Full wwPDB X-ray Structure Validation Report (i)

Jul 31, 2023 – 04:04 AM EDT

PDB ID	:	1VKL
Title	:	RABBIT MUSCLE PHOSPHOGLUCOMUTASE
Authors	:	Ray Junior, W.J.; Baranidharan, S.; Liu, Y.
Deposited on	:	1996-07-03
Resolution	:	2.70 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:

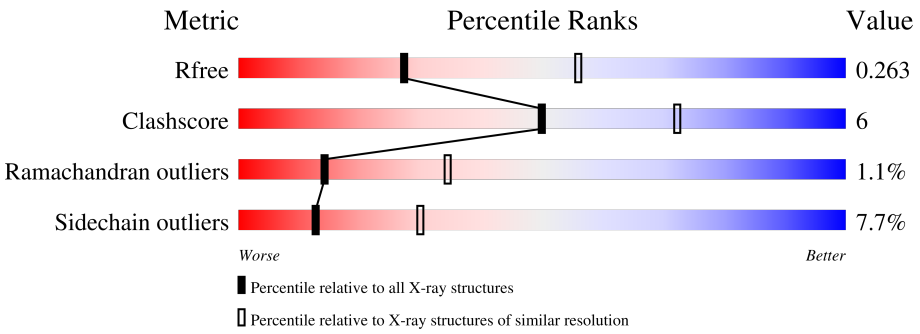
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.34
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

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 2.70 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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)

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%

Mol	Chain	Length	Quality of chain
1	A	561	76% 20% • •
1	B	561	77% 19% • •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 9019 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 PHOSPHOGLUCOMUTASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	561	4333	2753	743	820	1	16	0	0	0
1	B	561	4333	2753	743	820	1	16	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	116	SEP	SER	conflict	UNP P00949
B	116	SEP	SER	conflict	UNP P00949

- Molecule 2 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

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

- Molecule 3 is water.

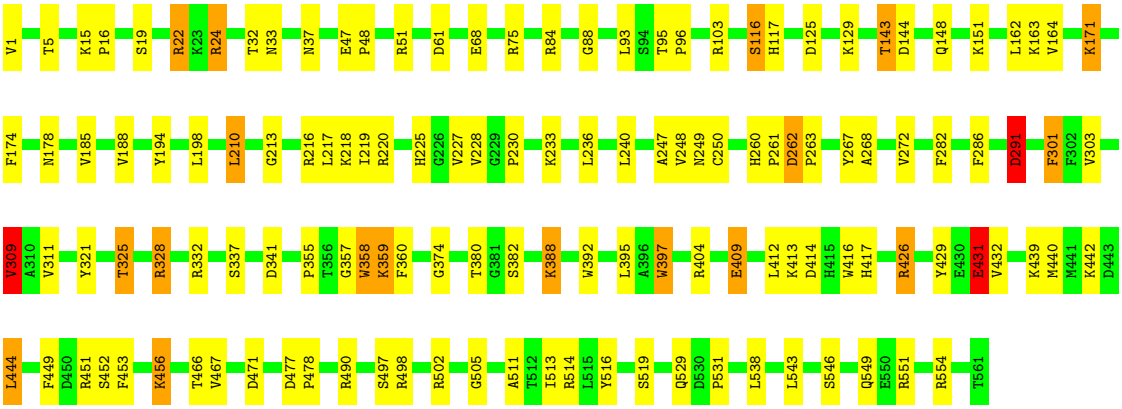
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	143	143	143	0	0
3	B	208	208	208	0	0

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. 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. 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.

