



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:26 AM UTC

PDB ID : 3LGD / pdb_00003lgd
Title : Crystal structure of human adenosine deaminase growth factor, adenosine deaminase type 2 (ADA2)
Authors : Zavialov, A.V.
Deposited on : 2010-01-20
Resolution : 2.00 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

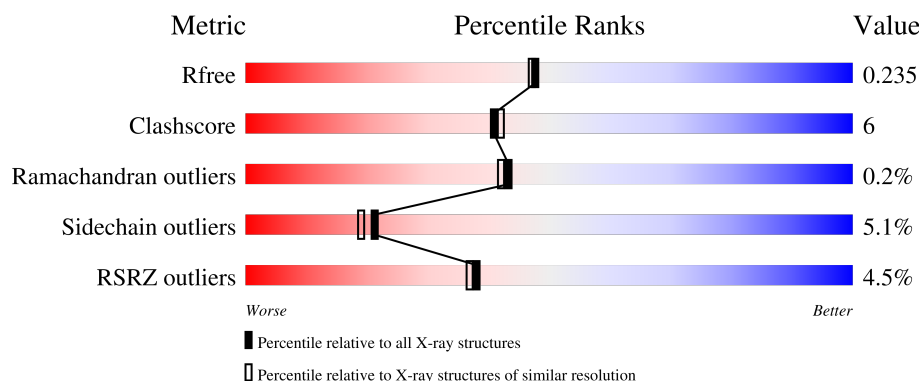
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

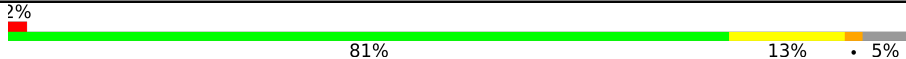
The reported resolution of this entry is 2.00 Å.

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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	508	
1	B	508	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	B	550	X	-	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8743 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 Adenosine deaminase CECR1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	482	Total	C	N	O	S	0	0	0
			3927	2529	675	696	27			
1	B	482	Total	C	N	O	S	0	0	0
			3931	2532	676	696	27			

There are 50 discrepancies between the modelled and reference sequences:

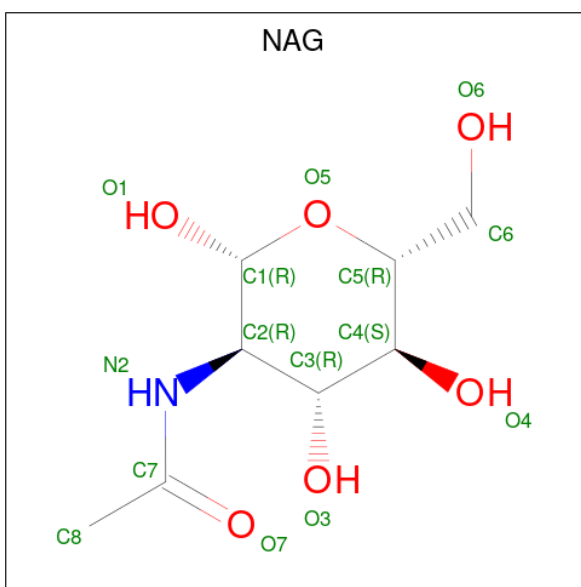
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP Q9NZK5
A	2	GLY	-	expression tag	UNP Q9NZK5
A	486	GLY	-	expression tag	UNP Q9NZK5
A	487	SER	-	expression tag	UNP Q9NZK5
A	488	LEU	-	expression tag	UNP Q9NZK5
A	489	HIS	-	expression tag	UNP Q9NZK5
A	490	HIS	-	expression tag	UNP Q9NZK5
A	491	ILE	-	expression tag	UNP Q9NZK5
A	492	LEU	-	expression tag	UNP Q9NZK5
A	493	ASP	-	expression tag	UNP Q9NZK5
A	494	ALA	-	expression tag	UNP Q9NZK5
A	495	GLN	-	expression tag	UNP Q9NZK5
A	496	LYS	-	expression tag	UNP Q9NZK5
A	497	MET	-	expression tag	UNP Q9NZK5
A	498	VAL	-	expression tag	UNP Q9NZK5
A	499	TRP	-	expression tag	UNP Q9NZK5
A	500	ASN	-	expression tag	UNP Q9NZK5
A	501	HIS	-	expression tag	UNP Q9NZK5
A	502	ARG	-	expression tag	UNP Q9NZK5
A	503	HIS	-	expression tag	UNP Q9NZK5
A	504	HIS	-	expression tag	UNP Q9NZK5
A	505	HIS	-	expression tag	UNP Q9NZK5
A	506	HIS	-	expression tag	UNP Q9NZK5
A	507	HIS	-	expression tag	UNP Q9NZK5
A	508	HIS	-	expression tag	UNP Q9NZK5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1	GLY	-	expression tag	UNP Q9NZK5
B	2	GLY	-	expression tag	UNP Q9NZK5
B	486	GLY	-	expression tag	UNP Q9NZK5
B	487	SER	-	expression tag	UNP Q9NZK5
B	488	LEU	-	expression tag	UNP Q9NZK5
B	489	HIS	-	expression tag	UNP Q9NZK5
B	490	HIS	-	expression tag	UNP Q9NZK5
B	491	ILE	-	expression tag	UNP Q9NZK5
B	492	LEU	-	expression tag	UNP Q9NZK5
B	493	ASP	-	expression tag	UNP Q9NZK5
B	494	ALA	-	expression tag	UNP Q9NZK5
B	495	GLN	-	expression tag	UNP Q9NZK5
B	496	LYS	-	expression tag	UNP Q9NZK5
B	497	MET	-	expression tag	UNP Q9NZK5
B	498	VAL	-	expression tag	UNP Q9NZK5
B	499	TRP	-	expression tag	UNP Q9NZK5
B	500	ASN	-	expression tag	UNP Q9NZK5
B	501	HIS	-	expression tag	UNP Q9NZK5
B	502	ARG	-	expression tag	UNP Q9NZK5
B	503	HIS	-	expression tag	UNP Q9NZK5
B	504	HIS	-	expression tag	UNP Q9NZK5
B	505	HIS	-	expression tag	UNP Q9NZK5
B	506	HIS	-	expression tag	UNP Q9NZK5
B	507	HIS	-	expression tag	UNP Q9NZK5
B	508	HIS	-	expression tag	UNP Q9NZK5

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

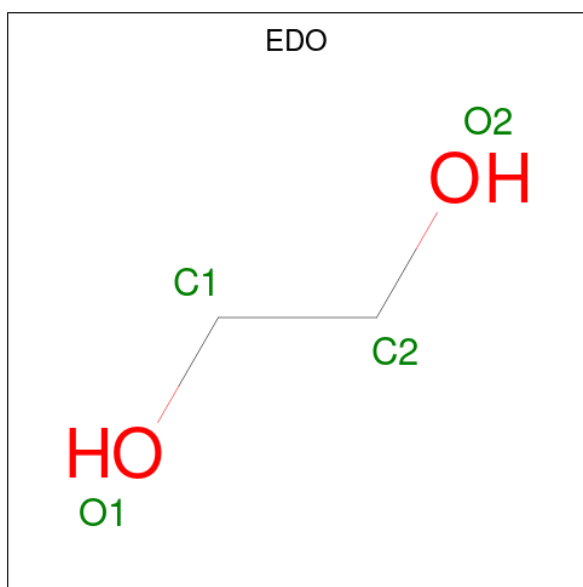


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

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

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

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is UNKNOWN ATOM OR ION (CCD ID: UNX) (formula: X).

