



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:57 PM UTC

PDB ID : 4AI9 / pdb_00004ai9
Title : JMJD2A Complexed with Daminozide
Authors : Chowdhury, R.; Schofield, C.J.
Deposited on : 2012-02-08
Resolution : 2.25 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 : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

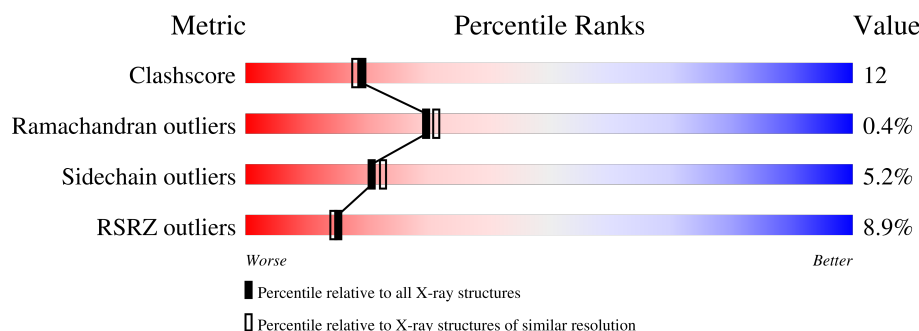
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	381	
1	B	381	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6324 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 LYSINE-SPECIFIC DEMETHYLASE 4A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	348	Total	C	N	O	S	0	3	0
			2872	1863	483	511	15			
1	B	349	Total	C	N	O	S	0	1	0
			2839	1841	474	509	15			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	expression tag	UNP O75164
A	-20	HIS	-	expression tag	UNP O75164
A	-19	HIS	-	expression tag	UNP O75164
A	-18	HIS	-	expression tag	UNP O75164
A	-17	HIS	-	expression tag	UNP O75164
A	-16	HIS	-	expression tag	UNP O75164
A	-15	HIS	-	expression tag	UNP O75164
A	-14	SER	-	expression tag	UNP O75164
A	-13	SER	-	expression tag	UNP O75164
A	-12	GLY	-	expression tag	UNP O75164
A	-11	VAL	-	expression tag	UNP O75164
A	-10	ASP	-	expression tag	UNP O75164
A	-9	LEU	-	expression tag	UNP O75164
A	-8	GLY	-	expression tag	UNP O75164
A	-7	THR	-	expression tag	UNP O75164
A	-6	GLU	-	expression tag	UNP O75164
A	-5	ASN	-	expression tag	UNP O75164
A	-4	LEU	-	expression tag	UNP O75164
A	-3	TYR	-	expression tag	UNP O75164
A	-2	PHE	-	expression tag	UNP O75164
A	-1	GLN	-	expression tag	UNP O75164
A	0	SER	-	expression tag	UNP O75164
B	-21	MET	-	expression tag	UNP O75164
B	-20	HIS	-	expression tag	UNP O75164
B	-19	HIS	-	expression tag	UNP O75164

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	HIS	-	expression tag	UNP O75164
B	-17	HIS	-	expression tag	UNP O75164
B	-16	HIS	-	expression tag	UNP O75164
B	-15	HIS	-	expression tag	UNP O75164
B	-14	SER	-	expression tag	UNP O75164
B	-13	SER	-	expression tag	UNP O75164
B	-12	GLY	-	expression tag	UNP O75164
B	-11	VAL	-	expression tag	UNP O75164
B	-10	ASP	-	expression tag	UNP O75164
B	-9	LEU	-	expression tag	UNP O75164
B	-8	GLY	-	expression tag	UNP O75164
B	-7	THR	-	expression tag	UNP O75164
B	-6	GLU	-	expression tag	UNP O75164
B	-5	ASN	-	expression tag	UNP O75164
B	-4	LEU	-	expression tag	UNP O75164
B	-3	TYR	-	expression tag	UNP O75164
B	-2	PHE	-	expression tag	UNP O75164
B	-1	GLN	-	expression tag	UNP O75164
B	0	SER	-	expression tag	UNP O75164

