



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 17, 2023 – 09:40 pm GMT

PDB ID : 4BJU
Title : Genetic and structural validation of *Aspergillus fumigatus* N- acetylphosphog
lucosamine mutase as an antifungal target
Authors : Fang, W.; Raimi, O.G.; Hurtado Guerrero, R.; van Aalten, D.M.F.
Deposited on : 2013-04-19
Resolution : 2.35 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

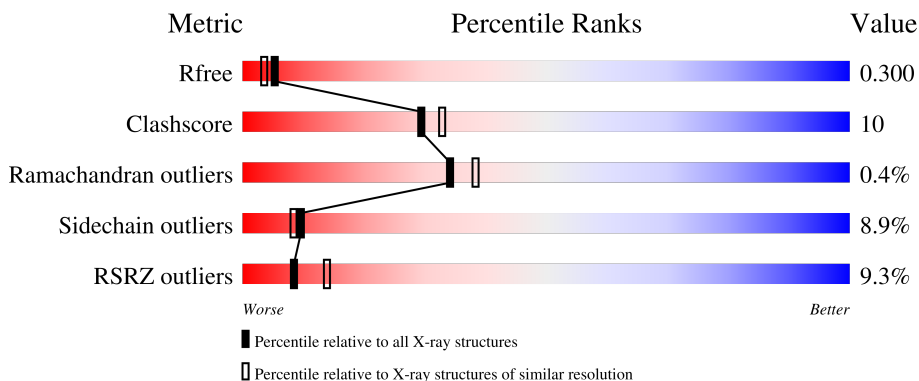
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 2.35 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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	549	
1	B	549	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 8388 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 N-ACETYLGLUCOSAMINE-PHOSPHATE MUTASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	548	Total	C	N	O	P	S	0	0	0
			4194	2635	726	815	1	17			
1	B	542	Total	C	N	O	P	S	0	0	0
			4157	2612	720	807	1	17			

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	VAL	deletion	UNP B0XPI4
A	?	-	SER	deletion	UNP B0XPI4
A	?	-	SER	deletion	UNP B0XPI4
A	?	-	TYR	deletion	UNP B0XPI4
A	?	-	GLY	deletion	UNP B0XPI4
A	?	-	THR	deletion	UNP B0XPI4
A	?	-	PHE	deletion	UNP B0XPI4
A	?	-	ASP	deletion	UNP B0XPI4
A	?	-	GLY	deletion	UNP B0XPI4
A	?	-	GLY	deletion	UNP B0XPI4
A	?	-	MET	deletion	UNP B0XPI4
A	?	-	LYS	deletion	UNP B0XPI4
A	?	-	GLY	deletion	UNP B0XPI4
A	?	-	GLU	deletion	UNP B0XPI4
A	?	-	PHE	deletion	UNP B0XPI4
A	?	-	ALA	deletion	UNP B0XPI4
A	?	-	ASP	deletion	UNP B0XPI4
A	291	LEU	VAL	conflict	UNP B0XPI4
A	467	GLU	ASP	conflict	UNP B0XPI4
B	?	-	VAL	deletion	UNP B0XPI4
B	?	-	SER	deletion	UNP B0XPI4
B	?	-	SER	deletion	UNP B0XPI4
B	?	-	TYR	deletion	UNP B0XPI4
B	?	-	GLY	deletion	UNP B0XPI4
B	?	-	THR	deletion	UNP B0XPI4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	PHE	deletion	UNP B0XPI4
B	?	-	ASP	deletion	UNP B0XPI4
B	?	-	GLY	deletion	UNP B0XPI4
B	?	-	GLY	deletion	UNP B0XPI4
B	?	-	MET	deletion	UNP B0XPI4
B	?	-	LYS	deletion	UNP B0XPI4
B	?	-	GLY	deletion	UNP B0XPI4
B	?	-	GLU	deletion	UNP B0XPI4
B	?	-	PHE	deletion	UNP B0XPI4
B	?	-	ALA	deletion	UNP B0XPI4
B	?	-	ASP	deletion	UNP B0XPI4
B	291	LEU	VAL	conflict	UNP B0XPI4
B	467	GLU	ASP	conflict	UNP B0XPI4

