



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 13, 2026 – 02:29 pm BST

PDB ID : 4BKM / pdb_00004bkm
Title : Crystal structure of the murine AUM (phosphoglycolate phosphatase) capping domain as a fusion protein with the catalytic core domain of murine chronophin (pyridoxal phosphate phosphatase)
Authors : Knobloch, G.; Seifried, A.; Gohla, A.; Schindelin, H.
Deposited on : 2013-04-26
Resolution : 2.65 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

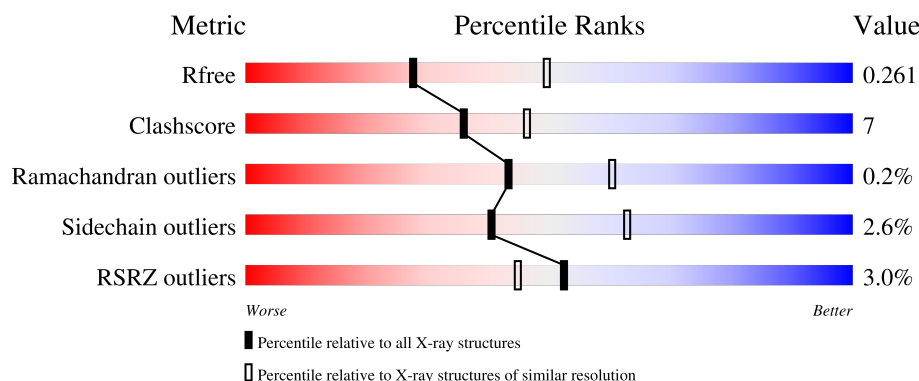
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	309	3% 82% 16% ..
1	B	309	2% 80% 17% ..
1	C	309	2% 84% 13% ..
1	D	309	5% 83% 15% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 18782 atoms, of which 9332 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.

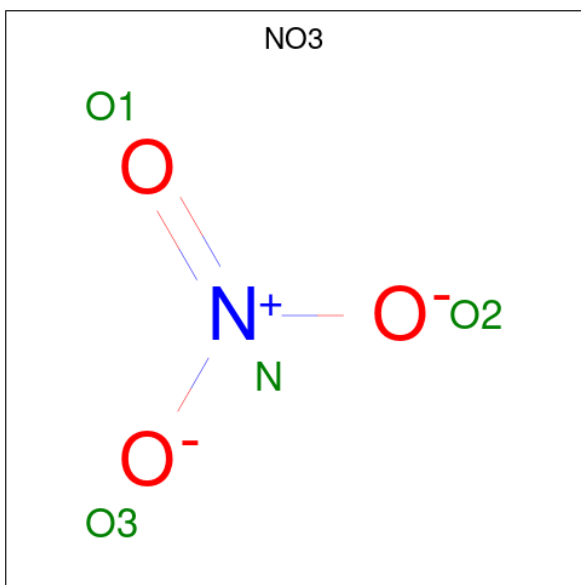
- Molecule 1 is a protein called PYRIDOXAL PHOSPHATE PHOSPHATASE, PHOSPHO-GLYCOLATE PHOSPHATASE, PYRIDOXAL PHOSPHATE PHOSPHATASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	304	Total	C	H	N	O	S	0	0	0
			4642	1454	2333	416	424	15			
1	B	304	Total	C	H	N	O	S	0	0	0
			4642	1454	2333	416	424	15			
1	C	304	Total	C	H	N	O	S	0	0	0
			4642	1454	2333	416	424	15			
1	D	304	Total	C	H	N	O	S	0	0	0
			4642	1454	2333	416	424	15			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 3 is NITRATE ION (CCD ID: NO3) (formula: NO₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	N	O	0	0
			4	1	3		
3	A	1	Total	N	O	0	0
			4	1	3		

- Molecule 4 is water.

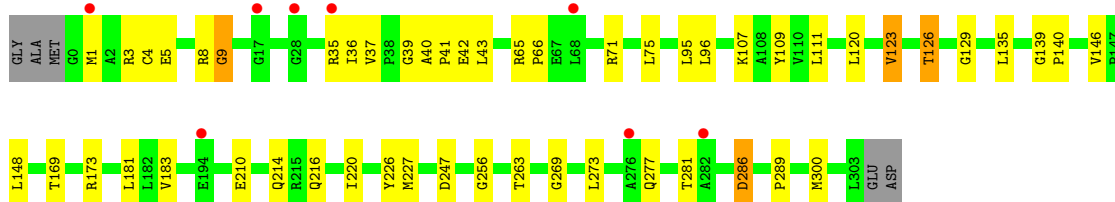
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	58	Total	O	0	0
			58	58		
4	B	52	Total	O	0	0
			52	52		
4	C	43	Total	O	0	0
			43	43		
4	D	49	Total	O	0	0
			49	49		

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.