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

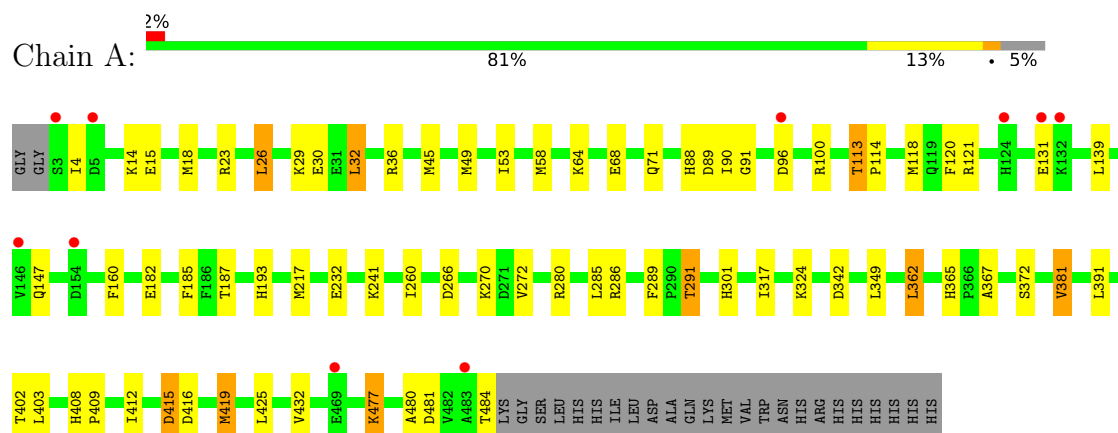
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	383	Total	O	0	0
			383	383		
6	B	406	Total	O	0	0
			406	406		

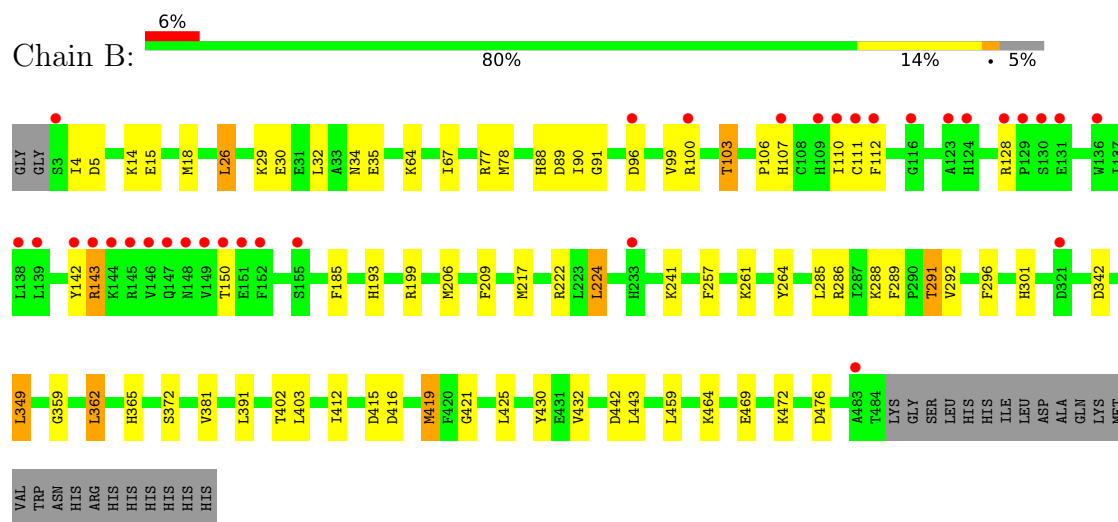
3 Residue-property plots [i](#)

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: Adenosine deaminase CECR1



• Molecule 1: Adenosine deaminase CECR1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	63.21Å 73.10Å 80.66Å 113.38° 94.18° 92.16°	Depositor
Resolution (Å)	39.68 – 2.00 39.68 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.5 (39.68-2.00) 97.5 (39.68-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.185 , 0.234 0.186 , 0.235	Depositor DCC
R_{free} test set	4277 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	23.9	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 57.6	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	0.95	EDS
Total number of atoms	8743	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.71% 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: UNX, NAG, EDO, ZN

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	0.82	0/4028	0.90	3/5447 (0.1%)
1	B	0.81	0/4032	0.91	2/5451 (0.0%)
All	All	0.82	0/8060	0.91	5/10898 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	89	ASP	N-CA-C	5.68	118.20	111.33
1	A	362	LEU	N-CA-C	5.50	117.27	111.28
1	B	143	ARG	N-CA-C	5.22	117.05	111.36
1	A	381	VAL	CB-CA-C	5.13	117.81	110.84
1	B	89	ASP	N-CA-C	5.06	117.45	111.33