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

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

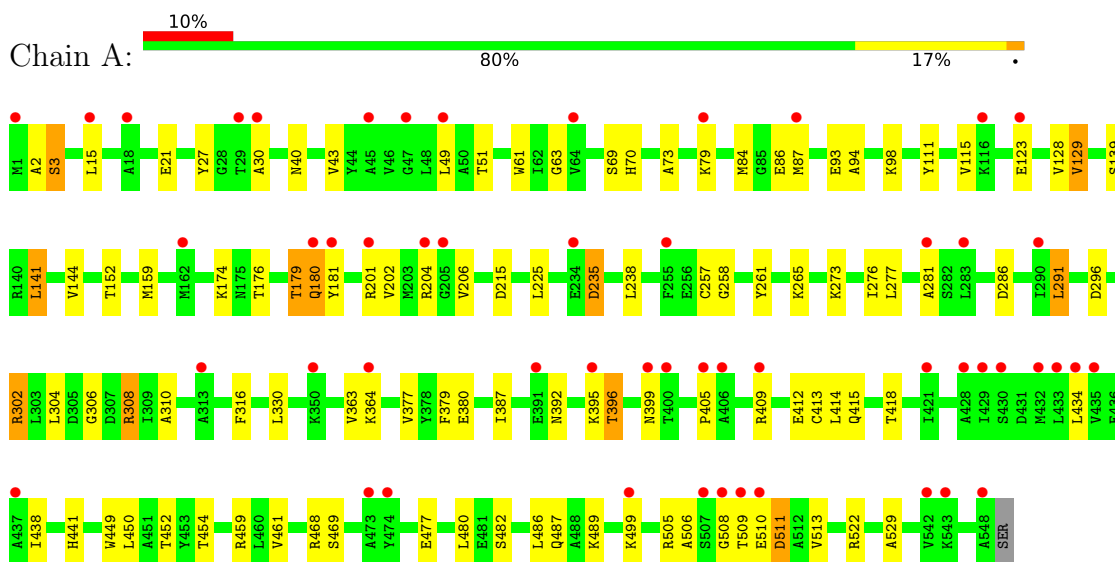
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	16	Total O 16 16	0	0
3	B	19	Total O 19 19	0	0

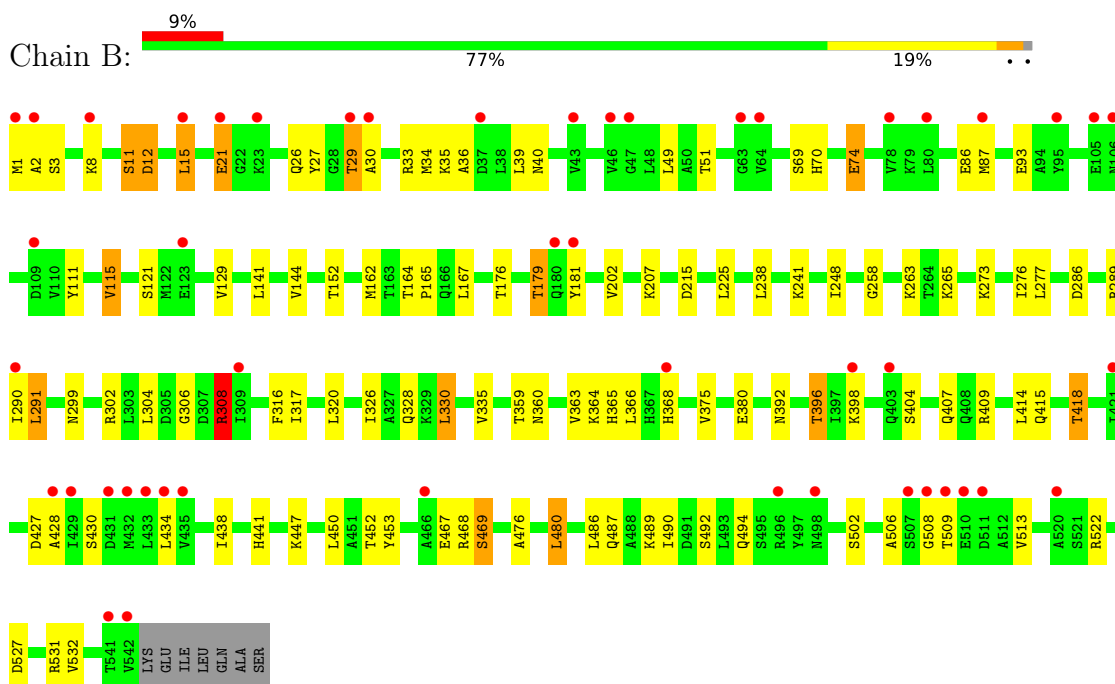
3 Residue-property plots [i](#)