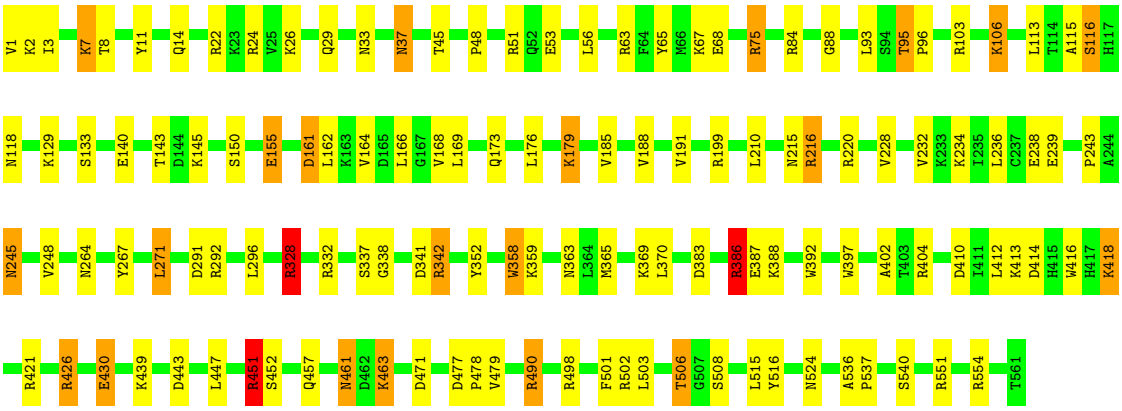
• Molecule 1: PHOSPHOGLUCOMUTASE

Chain A:



• Molecule 1: PHOSPHOGLUCOMUTASE

Chain B:



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 – 2.70 6.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	92.1 (6.00-2.70) 97.2 (6.00-2.70)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.16 (at 2.69Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.170 , 0.210 0.242 , 0.263	Depositor DCC
R_{free} test set	3838 reflections (10.05%)	wwPDB-VP
Wilson B-factor (Å^2)	36.2	Xtriage
Anisotropy	0.305	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 99.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	9019	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.37% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: NI, 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	0.72	0/4409	1.50	47/5958 (0.8%)
1	B	0.75	0/4409	1.54	51/5958 (0.9%)
All	All	0.74	0/8818	1.52	98/11916 (0.8%)

There are no bond length outliers.

