



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2021 – 03:20 PM EDT

PDB ID : 7JZ4
Title : Crystal structure of broadly Plasmodium RIFIN reactive LAIR1-inserted antibody MGD21
Authors : Xu, K.; Kwong, P.D.
Deposited on : 2020-09-01
Resolution : 2.75 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 following versions of software and data (see [references ⓘ](#)) 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 : 2.23.1
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) : 2.23.1

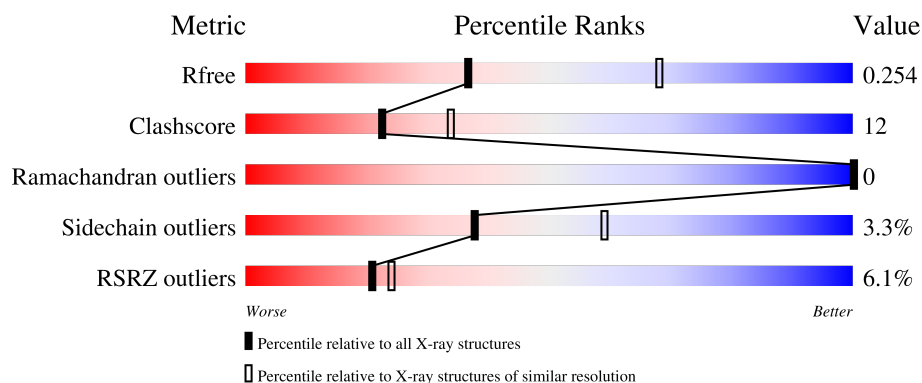
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1271 (2.76-2.72)
Clashscore	141614	1322 (2.76-2.72)
Ramachandran outliers	138981	1297 (2.76-2.72)
Sidechain outliers	138945	1298 (2.76-2.72)
RSRZ outliers	127900	1243 (2.76-2.72)

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	364	<div> <div>12%</div> <div> <div></div> <div>71%</div> <div>26%</div> <div>..</div> </div> </div>
1	C	364	<div> <div>3%</div> <div> <div></div> <div>67%</div> <div>22%</div> <div>• 10%</div> </div> </div>
2	B	213	<div> <div>3%</div> <div> <div></div> <div>80%</div> <div>18%</div> <div>•</div> </div> </div>
2	D	213	<div> <div>4%</div> <div> <div></div> <div>76%</div> <div>24%</div> </div> </div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8516 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.

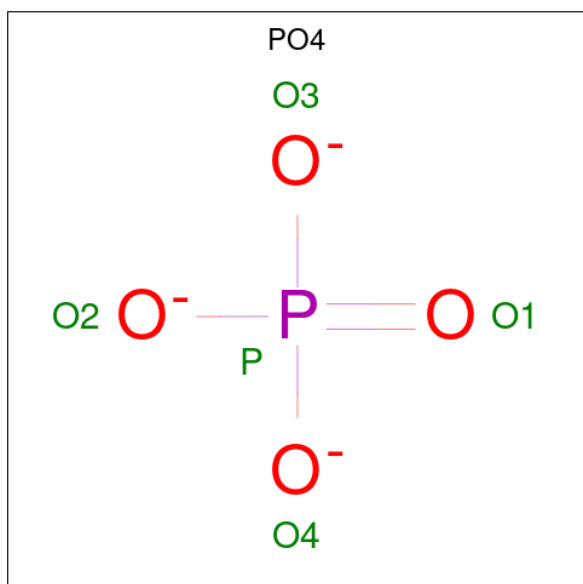
- Molecule 1 is a protein called MGD21 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	355	Total	C	N	O	S	0	0	0
			2701	1692	462	538	9			
1	C	328	Total	C	N	O	S	0	0	0
			2494	1566	428	492	8			

- Molecule 2 is a protein called MGD21 light chain.

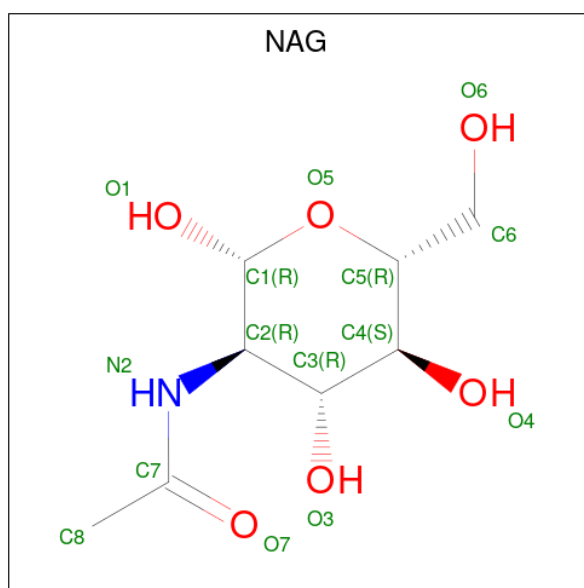
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	213	Total	C	N	O	S	0	0	0
			1629	1015	281	326	7			
2	D	213	Total	C	N	O	S	0	0	0
			1629	1015	281	326	7			