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: N-ACETYLGLUCOSAMINE-PHOSPHATE MUTASE



• Molecule 1: N-ACETYLGLUCOSAMINE-PHOSPHATE MUTASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.70Å 86.57Å 185.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.69 – 2.35 24.68 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.9 (24.69-2.35) 100.0 (24.68-2.35)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 2.36Å)	Xtrriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.218 , 0.277 0.245 , 0.300	Depositor DCC
R_{free} test set	1048 reflections (2.06%)	wwPDB-VP
Wilson B-factor (Å ²)	38.7	Xtrriage
Anisotropy	0.263	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 21.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8388	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SEP, MG

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	0.47	0/4253	0.66	1/5760 (0.0%)
1	B	0.48	0/4216	0.71	5/5709 (0.1%)
All	All	0.47	0/8469	0.69	6/11469 (0.1%)

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	1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	286	ASP	CB-CG-OD1	6.18	123.86	118.30
1	B	308	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	B	289	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	A	286	ASP	CB-CG-OD1	5.46	123.22	118.30
1	B	308	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	B	414	LEU	CA-CB-CG	5.07	126.95	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	257	CYS	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	A	4194	0	4192	86	0
1	B	4157	0	4164	73	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	16	0	0	0	0
3	B	19	0	0	1	0
All	All	8388	0	8356	159	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 (159) 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:201:ARG:HE	1:A:204:ARG:NH1	1.07	1.52
1:A:201:ARG:NE	1:A:204:ARG:NH1	1.80	1.26
1:A:415:GLN:O	1:A:418:THR:HG22	1.41	1.19
1:B:87:MET:CE	1:B:363:VAL:HG23	1.71	1.18
1:A:93:GLU:OE2	1:A:364:LYS:NZ	1.79	1.15
1:A:395:LYS:NZ	1:A:399:ASN:HD21	1.45	1.13
1:A:395:LYS:CE	1:A:399:ASN:HD21	1.61	1.13
1:A:395:LYS:CE	1:A:399:ASN:ND2	2.16	1.07
1:A:395:LYS:HE3	1:A:399:ASN:ND2	1.70	1.05
1:A:87:MET:CE	1:A:363:VAL:HG23	1.91	1.00
