Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 11:39 AM GMT

PDB ID	:	3PMG
Title	:	STRUCTURE OF RABBIT MUSCLE PHOSPHOGLUCOMUTASE AT 2.4 ANGSTROMS RESOLUTION. USE OF FREEZING POINT DEPRESSANT AND REDUCED TEMPERATURE TO ENHANCE DIFFRACTIVITY
Authors	:	Ray Junior, W.J.; Liu, Y.; Baranidharan, S.
Deposited on	:	1995-03-02
Resolution	:	2.40 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
http://wwpdb.org/validation/2016/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:

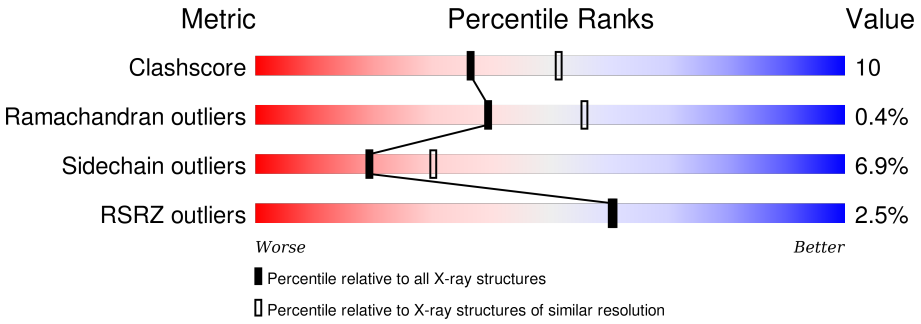
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.40 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))
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	A	561	4% 66% 28% 5%
1	B	561	% 73% 21% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12092 atoms, of which 2930 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 ALPHA-D-GLUCOSE-1,6-BISPHOSPHATE.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	561	Total	C	H	N	O	P	S	0	0	0
			5304	2753	971	743	820	1	16			
1	B	561	Total	C	H	N	O	P	S	0	0	0
			5304	2753	971	743	820	1	16			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is water.

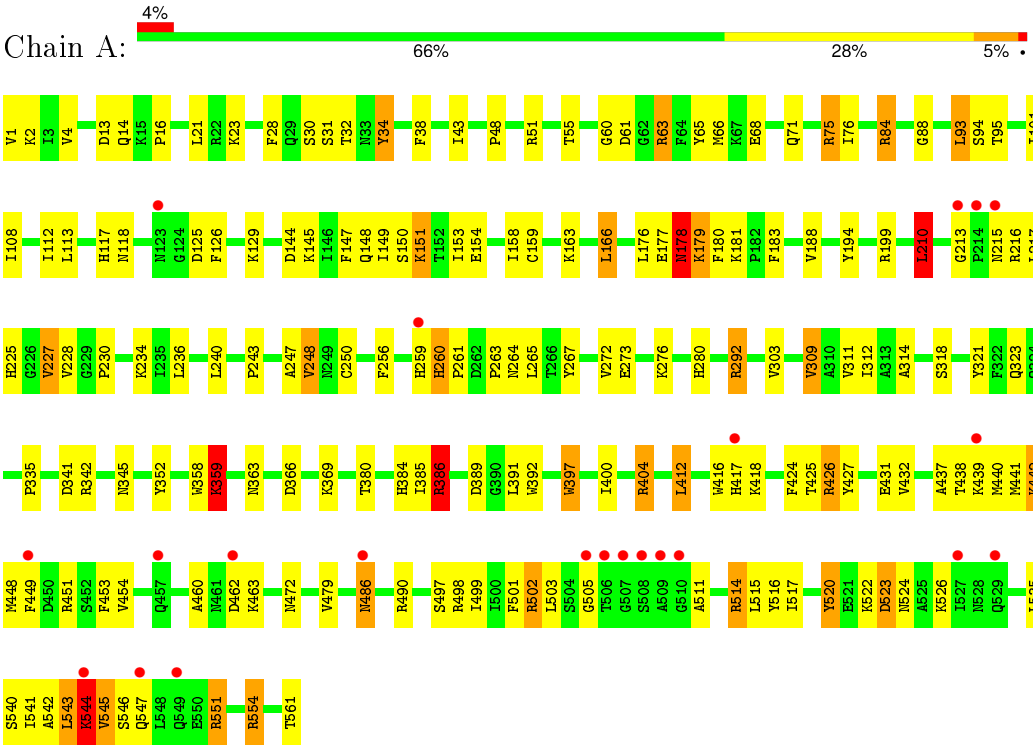
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	201	Total	H	O	0	0
			603	402	201		
3	B	293	Total	H	O	0	0
			879	586	293		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

