Full wwPDB X-ray Structure Validation Report (i)

Oct 15, 2023 – 01:21 PM EDT

PDB ID	:	8E0W
Title	:	Crystal structure of mouse APCDD1 in P1 space group
Authors	:	Hsieh, F.L.; Chang, T.H.; Gabelli, S.B.; Nathans, J.
Deposited on	:	2022-08-09
Resolution	:	2.15 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 (i) 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 (1)) were used in the production of this report:

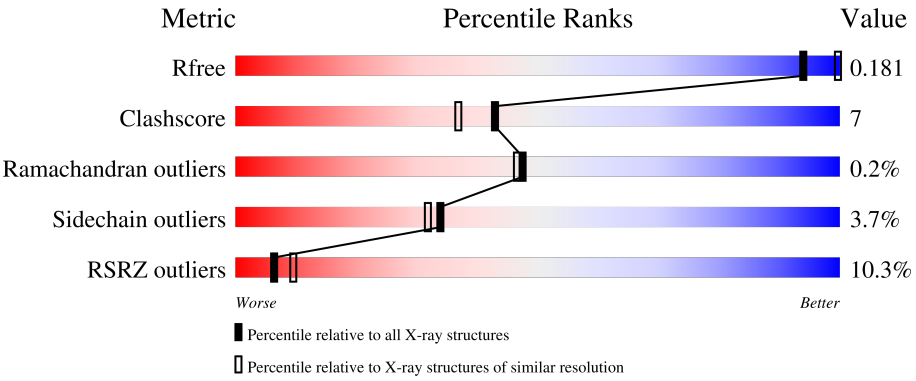
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.15 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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 <=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	468	8% 76% 12% • 11%
1	B	468	10% 69% 16% • 13%

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	502	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7002 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.

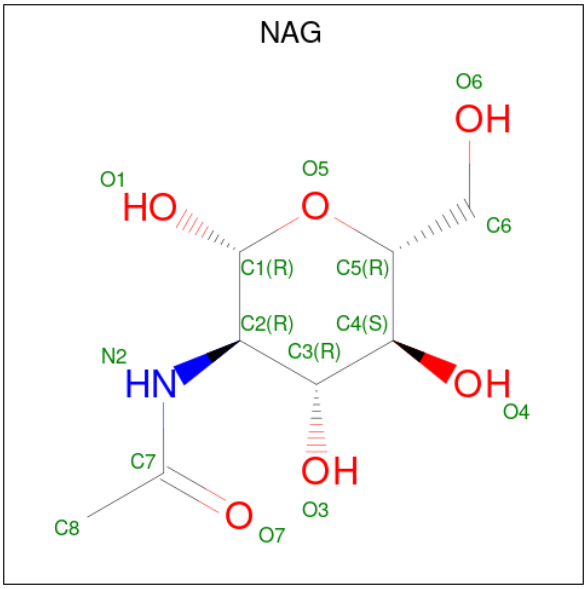
- Molecule 1 is a protein called Protein APCDD1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	418	Total	C	N	O	S	0	0	0
			3373	2127	614	610	22			
1	B	409	Total	C	N	O	S	0	3	0
			3343	2109	610	602	22			

There are 24 discrepancies between the modelled and reference sequences:

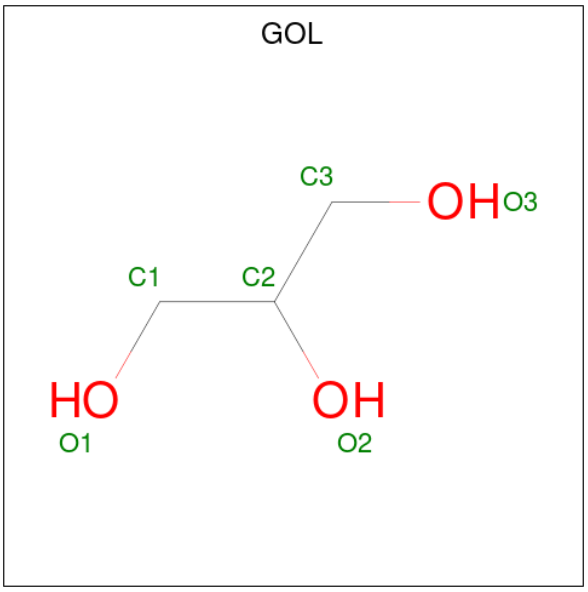
Chain	Residue	Modelled	Actual	Comment	Reference
A	24	GLU	-	expression tag	UNP Q3U128
A	25	THR	-	expression tag	UNP Q3U128
A	26	GLY	-	expression tag	UNP Q3U128
A	483	THR	-	expression tag	UNP Q3U128
A	484	HIS	-	expression tag	UNP Q3U128
A	485	HIS	-	expression tag	UNP Q3U128
A	486	HIS	-	expression tag	UNP Q3U128
A	487	HIS	-	expression tag	UNP Q3U128
A	488	HIS	-	expression tag	UNP Q3U128
A	489	HIS	-	expression tag	UNP Q3U128
A	490	HIS	-	expression tag	UNP Q3U128
A	491	HIS	-	expression tag	UNP Q3U128
B	24	GLU	-	expression tag	UNP Q3U128
B	25	THR	-	expression tag	UNP Q3U128
B	26	GLY	-	expression tag	UNP Q3U128
B	483	THR	-	expression tag	UNP Q3U128
B	484	HIS	-	expression tag	UNP Q3U128
B	485	HIS	-	expression tag	UNP Q3U128
B	486	HIS	-	expression tag	UNP Q3U128
B	487	HIS	-	expression tag	UNP Q3U128
B	488	HIS	-	expression tag	UNP Q3U128
B	489	HIS	-	expression tag	UNP Q3U128
B	490	HIS	-	expression tag	UNP Q3U128
B	491	HIS	-	expression tag	UNP Q3U128

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (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 GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 5 is water.

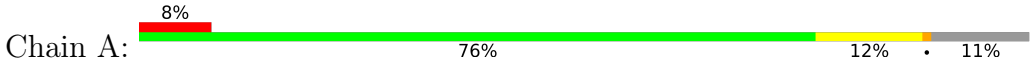
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	97	Total O 97 97	0	0
5	B	85	Total O 85 85	0	0

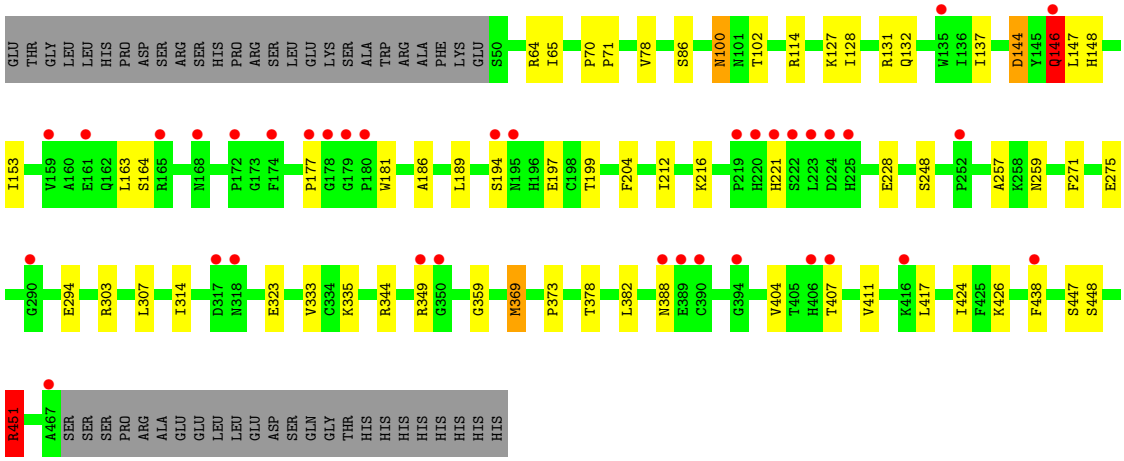
3 Residue-property plots (i)