1:B:87:MET:HE2	1:B:363:VAL:HG23	1.44	0.99
1:B:364:LYS:O	1:B:368:HIS:CD2	2.16	0.98
1:A:201:ARG:HE	1:A:204:ARG:HH11	1.09	0.96
1:B:93:GLU:OE2	1:B:364:LYS:NZ	1.98	0.96
1:B:364:LYS:O	1:B:368:HIS:HD2	1.46	0.96
1:A:176:THR:O	1:A:179:THR:HB	1.67	0.94
1:B:29:THR:HG23	1:B:364:LYS:HE3	1.48	0.93
1:B:87:MET:HE1	1:B:363:VAL:HG23	1.55	0.89
1:A:87:MET:HE1	1:A:363:VAL:HG23	1.52	0.88
1:A:449:TRP:O	1:A:452:THR:HG22	1.73	0.87
1:A:201:ARG:NE	1:A:204:ARG:HH12	1.72	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:THR:CG2	1:B:364:LYS:HE3	2.07	0.84
1:B:398:LYS:HG2	1:B:415:GLN:OE1	1.80	0.82
1:A:405:PRO:O	1:A:409:ARG:HG3	1.79	0.81
1:A:201:ARG:NE	1:A:204:ARG:HH11	1.70	0.79
1:B:468:ARG:HG3	1:B:506:ALA:HB1	1.63	0.79
1:A:392:ASN:O	1:A:396:THR:HG23	1.83	0.79
1:B:392:ASN:O	1:B:396:THR:HG23	1.83	0.78
1:A:30:ALA:HA	1:A:79:LYS:HD2	1.64	0.78
1:A:395:LYS:HE3	1:A:399:ASN:HD22	1.44	0.78
1:A:84:MET:HE1	1:A:181:TYR:HE1	1.49	0.77
1:A:176:THR:HG22	1:A:181:TYR:CE1	2.21	0.75
1:B:480:LEU:H	1:B:487:GLN:NE2	1.84	0.75
1:A:181:TYR:CD1	1:A:181:TYR:O	2.41	0.74
1:A:87:MET:CE	1:A:363:VAL:CG2	2.65	0.74
1:B:87:MET:CE	1:B:363:VAL:CG2	2.61	0.73
1:A:87:MET:HE2	1:A:363:VAL:HG23	1.69	0.73
1:A:201:ARG:HB3	1:A:204:ARG:HH12	1.55	0.71
1:B:415:GLN:O	1:B:418:THR:HB	1.90	0.71
1:A:395:LYS:NZ	1:A:399:ASN:ND2	2.30	0.70
1:A:84:MET:HE1	1:A:181:TYR:CE1	2.27	0.70
1:A:468:ARG:HD2	1:A:508:GLY:H	1.57	0.69
1:B:480:LEU:H	1:B:487:GLN:HE21	1.41	0.68
1:A:179:THR:HG22	1:A:181:TYR:H	1.56	0.68
1:B:304:LEU:HD23	1:B:308:ARG:HG2	1.77	0.66
1:A:176:THR:CG2	1:A:181:TYR:CE1	2.79	0.66
1:A:201:ARG:HB3	1:A:204:ARG:NH1	2.10	0.66
1:A:27:TYR:OH	1:A:79:LYS:HG3	1.95	0.65
1:A:87:MET:HE2	1:A:363:VAL:CG2	2.26	0.65
1:A:215:ASP:OD2	1:A:258:GLY:HA2	1.97	0.63
1:B:359:THR:OG1	1:B:366:LEU:HD23	1.98	0.63
1:A:510:GLU:O	1:A:511:ASP:HB2	1.97	0.63
1:A:201:ARG:HE	1:A:204:ARG:CZ	2.04	0.62
1:B:179:THR:CG2	1:B:181:TYR:H	2.13	0.61
1:B:468:ARG:HD2	1:B:508:GLY:CA	2.30	0.61
1:A:202:VAL:O	1:A:441:HIS:HE1	1.84	0.61
1:A:201:ARG:CD	1:A:204:ARG:HH11	2.14	0.60
1:A:201:ARG:CD	1:A:204:ARG:NH1	2.64	0.60
1:B:179:THR:HG23	1:B:181:TYR:H	1.66	0.59
1:A:179:THR:CG2	1:A:181:TYR:H	2.15	0.59
1:B:360:ASN:OD1	1:B:476:ALA:HA	2.01	0.59