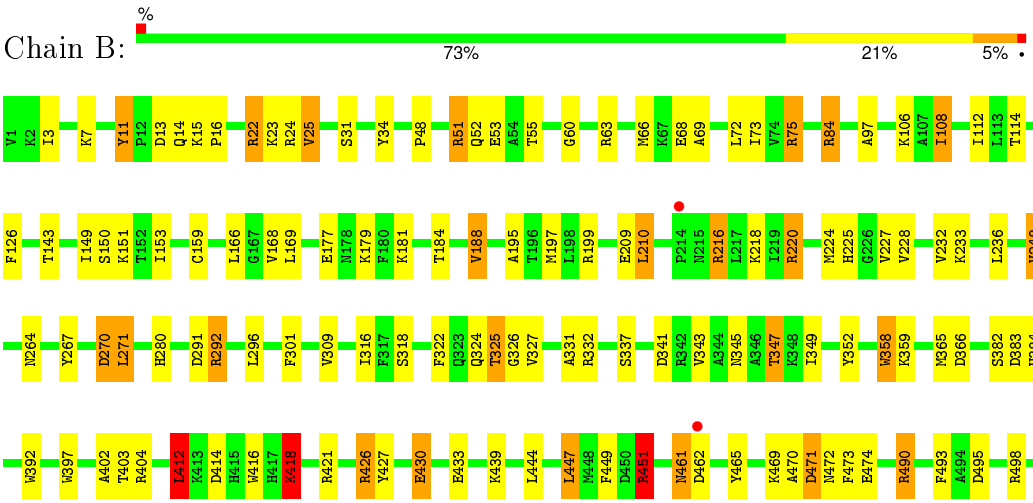
- Molecule 1: ALPHA-D-GLUCOSE-1,6-BISPHOSPHATE

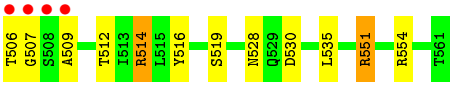
Chain A:



- Molecule 1: ALPHA-D-GLUCOSE-1,6-BISPHOSPHATE

Chain B:




T506
G507
S508
A509
T512
I513
R514
L515
Y516
S519
N528
Q529
D530
L535
R551
R554
T561

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	174.42Å 174.42Å 101.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.40 9.87 – 2.28	Depositor EDS
% Data completeness (in resolution range)	87.0 (6.00-2.40) 77.7 (9.87-2.28)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.40 (at 2.28Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.163 , 0.191 0.156 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	26.0	Xtriage
Anisotropy	0.394	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.48 , 111.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 54817 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12092	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: MG, SEP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.95	0/4409	1.77	80/5958 (1.3%)
1	B	1.01	1/4409 (0.0%)	1.82	91/5958 (1.5%)
All	All	0.98	1/8818 (0.0%)	1.80	171/11916 (1.4%)

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	A	0	2
1	B	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	358	TRP	CG-CD2	-5.72	1.33	1.43