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	3927	0	3920	49	0
1	B	3931	0	3931	56	0
2	A	42	0	39	0	0
2	B	42	0	39	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	4	0	6	0	0
4	B	4	0	6	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	383	0	0	10	0
6	B	406	0	0	15	1
All	All	8743	0	7941	103	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (103) 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:402:THR:HG21	6:B:765:HOH:O	1.57	1.05
1:B:91:GLY:HA2	1:B:419:MET:HE1	1.42	1.00
1:B:469:GLU:HG2	6:B:799:HOH:O	1.64	0.95
1:A:91:GLY:CA	1:A:419:MET:HE1	1.99	0.92
1:B:209:PHE:HB2	1:B:217:MET:HE2	1.52	0.91
1:B:91:GLY:CA	1:B:419:MET:HE1	2.03	0.89
1:A:91:GLY:HA2	1:A:419:MET:HE1	1.55	0.88
1:A:53:ILE:HG23	1:A:58:MET:HE1	1.62	0.80
1:B:209:PHE:CB	1:B:217:MET:HE2	2.11	0.79
1:A:113:THR:HG22	1:A:114:PRO:HD2	1.65	0.77
1:A:419:MET:N	1:A:419:MET:HE2	2.02	0.75
1:B:209:PHE:HB2	1:B:217:MET:CE	2.16	0.75
1:A:301:HIS:HE1	6:A:788:HOH:O	1.70	0.75
1:B:206:MET:HA	1:B:217:MET:HE1	1.69	0.73
1:B:103:THR:CG2	1:B:143:ARG:HH22	2.04	0.70
1:A:412:ILE:HD12	1:A:432:VAL:HG21	1.74	0.70
1:B:35:GLU:HG2	6:B:751:HOH:O	1.90	0.70
1:B:99:VAL:O	1:B:103:THR:HG22	1.92	0.69
1:A:90:ILE:HD11	1:A:185:PHE:HD1	1.58	0.68
1:B:103:THR:HG23	1:B:143:ARG:HH22	1.59	0.67
1:A:419:MET:H	1:A:419:MET:CE	2.07	0.67
1:B:301:HIS:HE1	6:B:675:HOH:O	1.77	0.66
1:B:199:ARG:NH2	6:B:805:HOH:O	2.13	0.66
1:A:26:LEU:HG	1:A:30:GLU:HB3	1.79	0.64
1:A:118:MET:CE	1:A:160:PHE:HE1	2.11	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:MET:N	1:A:419:MET:CE	2.60	0.64
1:B:217:MET:HE3	1:B:257:PHE:CZ	2.32	0.63
1:B:419:MET:HE3	1:B:419:MET:H	1.64	0.63
1:A:477:LYS:HE2	1:A:481:ASP:OD2	1.98	0.62
1:A:91:GLY:HA3	1:A:419:MET:HE1	1.78	0.62
1:B:286:ARG:HD3	6:B:544:HOH:O	2.00	0.62
2:B:650:NAG:H81	6:B:752:HOH:O	2.00	0.61
1:A:118:MET:HE3	1:A:160:PHE:HE1	1.65	0.61
1:A:324:LYS:CB	6:A:811:HOH:O	2.49	0.59
1:A:480:ALA:HA	6:A:845:HOH:O	2.01	0.59
1:B:110:ILE:HG22	6:B:551:HOH:O	2.01	0.59
1:A:365:HIS:HD2	1:B:15:GLU:OE1	1.85	0.59
1:A:266:ASP:OD1	1:A:270:LYS:HE2	2.04	0.57
1:A:419:MET:H	1:A:419:MET:HE3	1.67	0.57
1:B:34:ASN:ND2	1:B:443:LEU:H	2.04	0.56
1:B:90:ILE:HD11	1:B:185:PHE:HD1	1.70	0.56
1:A:88:HIS:CD2	1:A:415:ASP:OD1	2.59	0.56
1:A:4:ILE:HD12	6:B:671:HOH:O	2.05	0.55
1:B:419:MET:N	1:B:419:MET:CE	2.69	0.55
1:B:77:ARG:HG3	1:B:77:ARG:HH11	1.72	0.54
1:B:142:TYR:HB2	6:B:551:HOH:O	2.07	0.54
1:A:280:ARG:NH1	1:A:317:ILE:HD13	2.23	0.54