1:B:202:VAL:O	1:B:441:HIS:HE1	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:365:HIS:NE2	3:B:2016:HOH:O	2.32	0.59
1:B:34:MET:HG2	1:B:39:LEU:HD13	1.85	0.58
1:B:215:ASP:OD2	1:B:258:GLY:CA	2.51	0.58
1:B:215:ASP:OD2	1:B:258:GLY:HA2	2.03	0.58
1:B:468:ARG:HD2	1:B:508:GLY:HA2	1.86	0.58
1:B:276:ILE:HG22	1:B:277:LEU:HG	1.86	0.57
1:A:395:LYS:HZ1	1:A:399:ASN:HD21	1.46	0.56
1:A:395:LYS:CD	1:A:399:ASN:ND2	2.68	0.56
1:A:395:LYS:HZ2	1:A:399:ASN:HD21	1.47	0.55
1:A:468:ARG:HB2	1:A:511:ASP:HA	1.89	0.55
1:B:2:ALA:HB1	1:B:3:SER:HB2	1.88	0.55
1:A:477:GLU:HB3	1:A:505:ARG:HD2	1.90	0.54
1:B:326:ILE:HD12	1:B:330:LEU:HD22	1.90	0.54
1:A:111:TYR:O	1:A:115:VAL:HG13	2.06	0.54
1:A:84:MET:CE	1:A:181:TYR:CE1	2.91	0.54
1:A:204:ARG:HH22	1:A:412:GLU:HB3	1.73	0.54
1:B:35:LYS:HE3	1:B:74:GLU:HG3	1.89	0.53
1:A:276:ILE:HG22	1:A:277:LEU:HG	1.90	0.53
1:B:494:GLN:NE2	1:B:502:SER:H	2.06	0.53
1:B:27:TYR:HD1	1:B:93:GLU:HG2	1.74	0.52
1:A:480:LEU:H	1:A:487:GLN:HE21	1.57	0.52
1:A:235:ASP:OD1	1:A:235:ASP:N	2.42	0.52
1:B:87:MET:HE2	1:B:363:VAL:CG2	2.29	0.52
1:A:449:TRP:O	1:A:452:THR:CG2	2.53	0.51
1:B:306:GLY:HA3	1:B:380:GLU:O	2.11	0.51
1:B:263:LYS:HB2	1:B:291:LEU:HD21	1.93	0.50
1:A:310:ALA:HB2	1:A:379:PHE:HB2	1.94	0.50
1:B:51:THR:HG21	1:B:152:THR:HB	1.93	0.50
1:A:480:LEU:H	1:A:487:GLN:NE2	2.10	0.50
1:A:180:GLN:HE21	1:A:180:GLN:HA	1.76	0.49
1:A:468:ARG:HG2	1:A:506:ALA:HB1	1.95	0.49
1:A:94:ALA:O	1:A:98:LYS:HG3	2.13	0.49
1:B:176:THR:O	1:B:179:THR:HB	2.13	0.49
1:B:162:MET:CE	1:B:167:LEU:HA	2.43	0.49
1:A:201:ARG:CB	1:A:204:ARG:NH1	2.76	0.48
1:B:290:ILE:HB	1:B:428:ALA:HB1	1.95	0.48
1:B:276:ILE:HD11	1:B:299:ASN:OD1	2.13	0.48
1:A:176:THR:CG2	1:A:181:TYR:HE1	2.26	0.48
1:A:202:VAL:O	1:A:441:HIS:CE1	2.66	0.48
1:A:204:ARG:NH2	1:A:412:GLU:HB3	2.28	0.48
1:B:30:ALA:HB1	1:B:33:ARG:NH2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:427:ASP:HB3	1:B:430:SER:HB3	1.96	0.47
1:B:468:ARG:HH11	1:B:508:GLY:HA2	1.79	0.47
1:A:215:ASP:OD2	1:A:258:GLY:CA	2.63	0.47
1:B:215:ASP:OD2	1:B:258:GLY:HA3	2.14	0.47
1:B:494:GLN:HE21	1:B:502:SER:H	1.63	0.47
1:B:164:THR:HB	1:B:165:PRO:HD3	1.95	0.47
1:B:87:MET:SD	1:B:363:VAL:CG2	3.03	0.46
1:B:308:ARG:NH2	1:B:453:TYR:O	2.43	0.46
1:B:404:SER:OG	1:B:407:GLN:HB2	2.14	0.46