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 5 4 1	0	0
3	A	1	Total O P 5 4 1	0	0
3	A	1	Total O P 5 4 1	0	0
3	B	1	Total O P 5 4 1	0	0
3	C	1	Total O P 5 4 1	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C N O 14 8 1 5	0	0
4	D	1	Total C N O 14 8 1 5	0	0

- Molecule 5 is water.

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

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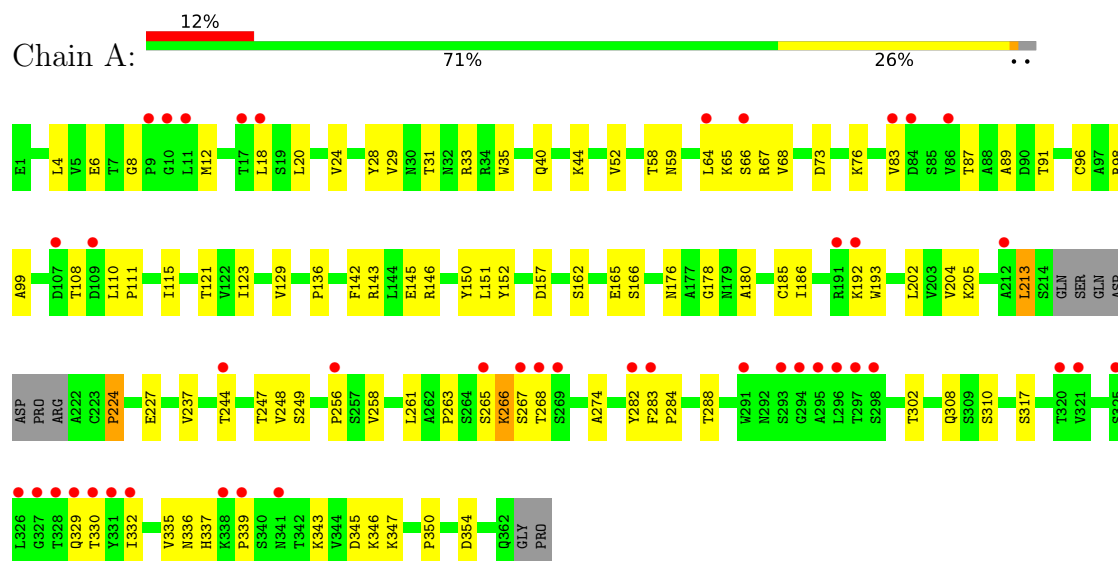
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	5	Total	O	0	0
			5	5		

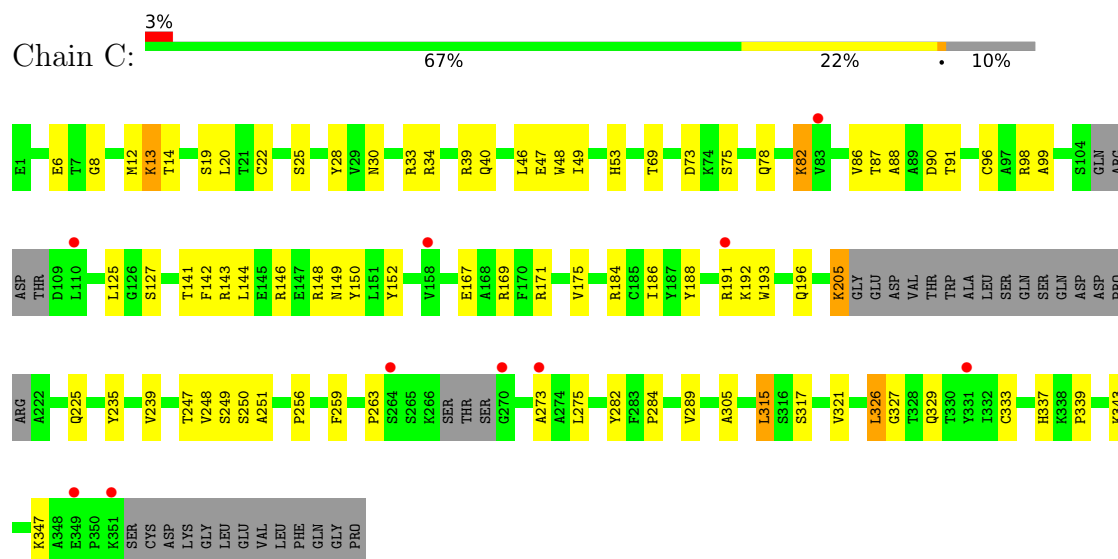
3 Residue-property plots [i](#)

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.