- Molecule 2 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

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

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Zn 1 1	0	0
3	B	1	Total Zn 1 1	0	0

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

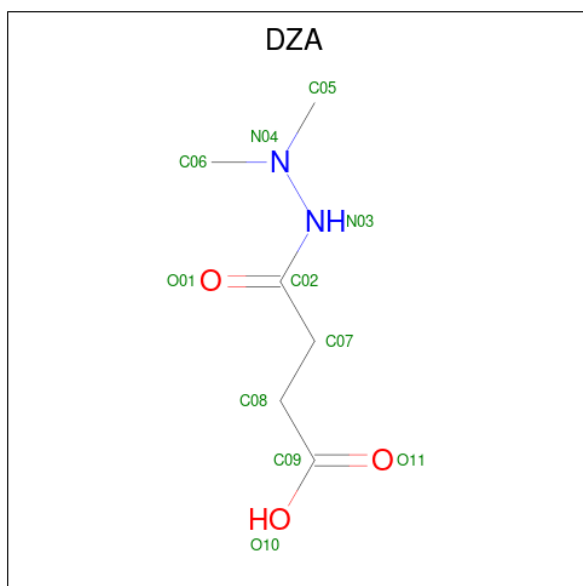
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Cl 1 1	0	0

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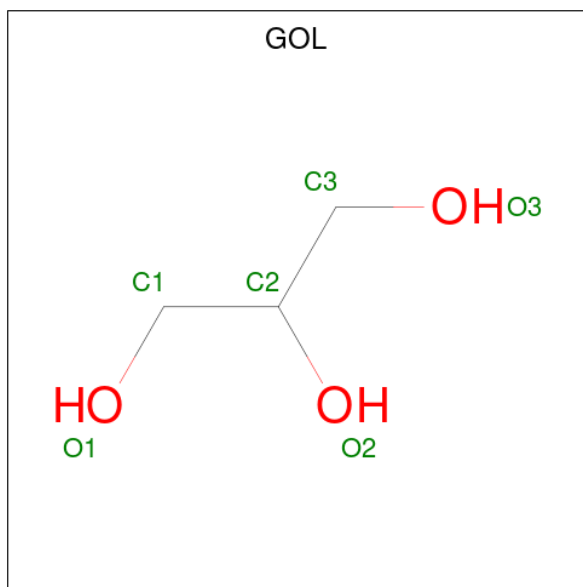
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	Cl		0	0
			1	1			

- Molecule 5 is DAMINOZIDE (CCD ID: DZA) (formula: $C_6H_{12}N_2O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			11	6	2	3		
5	A	1	Total	C	N	O	0	0
			11	6	2	3		
5	B	1	Total	C	N	O	0	0
			11	6	2	3		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			6	3	3		

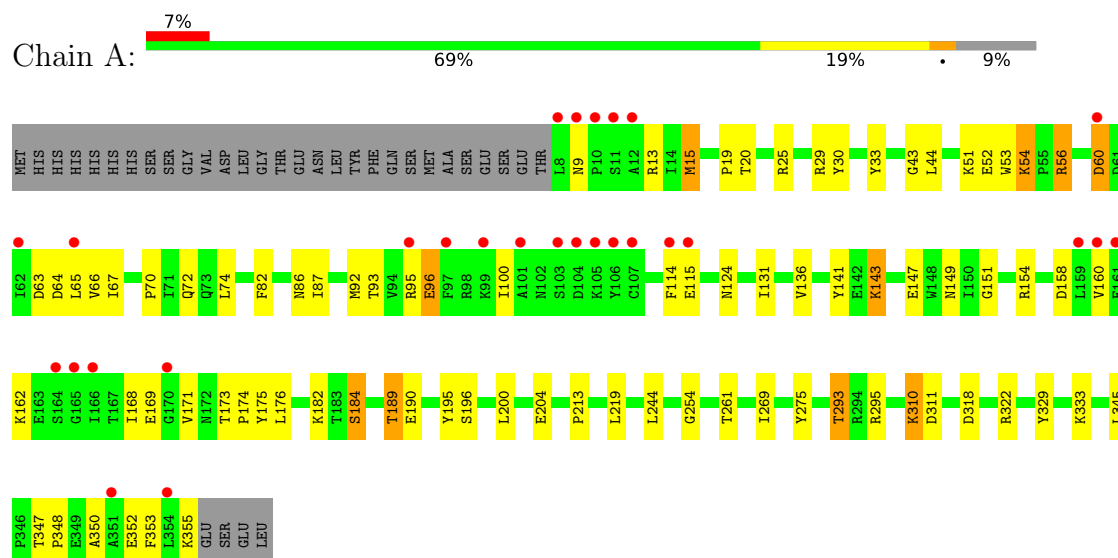
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	265	Total	O	0	0
			265	265		
7	B	303	Total	O	0	0
			303	303		