1:B:34:ASN:HD21	1:B:442:ASP:HB2	1.72	0.54
1:A:286:ARG:HD3	6:A:778:HOH:O	2.09	0.53
1:B:342:ASP:OD1	1:B:365:HIS:HE1	1.91	0.52
1:B:217:MET:HE3	1:B:257:PHE:HZ	1.74	0.52
1:B:472:LYS:NZ	1:B:476:ASP:OD1	2.43	0.52
1:A:118:MET:HE2	1:A:187:THR:HG21	1.91	0.51
1:B:88:HIS:HB2	1:B:416:ASP:OD1	2.11	0.50
1:B:26:LEU:HG	1:B:30:GLU:HB3	1.94	0.50
1:A:53:ILE:HA	1:A:58:MET:CE	2.42	0.49
1:A:342:ASP:OD2	1:A:365:HIS:HE1	1.96	0.49
1:A:118:MET:HE3	1:A:120:PHE:HE2	1.77	0.49
1:B:291:THR:HG22	1:B:292:VAL:HG23	1.95	0.48
1:A:182:GLU:HG2	6:A:543:HOH:O	2.13	0.48
1:B:111:CYS:SG	1:B:112:PHE:N	2.88	0.47
1:B:217:MET:HE3	1:B:257:PHE:CE1	2.50	0.47
1:B:419:MET:HE3	1:B:419:MET:N	2.27	0.47
1:B:419:MET:N	1:B:419:MET:HE2	2.30	0.47
1:A:118:MET:CE	1:A:160:PHE:CE1	2.95	0.47
1:A:291:THR:HG22	6:A:770:HOH:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:ASP:HB3	1:A:419:MET:HE3	1.98	0.46
1:B:349:LEU:HD21	1:B:372:SER:HB3	1.97	0.46
1:B:412:ILE:HD12	1:B:432:VAL:HG21	1.97	0.46
1:A:32:LEU:O	1:A:36:ARG:HG3	2.16	0.46
1:A:118:MET:HE3	1:A:120:PHE:CE2	2.51	0.46
1:A:217:MET:HB2	1:A:260:ILE:HG22	1.96	0.46
1:A:45:MET:O	1:A:49:MET:HG3	2.16	0.46
1:B:14:LYS:O	1:B:18:MET:HG2	2.15	0.46
1:B:193:HIS:HE1	6:B:832:HOH:O	1.99	0.46
1:B:291:THR:HB	6:B:694:HOH:O	2.16	0.46
1:A:90:ILE:CD1	1:A:185:PHE:HD1	2.28	0.45
1:B:264:TYR:O	1:B:296:PHE:HA	2.17	0.45
1:A:14:LYS:O	1:A:18:MET:HG2	2.17	0.45
1:A:53:ILE:HA	1:A:58:MET:HE3	1.99	0.45
1:A:193:HIS:HE1	6:A:570:HOH:O	1.99	0.45
1:B:90:ILE:HD11	1:B:185:PHE:CD1	2.50	0.44
1:A:241:LYS:HE2	1:A:289:PHE:HE1	1.83	0.44
1:B:106:PRO:HB2	1:B:107:HIS:CD2	2.53	0.44
1:B:342:ASP:OD1	1:B:365:HIS:CE1	2.70	0.44
1:B:64:LYS:HE3	1:B:421:GLY:O	2.17	0.44
1:A:15:GLU:OE1	1:B:365:HIS:HD2	2.00	0.44
1:A:64:LYS:HE2	1:A:68:GLU:OE2	2.17	0.43
1:B:459:LEU:O	1:B:464:LYS:HE3	2.18	0.43
1:B:67:ILE:HG12	1:B:430:TYR:CE1	2.54	0.43
1:B:359:GLY:O	1:B:362:LEU:HB2	2.18	0.43
1:B:288:LYS:HD3	1:B:289:PHE:CE2	2.54	0.42
1:A:29:LYS:HG2	6:A:845:HOH:O	2.19	0.42
1:B:261:LYS:HE3	6:B:719:HOH:O	2.18	0.42
1:B:78:MET:HE3	6:B:855:HOH:O	2.20	0.42
1:A:23:ARG:NE	6:A:872:HOH:O	2.52	0.42
1:A:408:HIS:CG	1:A:409:PRO:HD2	2.56	0.41
1:B:222:ARG:HB3	1:B:224:LEU:HD13	2.02	0.41
1:B:241:LYS:HE3	6:B:913:HOH:O	2.20	0.41
1:B:261:LYS:HE2	1:B:459:LEU:HD23	2.03	0.41
1:A:113:THR:CG2	1:A:114:PRO:HD2	2.43	0.41
1:A:71:GLN:HG2	6:A:619:HOH:O	2.21	0.40
1:A:367:ALA:HB3	1:B:15:GLU:HG3	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:801:HOH:O	6:B:838:HOH:O[1_655]	2.07	0.13