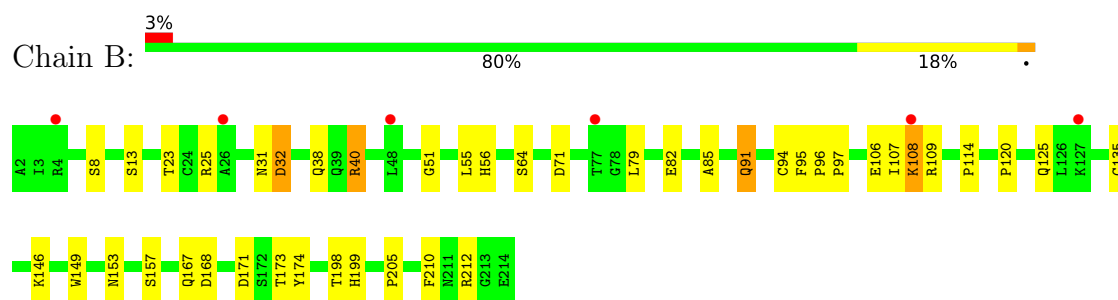
• Molecule 1: MGD21 heavy chain



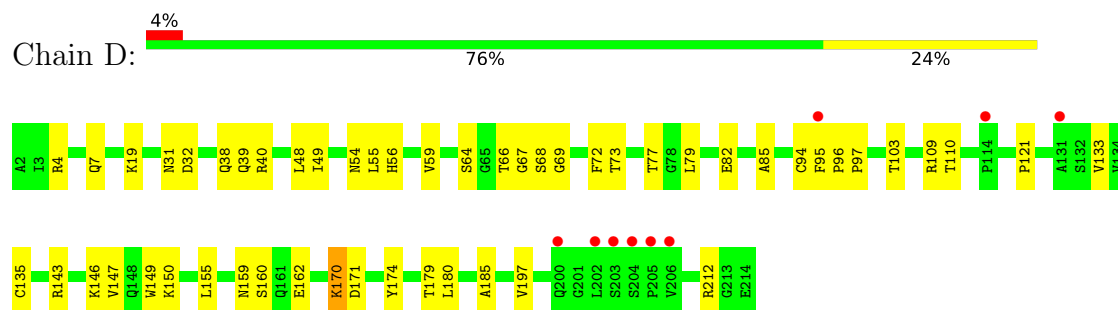
• Molecule 1: MGD21 heavy chain



• Molecule 2: MGD21 light chain



• Molecule 2: MGD21 light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.93Å 81.10Å 111.56Å 90.00° 94.03° 90.00°	Depositor
Resolution (Å)	38.93 – 2.75 38.93 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.2 (38.93-2.75) 99.2 (38.93-2.75)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.11.1 _2575	Depositor
R, R_{free}	0.194 , 0.249 0.200 , 0.254	Depositor DCC
R_{free} test set	1844 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	67.9	Xtriage
Anisotropy	0.312	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 54.9	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	8516	wwPDB-VP
Average B, all atoms (Å ²)	82.0	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.*

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: NAG, PO4

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	0.32	0/2761	0.58	2/3762 (0.1%)
1	C	0.30	0/2549	0.52	0/3471
2	B	0.34	0/1665	0.60	2/2258 (0.1%)
2	D	0.34	0/1665	0.61	0/2258
All	All	0.32	0/8640	0.57	4/11749 (0.0%)

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 (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	213	LEU	CA-CB-CG	6.43	130.08	115.30
2	B	32	ASP	CB-CG-OD1	5.58	123.32	118.30
2	B	108	LYS	CA-CB-CG	5.24	124.93	113.40
1	A	261	LEU	C-N-CA	5.21	134.73	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	224	PRO	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	2701	0	2650	68	0
1	C	2494	0	2455	59	0
2	B	1629	0	1573	30	0
2	D	1629	0	1574	46	0
3	A	15	0	0	0	0
3	B	5	0	0	1	0
3	C	5	0	0	0	0
4	B	14	0	13	0	0
4	D	14	0	13	5	0
5	A	4	0	0	0	0
5	B	1	0	0	0	0
5	C	5	0	0	0	0
All	All	8516	0	8278	194	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 12.