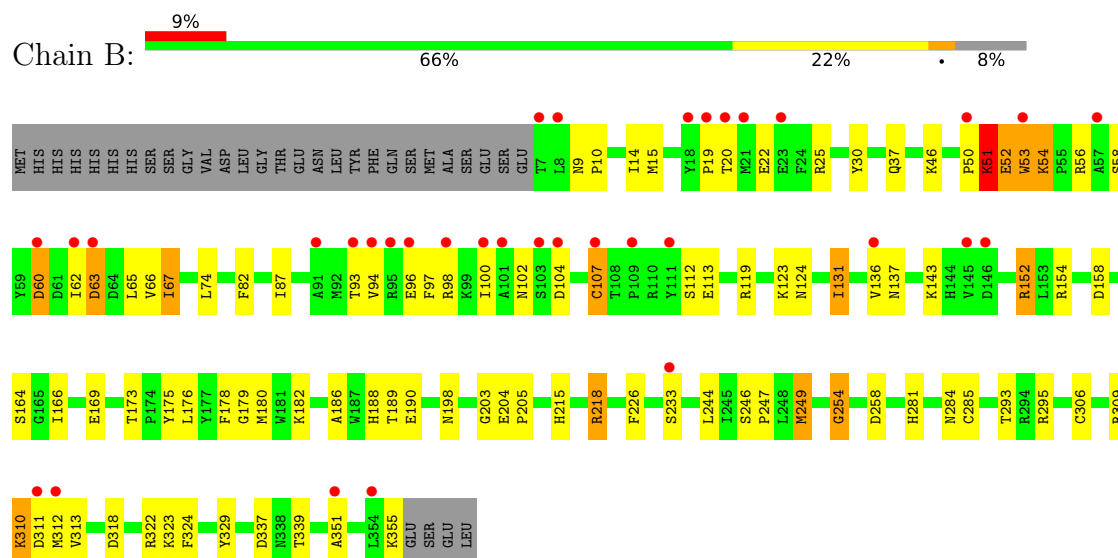
3 Residue-property plots

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: LYSINE-SPECIFIC DEMETHYLASE 4A



• Molecule 1: LYSINE-SPECIFIC DEMETHYLASE 4A



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	100.48Å 149.75Å 57.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.62 – 2.25 45.62 – 2.25	Depositor EDS
% Data completeness (in resolution range)	95.6 (45.62-2.25) 90.4 (45.62-2.25)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 2.24Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.216 , 0.237 0.229 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	36.8	Xtriage
Anisotropy	0.356	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 49.3	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	6324	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.89% 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: GOL, NI, ZN, DZA, CL

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	0.48	1/2969 (0.0%)	1.01	10/4018 (0.2%)
1	B	0.47	0/2929	1.06	18/3970 (0.5%)
All	All	0.48	1/5898 (0.0%)	1.03	28/7988 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	15	MET	SD-CE	-6.47	1.63	1.79