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	480/508 (94%)	474 (99%)	5 (1%)	1 (0%)	43	42
1	B	480/508 (94%)	474 (99%)	5 (1%)	1 (0%)	43	42
All	All	960/1016 (94%)	948 (99%)	10 (1%)	2 (0%)	43	42

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	415	ASP
1	B	415	ASP

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	429/452 (95%)	405 (94%)	24 (6%)	19	16
1	B	430/452 (95%)	410 (95%)	20 (5%)	23	22
All	All	859/904 (95%)	815 (95%)	44 (5%)	21	19

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	LEU
1	A	32	LEU
1	A	96	ASP
1	A	100	ARG
1	A	113	THR
1	A	121	ARG
1	A	131	GLU
1	A	139	LEU
1	A	147	GLN
1	A	232	GLU
1	A	272	VAL
1	A	285	LEU
1	A	291	THR
1	A	349	LEU
1	A	362	LEU
1	A	372	SER
1	A	381	VAL
1	A	391	LEU
1	A	402	THR
1	A	403	LEU
1	A	419	MET
1	A	425	LEU
1	A	477	LYS
1	A	484	THR
1	B	4	ILE
1	B	5	ASP
1	B	26	LEU
1	B	29	LYS
1	B	32	LEU
1	B	96	ASP
1	B	100	ARG
1	B	103	THR
1	B	128	ARG
1	B	150	THR
1	B	224	LEU
1	B	285	LEU
1	B	291	THR
1	B	349	LEU
1	B	362	LEU
1	B	381	VAL
1	B	391	LEU
1	B	403	LEU
1	B	419	MET

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Mol	Chain	Res	Type
1	B	425	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	HIS
1	A	165	GLN
1	A	174	GLN
1	A	193	HIS
1	A	301	HIS
1	A	337	GLN
1	A	365	HIS
1	A	397	ASN
1	A	448	GLN
1	B	34	ASN
1	B	166	HIS
1	B	174	GLN
1	B	193	HIS
1	B	301	HIS
1	B	365	HIS
1	B	397	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 12 ligands modelled in this entry, 2 are monoatomic and 2 are unknown - leaving 8 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
2	NAG	A	550	1	14,14,15	0.58	0	17,19,21	1.65	3 (17%)
4	EDO	B	950	-	3,3,3	0.30	0	2,2,2	0.59	0
2	NAG	A	650	1	14,14,15	0.61	0	17,19,21	1.05	1 (5%)
2	NAG	A	750	1	14,14,15	0.43	0	17,19,21	0.97	0
2	NAG	B	550	1	14,14,15	0.50	0	17,19,21	1.22	1 (5%)
2	NAG	B	650	1	14,14,15	0.71	1 (7%)	17,19,21	1.53	2 (11%)
2	NAG	B	750	1	14,14,15	0.40	0	17,19,21	0.80	0
4	EDO	A	950	-	3,3,3	0.24	0	2,2,2	1.08	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
2	NAG	A	550	1	-	0/6/23/26	0/1/1/1
4	EDO	B	950	-	-	1/1/1/1	-
2	NAG	A	650	1	-	0/6/23/26	0/1/1/1
2	NAG	A	750	1	-	0/6/23/26	0/1/1/1
2	NAG	B	550	1	1/1/5/7	1/6/23/26	0/1/1/1
2	NAG	B	650	1	-	2/6/23/26	0/1/1/1
2	NAG	B	750	1	-	0/6/23/26	0/1/1/1
4	EDO	A	950	-	-	0/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	650	NAG	C1-C2	2.03	1.55	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	550	NAG	C4-C3-C2	4.22	117.20	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	550	NAG	C3-C4-C5	3.82	117.16	110.23
2	B	650	NAG	C3-C4-C5	-3.61	103.68	110.23
2	B	650	NAG	O5-C5-C6	3.17	113.83	107.66
2	B	550	NAG	C1-O5-C5	3.10	116.33	112.19
2	A	650	NAG	C4-C3-C2	2.54	114.74	111.02
2	A	550	NAG	O5-C1-C2	-2.25	107.82	111.29