1:A:40:ASN:O	1:A:144:VAL:HG11	2.16	0.46
1:B:468:ARG:HD2	1:B:508:GLY:N	2.31	0.46
1:A:51:THR:HG21	1:A:152:THR:HB	1.97	0.45
1:A:306:GLY:HA3	1:A:380:GLU:O	2.16	0.45
1:A:2:ALA:HB1	1:A:3:SER:HB2	1.99	0.45
1:B:29:THR:HG23	1:B:364:LYS:CE	2.32	0.45
1:B:8:LYS:O	1:B:12:ASP:HB2	2.16	0.45
1:A:261:TYR:CD1	1:A:261:TYR:C	2.90	0.44
1:B:27:TYR:CD1	1:B:93:GLU:HG2	2.53	0.44
1:A:459:ARG:HD3	1:A:529:ALA:HB3	2.00	0.44
1:B:111:TYR:O	1:B:115:VAL:HG13	2.18	0.44
1:A:179:THR:CG2	1:A:180:GLN:N	2.81	0.44
1:A:316:PHE:CD2	1:A:438:ILE:HG12	2.53	0.44
1:A:30:ALA:O	1:A:79:LYS:HB2	2.18	0.44
1:A:61:TRP:CE2	1:A:174:LYS:HE3	2.53	0.44
1:B:452:THR:HG23	1:B:453:TYR:CD2	2.53	0.44
1:A:510:GLU:O	1:A:511:ASP:CB	2.66	0.43
1:B:36:ALA:O	1:B:39:LEU:HB2	2.18	0.43
1:A:43:VAL:HG21	1:A:141:LEU:HG	2.00	0.43
1:A:176:THR:HG21	1:A:181:TYR:CE1	2.54	0.43
1:B:276:ILE:CD1	1:B:299:ASN:OD1	2.66	0.43
1:B:304:LEU:CD2	1:B:308:ARG:HG2	2.46	0.43
1:B:320:LEU:HD23	1:B:320:LEU:HA	1.92	0.43
1:B:527:ASP:O	1:B:531:ARG:HG3	2.18	0.43
1:B:162:MET:HE3	1:B:167:LEU:HA	2.01	0.43
1:B:468:ARG:NH1	1:B:508:GLY:HA2	2.33	0.43
1:A:129:VAL:HG12	1:A:159:MET:HG2	2.01	0.42
1:B:335:VAL:HG12	1:B:366:LEU:HD22	2.01	0.42
1:B:467:GLU:HG2	1:B:469:SER:HB3	2.01	0.42
1:B:316:PHE:CD2	1:B:438:ILE:HG12	2.54	0.42
1:A:179:THR:HG22	1:A:181:TYR:N	2.29	0.42
1:A:395:LYS:HD2	1:A:399:ASN:ND2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:317:ILE:HG21	1:B:375:VAL:HG11	2.02	0.41
1:B:490:ILE:HG12	1:B:532:VAL:HG13	2.01	0.41
1:A:181:TYR:O	1:A:181:TYR:CG	2.71	0.41
1:A:377:VAL:HG22	1:A:387:ILE:HG12	2.02	0.41
1:A:468:ARG:HD2	1:A:508:GLY:N	2.31	0.41
1:B:34:MET:CG	1:B:39:LEU:HD13	2.49	0.41
1:A:296:ASP:OD2	1:A:302:ARG:NH1	2.41	0.41
1:A:316:PHE:CG	1:A:438:ILE:HG12	2.56	0.41
1:B:40:ASN:O	1:B:144:VAL:HG11	2.21	0.41
1:A:63:GLY:HA2	1:A:129:VAL:O	2.21	0.41
1:B:1:MET:HG2	1:B:2:ALA:N	2.35	0.41
1:A:304:LEU:HA	1:A:308:ARG:HG2	2.04	0.40
1:B:11:SER:O	1:B:15:LEU:HD23	2.21	0.40
1:A:281:ALA:HA	1:A:291:LEU:O	2.21	0.40
1:B:87:MET:HE1	1:B:364:LYS:N	2.36	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	545/549 (99%)	521 (96%)	21 (4%)	3 (1%)	25 27
1	B	539/549 (98%)	518 (96%)	20 (4%)	1 (0%)	47 56
All	All	1084/1098 (99%)	1039 (96%)	41 (4%)	4 (0%)	34 38