All (171) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	490	ARG	NE-CZ-NH1	21.14	130.87	120.30
1	A	199	ARG	NE-CZ-NH2	-20.45	110.07	120.30
1	B	490	ARG	NE-CZ-NH2	-18.62	110.99	120.30
1	A	386	ARG	NE-CZ-NH1	18.12	129.36	120.30
1	A	199	ARG	NE-CZ-NH1	15.83	128.22	120.30
1	A	328	ARG	NE-CZ-NH2	-15.39	112.61	120.30
1	B	514	ARG	NE-CZ-NH2	-14.20	113.20	120.30
1	B	426	ARG	NE-CZ-NH1	10.90	125.75	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	514	ARG	NE-CZ-NH1	10.42	125.51	120.30
1	A	514	ARG	NE-CZ-NH2	-10.26	115.17	120.30
1	B	22	ARG	NE-CZ-NH1	10.19	125.39	120.30
1	B	426	ARG	NE-CZ-NH2	-10.17	115.22	120.30
1	A	426	ARG	NE-CZ-NH1	10.14	125.37	120.30
1	B	352	TYR	CB-CG-CD1	-10.00	115.00	121.00
1	B	75	ARG	NE-CZ-NH2	-9.81	115.40	120.30
1	B	220	ARG	NE-CZ-NH1	9.81	125.20	120.30
1	A	554	ARG	NE-CZ-NH1	9.48	125.04	120.30
1	B	224	MET	CG-SD-CE	-9.22	85.45	100.20
1	A	386	ARG	NE-CZ-NH2	-9.20	115.70	120.30
1	B	397	TRP	CD1-CG-CD2	9.20	113.66	106.30
1	B	199	ARG	NE-CZ-NH2	-9.18	115.71	120.30
1	B	416	TRP	CD1-CG-CD2	9.12	113.60	106.30
1	A	397	TRP	CD1-CG-CD2	9.08	113.56	106.30
1	A	392	TRP	CD1-CG-CD2	8.95	113.46	106.30
1	B	51	ARG	NE-CZ-NH1	8.87	124.74	120.30
1	A	404	ARG	NE-CZ-NH2	-8.83	115.88	120.30
1	B	392	TRP	CD1-CG-CD2	8.77	113.31	106.30
1	A	84	ARG	NE-CZ-NH1	8.76	124.68	120.30
1	B	418	LYS	CA-CB-CG	8.56	132.23	113.40
1	A	220	ARG	NE-CZ-NH1	8.47	124.53	120.30
1	A	392	TRP	CE2-CD2-CG	-8.39	100.58	107.30
1	B	404	ARG	NE-CZ-NH2	-8.36	116.12	120.30
1	B	392	TRP	CE2-CD2-CG	-8.23	100.72	107.30
1	A	309	VAL	CB-CA-C	-8.11	96.00	111.40
1	A	498	ARG	NE-CZ-NH1	7.85	124.22	120.30
1	B	430	GLU	CA-C-N	7.82	134.40	117.20
1	B	358	TRP	CD1-CG-CD2	7.81	112.55	106.30
1	A	328	ARG	NE-CZ-NH1	7.79	124.19	120.30
1	B	24	ARG	NE-CZ-NH2	-7.75	116.42	120.30
1	A	51	ARG	NE-CZ-NH2	-7.75	116.42	120.30
1	B	358	TRP	CE2-CD2-CG	-7.57	101.25	107.30
1	B	309	VAL	CA-CB-CG2	-7.52	99.63	110.90
1	A	397	TRP	CE2-CD2-CG	-7.51	101.30	107.30
1	A	386	ARG	NH1-CZ-NH2	-7.48	111.17	119.40
1	A	220	ARG	NE-CZ-NH2	-7.45	116.57	120.30
1	B	507	GLY	CA-C-N	-7.43	100.84	117.20
1	B	397	TRP	CE2-CD2-CG	-7.42	101.37	107.30
1	B	430	GLU	O-C-N	-7.41	110.84	122.70
1	B	270	ASP	CB-CG-OD2	-7.34	111.69	118.30
1	B	514	ARG	CG-CD-NE	-7.25	96.59	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	255	ASP	CB-CG-OD1	7.18	124.76	118.30
1	A	342	ARG	NE-CZ-NH1	7.16	123.88	120.30
1	B	427	TYR	CB-CG-CD2	-7.07	116.76	121.00
1	A	352	TYR	CB-CG-CD1	-7.03	116.78	121.00
1	A	51	ARG	NE-CZ-NH1	6.97	123.78	120.30
1	B	551	ARG	CG-CD-NE	-6.96	97.17	111.80
1	A	426	ARG	NE-CZ-NH2	-6.89	116.85	120.30
1	B	220	ARG	NE-CZ-NH2	-6.88	116.86	120.30
1	B	462	ASP	N-CA-CB	-6.81	98.34	110.60
1	B	199	ARG	NE-CZ-NH1	6.77	123.69	120.30
1	A	412	LEU	CA-CB-CG	-6.74	99.79	115.30
1	B	25	VAL	CG1-CB-CG2	-6.68	100.21	110.90
1	B	248	VAL	CG1-CB-CG2	-6.64	100.27	110.90
1	A	188	VAL	N-CA-CB	-6.62	96.95	111.50
1	A	416	TRP	CD1-CG-CD2	6.58	111.56	106.30
1	B	430	GLU	N-CA-C	6.56	128.72	111.00
1	B	412	LEU	CA-CB-CG	-6.51	100.32	115.30
1	A	224	MET	CG-SD-CE	-6.48	89.83	100.20
1	B	530	ASP	CB-CG-OD1	6.47	124.13	118.30
1	B	551	ARG	NE-CZ-NH2	-6.47	117.07	120.30
1	B	216	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	A	358	TRP	CD1-CG-CD2	6.43	111.44	106.30
1	A	75	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	A	210	LEU	CA-CB-CG	6.37	129.96	115.30
1	A	514	ARG	CG-CD-NE	-6.37	98.42	111.80
1	A	502	ARG	NE-CZ-NH2	-6.37	117.12	120.30
1	A	397	TRP	CG-CD1-NE1	-6.35	103.75	110.10
1	B	416	TRP	CE2-CD2-CG	-6.33	102.24	107.30
1	B	498	ARG	NE-CZ-NH2	-6.25	117.18	120.30
1	B	358	TRP	CE2-CD2-CE3	6.14	126.07	118.70
1	B	397	TRP	CG-CD1-NE1	-6.13	103.97	110.10
1	A	30	SER	N-CA-C	6.11	127.50	111.00
1	A	63	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	A	490	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	A	544	LYS	CA-CB-CG	6.03	126.67	113.40
1	B	416	TRP	CG-CD1-NE1	-6.01	104.09	110.10
1	B	151	LYS	CA-CB-CG	5.99	126.58	113.40