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	421	ARG	NE-CZ-NH2	-10.70	114.95	120.30
1	B	451	ARG	NE-CZ-NH2	-10.33	115.13	120.30
1	B	22	ARG	NE-CZ-NH1	10.28	125.44	120.30
1	B	421	ARG	NE-CZ-NH1	9.84	125.22	120.30
1	B	426	ARG	NE-CZ-NH2	-9.30	115.65	120.30
1	B	51	ARG	NE-CZ-NH2	-8.83	115.88	120.30
1	A	392	TRP	CD1-CG-CD2	8.79	113.33	106.30
1	A	392	TRP	CE2-CD2-CG	-8.75	100.30	107.30
1	A	328	ARG	NE-CZ-NH1	-8.72	115.94	120.30
1	B	416	TRP	CD1-CG-CD2	8.65	113.22	106.30
1	B	24	ARG	NE-CZ-NH2	-8.21	116.20	120.30
1	B	498	ARG	NE-CZ-NH2	-8.20	116.20	120.30
1	B	397	TRP	CD1-CG-CD2	8.03	112.72	106.30
1	A	220	ARG	NE-CZ-NH2	-7.98	116.31	120.30
1	A	451	ARG	NE-CZ-NH2	-7.85	116.37	120.30
1	A	404	ARG	NE-CZ-NH2	-7.82	116.39	120.30
1	B	392	TRP	CD1-CG-CD2	7.82	112.56	106.30
1	A	514	ARG	NE-CZ-NH1	7.80	124.20	120.30
1	A	75	ARG	NE-CZ-NH2	-7.78	116.41	120.30
1	B	386	ARG	NE-CZ-NH1	7.74	124.17	120.30
1	B	392	TRP	CE2-CD2-CG	-7.66	101.17	107.30
1	B	397	TRP	CE2-CD2-CG	-7.66	101.17	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	426	ARG	NE-CZ-NH1	7.58	124.09	120.30
1	B	22	ARG	NH1-CZ-NH2	-7.54	111.10	119.40
1	B	416	TRP	CE2-CD2-CG	-7.49	101.31	107.30
1	B	328	ARG	NE-CZ-NH2	7.47	124.04	120.30
1	B	554	ARG	NE-CZ-NH2	-7.47	116.57	120.30
1	A	328	ARG	NE-CZ-NH2	7.46	124.03	120.30
1	A	397	TRP	CE2-CD2-CG	-7.46	101.33	107.30
1	B	63	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	B	332	ARG	NE-CZ-NH1	7.42	124.01	120.30
1	A	22	ARG	NE-CZ-NH2	-7.37	116.62	120.30
1	A	397	TRP	CD1-CG-CD2	7.36	112.19	106.30
1	A	416	TRP	CD1-CG-CD2	7.27	112.12	106.30
1	B	490	ARG	NE-CZ-NH2	-7.27	116.66	120.30
1	B	551	ARG	NE-CZ-NH2	-7.27	116.67	120.30
1	B	216	ARG	NE-CZ-NH2	-7.22	116.69	120.30
1	A	358	TRP	CE2-CD2-CG	-7.16	101.57	107.30
1	A	392	TRP	CG-CD2-CE3	7.06	140.25	133.90
1	A	404	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	A	416	TRP	CE2-CD2-CG	-6.67	101.96	107.30
1	A	51	ARG	NE-CZ-NH2	-6.67	116.97	120.30
1	A	24	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	B	358	TRP	CD1-CG-CD2	6.66	111.63	106.30
1	A	392	TRP	CB-CG-CD1	-6.65	118.35	127.00
1	B	358	TRP	CE2-CD2-CG	-6.53	102.08	107.30
1	A	194	TYR	CB-CG-CD1	-6.42	117.15	121.00
1	A	358	TRP	CD1-CG-CD2	6.41	111.43	106.30
1	B	24	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	B	65	TYR	CB-CG-CD1	-6.38	117.17	121.00
1	A	220	ARG	NE-CZ-NH1	6.37	123.49	120.30
1	A	498	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	A	84	ARG	NE-CZ-NH1	-6.16	117.22	120.30
1	B	95	THR	CA-CB-OG1	-6.08	96.24	109.00
1	B	451	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	B	22	ARG	CB-CG-CD	6.07	127.39	111.60
1	B	22	ARG	NE-CZ-NH2	6.06	123.33	120.30
1	A	502	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	B	418	LYS	CA-CB-CG	6.04	126.68	113.40
1	B	210	LEU	CA-CB-CG	6.01	129.13	115.30
1	B	471	ASP	CB-CG-OD1	5.98	123.68	118.30
1	B	95	THR	CA-CB-CG2	5.95	120.72	112.40
1	B	26	LYS	CA-CB-CG	-5.89	100.45	113.40
1	B	502	ARG	NE-CZ-NH1	5.85	123.23	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	332	ARG	NE-CZ-NH1	-5.82	117.39	120.30
1	A	490	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	A	260	HIS	CA-CB-CG	5.82	123.50	113.60
1	B	342	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	A	309	VAL	CB-CA-C	-5.74	100.48	111.40
1	A	260	HIS	CB-CA-C	-5.72	98.96	110.40
1	B	352	TYR	CB-CG-CD1	-5.71	117.57	121.00
1	B	168	VAL	CA-CB-CG2	-5.68	102.37	110.90
1	B	56	LEU	CA-CB-CG	5.64	128.27	115.30
1	A	103	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	A	498	ARG	CA-CB-CG	5.54	125.59	113.40
1	A	32	THR	CA-CB-CG2	5.53	120.14	112.40
1	A	451	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	A	291	ASP	CB-CG-OD2	-5.48	113.37	118.30
1	B	75	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	A	332	ARG	NE-CZ-NH2	5.47	123.03	120.30
1	B	498	ARG	NE-CZ-NH1	5.45	123.02	120.30
1	B	490	ARG	NE-CZ-NH1	5.45	123.02	120.30
1	B	397	TRP	CG-CD2-CE3	5.40	138.76	133.90
1	A	358	TRP	CA-CB-CG	-5.35	103.53	113.70
1	A	262	ASP	CB-CG-OD2	5.25	123.02	118.30
1	A	171	LYS	CA-CB-CG	5.21	124.87	113.40
1	A	129	LYS	CB-CG-CD	-5.21	98.05	111.60
1	B	404	ARG	NE-CZ-NH2	5.19	122.89	120.30
1	A	498	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	B	498	ARG	CA-CB-CG	5.18	124.79	113.40
1	A	188	VAL	N-CA-CB	-5.15	100.17	111.50
1	A	24	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	B	463	LYS	CA-C-N	-5.09	106.00	117.20
1	A	444	LEU	CA-CB-CG	5.08	127.00	115.30
1	A	358	TRP	CB-CG-CD1	-5.04	120.45	127.00
1	B	245	ASN	CB-CG-ND2	5.03	128.78	116.70
1	A	426	ARG	NE-CZ-NH1	5.01	122.81	120.30
1	B	11	TYR	CB-CG-CD1	-5.00	118.00	121.00

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	A	4333	0	4331	56	0
1	B	4333	0	4331	45	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	143	0	0	4	0
3	B	208	0	0	3	0
All	All	9019	0	8662	101	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 6.