All (194) 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)
2:D:31:ASN:HD21	4:D:301:NAG:C1	1.15	1.58
2:D:31:ASN:ND2	4:D:301:NAG:C1	1.79	1.44
1:A:146:ARG:HG3	1:A:146:ARG:HH11	1.24	0.97
2:B:106:GLU:HB2	2:B:167:GLN:HE22	1.29	0.93
2:D:31:ASN:CG	4:D:301:NAG:C1	2.35	0.93
1:C:13:LYS:HZ1	1:C:250:SER:C	1.77	0.88
2:D:121:PRO:HD3	2:D:133:VAL:HG12	1.58	0.85
1:A:40:GLN:HE22	2:D:39:GLN:HE22	1.23	0.84
1:A:146:ARG:NH2	1:A:180:ALA:O	2.10	0.83
1:A:87:THR:HG22	1:A:89:ALA:H	1.43	0.83
1:A:332:ILE:HG13	1:A:347:LYS:HB2	1.65	0.78
1:C:91:THR:HG23	1:C:247:THR:HA	1.67	0.76
2:D:212:ARG:HG2	2:D:212:ARG:HH11	1.51	0.76
1:A:150:TYR:O	1:A:151:LEU:HD22	1.88	0.74
2:B:212:ARG:HH11	2:B:212:ARG:HG2	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:13:LYS:NZ	1:C:250:SER:C	2.41	0.72
1:A:146:ARG:HG3	1:A:146:ARG:NH1	1.98	0.71
1:C:39:ARG:HB3	1:C:49:ILE:HD11	1.70	0.71
2:D:31:ASN:OD1	4:D:301:NAG:C1	2.38	0.71
2:D:109:ARG:NH1	2:D:110:THR:O	2.25	0.69
1:A:258:VAL:HG21	1:A:335:VAL:HG11	1.75	0.68
1:A:266:LYS:O	1:A:266:LYS:HD2	1.93	0.68
1:C:13:LYS:HZ1	1:C:251:ALA:N	1.92	0.67
1:C:39:ARG:NH2	1:C:90:ASP:HA	2.11	0.66
1:A:284:PRO:HD2	1:A:337:HIS:CE1	2.31	0.66
1:A:336:ASN:HB2	1:A:343:LYS:HZ2	1.61	0.64
1:C:186:ILE:HD13	1:C:193:TRP:CZ3	2.33	0.64
2:B:167:GLN:NE2	2:B:174:TYR:OH	2.31	0.63
2:D:212:ARG:HG2	2:D:212:ARG:NH1	2.13	0.62
1:A:91:THR:HG23	1:A:247:THR:HA	1.80	0.62
1:A:176:ASN:OD1	1:A:178:GLY:N	2.33	0.62
2:D:170:LYS:HG3	2:D:171:ASP:N	2.15	0.62
1:A:31:THR:HG23	1:A:33:ARG:HG2	1.81	0.62
1:A:162:SER:OG	1:A:165:GLU:HG2	2.00	0.61
1:A:180:ALA:HB2	1:A:204:VAL:HG23	1.82	0.61
1:C:40:GLN:HB2	1:C:46:LEU:HD23	1.83	0.61
1:C:305:ALA:HA	1:C:315:LEU:HB3	1.83	0.61
1:C:13:LYS:HZ1	1:C:250:SER:CA	2.14	0.60
1:A:146:ARG:HH11	1:A:146:ARG:CG	2.05	0.60
1:A:157:ASP:OD2	1:A:157:ASP:O	2.19	0.60
2:B:171:ASP:N	2:B:171:ASP:OD1	2.33	0.60
2:D:68:SER:OG	2:D:69:GLY:N	2.34	0.60
1:A:283:PHE:HB3	1:A:284:PRO:HD3	1.85	0.58
1:C:326:LEU:HG	1:C:327:GLY:H	1.67	0.58
1:C:14:THR:OG1	1:C:249:SER:O	2.17	0.58
2:B:40:ARG:HG3	2:B:85:ALA:HB2	1.86	0.58
1:C:12:MET:O	1:C:248:VAL:HA	2.04	0.58
1:C:39:ARG:HH22	1:C:90:ASP:HA	1.67	0.57
1:C:143:ARG:HD2	1:C:186:ILE:HD11	1.86	0.57
2:B:25:ARG:NE	2:B:71:ASP:OD1	2.38	0.57
2:B:212:ARG:HG2	2:B:212:ARG:NH1	2.18	0.57
1:A:4:LEU:HD22	1:A:24:VAL:HG22	1.87	0.56
1:A:44:LYS:O	1:A:44:LYS:HG3	2.05	0.56
2:B:38:GLN:NE2	3:B:302:PO4:O1	2.29	0.56
2:B:146:LYS:HB3	2:B:198:THR:HB	1.86	0.56
1:C:34:ARG:HD3	1:C:53:HIS:CD2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:ARG:NH1	1:A:146:ARG:CG	2.66	0.56
1:A:123:ILE:HG13	1:A:129:VAL:HB	1.87	0.56
1:A:227:GLU:HB3	2:D:95:PHE:HB2	1.86	0.56
1:C:186:ILE:CG2	1:C:196:GLN:HA	2.35	0.56
2:D:160:SER:HA	2:D:179:THR:O	2.07	0.55
1:A:99:ALA:HA	1:A:237:VAL:HA	1.88	0.55
2:D:19:LYS:HB2	2:D:77:THR:HA	1.88	0.55
2:B:171:ASP:OD2	2:B:173:THR:OG1	2.21	0.55
2:B:95:PHE:O	2:B:97:PRO:HD3	2.07	0.55
2:D:143:ARG:HG2	2:D:174:TYR:CD2	2.42	0.55
2:D:133:VAL:HG22	2:D:180:LEU:HB3	1.89	0.54