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	550	NAG	C1

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	650	NAG	C8-C7-N2-C2
2	B	650	NAG	O7-C7-N2-C2
2	B	550	NAG	C4-C5-C6-O6
4	B	950	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	650	NAG	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	482/508 (94%)	0.03	10 (2%) 63 63	12, 24, 41, 59	0
1	B	482/508 (94%)	0.17	33 (6%) 23 22	12, 24, 51, 74	0
All	All	964/1016 (94%)	0.10	43 (4%) 38 37	12, 24, 47, 74	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	146	VAL	6.6
1	B	147	GLN	4.4
1	B	149	VAL	4.3
1	B	151	GLU	3.8
1	B	131	GLU	3.4
1	B	142	TYR	3.3
1	B	139	LEU	3.1
1	B	144	LYS	3.1
1	B	136	TRP	3.0
1	B	233	HIS	3.0
1	B	148	ASN	3.0
1	B	129	PRO	2.9
1	B	152	PHE	2.8
1	B	109	HIS	2.7
1	B	321	ASP	2.7
1	B	96	ASP	2.6
1	B	143	ARG	2.6
1	B	124	HIS	2.6
1	B	138	LEU	2.6
1	B	111	CYS	2.5
1	A	483	ALA	2.5
1	B	130	SER	2.5
1	A	154	ASP	2.4
1	B	110	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	155	SER	2.4
1	A	96	ASP	2.4
1	B	150	THR	2.3
1	B	145	ARG	2.3
1	B	116	GLY	2.3
1	A	3	SER	2.2
1	B	123	ALA	2.2
1	B	112	PHE	2.2
1	B	107	HIS	2.2
1	B	3	SER	2.2
1	A	131	GLU	2.2
1	A	124	HIS	2.2
1	B	483	ALA	2.1
1	A	146	VAL	2.1
1	B	128	ARG	2.1
1	A	5	ASP	2.1
1	B	100	ARG	2.1
1	A	132	LYS	2.1
1	A	469	GLU	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	NAG	A	550	14/15	0.79	0.14	48,52,53,54	0
2	NAG	B	650	14/15	0.79	0.12	44,46,50,53	0
2	NAG	A	650	14/15	0.80	0.13	44,48,49,51	0
2	NAG	B	550	14/15	0.84	0.11	43,46,47,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	A	750	14/15	0.86	0.11	41,43,47,49	0
5	UNX	B	951	1/1	0.87	0.54	29,29,29,29	0
2	NAG	B	750	14/15	0.89	0.09	40,42,45,45	0
5	UNX	A	951	1/1	0.90	0.55	25,25,25,25	0
4	EDO	B	950	4/4	0.93	0.12	18,19,21,23	0
4	EDO	A	950	4/4	0.94	0.12	22,25,27,27	0
3	ZN	A	850	1/1	0.99	0.04	30,30,30,30	0
3	ZN	B	850	1/1	0.99	0.06	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.