Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:15 AM GMT

PDB ID	:	3LGD
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

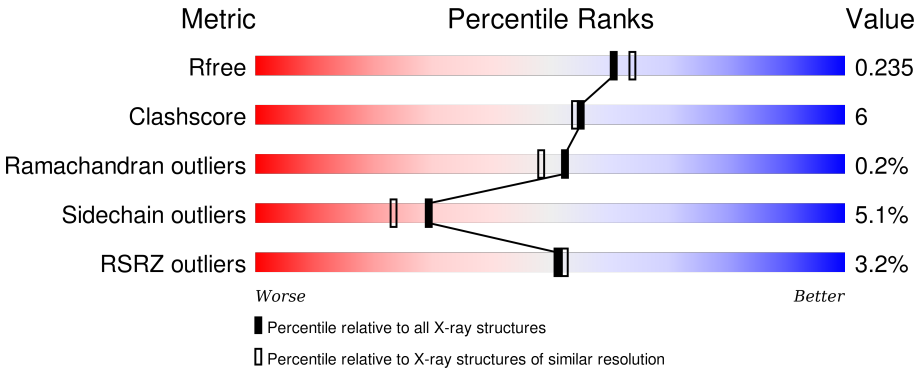
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	2% 81% 12% • 5%
1	B	508	4% 80% 13% • 5%

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	A	650	-	-	-	X
2	NAG	A	750	-	-	-	X
2	NAG	B	550	X	-	-	-
2	NAG	B	650	-	-	-	X
5	UNX	A	951	-	-	-	X
5	UNX	B	951	-	-	-	X

2 Entry composition (i)

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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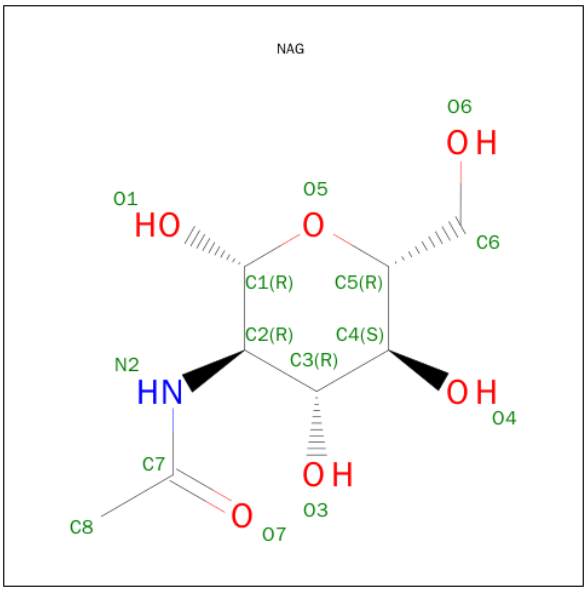
Chain	Residue	Modelled	Actual	Comment	Reference
B	1	GLY	-	EXPRESSION TAG	UNP Q9NZK5
B	2	GLY	-	EXPRESSION TAG	UNP Q9NZK5
B	486	GLY	-	EXPRESSION TAG	UNP Q9NZK5
B	487	SER	-	EXPRESSION TAG	UNP Q9NZK5
B	488	LEU	-	EXPRESSION TAG	UNP Q9NZK5
B	489	HIS	-	EXPRESSION TAG	UNP Q9NZK5
B	490	HIS	-	EXPRESSION TAG	UNP 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 SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

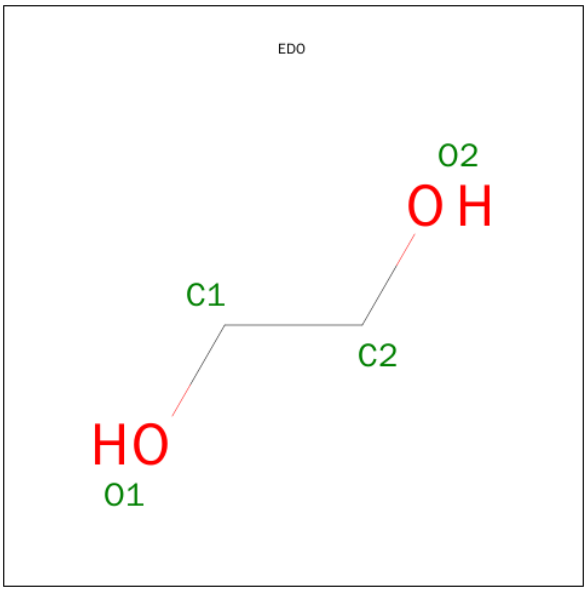


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 5 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

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

- Molecule 6 is water.