1:A:308:GLN:HG3	1:A:310:SER:HB3	1.90	0.54
1:A:59:ASN:HB3	2:D:95:PHE:HE2	1.72	0.54
1:A:8:GLY:HA3	1:A:20:LEU:HD23	1.89	0.53
1:C:273:ALA:HB3	1:C:321:VAL:HG23	1.91	0.53
2:D:82:GLU:OE2	2:D:82:GLU:N	2.36	0.53
2:B:95:PHE:HB3	2:B:96:PRO:HD3	1.90	0.53
1:A:73:ASP:OD1	1:A:76:LYS:HG3	2.08	0.53
2:B:40:ARG:HH12	2:B:82:GLU:HB2	1.73	0.53
1:C:34:ARG:HB2	1:C:99:ALA:HB3	1.90	0.53
2:B:13:SER:HB2	2:B:108:LYS:HD2	1.90	0.53
2:B:205:PRO:HG2	2:D:185:ALA:HB1	1.91	0.52
1:A:345:ASP:N	1:A:345:ASP:OD1	2.42	0.52
1:C:263:PRO:HG3	1:C:275:LEU:HB3	1.91	0.52
1:C:256:PRO:HB3	1:C:282:TYR:HB3	1.91	0.52
2:D:31:ASN:HD21	4:D:301:NAG:C2	2.11	0.51
2:B:31:ASN:O	2:B:32:ASP:HB3	2.10	0.51
1:A:18:LEU:HB3	1:A:83:VAL:HG13	1.93	0.51
1:A:336:ASN:CB	1:A:343:LYS:HZ2	2.22	0.50
2:D:171:ASP:N	2:D:171:ASP:OD1	2.38	0.50
1:C:143:ARG:HB3	1:C:186:ILE:CD1	2.42	0.50
1:C:13:LYS:NZ	1:C:250:SER:CA	2.74	0.50
1:C:73:ASP:OD1	1:C:75:SER:N	2.44	0.50
2:D:49:ILE:HG23	2:D:54:ASN:O	2.12	0.49
1:C:284:PRO:O	1:C:337:HIS:NE2	2.39	0.49
1:C:144:LEU:O	1:C:152:TYR:HA	2.13	0.48
1:C:186:ILE:HG23	1:C:196:GLN:HA	1.94	0.48
1:A:28:TYR:O	1:A:31:THR:HG22	2.14	0.48
1:C:186:ILE:HD12	1:C:186:ILE:O	2.13	0.48
1:A:256:PRO:HB3	1:A:282:TYR:HB3	1.96	0.48
1:C:167:GLU:OE1	1:C:169:ARG:NH1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:GLU:HB2	1:A:244:THR:OG1	2.13	0.48
1:C:87:THR:OG1	1:C:88:ALA:N	2.46	0.48
2:B:135:CYS:HB2	2:B:149:TRP:CH2	2.49	0.47
2:D:147:VAL:HG22	2:D:162:GLU:OE2	2.14	0.47
2:D:170:LYS:HG3	2:D:171:ASP:H	1.77	0.47
2:D:38:GLN:HB2	2:D:48:LEU:HD11	1.96	0.47
1:C:13:LYS:HA	1:C:13:LYS:CE	2.43	0.47
2:D:66:THR:HG22	2:D:73:THR:HB	1.97	0.47
1:C:34:ARG:HG3	1:C:235:TYR:CD2	2.49	0.47
1:C:326:LEU:HG	1:C:327:GLY:N	2.28	0.47
1:C:337:HIS:CE1	1:C:339:PRO:HB2	2.49	0.47
1:A:64:LEU:O	1:A:68:VAL:HG22	2.14	0.47
1:A:224:PRO:HD2	2:D:94:CYS:SG	2.55	0.47
1:C:28:TYR:CE1	1:C:30:ASN:HB3	2.50	0.47
1:A:111:PRO:HD2	1:A:136:PRO:HG3	1.97	0.46
1:C:39:ARG:HG2	1:C:47:GLU:HB3	1.98	0.46
1:C:171:ARG:HH11	1:C:171:ARG:HG3	1.81	0.46
1:C:205:LYS:HD2	1:C:205:LYS:HA	1.72	0.46
1:A:267:SER:O	1:A:268:THR:OG1	2.29	0.46
1:A:288:THR:HB	1:A:336:ASN:OD1	2.16	0.46
2:B:32:ASP:OD1	2:B:32:ASP:O	2.34	0.46
1:C:146:ARG:O	1:C:150:TYR:HA	2.15	0.46
1:A:66:SER:OG	1:A:67:ARG:HG2	2.16	0.46
1:A:150:TYR:C	1:A:151:LEU:HD22	2.35	0.46
1:C:86:VAL:HA	1:C:90:ASP:OD2	2.15	0.46
2:D:143:ARG:HD3	2:D:174:TYR:CE1	2.51	0.46
1:C:289:VAL:HG21	1:C:317:SER:CB	2.46	0.46
2:D:95:PHE:O	2:D:97:PRO:HD3	2.16	0.45
1:C:13:LYS:NZ	1:C:250:SER:HA	2.31	0.45
1:A:145:GLU:OE1	1:A:150:TYR:OH	2.27	0.45
2:D:56:HIS:O	2:D:59:VAL:HG22	2.16	0.45
1:C:148:ARG:HG3	1:C:149:ASN:N	2.32	0.45
1:C:69:THR:OG1	1:C:82:LYS:HG2	2.16	0.45
1:A:186:ILE:HG12	1:A:193:TRP:CE3	2.51	0.45
2:B:32:ASP:OD1	2:B:51:GLY:O	2.34	0.45
1:C:98:ARG:HB3	1:C:239:VAL:HG13	1.98	0.45
1:A:336:ASN:HB2	1:A:343:LYS:NZ	2.31	0.44
1:C:8:GLY:HA3	1:C:20:LEU:HD23	1.99	0.44
2:B:120:PRO:HB3	2:B:210:PHE:CE1	2.52	0.44
2:D:7:GLN:NE2	2:D:103:THR:HG23	2.31	0.44