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	189	THR	N-CA-C	-8.39	97.81	110.14
1	B	189	THR	N-CA-C	-8.26	97.17	109.81
1	B	25	ARG	N-CA-C	8.13	120.15	111.28
1	B	62	ILE	N-CA-C	7.30	121.19	112.80
1	A	20	THR	N-CA-C	-7.03	101.46	110.53
1	B	313	VAL	N-CA-C	6.90	118.24	108.93
1	B	67	ILE	CA-C-N	6.87	126.55	119.82
1	B	67	ILE	C-N-CA	6.87	126.55	119.82
1	B	20	THR	N-CA-C	-6.81	102.04	110.41
1	B	293	THR	N-CA-C	-6.55	99.38	109.14
1	A	25	ARG	N-CA-C	6.54	119.24	111.33
1	B	53	TRP	N-CA-C	6.08	118.82	110.24
1	B	249	MET	N-CA-C	-5.97	104.85	111.36
1	A	293	THR	N-CA-C	-5.97	100.50	108.74
1	B	60	ASP	N-CA-C	5.88	120.61	113.38
1	A	184	SER	N-CA-C	5.85	119.09	109.85
1	B	254	GLY	CA-C-N	-5.78	118.43	122.59
1	B	254	GLY	C-N-CA	-5.78	118.43	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	67	ILE	N-CA-C	-5.62	96.74	108.88
1	A	254	GLY	CA-C-N	-5.41	118.70	122.59
1	A	254	GLY	C-N-CA	-5.41	118.70	122.59
1	B	124	ASN	N-CA-C	5.26	119.66	112.88
1	B	323	LYS	N-CA-C	5.23	118.12	111.69
1	B	107	CYS	N-CA-C	5.19	117.39	110.53
1	A	60	ASP	N-CA-C	5.15	120.20	113.30
1	B	166	ILE	N-CA-C	5.15	116.16	108.54
1	A	124	ASN	N-CA-C	5.13	119.49	112.88
1	A	67	ILE	N-CA-C	-5.01	98.05	108.88