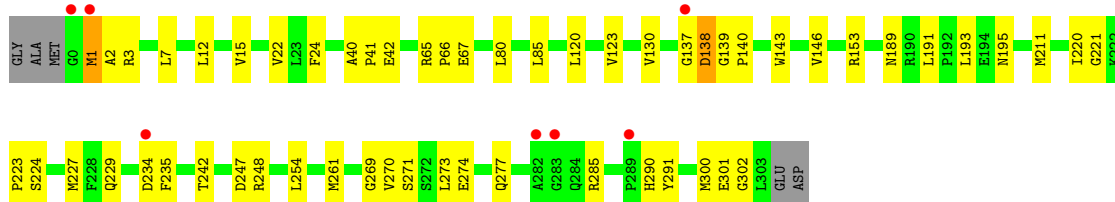
- Molecule 1: PYRIDOXAL PHOSPHATE PHOSPHATASE, PHOSPHOGLYCOLATE PHOSPHATASE, PYRIDOXAL PHOSPHATE PHOSPHATASE

Chain A: 



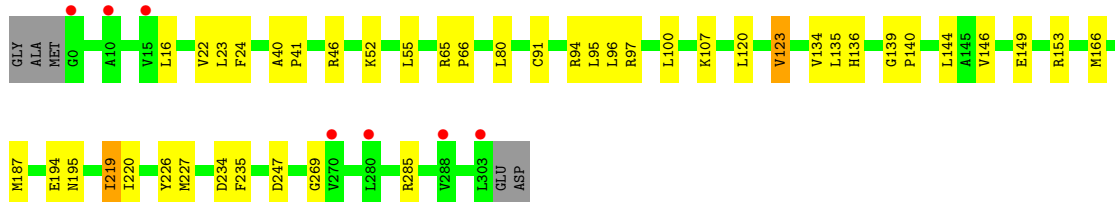
- Molecule 1: PYRIDOXAL PHOSPHATE PHOSPHATASE, PHOSPHOGLYCOLATE PHOSPHATASE, PYRIDOXAL PHOSPHATE PHOSPHATASE

Chain B: 

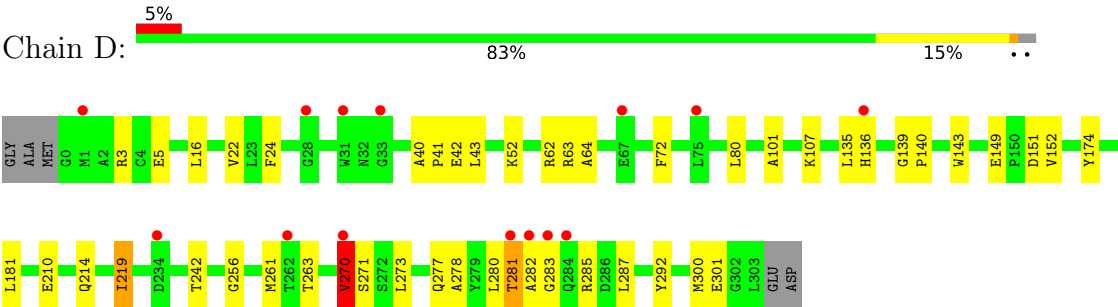


- Molecule 1: PYRIDOXAL PHOSPHATE PHOSPHATASE, PHOSPHOGLYCOLATE PHOSPHATASE, PYRIDOXAL PHOSPHATE PHOSPHATASE

Chain C: 



- Molecule 1: PYRIDOXAL PHOSPHATE PHOSPHATASE, PHOSPHOGLYCOLATE PHOSPHATASE, PYRIDOXAL PHOSPHATE PHOSPHATASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	67.50Å 91.96Å 105.92Å 90.00° 90.20° 90.00°	Depositor
Resolution (Å)	41.74 – 2.65 41.74 – 2.65	Depositor EDS
% Data completeness (in resolution range)	95.3 (41.74-2.65) 95.8 (41.74-2.65)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.198 , 0.256 0.207 , 0.261	Depositor DCC
R_{free} test set	1836 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	(Not available)	Xtriage
Anisotropy	(Not available)	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 74.4	EDS
L-test for twinning ¹	$\langle L \rangle =$ (Not available), $\langle L^2 \rangle =$ (Not available)	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18782	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *(Not available)*