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: Protein APCDD1

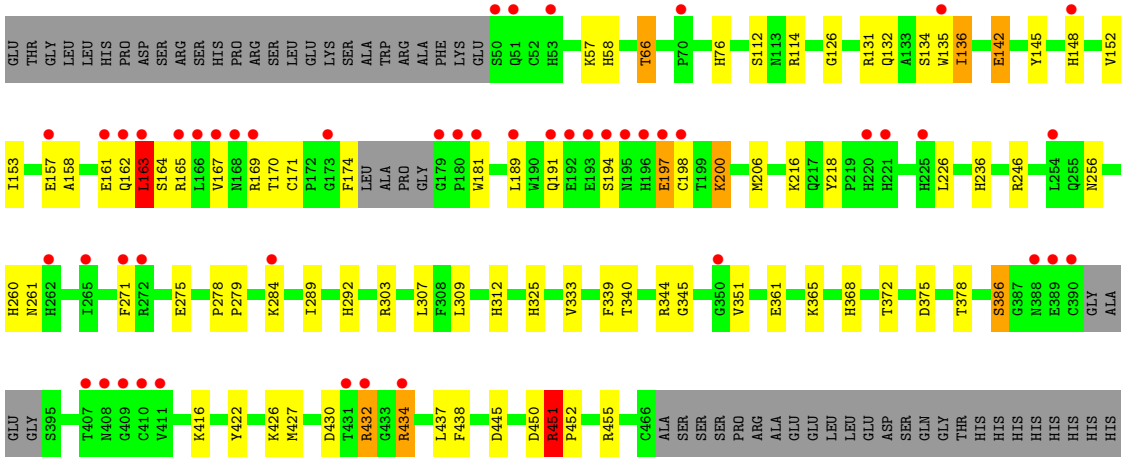
Chain A:





• Molecule 1: Protein APCDD1

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	50.34Å 65.60Å 79.69Å 74.50° 76.82° 72.23°	Depositor
Resolution (Å)	33.93 – 2.15 33.93 – 2.15	Depositor EDS
% Data completeness (in resolution range)	68.2 (33.93-2.15) 68.2 (33.93-2.15)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.32 (at 2.16Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.179 , 0.220 0.186 , 0.181	Depositor DCC
R_{free} test set	2000 reflections (5.87%)	wwPDB-VP
Wilson B-factor (Å^2)	41.6	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 34.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7002	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.44% 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, 0.333 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: CL, GOL, NAG

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	0.42	0/3473	0.66	4/4718 (0.1%)
1	B	0.54	6/3447 (0.2%)	1.03	19/4679 (0.4%)
All	All	0.48	6/6920 (0.1%)	0.86	23/9397 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	3
All	All	0	4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	261[A]	ASN	C-O	6.94	1.36	1.23
1	B	261[B]	ASN	C-O	6.94	1.36	1.23
1	B	292[A]	HIS	C-O	6.77	1.36	1.23
1	B	292[B]	HIS	C-O	6.77	1.36	1.23
1	B	142	GLU	CD-OE1	5.41	1.31	1.25
1	B	432	ARG	CZ-NH1	-5.10	1.26	1.33