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	511	ASP
1	A	21	GLU
1	A	73	ALA

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Mol	Chain	Res	Type
1	B	21	GLU

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	438/442 (99%)	401 (92%)	37 (8%)	11	10
1	B	436/442 (99%)	395 (91%)	41 (9%)	8	8
All	All	874/884 (99%)	796 (91%)	78 (9%)	9	8

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	15	LEU
1	A	49	LEU
1	A	70	HIS
1	A	86	GLU
1	A	123	GLU
1	A	128	VAL
1	A	129	VAL
1	A	139	SER
1	A	141	LEU
1	A	179	THR
1	A	180	GLN
1	A	206	VAL
1	A	225	LEU
1	A	235	ASP
1	A	238	LEU
1	A	265	LYS
1	A	273	LYS
1	A	291	LEU
1	A	302	ARG
1	A	308	ARG
1	A	330	LEU

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Mol	Chain	Res	Type
1	A	396	THR
1	A	413	CYS
1	A	414	LEU
1	A	434	LEU
1	A	450	LEU
1	A	454	THR
1	A	461	VAL
1	A	469	SER
1	A	482	SER
1	A	486	LEU
1	A	489	LYS
1	A	499	LYS
1	A	509	THR
1	A	513	VAL
1	A	522	ARG
1	B	11	SER
1	B	12	ASP
1	B	15	LEU
1	B	21	GLU
1	B	26	GLN
1	B	29	THR
1	B	49	LEU
1	B	70	HIS
1	B	74	GLU
1	B	86	GLU
1	B	115	VAL
1	B	121	SER
1	B	129	VAL
1	B	141	LEU
1	B	179	THR
1	B	207	LYS
1	B	225	LEU
1	B	238	LEU
1	B	241	LYS
1	B	248	ILE
1	B	265	LYS
1	B	273	LYS
1	B	291	LEU
1	B	302	ARG
1	B	308	ARG
1	B	328	GLN
1	B	330	LEU

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Mol	Chain	Res	Type
1	B	396	THR
1	B	409	ARG
1	B	418	THR
1	B	434	LEU
1	B	447	LYS
1	B	450	LEU
1	B	469	SER
1	B	480	LEU
1	B	486	LEU
1	B	489	LYS
1	B	492	SER
1	B	509	THR
1	B	513	VAL
1	B	522	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	180	GLN
1	A	266	GLN
1	A	336	GLN
1	A	399	ASN
1	A	408	GLN
1	A	441	HIS
1	A	487	GLN
1	A	494	GLN
1	B	16	GLN
1	B	70	HIS
1	B	124	ASN
1	B	249	ASN
1	B	328	GLN
1	B	368	HIS
1	B	407	GLN
1	B	441	HIS
1	B	487	GLN
1	B	494	GLN

5.3.3 RNA [i](#)

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	69	2,1	8,9,10	0.65	0	8,12,14	1.47	3 (37%)
1	SEP	B	69	2,1	8,9,10	0.66	0	8,12,14	1.47	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	69	2,1	-	4/5/8/10	-
1	SEP	B	69	2,1	-	4/5/8/10	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	69	SEP	O2P-P-OG	-2.40	100.34	106.73
1	A	69	SEP	O2P-P-OG	-2.39	100.36	106.73
1	B	69	SEP	O3P-P-O2P	2.19	116.00	107.64
1	A	69	SEP	O3P-P-O2P	2.16	115.88	107.64
1	A	69	SEP	O2P-P-O1P	2.03	118.63	110.68

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	69	SEP	CB-OG-P-O2P
1	A	69	SEP	CB-OG-P-O3P
1	B	69	SEP	CB-OG-P-O2P

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Mol	Chain	Res	Type	Atoms
1	B	69	SEP	CB-OG-P-O3P
1	A	69	SEP	CB-OG-P-O1P
1	B	69	SEP	CB-OG-P-O1P
1	A	69	SEP	N-CA-CB-OG
1	B	69	SEP	N-CA-CB-OG

There are no ring outliers.

No monomer is involved in short contacts.