All (101) 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:357:GLY:HA3	1:A:359:LYS:HE3	1.64	0.79
1:B:426:ARG:HG3	1:B:516:TYR:CD1	2.31	0.66
1:A:429:TYR:HB2	1:A:513:ILE:HB	1.79	0.65
1:A:426:ARG:HG3	1:A:516:TYR:CD1	2.33	0.64
1:B:45:THR:HB	1:B:145:LYS:HE3	1.80	0.62
1:A:453:PHE:HA	1:A:456:LYS:HZ1	1.64	0.61
1:A:236:LEU:HD23	1:A:240:LEU:HD12	1.83	0.61
1:A:16:PRO:HB2	1:A:143:THR:HG22	1.83	0.60
1:A:453:PHE:HA	1:A:456:LYS:NZ	2.18	0.59
1:B:14:GLN:HE21	1:B:150:SER:HB2	1.69	0.57
1:A:33:ASN:HB3	1:A:37:ASN:ND2	2.21	0.56
1:B:3:ILE:HD12	1:B:179:LYS:HE3	1.86	0.56
1:B:264:ASN:HD21	1:B:267:TYR:HD2	1.54	0.56
1:A:61:ASP:HA	1:A:227:VAL:HB	1.87	0.56
1:B:271:LEU:HD13	1:B:296:LEU:HD12	1.89	0.55
1:A:164:VAL:HG12	1:A:174:PHE:CZ	2.42	0.54
1:A:88:GLY:HA3	1:A:93:LEU:HD13	1.88	0.54
1:B:88:GLY:HA3	1:B:93:LEU:HD13	1.90	0.54
1:A:303:VAL:HG13	1:A:412:LEU:HD11	1.91	0.53
1:B:115:ALA:O	1:B:118:ASN:HB2	2.10	0.52
1:A:432:VAL:HG22	1:A:511:ALA:O	2.09	0.52
1:B:232:VAL:HG13	1:B:236:LEU:HD12	1.91	0.52
1:A:449:PHE:HE1	1:A:471:ASP:HA	1.75	0.51
1:B:68:GLU:HB2	3:B:719:HOH:O	2.11	0.51
1:B:7:LYS:HA	1:B:155:GLU:HB3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:TYR:O	1:A:325:THR:HB	2.12	0.50
1:B:33:ASN:HB3	1:B:37:ASN:ND2	2.27	0.50
1:A:148:GLN:OE1	1:A:151:LYS:NZ	2.45	0.49
1:B:129:LYS:NZ	1:B:387:GLU:OE1	2.45	0.49
1:A:325:THR:HG23	1:A:328:ARG:NH1	2.28	0.49
1:B:410:ASP:O	1:B:414:ASP:HB2	2.13	0.48
1:A:440:MET:O	1:A:444:LEU:HB2	2.14	0.48
1:B:451:ARG:HD3	1:B:451:ARG:H	1.79	0.48
1:B:164:VAL:HG11	1:B:185:VAL:HG11	1.96	0.47
1:B:402:ALA:HB3	3:B:666:HOH:O	2.12	0.47
1:A:225:HIS:HD2	3:A:678:HOH:O	1.96	0.47
1:B:2:LYS:HZ3	1:B:161:ASP:CG	2.17	0.47
1:B:228:VAL:HG12	1:B:232:VAL:HG23	1.96	0.47
1:A:117:HIS:HA	1:A:261:PRO:HG2	1.97	0.47
1:A:24:ARG:HA	1:A:125:ASP:HA	1.96	0.47
1:A:210:LEU:HD22	1:A:217:LEU:HB2	1.97	0.47
1:B:413:LYS:NZ	3:B:765:HOH:O	2.48	0.46
1:B:501:PHE:CE1	1:B:515:LEU:HD13	2.51	0.46
1:A:497:SER:HB3	1:A:538:LEU:HD11	1.98	0.46
1:A:519:SER:HB3	1:A:538:LEU:HD12	1.97	0.46
1:A:163:LYS:NZ	3:A:582:HOH:O	2.48	0.45
1:B:328:ARG:HH21	1:B:328:ARG:HG2	1.80	0.45
1:A:164:VAL:HG11	1:A:185:VAL:HG21	1.98	0.45
1:A:309:VAL:HG21	1:A:374:GLY:HA3	1.97	0.45
1:B:383:ASP:O	1:B:386:ARG:NH2	2.50	0.45
1:A:219:ILE:HG22	1:A:282:PHE:HB3	1.99	0.45
1:B:338:GLY:HA2	1:B:341:ASP:OD1	2.17	0.44