1	A	166	LEU	CA-CB-CG	5.98	129.05	115.30
1	A	358	TRP	CE2-CD2-CE3	5.98	125.87	118.70
1	B	472	ASN	N-CA-C	-5.94	94.97	111.00
1	A	397	TRP	CG-CD2-CE3	5.91	139.22	133.90
1	A	454	VAL	CG1-CB-CG2	-5.88	101.50	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	188	VAL	CA-CB-CG2	-5.88	102.08	110.90
1	A	358	TRP	CE2-CD2-CG	-5.87	102.61	107.30
1	B	11	TYR	CB-CG-CD2	-5.84	117.49	121.00
1	A	554	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	A	65	TYR	CB-CG-CD1	-5.80	117.52	121.00
1	B	502	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	B	352	TYR	CB-CG-CD2	5.75	124.45	121.00
1	A	292	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	B	528	ASN	CA-CB-CG	-5.68	100.89	113.40
1	B	421	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	A	148	GLN	OE1-CD-NE2	-5.68	108.84	121.90
1	B	386	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	B	55	THR	OG1-CB-CG2	-5.63	97.05	110.00
1	A	416	TRP	CE2-CD2-CG	-5.62	102.80	107.30
1	A	260	HIS	CB-CA-C	-5.61	99.19	110.40
1	B	332	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	A	328	ARG	CB-CA-C	-5.58	99.25	110.40
1	A	551	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	B	168	VAL	CG1-CB-CG2	-5.58	101.98	110.90
1	B	108	ILE	CA-CB-CG1	-5.56	100.43	111.00
1	A	314	ALA	O-C-N	-5.56	113.81	122.70
1	B	554	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	B	347	THR	CA-CB-CG2	5.52	120.13	112.40
1	B	228	VAL	CG1-CB-CG2	-5.51	102.08	110.90
1	A	463	LYS	N-CA-C	5.51	125.88	111.00
1	B	498	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	B	291	ASP	CB-CG-OD2	5.50	123.25	118.30
1	A	397	TRP	CB-CG-CD1	-5.48	119.88	127.00
1	B	51	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	B	309	VAL	CA-CB-CG1	5.48	119.12	110.90
1	B	509	ALA	CA-C-N	-5.47	105.25	116.20
1	A	359	LYS	CB-CA-C	-5.47	99.47	110.40
1	B	461	ASN	OD1-CG-ND2	-5.46	109.34	121.90
1	A	391	LEU	CB-CG-CD2	-5.45	101.73	111.00
1	A	427	TYR	CB-CG-CD2	-5.43	117.74	121.00
1	B	188	VAL	N-CA-CB	-5.43	99.56	111.50
1	B	13	ASP	N-CA-C	5.39	125.56	111.00
1	B	75	ARG	CA-CB-CG	-5.38	101.55	113.40
1	B	13	ASP	N-CA-CB	-5.38	100.92	110.60
1	B	327	VAL	CG1-CB-CG2	-5.36	102.33	110.90
1	B	471	ASP	CB-CG-OD2	5.35	123.12	118.30
1	A	84	ARG	CB-CG-CD	-5.33	97.75	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	325	THR	O-C-N	-5.32	114.15	123.20
1	A	108	ILE	CA-CB-CG1	-5.31	100.90	111.00
1	B	324	GLN	CA-CB-CG	-5.30	101.74	113.40
1	A	520	TYR	CB-CG-CD2	-5.29	117.83	121.00
1	B	97	ALA	CA-C-N	5.29	128.83	117.20
1	B	84	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	A	43	ILE	CB-CG1-CD1	-5.25	99.19	113.90
1	B	345	ASN	CB-CG-ND2	5.25	129.31	116.70
1	B	358	TRP	CD2-CE3-CZ3	-5.25	111.97	118.80
1	B	24	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	B	451	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	A	1	VAL	CG1-CB-CG2	-5.23	102.54	110.90
1	A	318	SER	CB-CA-C	-5.22	100.18	110.10
1	B	507	GLY	O-C-N	5.20	131.01	122.70
1	A	178	ASN	CB-CG-ND2	5.19	129.16	116.70
1	A	412	LEU	CB-CG-CD2	-5.19	102.17	111.00
1	B	495	ASP	CB-CG-OD2	5.18	122.97	118.30
1	A	95	THR	CA-CB-CG2	5.18	119.65	112.40
1	B	331	ALA	CB-CA-C	-5.16	102.36	110.10
1	B	474	GLU	N-CA-CB	-5.16	101.31	110.60
1	B	345	ASN	OD1-CG-ND2	-5.15	110.06	121.90
1	A	32	THR	CA-CB-CG2	5.14	119.59	112.40
1	A	34	TYR	CB-CG-CD1	-5.12	117.93	121.00
1	A	392	TRP	CB-CG-CD1	-5.12	120.35	127.00
1	A	248	VAL	O-C-N	-5.11	114.52	122.70
1	B	195	ALA	O-C-N	-5.11	114.52	122.70
1	A	292	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	B	259	HIS	CA-CB-CG	-5.10	104.94	113.60
1	A	325	THR	CA-CB-OG1	-5.09	98.30	109.00
1	A	345	ASN	CB-CG-ND2	5.08	128.90	116.70
1	A	345	ASN	OD1-CG-ND2	-5.07	110.25	121.90
1	A	13	ASP	N-CA-C	5.05	124.64	111.00
1	A	523	ASP	CA-C-N	-5.03	106.14	117.20
1	A	260	HIS	CA-CB-CG	5.02	122.14	113.60
1	B	292	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	A	392	TRP	CG-CD2-CE3	5.01	138.41	133.90
1	B	248	VAL	CA-CB-CG1	5.00	118.40	110.90