¹Theoretical 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: MG, NO3

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	0.34	0/2351	0.74	2/3190 (0.1%)
1	B	0.34	0/2351	0.75	3/3190 (0.1%)
1	C	0.33	0/2351	0.72	2/3190 (0.1%)
1	D	0.34	0/2351	0.77	5/3190 (0.2%)
All	All	0.34	0/9404	0.75	12/12760 (0.1%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	139	GLY	CA-C-N	7.55	127.09	119.24
1	C	139	GLY	C-N-CA	7.55	127.09	119.24
1	B	1	MET	N-CA-C	7.36	120.24	110.53
1	D	139	GLY	CA-C-N	6.57	126.07	119.24
1	D	139	GLY	C-N-CA	6.57	126.07	119.24
1	A	139	GLY	CA-C-N	6.47	125.97	119.24
1	A	139	GLY	C-N-CA	6.47	125.97	119.24
1	B	139	GLY	CA-C-N	6.32	125.81	119.24
1	B	139	GLY	C-N-CA	6.32	125.81	119.24
1	D	270	VAL	N-CA-C	5.22	115.33	110.42
1	D	64	ALA	N-CA-C	5.20	117.24	110.53
1	D	280	LEU	N-CA-C	-5.07	105.76	111.28

There are no chirality outliers.

There are no planarity outliers.

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	2309	2333	2329	34	0
1	B	2309	2333	2329	42	0
1	C	2309	2333	2329	27	0
1	D	2309	2333	2329	33	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	8	0	0	1	0
4	A	58	0	0	4	0
4	B	52	0	0	5	0
4	C	43	0	0	4	0
4	D	49	0	0	0	0
All	All	9450	9332	9316	136	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 7.