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

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, 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	547/549 (99%)	0.57	53 (9%) 7 12	14, 25, 42, 83	0
1	B	541/549 (98%)	0.50	48 (8%) 9 14	7, 20, 36, 50	0
All	All	1088/1098 (99%)	0.54	101 (9%) 8 14	7, 22, 39, 83	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	542	VAL	6.5
1	B	509	THR	5.6
1	A	181	TYR	4.8
1	B	508	GLY	4.7
1	B	123	GLU	4.7
1	A	509	THR	4.5
1	B	1	MET	4.5
1	B	510	GLU	4.5
1	A	1	MET	4.4
1	A	434	LEU	4.0
1	B	398	LYS	3.9
1	A	430	SER	3.8
1	A	234	GLU	3.8
1	A	433	LEU	3.7
1	B	466	ALA	3.6
1	B	434	LEU	3.6
1	B	46	VAL	3.6
1	A	116	LYS	3.5
1	A	123	GLU	3.5
1	B	109	ASP	3.4
1	B	87	MET	3.4
1	A	409	ARG	3.4
1	A	79	LYS	3.3
1	A	364	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	368	HIS	3.2
1	A	29	THR	3.2
1	B	29	THR	3.1
1	A	508	GLY	3.1
1	B	435	VAL	3.0
1	B	507	SER	3.0
1	B	181	TYR	3.0
1	B	105	GLU	2.9
1	B	541	THR	2.9
1	A	428	ALA	2.9
1	A	255	PHE	2.9
1	B	64	VAL	2.9
1	B	290	ILE	2.8
1	A	313	ALA	2.8
1	A	548	ALA	2.7
1	B	106	ASN	2.7
1	A	542	VAL	2.7
1	B	15	LEU	2.7
1	A	15	LEU	2.7
1	A	64	VAL	2.7
1	B	30	ALA	2.6
1	B	80	LEU	2.6
1	A	395	LYS	2.6
1	A	405	PRO	2.6
1	A	406	ALA	2.6
1	A	399	ASN	2.6
1	A	391	GLU	2.6
1	A	87	MET	2.6
1	B	432	MET	2.6
1	B	433	LEU	2.5
1	A	499	LYS	2.5
1	A	162	MET	2.5
1	A	429	ILE	2.5
1	B	37	ASP	2.5
1	A	205	GLY	2.4
1	A	432	MET	2.4
1	A	45	ALA	2.4
1	A	180	GLN	2.4
1	A	290	ILE	2.4
1	B	431	ASP	2.3
1	A	47	GLY	2.3
1	A	510	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	63	GLY	2.3
1	B	429	ILE	2.3
1	B	95	TYR	2.3
1	B	8	LYS	2.3
1	B	511	ASP	2.2
1	B	2	ALA	2.2
1	A	49	LEU	2.2
1	A	350	LYS	2.2
1	A	543	LYS	2.2
1	A	435	VAL	2.2
1	A	204	ARG	2.2
1	B	421	ILE	2.2
1	B	498	ASN	2.2
1	A	473	ALA	2.2
1	B	180	GLN	2.2
1	A	474	TYR	2.2
1	B	21	GLU	2.2
1	B	78	VAL	2.2
1	A	437	ALA	2.2
1	B	428	ALA	2.2
1	A	507	SER	2.2
1	B	403	GLN	2.2
1	B	43	VAL	2.1
1	A	281	ALA	2.1
1	A	18	ALA	2.1
1	A	400	THR	2.1
1	A	421	ILE	2.1
1	A	283	LEU	2.1
1	A	30	ALA	2.1
1	B	520	ALA	2.1
1	B	496	ARG	2.1
1	B	309	ILE	2.0
1	B	23	LYS	2.0
1	B	47	GLY	2.0
1	A	201	ARG	2.0

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

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(\AA^2)	Q<0.9
1	SEP	A	69	10/11	0.91	0.14	23,25,28,29	0
1	SEP	B	69	10/11	0.91	0.13	22,24,25,26	0

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, 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(\AA^2)	Q<0.9
2	MG	A	998	1/1	0.95	0.34	5,5,5,5	0
2	MG	B	998	1/1	0.96	0.28	5,5,5,5	0

6.5 Other polymers [i](#)

There are no such residues in this entry.