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	194	TYR	Sidechain
1	A	386	ARG	Sidechain
1	B	514	ARG	Sidechain

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	A	4333	971	4331	92	0
1	B	4333	971	4331	73	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	201	402	0	17	0
3	B	293	586	0	15	0
All	All	9162	2930	8662	165	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 10.

All (165) 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:A:63:ARG:HD2	3:A:758:HOH:O	1.77	0.84
1:B:383:ASP:HB2	1:B:386:ARG:NH2	1.94	0.83
1:A:280:HIS:HD2	3:A:753:HOH:O	1.65	0.78
1:A:112:ILE:HD12	1:A:129:LYS:HD3	1.68	0.74
1:B:365:MET:HB3	1:B:386:ARG:NH2	2.03	0.73
1:B:383:ASP:HB2	1:B:386:ARG:HH21	1.56	0.70
1:B:471:ASP:OD1	1:B:490:ARG:HD3	1.91	0.69
1:B:325:THR:HG22	1:B:326:GLY:O	1.92	0.69
1:A:359:LYS:HE2	3:A:644:HOH:O	1.92	0.69
1:A:178:ASN:HB2	3:A:714:HOH:O	1.93	0.69
1:A:547:GLN:HB2	1:A:551:ARG:NH1	2.10	0.67
1:B:444:LEU:HD12	1:B:447:LEU:HD22	1.80	0.64
1:B:473:PHE:HB2	1:B:490:ARG:HD2	1.81	0.63
1:B:68:GLU:HB2	3:B:773:HOH:O	1.97	0.63
1:B:280:HIS:HD2	3:B:643:HOH:O	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:382:SER:OG	1:B:384:HIS:HD2	1.81	0.63
1:A:437:ALA:HB1	1:A:503:LEU:HD11	1.82	0.62
1:A:259:HIS:NE2	1:A:267:TYR:HD1	1.98	0.61
1:A:272:VAL:O	1:A:276:LYS:HG2	2.01	0.60
1:A:321:TYR:O	1:A:325:THR:HB	2.01	0.60
1:A:384:HIS:HE1	1:A:389:ASP:OD2	1.86	0.59
1:A:384:HIS:CE1	1:A:385:ILE:HG12	2.38	0.58
1:A:440:MET:HG3	1:A:546:SER:O	2.01	0.58
1:A:505:GLY:HA2	1:A:511:ALA:HA	1.86	0.58
1:A:247:ALA:HB1	1:A:250:CYS:SG	2.44	0.58
1:B:220:ARG:NH1	1:B:248:VAL:HG21	2.19	0.58
1:B:75:ARG:HD2	1:B:159:CYS:O	2.04	0.58
1:B:11:TYR:OH	1:B:31:SER:HB3	2.04	0.57
1:A:499:ILE:HD13	1:A:542:ALA:HB2	1.87	0.57
1:B:197:MET:HA	3:B:576:HOH:O	2.03	0.57
1:B:426:ARG:HG3	1:B:516:TYR:CD2	2.40	0.57
1:B:451:ARG:H	1:B:451:ARG:HD3	1.71	0.56
1:B:384:HIS:HE1	1:B:389:ASP:OD2	1.88	0.55
1:A:499:ILE:HD11	1:A:538:LEU:HD22	1.88	0.55
1:B:318:SER:HB2	1:B:403:THR:HG21	1.89	0.55
1:A:426:ARG:HG3	1:A:516:TYR:CE2	2.41	0.54
1:B:15:LYS:HB3	1:B:15:LYS:NZ	2.22	0.54
1:A:536:ALA:HB3	1:A:537:PRO:HD3	1.90	0.54
1:A:147:PHE:CZ	1:A:151:LYS:HD2	2.43	0.54
1:A:554:ARG:NH1	3:A:763:HOH:O	2.34	0.54
1:A:448:MET:HA	1:A:453:PHE:CD2	2.44	0.53
1:B:16:PRO:HG2	1:B:143:THR:HB	1.91	0.53
1:A:228:VAL:HG12	3:A:627:HOH:O	2.08	0.53
1:A:55:THR:OG1	1:A:84:ARG:HD3	2.09	0.53
1:B:14:GLN:HE21	1:B:150:SER:HB2	1.73	0.52
1:B:69:ALA:O	1:B:73:ILE:HG13	2.09	0.52
1:B:106:LYS:HD3	3:B:787:HOH:O	2.10	0.52
1:B:53:GLU:HG2	3:B:805:HOH:O	2.08	0.52
1:A:31:SER:HB2	1:A:34:TYR:HB2	1.92	0.51
1:B:117:HIS:HB3	1:B:292:ARG:HH21	1.75	0.51