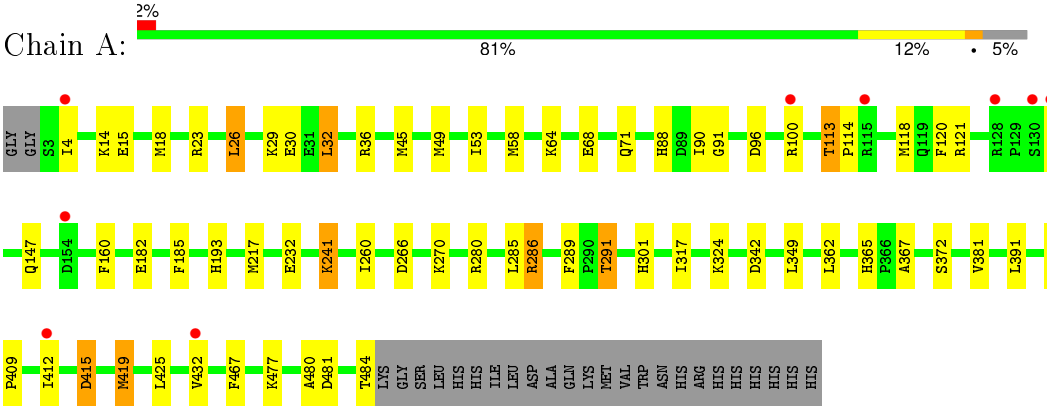
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	383	Total O 383 383	0	0
6	B	406	Total O 406 406	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

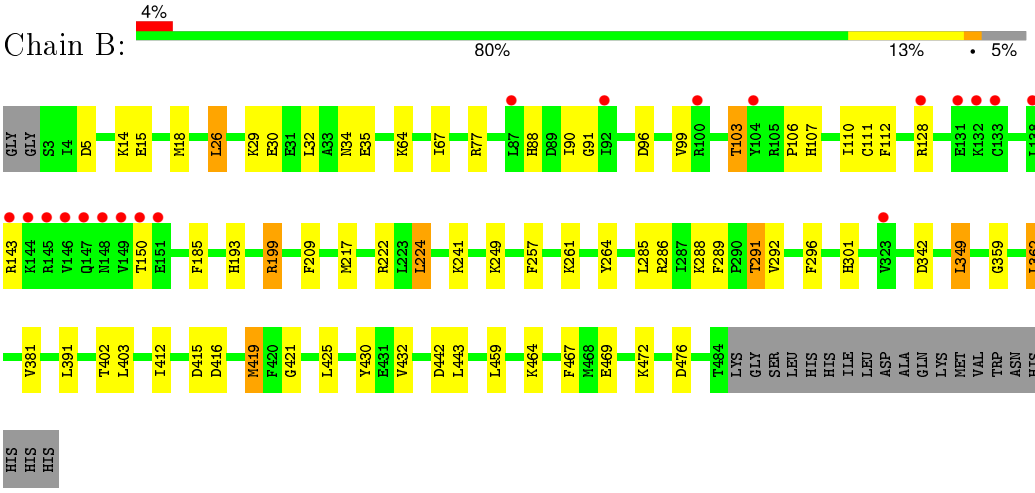
- Molecule 1: Adenosine deaminase CECR1

Chain A:



- Molecule 1: Adenosine deaminase CECR1

Chain B:



4 Data and refinement statistics (i)

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 39.70 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.5 (39.68-2.00) 83.7 (39.70-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [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	4276 reflections (5.18%)	DCC
Wilson B-factor (Å^2)	23.9	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 65.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 86869 reflections	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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, ZN, NAG, EDO

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	0.66	0/4028	0.67	1/5447 (0.0%)
1	B	0.66	0/4032	0.68	1/5451 (0.0%)
All	All	0.66	0/8060	0.67	2/10898 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	199	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	A	286	ARG	NE-CZ-NH2	-5.03	117.78	120.30