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	2872	0	2807	58	0
1	B	2839	0	2751	74	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	22	0	22	6	0
5	B	11	0	11	3	0
6	B	6	0	8	1	0
7	A	265	0	0	11	0
7	B	303	0	0	13	0
All	All	6324	0	5599	133	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 (133) 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:218:ARG:HH11	1:B:218:ARG:HG2	1.05	1.14
1:A:56:ARG:HH11	1:A:56:ARG:HG3	1.19	1.02
1:A:136:VAL:CG2	1:A:176:LEU:HB2	1.95	0.96
1:B:324:PHE:HB3	6:B:701:GOL:H11	1.49	0.94
1:B:218:ARG:HG2	1:B:218:ARG:NH1	1.83	0.85
1:B:190:GLU:OE1	5:B:603:DZA:H051	1.77	0.85
1:B:136:VAL:CG2	1:B:176:LEU:HB2	2.08	0.83
1:B:93:THR:OG1	1:B:96:GLU:HG3	1.80	0.81
1:B:337:ASP:OD1	1:B:339:THR:HG23	1.84	0.78
1:A:56:ARG:HG3	1:A:56:ARG:NH1	1.95	0.78
1:A:136:VAL:HG23	1:A:176:LEU:HB2	1.64	0.78
1:B:136:VAL:HG23	1:B:176:LEU:HB2	1.66	0.77
1:B:104:ASP:HA	1:B:107:CYS:SG	2.29	0.73
1:A:70:PRO:HG2	1:A:92:MET:HE3	1.75	0.69
1:A:33:TYR:CE1	5:A:601:DZA:H072	2.29	0.68
1:B:218:ARG:HH11	1:B:218:ARG:CG	1.92	0.67
1:A:64:ASP:OD1	1:A:95:ARG:NH2	2.27	0.67
1:A:9:ASN:HB2	1:A:15:MET:CE	2.25	0.67
1:B:9:ASN:HB2	1:B:15:MET:CE	2.25	0.66
1:A:143:LYS:HE3	7:A:2142:HOH:O	1.97	0.64
1:B:15:MET:HE1	1:B:37:GLN:O	1.98	0.63
1:B:198:ASN:HB2	7:B:2190:HOH:O	1.97	0.63
1:A:43:GLY:HA3	7:A:2036:HOH:O	1.98	0.62
1:A:66:VAL:O	7:A:2063:HOH:O	2.16	0.60
1:B:295:ARG:HD2	7:B:2242:HOH:O	2.03	0.59
1:A:136:VAL:HG22	1:A:176:LEU:HB2	1.81	0.58
1:B:137:ASN:HD21	1:B:169:GLU:HG2	1.68	0.58
1:A:147:GLU:HA	7:A:2017:HOH:O	2.04	0.58
1:A:82:PHE:HB2	1:A:244:LEU:HB2	1.86	0.57
1:A:96:GLU:O	1:A:100:ILE:HG13	2.05	0.57
1:B:19:PRO:HB3	1:B:30:TYR:CZ	2.40	0.57
1:B:46:LYS:HE3	7:B:2017:HOH:O	2.05	0.56
1:B:53:TRP:O	1:B:54:LYS:HD2	2.05	0.56
1:B:136:VAL:HG22	1:B:176:LEU:O	2.05	0.56
1:B:218:ARG:NH2	1:B:254:GLY:O	2.38	0.56
1:B:137:ASN:ND2	1:B:169:GLU:HG2	2.21	0.56
1:B:351:ALA:O	1:B:355:LYS:HE2	2.06	0.56
1:A:9:ASN:HB2	1:A:15:MET:HE1	1.88	0.55
1:A:310:LYS:O	1:A:311:ASP:HB2	2.07	0.55
1:B:322:ARG:HG3	1:B:329:TYR:CE1	2.42	0.54
1:A:9:ASN:ND2	1:A:15:MET:HE3	2.22	0.54
1:B:19:PRO:O	1:B:50:PRO:HD3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:VAL:HG23	1:A:136:VAL:O	2.09	0.53
1:B:98:ARG:HG2	1:B:102:ASN:OD1	2.08	0.53
1:B:152:ARG:HG3	7:B:2151:HOH:O	2.08	0.53
1:B:63:ASP:N	1:B:63:ASP:OD1	2.41	0.52
1:A:352:GLU:HA	1:A:355:LYS:HE2	1.91	0.52
1:A:353:PHE:CZ	5:A:601:DZA:H053	2.45	0.52
1:B:164:SER:HA	7:B:2163:HOH:O	2.09	0.52
1:B:178:PHE:CE1	1:B:285:CYS:SG	3.00	0.52
1:A:13:ARG:HD2	7:A:2002:HOH:O	2.10	0.52
1:A:322[A]:ARG:HG3	1:A:329:TYR:CE1	2.44	0.52
1:B:137:ASN:HD21	1:B:169:GLU:CG	2.23	0.52
1:A:53:TRP:O	1:A:54:LYS:HD2	2.11	0.51
1:A:136:VAL:HG22	1:A:176:LEU:O	2.10	0.51
1:B:119:ARG:HG3	7:B:2108:HOH:O	2.10	0.51
1:A:56:ARG:NH1	1:A:56:ARG:CG	2.67	0.51
1:A:19:PRO:HB3	1:A:30:TYR:CZ	2.45	0.51
1:B:309:ARG:HB2	1:B:312:MET:HG2	1.92	0.51
1:A:151:GLY:HA2	1:A:174:PRO:HG3	1.92	0.51
1:B:215:HIS:HD2	7:B:2199:HOH:O	1.94	0.51
1:B:190:GLU:CD	5:B:603:DZA:H051	2.35	0.51
1:A:136:VAL:HG12	7:A:2064:HOH:O	2.10	0.51
1:B:66:VAL:HG12	7:B:2061:HOH:O	2.11	0.50
1:B:226:PHE:CZ	1:B:249:MET:HE3	2.47	0.50