All (136) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:MET:HE1	1:B:285:ARG:HD2	1.42	0.97
1:A:35:ARG:NH2	4:A:2008:HOH:O	2.16	0.77
1:B:1:MET:HE1	1:B:285:ARG:CD	2.15	0.76
1:A:216:GLN:O	4:A:2044:HOH:O	2.15	0.64
1:D:278:ALA:HA	1:D:281:THR:HB	1.81	0.62
1:C:195:ASN:ND2	4:C:2034:HOH:O	2.33	0.61
1:D:277:GLN:O	1:D:281:THR:N	2.32	0.60
1:B:1:MET:HG3	1:B:2:ALA:N	2.19	0.58
1:D:3:ARG:HD3	1:D:5:GLU:OE2	2.04	0.58
1:B:42:GLU:HB3	1:B:300:MET:HE1	1.87	0.57
1:D:277:GLN:O	1:D:281:THR:HB	2.05	0.57
1:D:285:ARG:N	1:D:285:ARG:HD3	2.19	0.57
1:A:3:ARG:HD3	1:A:5:GLU:OE2	2.04	0.56
1:A:286:ASP:N	1:A:286:ASP:OD1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:149:GLU:HB2	1:D:152:VAL:HG23	1.87	0.56
1:A:71:ARG:O	1:A:75:LEU:HD23	2.05	0.56
1:B:2:ALA:HA	1:B:290:HIS:HA	1.89	0.55
1:B:1:MET:CG	1:B:2:ALA:N	2.71	0.54
1:C:195:ASN:N	4:C:2032:HOH:O	2.37	0.54
1:B:195:ASN:ND2	4:B:2041:HOH:O	2.41	0.54
1:B:234:ASP:HB3	1:B:235:PHE:CD1	2.43	0.53
1:A:273:LEU:O	1:A:277:GLN:HG3	2.09	0.53
1:B:242:THR:HG22	1:B:261:MET:HE3	1.90	0.53
1:D:283:GLY:HA2	1:D:285:ARG:CZ	2.39	0.53
1:B:247:ASP:HB2	1:B:269:GLY:HA3	1.91	0.52
1:D:62:ARG:C	1:D:63:ARG:HG3	2.35	0.52
1:B:270:VAL:CG1	1:B:271:SER:N	2.72	0.52
1:B:1:MET:CE	1:B:285:ARG:HH11	2.22	0.52
1:C:247:ASP:HB2	1:C:269:GLY:HA3	1.91	0.52
1:A:183:VAL:CG1	1:A:220:ILE:HD11	2.39	0.52
3:A:1305:NO3:O2	4:A:2036:HOH:O	2.18	0.52
1:B:270:VAL:HG13	1:B:271:SER:N	2.25	0.51
1:D:22:VAL:HG11	1:D:24:PHE:CZ	2.46	0.51
1:C:123:VAL:O	1:C:123:VAL:HG13	2.09	0.51
1:D:278:ALA:O	1:D:282:ALA:N	2.43	0.51
1:A:43:LEU:N	1:A:300:MET:HE2	2.25	0.51
1:B:130:VAL:O	4:B:2023:HOH:O	2.18	0.51
1:B:211:MET:O	4:B:2044:HOH:O	2.18	0.51
1:B:1:MET:CE	1:B:285:ARG:CG	2.89	0.50
1:C:40:ALA:HB3	1:C:41:PRO:HD3	1.92	0.50
1:B:1:MET:HE1	1:B:285:ARG:HH11	1.76	0.50
1:D:42:GLU:HB2	1:D:300:MET:HE1	1.92	0.50
1:C:187:MET:HG2	1:C:219:ILE:HG13	1.94	0.50
1:D:277:GLN:O	1:D:281:THR:CB	2.60	0.50
1:B:1:MET:HE1	1:B:285:ARG:CG	2.42	0.50
1:C:65:ARG:N	1:C:66:PRO:CD	2.75	0.49
1:B:301:GLU:N	1:B:301:GLU:OE1	2.45	0.49
1:B:42:GLU:CB	1:B:300:MET:HE1	2.43	0.49
1:B:220:ILE:O	1:B:227:MET:HG2	2.13	0.48
1:C:135:LEU:HD12	1:C:166:MET:HE2	1.95	0.48
1:C:46:ARG:NH1	4:C:2008:HOH:O	2.47	0.48
1:B:273:LEU:O	1:B:277:GLN:HG3	2.14	0.47
1:B:189:ASN:ND2	4:B:2038:HOH:O	2.40	0.47
1:A:181:LEU:HD12	1:A:181:LEU:N	2.30	0.47
1:A:256:GLY:HA3	1:A:263:THR:HG22	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:107:LYS:HD2	1:D:151:ASP:HB2	1.96	0.47
1:C:107:LYS:NZ	1:C:149:GLU:OE1	2.48	0.47
1:D:278:ALA:CA	1:D:281:THR:HB	2.43	0.47
1:A:8:ARG:O	1:A:9:GLY:C	2.58	0.47
1:A:169:THR:HG23	4:A:2028:HOH:O	2.15	0.46
1:A:247:ASP:HB2	1:A:269:GLY:HA3	1.97	0.46
1:A:40:ALA:HB3	1:A:41:PRO:HD3	1.97	0.46
1:D:256:GLY:HA3	1:D:263:THR:HG22	1.97	0.46
1:B:22:VAL:HG11	1:B:24:PHE:CZ	2.51	0.46
1:C:134:VAL:HG11	1:C:136:HIS:CE1	2.51	0.46
1:D:270:VAL:HG12	1:D:271:SER:N	2.30	0.45
1:C:16:LEU:O	1:C:52:LYS:NZ	2.49	0.45
1:C:95:LEU:HD13	1:C:226:TYR:CE1	2.52	0.45
1:A:42:GLU:HB2	1:A:300:MET:HE1	1.99	0.45
1:B:7:LEU:HB2	1:B:291:TYR:HB3	1.98	0.45
1:A:109:TYR:CE1	1:A:129:GLY:HA3	2.51	0.45