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	51	0
1	B	3931	0	3931	51	0
2	A	42	0	39	0	0
2	B	42	0	39	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	4	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	14	1
All	All	8743	0	7941	100	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 (100) 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:209:PHE:HB2	1:B:217:MET:HE1	1.28	1.12
1:B:402:THR:HG21	6:B:765:HOH:O	1.57	1.05
1:B:91:GLY:HA2	1:B:419:MET:HE1	1.41	0.99
1:A:419:MET:HE3	1:A:419:MET:H	1.28	0.99
1:B:469:GLU:HG2	6:B:799:HOH:O	1.64	0.95
1:A:419:MET:N	1:A:419:MET:HE3	1.90	0.86
1:B:91:GLY:CA	1:B:419:MET:HE1	2.14	0.78
1:A:113:THR:HG22	1:A:114:PRO:HD2	1.65	0.77
1:A:301:HIS:HE1	6:A:788:HOH:O	1.70	0.75
1:B:419:MET:N	1:B:419:MET:HE2	2.03	0.73
1:A:91:GLY:CA	1:A:419:MET:HE1	2.22	0.70
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:91:GLY:HA3	1:A:419:MET:HE1	1.77	0.67
1:B:209:PHE:HB2	1:B:217:MET:CE	2.16	0.67
1:A:53:ILE:HA	1:A:58:MET:HE3	1.75	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:419:MET:CE	1:A:419:MET:H	2.07	0.65
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
1:A:419:MET:N	1:A:419:MET:CE	2.60	0.63
1:B:209:PHE:CB	1:B:217:MET:HE1	2.18	0.63
1:A:477:LYS:HE2	1:A:481:ASP:OD2	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:90:ILE:HD11	1:B:185:PHE:HD1	1.70	0.56
1:B:34:ASN:ND2	1:B:443:LEU:H	2.04	0.56
1:A:88:HIS:CD2	1:A:415:ASP:OD1	2.59	0.56
1:B:419:MET:N	1:B:419:MET:CE	2.69	0.55
1:A:4:ILE:HD12	6:B:671:HOH:O	2.05	0.55
1:B:142:TYR:HB2	6:B:551:HOH:O	2.07	0.54
1:B:77:ARG:HG3	1:B:77:ARG:HH11	1.72	0.54
1:B:34:ASN:HD21	1:B:442:ASP:HB2	1.72	0.54
1:A:280:ARG:NH1	1:A:317:ILE:HD13	2.23	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:472:LYS:NZ	1:B:476:ASP:OD1	2.43	0.52
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:118:MET:HE3	1:A:120:PHE:HE2	1.76	0.50
1:A:342:ASP:OD2	1:A:365:HIS:HE1	1.96	0.49
1:A:118:MET:HE1	1:A:160:PHE:CE1	2.47	0.49
1:B:291:THR:HG22	1:B:292:VAL:HG23	1.95	0.48
1:A:91:GLY:HA2	1:A:419:MET:CE	2.43	0.48
1:A:182:GLU:HG2	6:A:543:HOH:O	2.13	0.48
1:B:217:MET:HE3	1:B:257:PHE:CZ	2.50	0.47
1:B:111:CYS:SG	1:B:112:PHE:N	2.88	0.47
1:A:118:MET:HE3	1:A:160:PHE:HE1	1.78	0.47
1:A:291:THR:HG22	6:A:770:HOH:O	2.15	0.47
1:A:53:ILE:HA	1:A:58:MET:CE	2.42	0.47
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:217:MET:HB2	1:A:260:ILE:HG22	1.96	0.46
1:A:32:LEU:O	1:A:36:ARG:HG3	2.16	0.46
1:B:14:LYS:O	1:B:18:MET:HG2	2.15	0.46
1:A:45:MET:O	1:A:49:MET:HG3	2.16	0.46
1:B:291:THR:HB	6:B:694:HOH:O	2.16	0.46
1:B:193:HIS:HE1	6:B:832:HOH:O	1.99	0.46
1:A:90:ILE:CD1	1:A:185:PHE:HD1	2.28	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:ILE:CA	1:A:58:MET:HE3	2.44	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: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:B:419:MET:H	1:B:419:MET:CE	2.29	0.44
1:A:241:LYS:HE2	1:A:289:PHE:HE1	1.83	0.44
1:B:342:ASP:OD1	1:B:365:HIS:CE1	2.70	0.44
1:B:106:PRO:HB2	1:B:107:HIS:CD2	2.53	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:118:MET:HE1	1:A:160:PHE:HE1	1.83	0.43
1:A:64:LYS:HE2	1:A:68:GLU:OE2	2.17	0.43
1:A:91:GLY:HA2	1:A:419:MET:HE1	1.96	0.43
1:A:53:ILE:HG23	1:A:58:MET:HE3	1.99	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:A:118:MET:CE	1:A:160:PHE:CE1	2.95	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: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:261:LYS:HE2	1:B:459:LEU:HD23	2.03	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:A:113:THR:CG2	1:A:114:PRO:HD2	2.43	0.41
1:A:367:ALA:HB3	1:B:15:GLU:HG3	2.03	0.40
1:A:71:GLN:HG2	6:A:619:HOH:O	2.21	0.40
1:A:118:MET:HE3	1:A:120:PHE:CE2	2.54	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%)	52 48
1	B	480/508 (94%)	474 (99%)	5 (1%)	1 (0%)	52 48
All	All	960/1016 (94%)	948 (99%)	10 (1%)	2 (0%)	52 48

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%)	26 20
1	B	430/452 (95%)	410 (95%)	20 (5%)	32 27
All	All	859/904 (95%)	815 (95%)	44 (5%)	29 23

