



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 04:00 PM EDT

PDB ID : 2HY3 / pdb_00002hy3
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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

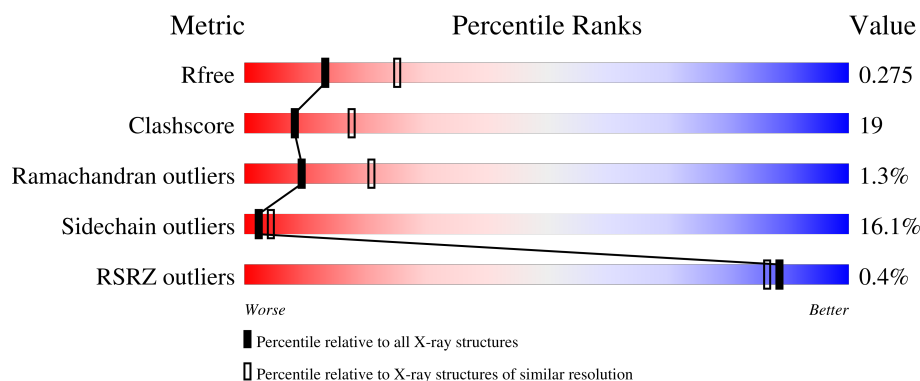
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	313	
1	B	313	

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	B	159	-	-	X	-

2 Entry composition

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.

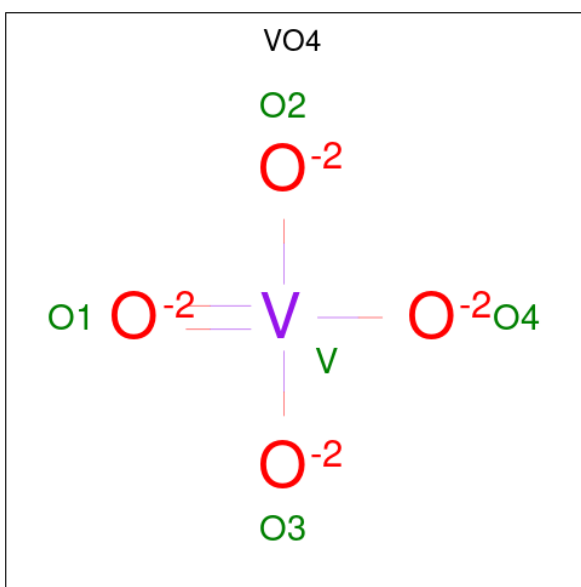
- Molecule 1 is a protein called Receptor-type tyrosine-protein phosphatase gamma.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	Se	0	0	0
			2251	1428	397	416	4	6			
1	B	276	Total	C	N	O	S	Se	0	0	0
			2250	1426	399	415	4	6			

There are 18 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is VANADATE ION (CCD ID: VO4) (formula: O₄V).



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

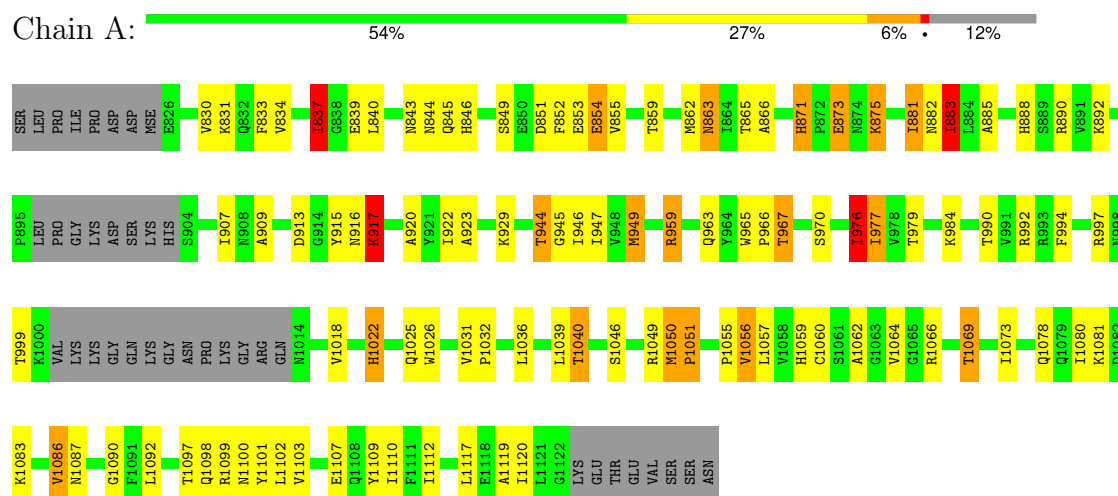
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	31	Total	O	0	0
			31	31		
3	B	19	Total	O	0	0
			19	19		

