	2.01	0.42
1:A:851:ASP:O	1:A:855:VAL:HG23	2.18	0.42
1:A:949:MSE:HE3	1:A:1059:HIS:HE1	1.84	0.42
1:A:915:TYR:O	1:A:915:TYR:CD2	2.72	0.42
1:B:1111:PHE:O	1:B:1112:ILE:C	2.57	0.42
1:B:883:ILE:O	1:B:883:ILE:HG13	2.18	0.42
1:B:946:ILE:HD11	1:B:948:VAL:HG23	2.02	0.41
1:A:1026:TRP:CE2	1:A:1032:PRO:HD3	2.55	0.41
1:A:922:ILE:HD11	1:A:1055:PRO:HG2	2.01	0.41
1:B:989:TYR:OH	1:B:1044:ARG:NH1	2.53	0.41
1:B:1058:VAL:HG12	1:B:1067:THR:HG23	2.02	0.41
1:A:881:ILE:H	1:A:881:ILE:CD1	2.33	0.41
1:A:923:ALA:HB3	1:A:1099:ARG:HD3	2.02	0.41
1:A:959:ARG:HG2	1:A:959:ARG:NH1	2.36	0.41
1:B:992:ARG:HD2	1:B:1020:GLN:OE1	2.21	0.41
1:B:1080:ILE:HD13	1:B:1080:ILE:HG23	1.54	0.41
1:B:859:THR:HG21	1:B:1096:ARG:HB3	2.01	0.41
1:A:976:ILE:HA	1:A:997:ARG:O	2.21	0.41
1:B:857:ARG:H	1:B:857:ARG:HG2	1.71	0.41
1:B:946:ILE:HD12	1:B:947:ILE:N	2.36	0.41
1:A:970:SER:OG	1:A:979:THR:OG1	2.30	0.41
1:A:853:GLU:O	1:A:854:GLU:C	2.59	0.41
1:A:965:TRP:HB2	1:A:966:PRO:HD2	2.03	0.41
1:A:946:ILE:HB	1:A:1056:VAL:HG22	2.02	0.40
1:A:977:ILE:HG21	1:A:977:ILE:HD13	1.64	0.40
1:A:875:LYS:HE2	1:A:881:ILE:CG2	2.51	0.40
1:A:881:ILE:N	1:A:881:ILE:HD13	2.36	0.40
1:B:1076:MSE:HE2	1:B:1086:VAL:CG1	2.52	0.40



$J \rightarrow J \rightarrow$						
Atom-1	Atom-2	$\begin{array}{l} {\rm Interatomic}\\ {\rm distance}~({\rm \AA}) \end{array}$	Clash overlap (Å)			
1:B:1080:ILE:CG2	1:B:1086:VAL:HG22	2.51	0.40			
1:A:839:GLU:OE1	1:A:839:GLU:HA	2.22	0.40			
1:B:1121:LEU:HA	1:B:1121:LEU:HD23	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	Percentiles
1	А	270/313~(86%)	251 (93%)	17~(6%)	2(1%)	22 43
1	В	270/313~(86%)	243 (90%)	22 (8%)	5(2%)	8 15
All	All	540/626~(86%)	494 (92%)	39~(7%)	7(1%)	12 24

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	863	ASN
1	В	1096	ARG
1	В	915	TYR
1	В	1103	VAL
1	А	1103	VAL
1	В	1027	PRO
1	В	1088	VAL

#### 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	246/273~(90%)	215~(87%)	31 (13%)	4 8
1	В	244/273~(89%)	206 (84%)	38 (16%)	2 4
All	All	490/546~(90%)	421 (86%)	69 (14%)	3 6

analysed, and the total number of residues.

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	831	LYS
1	А	837	ILE
1	А	840	LEU
1	А	854	GLU
1	А	859	THR
1	А	865	THR
1	А	873	GLU
1	А	875	LYS
1	А	881	ILE
1	А	883	ILE
1	А	907	ILE
1	А	916	ASN
1	А	917	LYS
1	А	944	THR
1	А	959	ARG
1	А	967	THR
1	А	984	LYS
1	А	990	THR
1	А	999	THR
1	А	1022	HIS
1	А	1025	GLN
1	А	1040	THR
1	А	1046	SER
1	А	1050	MSE
1	А	1057	LEU
1	A	1069	THR
1	А	1073	ILE
1	А	1086	VAL
1	А	1087	ASN
1	А	1092	LEU
1	А	1100	ASN
1	В	835	LYS
1	В	841	TYR
1	В	842	SER



Mol	Chain	Res	Type
1	В	853	GLU
1	В	859	THR
1	В	873	GLU
1	В	876	HIS
1	В	881	ILE
1	В	883	ILE
1	В	921	TYR
1	В	937	ARG
1	В	938	MSE
1	В	939	ILE
1	В	944	THR
1	В	946	ILE
1	В	950	ILE
1	В	959	ARG
1	В	962	ASP
1	В	977	ILE
1	В	990	THR
1	В	993	ARG
1	В	1015	GLU
1	В	1022	HIS
1	В	1040	THR
1	В	1044	ARG
1	В	1050	MSE
1	В	1053	THR
1	В	1057	LEU
1	В	1069	THR
1	В	1073	ILE
1	В	1080	ILE
1	В	1082	ASP
1	В	1084	SER
1	В	1092	LEU
1	В	1093	LYS
1	В	1097	THR
1	В	1100	ASN
1	В	1120	ILE

Continued from previous page...

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	832	GLN
1	А	843	ASN
1	А	871	HIS



Mol	Chain	Res	Type
1	А	888	HIS
1	А	963	GLN
1	А	1022	HIS
1	А	1079	GLN
1	А	1087	ASN
1	В	844	ASN
1	В	888	HIS
1	В	943	ASN
1	В	1022	HIS
1	В	1079	GLN

Continued from previous page...

#### 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)

2 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).

Mal	L Trupa Chain Dag Linl		Timle	Bond lengths			Bond angles		
IVIOI	туре	Chain	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ   #  Z  > 2
2	VO4	В	159	1	1,4,4	4.86	1 (100%)	-	
2	VO4	А	158	1	1,4,4	5.47	1 (100%)	-	



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	А	158	VO4	O1-V	5.47	1.95	1.63
2	В	159	VO4	01-V	4.86	1.91	1.63

All (2) bond length outliers are listed below:

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	В	159	VO4	3	0
2	А	158	VO4	1	0

#### 5.7 Other polymers (i)

There are no such residues in this entry.

#### 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



## 6 Fit of model and data (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	270/313~(86%)	-0.36	1 (0%) 9	92 91	29, 39, 50, 61	0
1	В	270/313~(86%)	-0.17	4 (1%) 7	73 70	23, 40, 48, 61	0
All	All	540/626~(86%)	-0.27	5 (0%) 8	84 82	23, 39, 49, 61	0

All (5) RSRZ outliers are listed below:

Mol	Chain	$\mathbf{Res}$	Type	RSRZ
1	В	1030	GLY	3.3
1	В	826	GLU	2.9
1	А	1030	GLY	2.5
1	В	1027	PRO	2.5
1	В	863	ASN	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	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
2	VO4	В	159	5/5	0.96	0.13	$55,\!56,\!59,\!61$	0
2	VO4	А	158	5/5	0.96	0.12	62,63,64,70	0

### 6.5 Other polymers (i)

There are no such residues in this entry.