1:B:12:LEU:HG	1:B:302:GLY:HA3	1.99	0.45
1:D:16:LEU:O	1:D:52:LYS:HE2	2.17	0.45
1:D:242:THR:HG22	1:D:261:MET:HE3	1.99	0.45
1:D:219:ILE:HD12	1:D:219:ILE:N	2.32	0.44
1:A:36:ILE:HG22	1:A:37:VAL:N	2.32	0.44
1:D:40:ALA:N	1:D:41:PRO:CD	2.81	0.44
1:A:4:CYS:HA	1:A:289:PRO:O	2.17	0.44
1:A:120:LEU:O	1:A:123:VAL:HG12	2.17	0.44
1:B:80:LEU:HD23	1:B:80:LEU:HA	1.93	0.44
1:D:40:ALA:HB3	1:D:41:PRO:HD3	2.00	0.44
1:D:43:LEU:N	1:D:300:MET:HE2	2.32	0.44
1:D:273:LEU:HD11	1:D:292:TYR:CE2	2.52	0.44
1:A:65:ARG:N	1:A:66:PRO:CD	2.81	0.44
1:C:23:LEU:HD13	1:C:55:LEU:HB2	1.99	0.44
1:A:1:MET:O	1:A:3:ARG:HG3	2.18	0.44
1:A:40:ALA:N	1:A:41:PRO:CD	2.80	0.44
1:A:183:VAL:CG1	1:A:220:ILE:CD1	2.95	0.44
1:C:247:ASP:OD1	4:C:2004:HOH:O	2.21	0.44
1:D:3:ARG:CD	1:D:5:GLU:OE2	2.65	0.44
1:B:221:GLY:O	1:B:224:SER:HB3	2.17	0.43
1:C:123:VAL:O	1:C:123:VAL:CG1	2.65	0.43
1:C:22:VAL:HG11	1:C:24:PHE:CZ	2.53	0.43
1:C:94:ARG:HD2	1:C:97:ARG:NH2	2.34	0.43
1:C:96:LEU:HD12	1:C:120:LEU:HD22	2.00	0.43
1:C:40:ALA:N	1:C:41:PRO:CD	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:219:ILE:N	1:D:219:ILE:CD1	2.80	0.43
1:C:220:ILE:CD1	1:C:220:ILE:N	2.82	0.43
1:D:242:THR:CG2	1:D:261:MET:HE3	2.48	0.43
1:A:140:PRO:HB3	1:B:193:LEU:HD21	1.99	0.43
1:A:183:VAL:HG13	1:A:220:ILE:HD11	2.00	0.43
1:B:248:ARG:HD2	1:B:270:VAL:HG11	2.00	0.43
1:B:67:GLU:OE2	4:B:2015:HOH:O	2.21	0.42
1:C:140:PRO:O	1:C:144:LEU:HD13	2.18	0.42
1:B:120:LEU:O	1:B:123:VAL:HG12	2.19	0.42
1:A:216:GLN:O	1:A:216:GLN:CG	2.68	0.42
1:B:40:ALA:N	1:B:41:PRO:CD	2.82	0.42
1:D:140:PRO:HA	1:D:143:TRP:CE3	2.54	0.42
1:C:146:VAL:HG23	1:C:146:VAL:O	2.19	0.42
1:D:72:PHE:CD1	1:D:80:LEU:CD1	3.02	0.42
1:D:152:VAL:HG21	1:D:174:TYR:CE1	2.55	0.42
1:B:40:ALA:HB3	1:B:41:PRO:HD3	2.02	0.42
1:B:12:LEU:HG	1:B:302:GLY:CA	2.49	0.42
1:B:223:PRO:HG3	1:B:254:LEU:HD23	2.00	0.42
1:C:91:CYS:SG	1:C:227:MET:HE3	2.59	0.42
1:A:109:TYR:CE2	1:A:111:LEU:HD11	2.55	0.42
1:A:39:GLY:O	1:A:300:MET:CE	2.68	0.42
1:B:65:ARG:NE	1:B:85:LEU:O	2.53	0.42
1:D:283:GLY:HA2	1:D:285:ARG:NE	2.35	0.42
1:A:220:ILE:O	1:A:227:MET:HG2	2.19	0.41
1:B:137:GLY:O	1:B:138:ASP:HB2	2.20	0.41
1:A:107:LYS:HG2	1:A:126:THR:HB	2.02	0.41
1:C:134:VAL:CG1	1:C:136:HIS:CE1	3.03	0.41
1:A:148:LEU:CD1	1:A:173:ARG:NH1	2.83	0.41
1:B:242:THR:CG2	1:B:261:MET:HE3	2.51	0.41
1:A:96:LEU:HD12	1:A:120:LEU:HD22	2.02	0.41
1:B:65:ARG:N	1:B:66:PRO:CD	2.83	0.41
1:C:220:ILE:N	1:C:220:ILE:HD12	2.36	0.41
1:A:210:GLU:O	1:A:214:GLN:N	2.54	0.41
1:B:146:VAL:O	1:B:146:VAL:HG13	2.20	0.41
1:C:234:ASP:HB3	1:C:235:PHE:CD1	2.56	0.41
1:D:181:LEU:HD12	1:D:181:LEU:N	2.36	0.41
1:A:95:LEU:HD13	1:A:226:TYR:CE1	2.57	0.40
1:B:140:PRO:HA	1:B:143:TRP:CE3	2.56	0.40
1:D:210:GLU:O	1:D:214:GLN:N	2.54	0.40
1:D:287:LEU:N	1:D:287:LEU:HD12	2.36	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	302/309 (98%)	295 (98%)	6 (2%)	1 (0%)	36	52
1	B	302/309 (98%)	295 (98%)	6 (2%)	1 (0%)	36	52
1	C	302/309 (98%)	295 (98%)	7 (2%)	0	100	100
1	D	302/309 (98%)	295 (98%)	6 (2%)	1 (0%)	36	52
All	All	1208/1236 (98%)	1180 (98%)	25 (2%)	3 (0%)	43	60