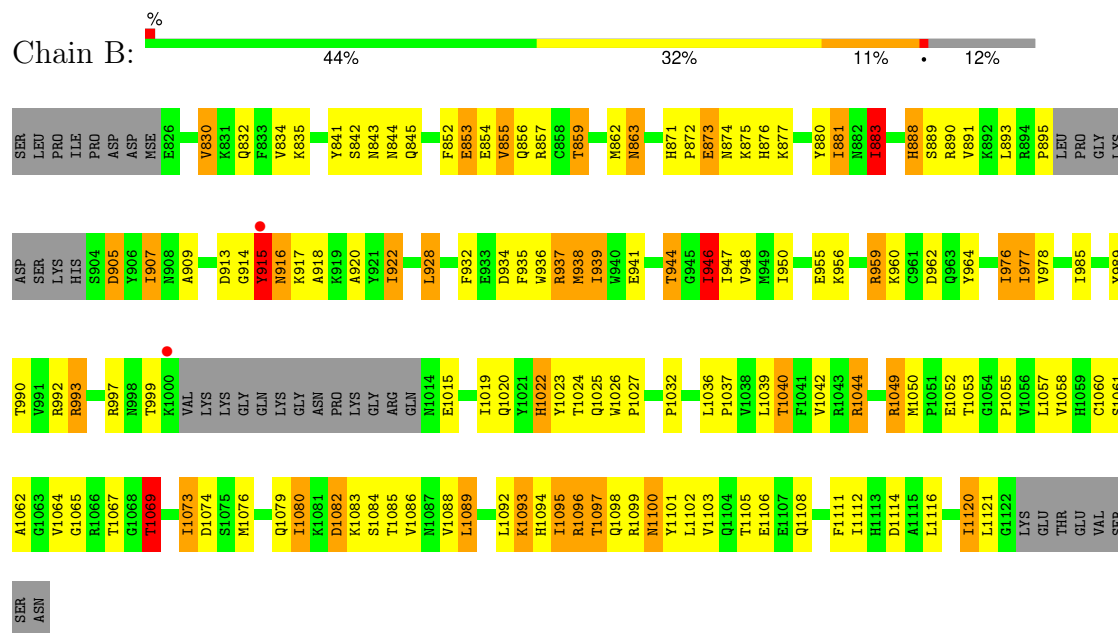
3 Residue-property plots [i](#)

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



- Molecule 1: Receptor-type tyrosine-protein phosphatase gamma



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	58.17Å 74.79Å 82.07Å 90.00° 99.58° 90.00°	Depositor
Resolution (Å)	17.00 – 2.60 17.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	81.9 (17.00-2.60) 81.7 (17.00-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 2.49Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.202 , 0.288 0.198 , 0.275	Depositor DCC
R_{free} test set	1021 reflections (4.14%)	wwPDB-VP
Wilson B-factor (Å ²)	49.3	Xtriage
Anisotropy	0.254	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 43.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.27	8/2296 (0.3%)	1.40	16/3100 (0.5%)
1	B	1.13	3/2294 (0.1%)	1.29	17/3097 (0.5%)
All	All	1.20	11/4590 (0.2%)	1.35	33/6197 (0.5%)

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	B	0	3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	885	ALA	C-O	-8.64	1.14	1.24
1	A	866	ALA	CA-CB	-8.06	1.47	1.53
1	B	1069	THR	CA-CB	7.04	1.64	1.53
1	B	883	ILE	CA-CB	6.43	1.61	1.54
1	B	976	ILE	CA-CB	6.25	1.61	1.54
1	A	909	ALA	CA-CB	-5.65	1.44	1.53
1	A	949	MSE	CA-C	-5.64	1.46	1.52
1	A	1018	VAL	CA-CB	-5.57	1.46	1.55
1	A	976	ILE	CA-CB	5.38	1.61	1.54
1	A	994	PHE	CA-C	-5.31	1.46	1.52
1	A	1064	VAL	CA-CB	5.03	1.62	1.55