2:D:68:SER:HA	2:D:72:PHE:CE1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:GLU:HG3	1:A:96:CYS:SG	2.58	0.44
2:B:107:ILE:HG13	2:B:167:GLN:OE1	2.17	0.44
1:A:186:ILE:HG12	1:A:193:TRP:HE3	1.83	0.44
1:A:136:PRO:O	1:A:166:SER:OG	2.21	0.44
1:A:115:ILE:HB	1:A:185:CYS:SG	2.58	0.43
1:A:265:SER:HB3	1:A:350:PRO:HB2	1.99	0.43
1:A:302:THR:HA	1:A:317:SER:HA	1.99	0.43
2:D:95:PHE:HB3	2:D:96:PRO:HD3	2.00	0.43
1:C:171:ARG:HG3	1:C:171:ARG:NH1	2.34	0.43
1:A:284:PRO:HD2	1:A:337:HIS:NE2	2.33	0.43
1:C:329:GLN:HE21	1:C:329:GLN:HB3	1.64	0.43
1:A:29:VAL:HA	1:A:35:TRP:CZ2	2.54	0.43
2:B:125:GLN:HG3	1:C:259:PHE:CE2	2.54	0.43
2:D:135:CYS:HB2	2:D:149:TRP:CH2	2.54	0.43
1:A:52:VAL:HG23	1:A:58:THR:HG22	2.00	0.42
2:B:55:LEU:HD23	2:B:56:HIS:O	2.19	0.42
2:B:97:PRO:HD2	1:C:48:TRP:CD2	2.54	0.42
2:B:168:ASP:HB3	2:B:171:ASP:OD1	2.19	0.42
2:D:109:ARG:HG2	2:D:110:THR:N	2.33	0.42
2:D:146:LYS:O	2:D:197:VAL:HA	2.19	0.42
1:C:127:SER:O	1:C:175:VAL:HG12	2.19	0.42
2:D:19:LYS:HB2	2:D:19:LYS:HE3	1.69	0.42
1:C:53:HIS:CD2	1:C:53:HIS:N	2.88	0.42
1:A:143:ARG:HD3	1:A:152:TYR:HB2	2.01	0.42
1:A:40:GLN:NE2	2:D:39:GLN:HE22	2.03	0.42
1:A:143:ARG:HD3	1:A:152:TYR:CD2	2.54	0.42
1:C:6:GLU:HG3	1:C:96:CYS:SG	2.60	0.42
1:A:99:ALA:HB2	1:A:237:VAL:HG12	2.00	0.42
1:A:284:PRO:HB2	1:A:339:PRO:HG2	2.01	0.42
2:D:79:LEU:HD23	2:D:79:LEU:HA	1.86	0.42
1:C:22:CYS:O	1:C:78:GLN:HB2	2.20	0.42
1:A:33:ARG:NH2	1:A:98:ARG:HH12	2.18	0.42
1:A:108:THR:C	1:A:110:LEU:H	2.22	0.42
1:A:329:GLN:OE1	1:A:330:THR:N	2.52	0.42
2:B:79:LEU:HD23	2:B:79:LEU:HA	1.84	0.42
1:C:141:THR:HB	1:C:188:TYR:HB3	2.02	0.42
1:C:98:ARG:HB3	1:C:239:VAL:CG1	2.50	0.41
1:A:67:ARG:O	1:A:83:VAL:HA	2.20	0.41
1:A:263:PRO:HB3	1:A:274:ALA:O	2.20	0.41
1:A:121:THR:O	1:A:202:LEU:HD12	2.21	0.41
1:A:346:LYS:HE2	1:A:346:LYS:HB2	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:114:PRO:HD3	2:B:199:HIS:ND1	2.36	0.41
2:B:153:ASN:HD21	2:D:159:ASN:ND2	2.18	0.41
1:C:13:LYS:HA	1:C:13:LYS:HE2	2.02	0.41
1:A:123:ILE:HG12	1:A:202:LEU:HD11	2.03	0.41
2:D:146:LYS:HA	2:D:146:LYS:HD3	1.74	0.41
1:C:33:ARG:CZ	1:C:98:ARG:NH1	2.84	0.41
2:B:91:GLN:HE22	2:B:94:CYS:H	1.69	0.41
2:D:40:ARG:HG2	2:D:85:ALA:HB2	2.01	0.41
2:D:67:GLY:HA3	2:D:72:PHE:HA	2.02	0.41
1:A:12:MET:O	1:A:248:VAL:HA	2.21	0.40
2:D:133:VAL:HG23	2:D:149:TRP:CH2	2.57	0.40
2:B:8:SER:HB2	2:B:23:THR:HG23	2.03	0.40
2:D:55:LEU:HD11	2:D:59:VAL:HG23	2.04	0.40
2:D:150:LYS:HE2	2:D:155:LEU:HD23	2.02	0.40
1:C:188:TYR:CZ	1:C:191:ARG:HA	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	351/364 (96%)	333 (95%)	18 (5%)	0	100	100
1	C	320/364 (88%)	306 (96%)	14 (4%)	0	100	100
2	B	211/213 (99%)	202 (96%)	9 (4%)	0	100	100
2	D	211/213 (99%)	202 (96%)	9 (4%)	0	100	100
All	All	1093/1154 (95%)	1043 (95%)	50 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	308/316 (98%)	300 (97%)	8 (3%)	46	66
1	C	284/316 (90%)	269 (95%)	15 (5%)	22	39
2	B	185/185 (100%)	180 (97%)	5 (3%)	44	65
2	D	185/185 (100%)	181 (98%)	4 (2%)	52	71
All	All	962/1002 (96%)	930 (97%)	32 (3%)	38	59