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	101	ALA
1	A	9	GLY
1	B	138	ASP

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	241/244 (99%)	235 (98%)	6 (2%)	42	64
1	B	241/244 (99%)	235 (98%)	6 (2%)	42	64
1	C	241/244 (99%)	234 (97%)	7 (3%)	37	58
1	D	241/244 (99%)	235 (98%)	6 (2%)	42	64
All	All	964/976 (99%)	939 (97%)	25 (3%)	40	63

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	123	VAL
1	A	126	THR
1	A	135	LEU
1	A	146	VAL
1	A	281	THR
1	A	286	ASP
1	B	3	ARG
1	B	15	VAL
1	B	153	ARG
1	B	191	LEU
1	B	229	GLN
1	B	274	GLU
1	C	80	LEU
1	C	100	LEU
1	C	123	VAL
1	C	153	ARG
1	C	194	GLU
1	C	219	ILE
1	C	285	ARG
1	D	135	LEU
1	D	136	HIS
1	D	219	ILE
1	D	270	VAL
1	D	281	THR
1	D	301	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	189	ASN
1	A	229	GLN
1	C	136	HIS
1	D	136	HIS
1	D	257	HIS

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

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	$\# Z > 2$
3	NO3	A	1305	-	1,3,3	3.54	1 (100%)	0,3,3	-	-
3	NO3	A	1306	-	1,3,3	3.57	1 (100%)	0,3,3	-	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1306	NO3	O1-N	3.57	1.40	1.24
3	A	1305	NO3	O1-N	3.54	1.40	1.24

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1305	NO3	1	0

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, 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	304/309 (98%)	0.36	8 (2%) 57 51	56, 86, 130, 225	0
1	B	304/309 (98%)	0.48	7 (2%) 61 54	51, 92, 145, 188	0
1	C	304/309 (98%)	0.39	7 (2%) 61 54	52, 89, 144, 167	0
1	D	304/309 (98%)	0.58	14 (4%) 37 29	57, 93, 149, 200	0
All	All	1216/1236 (98%)	0.45	36 (2%) 52 45	51, 90, 144, 225	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	234	ASP	4.9
1	D	282	ALA	4.6
1	D	283	GLY	3.4
1	B	137	GLY	2.9
1	B	289	PRO	2.9
1	B	1	MET	2.9
1	D	33	GLY	2.8
1	C	280	LEU	2.8
1	C	303	LEU	2.8
1	D	75	LEU	2.7
1	C	15	VAL	2.7
1	D	284	GLN	2.6
1	A	17	GLY	2.6
1	C	270	VAL	2.6
1	A	28	GLY	2.5
1	A	35	ARG	2.5
1	A	1	MET	2.5
1	A	282	ALA	2.4
1	A	276	ALA	2.4
1	B	234	ASP	2.3
1	D	1	MET	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	136	HIS	2.2
1	D	270	VAL	2.2
1	B	282	ALA	2.2
1	A	194	GLU	2.2
1	C	10	ALA	2.2
1	D	281	THR	2.1
1	D	28	GLY	2.1
1	D	67	GLU	2.1
1	C	288	VAL	2.1
1	D	31	TRP	2.0
1	D	262	THR	2.0
1	A	68	LEU	2.0
1	B	0	GLY	2.0
1	B	283	GLY	2.0
1	C	0	GLY	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	A	1304	1/1	0.87	0.13	88,88,88,88	0
2	MG	D	1304	1/1	0.93	0.11	67,67,67,67	0
2	MG	C	1304	1/1	0.95	0.07	61,61,61,61	0
2	MG	B	1304	1/1	0.95	0.07	59,59,59,59	0
3	NO3	A	1305	4/4	0.95	0.12	77,84,93,95	0
3	NO3	A	1306	4/4	0.95	0.11	64,73,81,96	0

6.5 Other polymers [i](#)

There are no such residues in this entry.