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	843	ASN	N-CA-C	10.33	125.59	111.54
1	A	1050	MSE	CA-C-N	10.16	129.78	119.82
1	A	1050	MSE	C-N-CA	10.16	129.78	119.82
1	B	917	LYS	CB-CA-C	9.70	130.18	111.17
1	B	918	ALA	N-CA-C	-8.31	95.86	109.40
1	A	1086	VAL	CB-CA-C	-7.55	97.58	111.18
1	B	917	LYS	N-CA-C	-7.52	97.62	108.60
1	B	830	VAL	N-CA-C	6.93	118.52	110.62
1	A	837	ILE	CB-CA-C	-6.89	101.99	112.05
1	A	1051	PRO	N-CA-C	6.54	122.42	113.98
1	B	895	PRO	N-CA-CB	6.37	110.01	103.00
1	B	1049	ARG	CB-CA-C	6.36	118.90	110.06
1	B	946	ILE	N-CA-C	6.25	117.29	108.17
1	A	977	ILE	CB-CA-C	-6.21	102.40	110.84
1	A	1036	LEU	CA-C-N	-5.99	112.69	119.28
1	A	1036	LEU	C-N-CA	-5.99	112.69	119.28
1	B	853	GLU	N-CA-C	-5.94	104.71	111.07
1	A	883	ILE	CB-CA-C	5.87	119.17	111.53
1	B	1042	VAL	N-CA-C	-5.75	104.90	110.42
1	B	1049	ARG	N-CA-C	-5.50	102.05	110.30
1	A	882	ASN	CA-C-N	-5.47	115.45	123.10
1	A	882	ASN	C-N-CA	-5.47	115.45	123.10
1	B	999	THR	N-CA-C	5.41	117.51	107.99
1	B	1089	LEU	N-CA-C	5.32	117.08	111.28
1	A	1040	THR	CB-CA-C	5.31	120.87	110.67
1	B	845	GLN	N-CA-C	-5.26	106.81	113.23
1	A	917	LYS	N-CA-C	-5.24	98.73	107.80
1	A	871	HIS	CA-C-N	5.22	126.36	119.84
1	A	871	HIS	C-N-CA	5.22	126.36	119.84
1	B	915	TYR	CB-CA-C	-5.19	100.09	110.42
1	B	863	ASN	N-CA-C	-5.13	104.31	111.39
1	B	1095	ILE	N-CA-C	5.09	117.41	111.05
1	B	916	ASN	N-CA-C	5.08	121.62	110.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