1:B:280:HIS:CD2	3:B:643:HOH:O	2.60	0.51
1:B:504:SER:OG	1:B:512:THR:HB	2.10	0.51
1:B:210:LEU:HG	1:B:402:ALA:HB2	1.93	0.51
1:B:271:LEU:HD13	1:B:296:LEU:HD12	1.92	0.51
1:B:60:GLY:HA3	1:B:66:MET:SD	2.52	0.50
1:A:256:PHE:CD1	1:A:261:PRO:HG3	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:449:PHE:CD1	1:A:449:PHE:N	2.78	0.50
1:A:145:LYS:O	1:A:149:ILE:HG13	2.11	0.50
1:A:425:THR:CG2	1:A:535:LEU:HD13	2.41	0.50
1:A:220:ARG:CZ	1:A:248:VAL:HG21	2.42	0.50
1:B:63:ARG:HD2	3:B:793:HOH:O	2.11	0.50
1:B:264:ASN:HD21	1:B:267:TYR:HD2	1.59	0.49
1:B:384:HIS:CE1	1:B:385:ILE:HG12	2.47	0.49
1:A:76:ILE:HG13	1:A:158:ILE:HD12	1.94	0.49
1:B:301:PHE:HE2	1:B:412:LEU:HD13	1.78	0.49
1:B:177:GLU:HB3	3:B:779:HOH:O	2.12	0.49
1:A:404:ARG:NH2	3:A:694:HOH:O	2.45	0.49
1:B:316:ILE:HG12	1:B:322:PHE:CD2	2.47	0.49
1:A:71:GLN:HB3	1:A:75:ARG:HH12	1.77	0.49
1:A:180:PHE:HB3	1:A:181:LYS:HD2	1.95	0.49
1:B:347:THR:HG22	1:B:349:ILE:HG12	1.95	0.48
1:A:425:THR:HG22	1:A:535:LEU:HD13	1.94	0.48
1:B:383:ASP:CB	1:B:386:ARG:HH21	2.25	0.48
1:A:369:LYS:HE2	3:A:737:HOH:O	2.13	0.48
1:A:259:HIS:CE1	1:A:260:HIS:O	2.65	0.48
1:A:539:ILE:HG22	1:A:543:LEU:HD22	1.94	0.48
1:A:71:GLN:HB3	1:A:75:ARG:NH1	2.28	0.48
1:B:280:HIS:CD2	1:B:280:HIS:N	2.82	0.48
1:B:225:HIS:HD2	3:B:767:HOH:O	1.96	0.48
1:A:460:ALA:HB3	1:A:537:PRO:HB3	1.96	0.47
1:B:470:ALA:HA	1:B:490:ARG:O	2.14	0.47
1:A:432:VAL:HG22	1:A:511:ALA:O	2.14	0.47
1:B:343:VAL:O	1:B:347:THR:HB	2.15	0.47
1:A:264:ASN:HB2	3:A:622:HOH:O	2.14	0.47
1:B:451:ARG:N	1:B:451:ARG:HD3	2.30	0.47
1:A:117:HIS:HB3	1:A:292:ARG:NH2	2.29	0.47
1:A:335:PRO:HG3	1:A:502:ARG:HD2	1.97	0.47
1:A:230:PRO:O	1:A:234:LYS:HB2	2.14	0.47
1:B:52:GLN:HG2	3:B:594:HOH:O	2.14	0.47
1:A:505:GLY:CA	1:A:511:ALA:HA	2.45	0.46
1:A:443:ASP:O	1:A:446:ALA:HB3	2.15	0.46
1:B:439:LYS:HE3	1:B:551:ARG:NE	2.30	0.46
1:B:181:LYS:HD3	3:B:592:HOH:O	2.14	0.46
1:B:414:ASP:O	1:B:418:LYS:HD2	2.15	0.46
1:B:365:MET:HB3	1:B:386:ARG:CZ	2.45	0.46
1:A:418:LYS:HE3	1:A:418:LYS:HB2	1.69	0.46
1:A:438:THR:O	1:A:442:LYS:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:HIS:HB3	1:B:292:ARG:NH2	2.31	0.46
1:B:366:ASP:OD1	1:B:386:ARG:NH1	2.45	0.46
1:B:68:GLU:CB	3:B:773:HOH:O	2.57	0.46
1:B:280:HIS:H	1:B:280:HIS:CD2	2.33	0.46
1:A:236:LEU:HD23	1:A:240:LEU:HD12	1.96	0.45
1:B:149:ILE:O	1:B:153:ILE:HB	2.16	0.45
1:A:61:ASP:HA	1:A:227:VAL:CG2	2.46	0.45
1:A:163:LYS:NZ	3:A:592:HOH:O	2.47	0.45
1:A:551:ARG:NH1	3:A:674:HOH:O	2.48	0.45
1:A:265:LEU:HD12	3:A:622:HOH:O	2.17	0.45
1:B:123:ASN:HB2	3:B:776:HOH:O	2.15	0.45
1:A:210:LEU:HD22	1:A:217:LEU:HB2	1.99	0.45