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	LYS
1	A	142	PHE
1	A	192	LYS
1	A	205	LYS
1	A	213	LEU
1	A	249	SER
1	A	266	LYS
1	A	354	ASP
2	B	40	ARG
2	B	64	SER
2	B	91	GLN
2	B	109	ARG
2	B	157	SER
2	D	4	ARG
2	D	32	ASP
2	D	64	SER
2	D	170	LYS
1	C	13	LYS
1	C	19	SER
1	C	25	SER
1	C	82	LYS
1	C	125	LEU
1	C	142	PHE
1	C	184	ARG

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Mol	Chain	Res	Type
1	C	192	LYS
1	C	205	LYS
1	C	225	GLN
1	C	315	LEU
1	C	326	LEU
1	C	333	CYS
1	C	343	LYS
1	C	347	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	337	HIS
2	B	153	ASN
2	B	167	GLN
2	D	31	ASN
2	D	138	ASN
1	C	3	GLN
1	C	140	GLN
1	C	329	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

7 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	$\# Z > 2$
4	NAG	B	301	2	14,14,15	1.24	1 (7%)	17,19,21	0.98	2 (11%)
3	PO4	A	401	-	4,4,4	0.91	0	6,6,6	0.46	0
3	PO4	A	403	-	4,4,4	0.93	0	6,6,6	0.42	0
3	PO4	A	402	-	4,4,4	0.90	0	6,6,6	0.46	0
4	NAG	D	301	-	14,14,15	1.68	1 (7%)	17,19,21	1.47	1 (5%)
3	PO4	B	302	-	4,4,4	0.92	0	6,6,6	0.47	0
3	PO4	C	401	-	4,4,4	0.90	0	6,6,6	0.41	0