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

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2251	0	2209	58	0
1	B	2250	0	2200	113	0
2	A	5	0	0	1	0
2	B	5	0	0	3	0
3	A	31	0	0	0	0
3	B	19	0	0	2	0
All	All	4561	0	4409	171	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 (171) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:915:TYR:OH	1:B:1082:ASP:OD2	1.59	1.19
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:915:TYR:OH	1:B:1082:ASP:CG	2.19	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: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:1082:ASP:OD1	1:B:1082:ASP:C	2.28	0.76
1:B:1073:ILE:HG13	1:B:1074:ASP:N	2.00	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:833:PHE:O	1:A:837:ILE:HG12	1.87	0.74
1:A:875:LYS:HZ3	1:A:875:LYS:HB3	1.53	0.73
1:A:875:LYS:HB3	1:A:875:LYS:NZ	2.05	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:HH11	1:B:993:ARG:CG	2.06	0.65
1:B:1095:ILE:C	1:B:1097:THR:H	2.04	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:1026:TRP:C	1:B:1026:TRP:CD1	2.76	0.62
1:B:977:ILE:CD1	1:B:997:ARG:HB3	2.30	0.62
1:B:920:ALA:C	1:B:1049:ARG:HH22	2.08	0.61
1:B:946:ILE:O	1:B:946:ILE:HG13	2.00	0.61
1:B:935:PHE:O	1:B:939:ILE:HG23	2.00	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
1:A:871:HIS:HD2	1:A:873:GLU:H	1.50	0.59
1:B:1076:MSE:HE3	1:B:1076:MSE:HA	1.84	0.59
1:B:977:ILE:HD11	1:B:997:ARG:CB	2.30	0.59
1:A:913:ASP:CG	1:A:1098:GLN:HE22	2.11	0.58
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:893:LEU:HD11	1:B:934:ASP:HB3	1.86	0.57
1:B:1100:ASN:HD22	1:B:1100:ASN:N	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:A:1087:ASN:HD22	1:A:1087:ASN:C	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:890:ARG:NH1	1:A:892:LYS:HE2	2.25	0.51
1:B:862:MSE:O	1:B:863:ASN:C	2.53	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:955:GLU:O	1:B:956:LYS:C	2.55	0.49
1:B:1036:LEU:O	1:B:1039:LEU:HB2	2.13	0.49
1:B:915:TYR:CG	1:B:916:ASN:N	2.80	0.49
1:A:830:VAL:O	1:A:834:VAL:HG22	2.12	0.49
1:A:862:MSE:O	1:A:863:ASN:C	2.56	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:HD13	1:A:881:ILE:H	1.77	0.48
1:B:1095:ILE:C	1:B:1097:THR:N	2.68	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:855:VAL:CG2	1:B:856:GLN:N	2.73	0.47
1:B:1064:VAL:HG23	1:B:1065:GLY:N	2.30	0.47
1:A:1101:TYR:O	1:A:1102:LEU:C	2.56	0.47
1:B:915:TYR:HA	3:B:7:HOH:O	2.15	0.47
1:B:1076:MSE:HE2	1:B:1086:VAL:HG13	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1080:ILE:HD12	1:B:1080:ILE:HG21	1.59	0.47
1:A:922:ILE:CD1	1:A:1055:PRO:HG2	2.44	0.47
1:B:1026:TRP:CD1	1:B:1026:TRP:O	2.67	0.46
1:B:1111:PHE:O	1:B:1112:ILE:C	2.57	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:A:853:GLU:O	1:A:854:GLU:C	2.59	0.45
1:B:830:VAL:O	1:B:834:VAL:HG23	2.17	0.45
1:B:1036:LEU:HB3	1:B:1037:PRO:CD	2.46	0.45
1:B:907:ILE:CG2	1:B:938:MSE:CE	2.77	0.45
1:B:1052:GLU:O	1:B:1052:GLU:HG3	2.16	0.45
1:B:891:VAL:HB	1:B:938:MSE:HE1	1.84	0.45
1:B:841:TYR:OH	1:B:1114:ASP:OD1	2.27	0.45
1:B:1080:ILE:HG22	1:B:1085:THR:O	2.17	0.45
1:A:846:HIS:HA	1:A:849:SER:HB3	1.99	0.44
1:B:881:ILE:H	1:B:881:ILE:HG13	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: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:CG	1:A:959:ARG:HH11	2.30	0.43
1:B:936:TRP:HB3	1:B:976:ILE:HG21	1.99	0.43
1:A:888:HIS:HE1	1:A:1097:THR:O	2.01	0.43
1:B:944:THR:HB	1:B:1055:PRO:O	2.18	0.43
1:B:1082:ASP:OD1	1:B:1083:LYS:N	2.50	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:B:1089:LEU:HD12	1:B:1093:LYS:HD2	2.00	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:B:993:ARG:HG2	1:B:1019:ILE:HG13	2.01	0.42
1:A:1080:ILE:O	1:A:1081:LYS:C	2.62	0.42
1:A:851:ASP:O	1:A:855:VAL:HG23	2.18	0.42
1:A:915:TYR:CD2	1:A:915:TYR:O	2.72	0.42
1:A:949:MSE:HE3	1:A:1059:HIS:HE1	1.84	0.42
1:B:883:ILE:HG13	1:B:883:ILE:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:946:ILE:HD11	1:B:948:VAL:HG23	2.02	0.41
1:A:922:ILE:HD11	1:A:1055:PRO:HG2	2.01	0.41
1:A:1026:TRP:CE2	1:A:1032:PRO:HD3	2.55	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:NH1	1:A:959:ARG:HG2	2.36	0.41
1:B:852:PHE:CE1	1:B:1105:THR:C	2.99	0.41
1:B:859:THR:HG21	1:B:1096:ARG:HB3	2.01	0.41
1:B:992:ARG:HD2	1:B:1020:GLN:OE1	2.21	0.41
1:B:1080:ILE:HG23	1:B:1080:ILE:HD13	1.54	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: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:B:913:ASP:CG	1:B:1098:GLN:HE22	2.29	0.40
1:B:1101:TYR:O	1:B:1102:LEU:C	2.64	0.40
1:A:875:LYS:HE2	1:A:881:ILE:CG2	2.51	0.40
1:A:881:ILE:HD13	1:A:881:ILE:N	2.36	0.40
1:B:1076:MSE:HE2	1:B:1086:VAL:CG1	2.52	0.40
1:B:1080:ILE:CG2	1:B:1086:VAL:HG22	2.51	0.40
1:A:839:GLU:HA	1:A:839:GLU:OE1	2.22	0.40
1:B:1121:LEU:HD23	1:B:1121:LEU:HA	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	A	270/313 (86%)	251 (93%)	17 (6%)	2 (1%)	18	38
1	B	270/313 (86%)	243 (90%)	22 (8%)	5 (2%)	6	13
All	All	540/626 (86%)	494 (92%)	39 (7%)	7 (1%)	9	21