1:B:519:SER:HB3	1:B:535:LEU:HD23	1.97	0.45
1:B:23:LYS:HE3	1:B:34:TYR:OH	2.16	0.45
1:B:218:LYS:HE2	1:B:218:LYS:HB3	1.85	0.45
1:A:441:MET:HG3	1:A:503:LEU:HD22	1.99	0.45
1:A:88:GLY:HA3	1:A:93:LEU:HD13	1.98	0.45
1:A:366:ASP:OD1	1:A:386:ARG:HD2	2.16	0.44
1:A:176:LEU:HD11	1:A:183:PHE:HB2	1.98	0.44
1:A:178:ASN:O	1:A:179:LYS:HG2	2.17	0.44
1:A:312:ILE:HA	1:A:400:ILE:HD11	1.99	0.44
1:B:465:TYR:HB3	1:B:493:PHE:CD1	2.53	0.44
1:A:426:ARG:HG3	1:A:516:TYR:CD2	2.53	0.44
1:B:232:VAL:O	1:B:236:LEU:HB2	2.18	0.44
1:B:84:ARG:HA	1:B:184:THR:O	2.18	0.44
1:A:101:ILE:O	1:A:105:ILE:HG12	2.18	0.44
1:A:520:TYR:CE2	1:A:522:LYS:HB2	2.53	0.44
1:B:112:ILE:HG22	1:B:114:THR:HG22	2.00	0.44
1:B:469:LYS:NZ	3:B:717:HOH:O	2.50	0.44
1:B:426:ARG:HG3	1:B:516:TYR:CE2	2.52	0.43
1:A:224:MET:HG2	3:A:612:HOH:O	2.18	0.43
1:A:28:PHE:CD2	1:A:126:PHE:HB3	2.53	0.43
1:B:551:ARG:HA	1:B:551:ARG:HD3	1.90	0.43
1:A:280:HIS:CD2	3:A:753:HOH:O	2.51	0.43
1:A:273:GLU:O	1:A:276:LYS:HB2	2.18	0.43
1:A:60:GLY:HA3	1:A:66:MET:SD	2.58	0.43
1:A:2:LYS:O	1:A:159:CYS:HA	2.19	0.43
1:B:382:SER:OG	1:B:384:HIS:CD2	2.66	0.43
1:A:523:ASP:OD2	1:A:526:LYS:HG3	2.17	0.43
1:A:225:HIS:HD2	3:A:713:HOH:O	2.00	0.43
1:A:363:ASN:HB3	1:A:479:VAL:HB	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:501:PHE:CE2	1:A:515:LEU:HD13	2.54	0.42
1:A:540:SER:O	1:A:544:LYS:HB2	2.19	0.42
1:A:537:PRO:O	1:A:541:ILE:HG13	2.20	0.42
1:A:14:GLN:HE21	1:A:150:SER:HB2	1.83	0.42
1:B:449:PHE:HE1	1:B:471:ASP:HA	1.85	0.42
1:B:3:ILE:HD12	1:B:179:LYS:HE3	2.01	0.42
1:B:325:THR:HG21	3:B:785:HOH:O	2.19	0.42
1:A:234:LYS:NZ	3:A:749:HOH:O	2.47	0.42
1:A:325:THR:O	1:A:328:ARG:NH2	2.53	0.41
1:A:497:SER:HB3	1:A:538:LEU:HD11	2.02	0.41
1:B:383:ASP:CB	1:B:386:ARG:NH2	2.77	0.41
1:A:14:GLN:O	1:A:16:PRO:HD3	2.21	0.41
1:B:31:SER:HB2	1:B:34:TYR:HB2	2.03	0.41
1:A:94:SER:HA	1:A:227:VAL:HG11	2.03	0.41
1:A:311:VAL:HG11	1:A:397:TRP:CH2	2.56	0.41
1:A:177:GLU:HG3	1:A:177:GLU:O	2.20	0.41
1:B:48:PRO:HA	1:B:51:ARG:CD	2.51	0.41
1:A:447:LEU:HD21	1:A:545:VAL:HG22	2.03	0.41
1:A:325:THR:HG22	1:A:326:GLY:O	2.21	0.40
1:B:25:VAL:HG22	1:B:126:PHE:HB2	2.02	0.40
1:A:303:VAL:HG22	1:A:412:LEU:CD1	2.52	0.40
1:A:424:PHE:HA	1:A:517:ILE:O	2.22	0.40
1:B:220:ARG:HH11	1:B:248:VAL:HG21	1.84	0.40
1:A:21:LEU:HD11	1:A:23:LYS:HE3	2.02	0.40
1:A:16:PRO:HG3	1:A:38:PHE:CZ	2.56	0.40
1:A:472:ASN:OD1	1:A:486:ASN:HA	2.21	0.40
1:A:104:LYS:NZ	3:A:605:HOH:O	2.52	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	558/561 (100%)	533 (96%)	22 (4%)	3 (0%)	34	48
1	B	558/561 (100%)	533 (96%)	24 (4%)	1 (0%)	52	69
All	All	1116/1122 (100%)	1066 (96%)	46 (4%)	4 (0%)	39	56