1:A:162:LYS:O	1:A:162:LYS:HG2	2.12	0.49
1:A:154:ARG:HA	1:A:158:ASP:OD2	2.13	0.49
1:B:154:ARG:NH2	7:B:2155:HOH:O	2.35	0.49
1:B:9:ASN:N	1:B:10:PRO:HD3	2.28	0.48
1:A:33:TYR:CD1	5:A:601:DZA:H072	2.49	0.47
1:A:169:GLU:HA	1:A:173:THR:OG1	2.15	0.47
1:B:56:ARG:HH11	1:B:56:ARG:HG3	1.80	0.47
1:A:114[B]:PHE:CE2	1:A:261:THR:HG21	2.50	0.47
1:B:136:VAL:HG23	1:B:136:VAL:O	2.14	0.47
1:A:63:ASP:OD1	1:A:63:ASP:N	2.48	0.46
1:B:154:ARG:HA	1:B:158:ASP:OD2	2.14	0.46
1:A:13:ARG:NH1	7:A:2003:HOH:O	2.49	0.46
1:A:29:ARG:NH1	1:A:352:GLU:OE2	2.49	0.46
1:A:86:ASN:ND2	7:A:2089:HOH:O	2.40	0.45
1:B:74:LEU:HD11	1:B:87:ILE:CD1	2.47	0.45
1:B:178:PHE:HE1	1:B:285:CYS:SG	2.40	0.45
1:A:195:TYR:CE1	1:A:293:THR:HG23	2.51	0.45
1:B:310:LYS:O	1:B:311:ASP:CB	2.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:GLU:O	1:B:100:ILE:HG13	2.17	0.45
1:B:97:PHE:HE2	1:B:179:GLY:O	1.98	0.45
1:B:169:GLU:HA	1:B:173:THR:OG1	2.17	0.45
1:B:107:CYS:HB2	7:B:2099:HOH:O	2.15	0.45
1:B:309:ARG:HB2	1:B:312:MET:CG	2.47	0.45
1:A:168:ILE:HB	1:A:171:VAL:HB	1.98	0.45
1:B:58:SER:HA	7:B:2055:HOH:O	2.16	0.44
1:B:306:CYS:SG	1:B:312:MET:HG3	2.56	0.44
5:A:601:DZA:O01	5:A:601:DZA:H063	2.16	0.44
1:A:72:GLN:HG2	1:A:74:LEU:CD1	2.48	0.44
1:A:196:SER:OG	5:A:605:DZA:H051	2.17	0.44
1:B:186:ALA:HA	1:B:244:LEU:HD23	1.99	0.44
1:B:112:SER:OG	1:B:113:GLU:N	2.51	0.44
1:B:188:HIS:NE2	5:B:603:DZA:H063	2.33	0.44
1:A:160:VAL:HG22	7:A:2238:HOH:O	2.18	0.43
1:A:219:LEU:HD23	1:A:275:TYR:CG	2.53	0.43
1:B:123:LYS:HD3	7:B:2127:HOH:O	2.19	0.43
1:A:9:ASN:CG	1:A:15:MET:HE3	2.44	0.43
1:B:60:ASP:N	1:B:60:ASP:OD1	2.51	0.43
1:B:74:LEU:HD11	1:B:87:ILE:HD11	2.01	0.43
1:B:154:ARG:NH1	7:B:2154:HOH:O	2.51	0.43
1:B:66:VAL:HG22	1:B:67:ILE:N	2.34	0.42
1:B:246:SER:HB2	1:B:247:PRO:HD2	2.01	0.42
1:B:52:GLU:H	1:B:52:GLU:HG3	1.60	0.42
1:B:351:ALA:O	1:B:355:LYS:CE	2.67	0.42
1:A:141:TYR:CE2	1:A:149:ASN:HA	2.55	0.41
1:A:295:ARG:HB2	1:A:347:THR:HA	2.01	0.41
1:B:205:PRO:HD2	1:B:281:HIS:HB2	2.02	0.41
1:A:204:GLU:HA	1:A:204:GLU:OE1	2.20	0.41
1:A:353:PHE:HZ	5:A:601:DZA:H053	1.85	0.41
1:B:94:VAL:O	1:B:97:PHE:N	2.53	0.41
1:B:218:ARG:NH1	1:B:218:ARG:CG	2.61	0.41
1:A:348:PRO:C	1:A:350:ALA:H	2.28	0.41
1:A:200:LEU:HD12	1:A:200:LEU:HA	1.93	0.41
1:B:51:LYS:H	1:B:51:LYS:HG2	1.60	0.41
1:A:74:LEU:HD13	1:A:87:ILE:HD12	2.03	0.41
1:B:56:ARG:HG3	1:B:56:ARG:NH1	2.35	0.41
1:B:203:GLY:HA3	1:B:284:ASN:HA	2.02	0.41
1:A:60:ASP:HA	7:A:2057:HOH:O	2.20	0.41
1:B:9:ASN:HB2	1:B:15:MET:HE1	2.01	0.41
1:A:44:LEU:HD12	1:A:269:ILE:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:ASN:CB	1:A:15:MET:CE	2.97	0.40
1:A:190:GLU:HG3	1:A:196:SER:HB3	2.02	0.40
1:B:14:ILE:HG13	1:B:258:ASP:HB3	2.02	0.40
1:B:131:ILE:O	1:B:180:MET:HE3	2.21	0.40
1:B:310:LYS:NZ	1:B:310:LYS:HB2	2.36	0.40
1:A:189:THR:HG23	1:A:275:TYR:CE1	2.56	0.40
1:A:295:ARG:HD2	7:A:2220:HOH:O	2.20	0.40
1:B:82:PHE:HB2	1:B:244:LEU:HB2	2.03	0.40
1:B:204:GLU:OE1	1:B:204:GLU:HA	2.21	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	349/381 (92%)	338 (97%)	10 (3%)	1 (0%)	36	40
1	B	348/381 (91%)	333 (96%)	13 (4%)	2 (1%)	21	21
All	All	697/762 (92%)	671 (96%)	23 (3%)	3 (0%)	30	31