1:A:355:PRO:HG2	1:A:360:PHE:CE2	2.52	0.44
1:B:359:LYS:H	1:B:359:LYS:HE2	1.82	0.44
1:A:268:ALA:O	1:A:272:VAL:HG23	2.18	0.44
1:A:311:VAL:HG11	1:A:397:TRP:CH2	2.52	0.44
1:A:456:LYS:NZ	1:A:456:LYS:HB3	2.34	0.43
1:B:363:ASN:O	1:B:479:VAL:HG21	2.18	0.43
1:A:248:VAL:HG22	1:A:249:ASN:ND2	2.33	0.43
1:A:440:MET:HG3	1:A:546:SER:O	2.18	0.43
1:B:342:ARG:HA	1:B:342:ARG:HD3	1.88	0.43
1:A:301:PHE:CE2	1:A:412:LEU:HD12	2.53	0.43
1:A:431:GLU:O	1:A:554:ARG:NH2	2.52	0.43
1:A:1:VAL:HG11	1:A:162:LEU:HD12	2.00	0.43
1:A:291:ASP:HB2	1:A:388:LYS:O	2.18	0.43
1:A:309:VAL:CG2	1:A:374:GLY:HA3	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:SEP:O1P	1:B:292:ARG:NH2	2.52	0.42
1:B:243:PRO:HB2	1:B:245:ASN:OD1	2.19	0.42
1:A:15:LYS:NZ	3:A:661:HOH:O	2.45	0.42
1:B:8:THR:HG22	1:B:155:GLU:HA	2.00	0.42
1:B:1:VAL:HG21	1:B:162:LEU:HD12	2.01	0.42
1:B:503:LEU:HG	1:B:506:THR:HA	2.02	0.42
1:B:191:VAL:HG21	1:B:234:LYS:HD2	2.02	0.42
1:A:505:GLY:HA2	1:A:511:ALA:HA	2.02	0.42
1:B:103:ARG:O	1:B:106:LYS:NZ	2.49	0.42
1:B:199:ARG:NH1	1:B:239:GLU:OE2	2.53	0.42
1:A:456:LYS:HB3	1:A:456:LYS:HZ3	1.85	0.41
1:A:198:LEU:HD13	1:A:395:LEU:HD12	2.03	0.41
1:B:3:ILE:HD11	1:B:176:LEU:HD13	2.02	0.41
1:B:439:LYS:HZ2	1:B:443:ASP:CG	2.23	0.41
1:A:116:SEP:OG	1:A:117:HIS:N	2.53	0.41
1:A:546:SER:O	1:A:551:ARG:NH1	2.54	0.41
1:A:233:LYS:NZ	3:A:650:HOH:O	2.53	0.41
1:A:409:GLU:OE2	1:A:413:LYS:NZ	2.54	0.41
1:B:84:ARG:HH11	1:B:84:ARG:HD2	1.71	0.41
1:B:291:ASP:OD1	1:B:388:LYS:NZ	2.54	0.41
1:A:227:VAL:O	1:A:230:PRO:HD2	2.21	0.41
1:B:95:THR:HB	1:B:96:PRO:HD3	2.02	0.41
1:B:365:MET:HG3	1:B:370:LEU:HD23	2.03	0.41
1:A:477:ASP:HA	1:A:478:PRO:HD3	1.82	0.41
1:A:15:LYS:HA	1:A:16:PRO:HD3	1.83	0.41
1:A:439:LYS:HE3	1:A:439:LYS:HB2	1.84	0.41
1:A:228:VAL:HG11	1:A:286:PHE:CD1	2.55	0.41
1:B:75:ARG:HH11	1:B:75:ARG:HD3	1.72	0.41
1:B:536:ALA:HB3	1:B:537:PRO:HD3	2.03	0.40
1:A:95:THR:HB	1:A:96:PRO:HD3	2.03	0.40
1:A:171:LYS:HE2	1:A:171:LYS:HB3	1.93	0.40
1:A:247:ALA:HB1	1:A:250:CYS:SG	2.62	0.40
1:A:262:ASP:O	1:A:267:TYR:HB2	2.21	0.40
1:B:477:ASP:HA	1:B:478:PRO:HD3	1.79	0.40
1:B:113:LEU:N	1:B:113:LEU:HD22	2.37	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%)	514 (92%)	38 (7%)	6 (1%)	14	34
1	B	558/561 (100%)	527 (94%)	25 (4%)	6 (1%)	14	34
All	All	1116/1122 (100%)	1041 (93%)	63 (6%)	12 (1%)	14	34