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

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Mol	Chain	Res	Type
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	241	LYS
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	467	PHE
1	A	484	THR
1	B	5	ASP
1	B	26	LEU
1	B	29	LYS
1	B	32	LEU
1	B	96	ASP
1	B	103	THR
1	B	128	ARG
1	B	150	THR
1	B	224	LEU
1	B	249	LYS
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
1	B	425	LEU
1	B	467	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	HIS
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	B	34	ASN
1	B	65	HIS
1	B	174	GLN
1	B	193	HIS
1	B	301	HIS
1	B	337	GLN
1	B	365	HIS
1	B	397	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 2 are unknown and 2 are monoatomic - 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	0.56	0	15,19,21	1.62	2 (13%)
2	NAG	A	650	1	14,14,15	0.58	0	15,19,21	1.08	2 (13%)
2	NAG	A	750	1	14,14,15	0.43	0	15,19,21	0.95	0
4	EDO	A	950	-	3,3,3	0.26	0	2,2,2	1.17	0
2	NAG	B	550	1	14,14,15	0.49	0	15,19,21	1.22	1 (6%)
2	NAG	B	650	1	14,14,15	0.68	0	15,19,21	1.53	2 (13%)
2	NAG	B	750	1	14,14,15	0.40	0	15,19,21	0.81	0
4	EDO	B	950	-	3,3,3	0.31	0	2,2,2	0.65	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
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
4	EDO	A	950	-	-	0/1/1/1	0/0/0/0
2	NAG	B	550	1	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	B	650	1	-	0/6/23/26	0/1/1/1
2	NAG	B	750	1	-	0/6/23/26	0/1/1/1
4	EDO	B	950	-	-	0/1/1/1	0/0/0/0

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	650	NAG	C3-C4-C5	-3.74	103.68	110.20
2	A	650	NAG	C1-O5-C5	2.00	114.79	112.25
2	A	650	NAG	C4-C3-C2	2.26	114.74	111.23
2	B	650	NAG	O5-C5-C6	3.00	113.83	107.35
2	B	550	NAG	C1-O5-C5	3.22	116.33	112.25
2	A	550	NAG	C4-C3-C2	3.84	117.20	111.23
2	A	550	NAG	C3-C4-C5	3.99	117.16	110.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	550	NAG	C1

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
2	B	650	NAG	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, 95^{th} 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%)	-0.14	10 (2%)	67	67	12, 24, 41, 59	0
1	B	482/508 (94%)	0.04	21 (4%)	38	39	12, 24, 51, 74	0
All	All	964/1016 (94%)	-0.05	31 (3%)	51	52	12, 24, 47, 74	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	147	GLN	8.3
1	B	149	VAL	8.3
1	B	146	VAL	8.0
1	B	131	GLU	5.5
1	B	148	ASN	4.3
1	B	128	ARG	4.0
1	A	131	GLU	4.0
1	B	150	THR	3.9
1	B	100	ARG	3.8
1	B	144	LYS	3.6
1	B	141	ASP	3.5
1	B	138	LEU	3.5
1	A	128	ARG	3.4
1	B	104	TYR	3.4
1	B	151	GLU	3.3
1	A	132	LYS	3.2
1	B	140	GLU	3.1
1	A	115	ARG	3.0
1	B	143	ARG	2.9
1	B	132	LYS	2.7
1	A	154	ASP	2.6
1	A	4	ILE	2.5
1	A	412	ILE	2.2
1	B	145	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	432	VAL	2.2
1	B	87	LEU	2.2
1	A	130	SER	2.1
1	B	133	CYS	2.1
1	B	323	VAL	2.1
1	A	100	ARG	2.1
1	B	92	ILE	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
5	UNX	A	951	1/1	0.94	0.83	23.86	25,25,25,25	0
5	UNX	B	951	1/1	0.93	0.87	23.05	29,29,29,29	0
2	NAG	A	650	14/15	0.82	0.19	4.46	44,48,49,51	0
2	NAG	A	750	14/15	0.86	0.22	3.01	41,43,47,49	0
2	NAG	B	650	14/15	0.82	0.25	2.92	44,46,50,53	0
2	NAG	B	750	14/15	0.91	0.14	0.46	40,42,45,45	0
4	EDO	A	950	4/4	0.94	0.13	-0.38	22,25,27,27	0
4	EDO	B	950	4/4	0.95	0.10	-2.06	18,19,21,23	0
3	ZN	A	850	1/1	0.99	0.07	-	30,30,30,30	0
2	NAG	A	550	14/15	0.81	0.22	-	48,52,53,54	0
3	ZN	B	850	1/1	0.99	0.05	-	30,30,30,30	0
2	NAG	B	550	14/15	0.78	0.19	-	43,46,47,48	0

6.5 Other polymers (i)

There are no such residues in this entry.