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	216	ARG
1	B	461	ASN
1	A	213	GLY
1	A	263	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 analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	461/461 (100%)	424 (92%)	37 (8%)	15	23
1	B	461/461 (100%)	434 (94%)	27 (6%)	24	38
All	All	922/922 (100%)	858 (93%)	64 (7%)	19	30

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	VAL
1	A	48	PRO
1	A	68	GLU
1	A	93	LEU
1	A	113	LEU
1	A	118	ASN
1	A	125	ASP
1	A	144	ASP
1	A	151	LYS
1	A	153	ILE
1	A	154	GLU
1	A	166	LEU

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Mol	Chain	Res	Type
1	A	178	ASN
1	A	179	LYS
1	A	210	LEU
1	A	215	ASN
1	A	220	ARG
1	A	227	VAL
1	A	243	PRO
1	A	309	VAL
1	A	323	GLN
1	A	341	ASP
1	A	359	LYS
1	A	380	THR
1	A	417	HIS
1	A	431	GLU
1	A	439	LYS
1	A	442	LYS
1	A	451	ARG
1	A	462	ASP
1	A	486	ASN
1	A	514	ARG
1	A	524	ASN
1	A	543	LEU
1	A	544	LYS
1	A	545	VAL
1	A	561	THR
1	B	7	LYS
1	B	22	ARG
1	B	72	LEU
1	B	108	ILE
1	B	166	LEU
1	B	169	LEU
1	B	188	VAL
1	B	209	GLU
1	B	210	LEU
1	B	216	ARG
1	B	227	VAL
1	B	233	LYS
1	B	270	ASP
1	B	271	LEU
1	B	325	THR
1	B	337	SER
1	B	341	ASP

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Mol	Chain	Res	Type
1	B	358	TRP
1	B	359	LYS
1	B	386	ARG
1	B	412	LEU
1	B	418	LYS
1	B	430	GLU
1	B	433	GLU
1	B	447	LEU
1	B	451	ARG
1	B	506	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	172	GLN
1	A	205	ASN
1	A	323	GLN
1	A	384	HIS
1	A	549	GLN
1	B	14	GLN
1	B	29	GLN
1	B	280	HIS
1	B	384	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\#\|Z\|>2$
1	SEP	A	116	1,2	8,9,10	1.29	1 (12%)	8,12,14	1.31	2 (25%)
1	SEP	B	116	1,2	8,9,10	1.18	1 (12%)	8,12,14	3.37	2 (25%)

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
1	SEP	A	116	1,2	-	0/6/8/10	0/0/0/0
1	SEP	B	116	1,2	-	0/6/8/10	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	116	SEP	P-OG	-2.88	1.50	1.60
1	A	116	SEP	P-OG	-2.53	1.51	1.60

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	116	SEP	OG-CB-CA	-8.81	100.76	108.27
1	B	116	SEP	O-C-CA	-2.98	117.72	125.49
1	A	116	SEP	OG-CB-CA	-2.33	106.28	108.27
1	A	116	SEP	O-C-CA	-2.14	119.91	125.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	A	560/561 (99%)	-0.48	22 (3%) 43 44	8, 30, 69, 90	0
1	B	560/561 (99%)	-0.82	6 (1%) 82 82	4, 21, 51, 80	0
All	All	1120/1122 (99%)	-0.65	28 (2%) 61 60	4, 26, 63, 90	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	506	THR	7.7
1	B	509	ALA	5.5
1	A	509	ALA	4.2
1	B	508	SER	4.2
1	A	507	GLY	4.0
1	A	214	PRO	3.8
1	A	510	GLY	3.6
1	A	508	SER	3.5
1	A	259	HIS	3.5
1	A	213	GLY	3.4
1	B	462	ASP	3.2
1	A	505	GLY	3.2
1	A	215	ASN	3.1
1	A	462	ASP	3.0
1	B	507	GLY	2.9
1	B	214	PRO	2.8
1	B	506	THR	2.7
1	A	547	GLN	2.5
1	A	529	GLN	2.5
1	A	449	PHE	2.4
1	A	417	HIS	2.4
1	A	527	ILE	2.4
1	A	486	ASN	2.3
1	A	123	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	457	GLN	2.2
1	A	549	GLN	2.1
1	A	439	LYS	2.1
1	A	544	LYS	2.1

6.2 Non-standard residues in protein, DNA, RNA chains (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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
1	SEP	B	116	10/11	0.88	0.18	-	0,40,53,54	0
1	SEP	A	116	10/11	0.93	0.14	-	0,45,60,61	0

6.3 Carbohydrates (i)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
2	MG	B	562	1/1	0.71	0.11	-0.66	28,28,28,28	0
2	MG	A	562	1/1	0.87	0.09	-1.13	51,51,51,51	0

6.5 Other polymers (i)

There are no such residues in this entry.