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	51	LYS
1	A	143	LYS
1	B	143	LYS

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	305/335 (91%)	288 (94%)	17 (6%)	19	20
1	B	299/335 (89%)	285 (95%)	14 (5%)	23	26
All	All	604/670 (90%)	573 (95%)	31 (5%)	21	23

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	LYS
1	A	52	GLU
1	A	54	LYS
1	A	56	ARG
1	A	65	LEU
1	A	93	THR
1	A	96	GLU
1	A	115	GLU
1	A	131	ILE
1	A	175	TYR
1	A	182	LYS
1	A	184	SER
1	A	213	PRO
1	A	310	LYS
1	A	318	ASP
1	A	333	LYS
1	A	345	LEU
1	B	22	GLU
1	B	51	LYS
1	B	52	GLU
1	B	54	LYS
1	B	63	ASP
1	B	65	LEU
1	B	131	ILE
1	B	152	ARG
1	B	175	TYR
1	B	182	LYS
1	B	218	ARG
1	B	233	SER
1	B	310	LYS
1	B	318	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such

sidechains are listed below:

Mol	Chain	Res	Type
1	B	72	GLN
1	B	84	GLN
1	B	137	ASN
1	B	338	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](#)

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 10 ligands modelled in this entry, 6 are monoatomic - leaving 4 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
5	DZA	A	601	-	10,10,10	7.33	1 (10%)	12,12,12	1.46	2 (16%)
5	DZA	A	605	2	10,10,10	7.36	2 (20%)	12,12,12	1.79	3 (25%)
5	DZA	B	603	2	10,10,10	7.44	2 (20%)	12,12,12	1.49	3 (25%)
6	GOL	B	701	-	5,5,5	0.50	0	5,5,5	0.21	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
5	DZA	A	601	-	-	3/9/9/9	-
5	DZA	A	605	2	-	4/9/9/9	-
5	DZA	B	603	2	-	2/9/9/9	-
6	GOL	B	701	-	-	0/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	603	DZA	N03-N04	-23.25	1.12	1.42
5	A	601	DZA	N03-N04	-22.97	1.12	1.42
5	A	605	DZA	N03-N04	-22.91	1.12	1.42
5	A	605	DZA	O10-C09	-2.28	1.23	1.30
5	B	603	DZA	O10-C09	-2.15	1.23	1.30

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	605	DZA	C02-N03-N04	-4.25	116.09	120.29
5	B	603	DZA	C07-C08-C09	-2.90	105.98	113.67
5	B	603	DZA	C02-N03-N04	-2.45	117.87	120.29
5	A	605	DZA	O11-C09-C08	-2.34	115.66	123.09
5	B	603	DZA	O11-C09-C08	-2.32	115.75	123.09
5	A	601	DZA	C02-N03-N04	-2.31	118.01	120.29
5	A	601	DZA	C06-N04-N03	2.23	111.06	109.03
5	A	605	DZA	C06-N04-N03	2.18	111.01	109.03