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
4	NAG	B	301	2	-	1/6/23/26	0/1/1/1
4	NAG	D	301	-	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	301	NAG	O5-C1	-6.07	1.34	1.43
4	B	301	NAG	C1-C2	4.37	1.58	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	301	NAG	C1-O5-C5	-5.55	104.68	112.19
4	B	301	NAG	C1-O5-C5	2.35	115.37	112.19
4	B	301	NAG	O5-C5-C4	-2.06	105.81	110.83

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	301	NAG	C4-C5-C6-O6
4	D	301	NAG	O5-C5-C6-O6
4	B	301	NAG	C1-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	301	NAG	5	0
3	B	302	PO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	355/364 (97%)	0.77	43 (12%) 4 4	41, 77, 148, 183	0
1	C	328/364 (90%)	0.36	10 (3%) 50 57	45, 78, 128, 164	0
2	B	213/213 (100%)	0.40	6 (2%) 53 60	54, 76, 108, 127	0
2	D	213/213 (100%)	0.52	9 (4%) 36 39	46, 76, 105, 127	0
All	All	1109/1154 (96%)	0.53	68 (6%) 21 24	41, 77, 128, 183	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	268	THR	6.9
2	B	26	ALA	5.0
1	A	265	SER	4.9
1	A	291	TRP	4.4
1	A	296	LEU	4.4
1	A	341	ASN	4.3
1	A	269	SER	4.1
1	A	328	THR	4.0
1	C	351	LYS	3.9
1	A	293	SER	3.8
1	A	297	THR	3.8
1	A	64	LEU	3.5
1	A	338	LYS	3.4
2	B	108	LYS	3.4
1	A	326	LEU	3.4
1	A	107	ASP	3.2
1	A	17	THR	3.2
1	C	191	ARG	3.1
1	A	191	ARG	3.1
1	A	11	LEU	3.1
1	A	295	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	327	GLY	3.0
1	A	84	ASP	3.0
2	D	202	LEU	3.0
1	A	86	VAL	3.0
1	A	325	SER	2.8
1	A	332	ILE	2.8
2	D	114	PRO	2.8
1	C	110	LEU	2.8
1	C	349	GLU	2.8
1	C	270	GLY	2.7
2	D	95	PHE	2.7
1	A	294	GLY	2.6
1	A	298	SER	2.6
2	D	204	SER	2.6
1	C	158	VAL	2.6
1	A	283	PHE	2.5
2	D	200	GLN	2.5
2	B	77	THR	2.4
1	A	267	SER	2.4
1	A	83	VAL	2.4
2	B	4	ARG	2.4
1	A	339	PRO	2.3
1	A	329	GLN	2.3
1	A	66	SER	2.3
1	A	192	LYS	2.3
1	A	282	TYR	2.3
1	A	331	TYR	2.3
2	D	203	SER	2.3
1	A	109	ASP	2.3
1	A	212	ALA	2.3
1	A	321	VAL	2.3
2	D	205	PRO	2.3
1	C	83	VAL	2.3
1	C	273	ALA	2.2
1	A	9	PRO	2.2
2	B	127	LYS	2.1
1	A	256	PRO	2.1
1	A	244	THR	2.1
1	C	331	TYR	2.1
2	B	48	LEU	2.1
1	A	320	THR	2.1
1	A	330	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	10	GLY	2.1
2	D	131	ALA	2.1
1	C	264	SER	2.1
2	D	206	VAL	2.1
1	A	18	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
4	NAG	B	301	14/15	0.79	0.35	115,137,150,153	0
3	PO4	A	401	5/5	0.83	0.29	151,153,154,158	0
3	PO4	A	403	5/5	0.84	0.27	201,202,203,207	0
3	PO4	C	401	5/5	0.88	0.10	159,160,160,161	0
4	NAG	D	301	14/15	0.88	0.20	109,124,128,129	0
3	PO4	B	302	5/5	0.89	0.73	232,232,233,233	0
3	PO4	A	402	5/5	0.90	0.12	155,155,157,159	0

6.5 Other polymers [i](#)

There are no such residues in this entry.