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	216	ARG
1	A	431	GLU
1	B	461	ASN
1	B	508	SER
1	A	467	VAL
1	B	133	SER
1	B	430	GLU
1	A	301	PHE
1	B	48	PRO
1	B	238	GLU
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%)	428 (93%)	33 (7%)	14	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	461/461 (100%)	423 (92%)	38 (8%)	11 26
All	All	922/922 (100%)	851 (92%)	71 (8%)	13 30

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	19	SER
1	A	22	ARG
1	A	47	GLU
1	A	48	PRO
1	A	68	GLU
1	A	143	THR
1	A	144	ASP
1	A	178	ASN
1	A	210	LEU
1	A	218	LYS
1	A	291	ASP
1	A	309	VAL
1	A	325	THR
1	A	337	SER
1	A	341	ASP
1	A	358	TRP
1	A	359	LYS
1	A	380	THR
1	A	382	SER
1	A	388	LYS
1	A	409	GLU
1	A	414	ASP
1	A	417	HIS
1	A	431	GLU
1	A	442	LYS
1	A	452	SER
1	A	456	LYS
1	A	466	THR
1	A	529	GLN
1	A	531	PRO
1	A	543	LEU
1	A	549	GLN
1	B	7	LYS
1	B	29	GLN
1	B	37	ASN

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Mol	Chain	Res	Type
1	B	53	GLU
1	B	67	LYS
1	B	106	LYS
1	B	140	GLU
1	B	143	THR
1	B	155	GLU
1	B	161	ASP
1	B	166	LEU
1	B	169	LEU
1	B	173	GLN
1	B	179	LYS
1	B	188	VAL
1	B	215	ASN
1	B	216	ARG
1	B	220	ARG
1	B	248	VAL
1	B	271	LEU
1	B	328	ARG
1	B	337	SER
1	B	358	TRP
1	B	369	LYS
1	B	386	ARG
1	B	412	LEU
1	B	418	LYS
1	B	430	GLU
1	B	447	LEU
1	B	451	ARG
1	B	452	SER
1	B	457	GLN
1	B	461	ASN
1	B	463	LYS
1	B	490	ARG
1	B	506	THR
1	B	524	ASN
1	B	540	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	37	ASN
1	A	249	ASN

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Mol	Chain	Res	Type
1	A	345	ASN
1	A	384	HIS
1	A	476	HIS
1	A	524	ASN
1	B	14	GLN
1	B	29	GLN
1	B	37	ASN
1	B	486	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)

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	B	116	2,1	8,9,10	1.42	1 (12%)	8,12,14	1.33	1 (12%)
1	SEP	A	116	2,1	8,9,10	1.79	2 (25%)	8,12,14	1.57	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	B	116	2,1	-	4/5/8/10	-
1	SEP	A	116	2,1	-	4/5/8/10	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	116	SEP	P-OG	-3.35	1.49	1.60
1	B	116	SEP	P-OG	-3.27	1.49	1.60
1	A	116	SEP	CB-CA	2.83	1.60	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	116	SEP	OG-CB-CA	3.16	111.22	108.14
1	B	116	SEP	P-OG-CB	-2.74	110.75	118.30
1	A	116	SEP	P-OG-CB	-2.34	111.85	118.30

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	116	SEP	N-CA-CB-OG
1	A	116	SEP	CB-OG-P-O2P
1	A	116	SEP	CB-OG-P-O3P
1	B	116	SEP	N-CA-CB-OG
1	B	116	SEP	CB-OG-P-O1P
1	B	116	SEP	CB-OG-P-O2P
1	B	116	SEP	CB-OG-P-O3P
1	A	116	SEP	CB-OG-P-O1P

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	116	SEP	1	0
1	A	116	SEP	1	0

5.5 Carbohydrates (i)

There are no monosaccharides 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 (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)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.