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	601	DZA	C02-N03-N04-C05
5	A	605	DZA	C02-N03-N04-C06
5	B	603	DZA	C07-C08-C09-O11
5	A	605	DZA	C07-C08-C09-O11
5	B	603	DZA	C07-C08-C09-O10
5	A	605	DZA	C07-C08-C09-O10
5	A	601	DZA	C07-C08-C09-O11
5	A	601	DZA	C07-C08-C09-O10
5	A	605	DZA	N03-C02-C07-C08

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	601	DZA	5	0
5	A	605	DZA	1	0
5	B	603	DZA	3	0
6	B	701	GOL	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	348/381 (91%)	0.64	28 (8%) 18 16	18, 40, 67, 85	11 (3%)
1	B	349/381 (91%)	0.69	34 (9%) 13 12	21, 41, 69, 84	10 (2%)
All	All	697/762 (91%)	0.66	62 (8%) 15 14	18, 41, 68, 85	21 (3%)

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	114[A]	PHE	4.6
1	B	93	THR	4.4
1	B	60	ASP	4.2
1	B	312	MET	4.2
1	A	164	SER	3.9
1	A	9	ASN	3.8
1	B	20	THR	3.8
1	B	7	THR	3.7
1	A	106	TYR	3.6
1	A	354	LEU	3.6
1	B	50	PRO	3.5
1	A	166	ILE	3.5
1	A	160	VAL	3.4
1	B	351	ALA	3.4
1	B	104	ASP	3.4
1	A	8	LEU	3.3
1	A	12	ALA	3.3
1	A	170	GLY	3.2
1	B	311	ASP	3.1
1	B	145	VAL	3.1
1	B	94	VAL	3.0
1	A	11	SER	2.9
1	A	65	LEU	2.9
1	A	104	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	62	ILE	2.8
1	B	53	TRP	2.7
1	A	159	LEU	2.7
1	A	95	ARG	2.7
1	A	60	ASP	2.7
1	A	10	PRO	2.7
1	A	161	GLU	2.7
1	A	62	ILE	2.6
1	B	354	LEU	2.6
1	A	351	ALA	2.6
1	B	100	ILE	2.6
1	B	98	ARG	2.6
1	B	19	PRO	2.6
1	B	111	TYR	2.6
1	B	107	CYS	2.5
1	B	18	TYR	2.5
1	B	103	SER	2.4
1	B	101	ALA	2.4
1	B	21	MET	2.4
1	A	99	LYS	2.3
1	A	101	ALA	2.3
1	B	96	GLU	2.3
1	A	107	CYS	2.3
1	B	146	ASP	2.3
1	A	105	LYS	2.3
1	B	63	ASP	2.2
1	B	57	ALA	2.2
1	B	136	VAL	2.2
1	B	95	ARG	2.2
1	A	165	GLY	2.2
1	B	109	PRO	2.2
1	B	233	SER	2.2
1	A	115	GLU	2.1
1	A	103	SER	2.1
1	B	91	ALA	2.1
1	B	8	LEU	2.1
1	A	97	PHE	2.0
1	B	23	GLU	2.0

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

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
5	DZA	A	601	11/11	0.74	0.20	82,83,84,84	11
4	CL	B	503	1/1	0.80	0.23	85,85,85,85	0
5	DZA	B	603	11/11	0.81	0.21	64,68,69,69	2
5	DZA	A	605	11/11	0.85	0.17	55,60,63,63	0
6	GOL	B	701	6/6	0.87	0.12	61,63,63,65	0
4	CL	A	503	1/1	0.90	0.10	76,76,76,76	0
2	NI	A	501	1/1	0.99	0.03	42,42,42,42	0
3	ZN	A	502	1/1	0.99	0.05	39,39,39,39	0
3	ZN	B	502	1/1	0.99	0.03	33,33,33,33	0
2	NI	B	501	1/1	1.00	0.02	37,37,37,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.