All (7) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	246/273 (90%)	210 (85%)	36 (15%)	3	6
1	B	244/273 (89%)	201 (82%)	43 (18%)	2	3
All	All	490/546 (90%)	411 (84%)	79 (16%)	2	4

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	831	LYS
1	A	837	ILE
1	A	840	LEU
1	A	854	GLU
1	A	859	THR
1	A	865	THR
1	A	873	GLU
1	A	875	LYS
1	A	881	ILE

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Mol	Chain	Res	Type
1	A	883	ILE
1	A	907	ILE
1	A	916	ASN
1	A	917	LYS
1	A	929	LYS
1	A	944	THR
1	A	959	ARG
1	A	967	THR
1	A	976	ILE
1	A	984	LYS
1	A	990	THR
1	A	999	THR
1	A	1022	HIS
1	A	1025	GLN
1	A	1040	THR
1	A	1046	SER
1	A	1056	VAL
1	A	1057	LEU
1	A	1069	THR
1	A	1073	ILE
1	A	1078	GLN
1	A	1083	LYS
1	A	1086	VAL
1	A	1092	LEU
1	A	1100	ASN
1	A	1107	GLU
1	A	1120	ILE
1	B	832	GLN
1	B	835	LYS
1	B	842	SER
1	B	853	GLU
1	B	855	VAL
1	B	859	THR
1	B	873	GLU
1	B	875	LYS
1	B	876	HIS
1	B	881	ILE
1	B	883	ILE
1	B	888	HIS
1	B	907	ILE
1	B	922	ILE
1	B	928	LEU

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Mol	Chain	Res	Type
1	B	937	ARG
1	B	938	MSE
1	B	939	ILE
1	B	944	THR
1	B	946	ILE
1	B	950	ILE
1	B	959	ARG
1	B	977	ILE
1	B	990	THR
1	B	993	ARG
1	B	1015	GLU
1	B	1022	HIS
1	B	1025	GLN
1	B	1040	THR
1	B	1044	ARG
1	B	1050	MSE
1	B	1053	THR
1	B	1057	LEU
1	B	1069	THR
1	B	1073	ILE
1	B	1080	ILE
1	B	1082	ASP
1	B	1084	SER
1	B	1092	LEU
1	B	1093	LYS
1	B	1097	THR
1	B	1100	ASN
1	B	1120	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	832	GLN
1	A	843	ASN
1	A	868	HIS
1	A	871	HIS
1	A	888	HIS
1	A	963	GLN
1	A	986	HIS
1	A	1022	HIS
1	A	1079	GLN
1	A	1087	ASN

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Mol	Chain	Res	Type
1	A	1108	GLN
1	B	844	ASN
1	B	863	ASN
1	B	888	HIS
1	B	943	ASN
1	B	1022	HIS
1	B	1079	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	VO4	A	158	-	0,4,4	-	-	-		
2	VO4	B	159	-	0,4,4	-	-	-		

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.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	158	VO4	1	0
2	B	159	VO4	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	270/313 (86%)	-0.50	0	100 100	29, 39, 50, 61	0
1	B	270/313 (86%)	-0.22	2 (0%)	84 82	23, 40, 48, 61	0
All	All	540/626 (86%)	-0.36	2 (0%)	88 86	23, 39, 49, 61	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	915	TYR	3.1
1	B	1000	LYS	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	VO4	A	158	5/5	0.95	0.12	62,63,64,70	0
2	VO4	B	159	5/5	0.95	0.14	55,56,59,61	0

6.5 Other polymers [i](#)

There are no such residues in this entry.