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	163	LEU	CB-CG-CD2	-36.12	49.59	111.00
1	B	451	ARG	CB-CG-CD	16.77	155.22	111.60
1	B	163	LEU	CB-CG-CD1	16.72	139.42	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	146	GLN	CA-CB-CG	-12.58	85.72	113.40
1	B	142	GLU	CA-CB-CG	10.43	136.35	113.40
1	B	432	ARG	CG-CD-NE	10.31	133.46	111.80
1	B	451	ARG	NE-CZ-NH1	-8.97	115.81	120.30
1	B	451	ARG	CD-NE-CZ	-8.42	111.82	123.60
1	B	142	GLU	CB-CA-C	6.87	124.14	110.40
1	B	163	LEU	CD1-CG-CD2	-6.39	91.33	110.50
1	B	432	ARG	NE-CZ-NH1	-6.33	117.13	120.30
1	A	451	ARG	CG-CD-NE	6.25	124.93	111.80
1	B	451	ARG	CA-CB-CG	-5.82	100.59	113.40
1	B	451	ARG	NE-CZ-NH2	5.63	123.12	120.30
1	B	434	ARG	CB-CG-CD	-5.46	97.40	111.60
1	B	261[A]	ASN	CA-C-O	5.40	131.44	120.10
1	B	261[B]	ASN	CA-C-O	5.40	131.44	120.10
1	B	292[A]	HIS	CA-C-O	5.37	131.37	120.10
1	B	292[B]	HIS	CA-C-O	5.37	131.37	120.10
1	B	434	ARG	CA-CB-CG	5.35	125.17	113.40
1	B	142	GLU	OE1-CD-OE2	-5.31	116.93	123.30
1	A	447	SER	C-N-CA	5.10	134.45	121.70
1	A	146	GLN	CB-CG-CD	5.06	124.75	111.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	451	ARG	Sidechain
1	B	432	ARG	Sidechain,Peptide
1	B	451	ARG	Sidechain

5.2 Too-close contacts (i)

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	3373	0	3214	32	1
1	B	3343	0	3185	59	0
2	A	42	0	39	1	0
2	B	42	0	39	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	6	0	7	0	0
3	B	12	0	16	3	1
4	A	1	0	0	1	0
4	B	1	0	0	1	0
5	A	97	0	0	0	0
5	B	85	0	0	2	0
All	All	7002	0	6500	91	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 7.

All (91) 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:A:146:GLN:HG3	1:A:147:LEU:N	1.76	0.98
1:B:197:GLU:O	1:B:200:LYS:NZ	2.09	0.86
1:B:66:THR:HG23	1:B:216:LYS:HB2	1.66	0.77
1:B:126:GLY:HA2	1:B:148:HIS:HB2	1.67	0.77
1:B:200:LYS:HD3	1:B:200:LYS:H	1.49	0.76
1:A:228:GLU:OE1	1:A:259:ASN:ND2	2.19	0.74
1:B:216:LYS:HB3	1:B:226:LEU:HD11	1.71	0.73
1:B:303:ARG:NH2	4:B:506:CL:CL	2.63	0.67
1:A:153:ILE:HD12	1:A:275:GLU:HB2	1.78	0.65
1:B:164:SER:HB3	1:B:181:TRP:HB2	1.77	0.65
1:B:375:ASP:OD1	1:B:378:THR:OG1	2.10	0.65
1:A:146:GLN:HG3	1:A:147:LEU:H	1.60	0.64
1:B:152:VAL:HG21	1:B:163:LEU:HD12	1.80	0.63
1:A:323:GLU:HG2	1:A:344:ARG:HG3	1.82	0.62
1:B:161:GLU:O	1:B:165:ARG:HG3	2.00	0.61
1:B:434:ARG:HH21	1:B:434:ARG:HG2	1.66	0.60
1:B:198:CYS:HA	1:B:200:LYS:NZ	2.17	0.59
1:B:236:HIS:CE1	3:B:505:GOL:H31	2.38	0.58
1:B:153:ILE:CD1	1:B:275:GLU:HB2	2.34	0.58
1:A:153:ILE:HG12	1:A:186:ALA:HA	1.86	0.57
1:A:137:ILE:HD11	1:A:248:SER:HA	1.85	0.57
1:B:134:SER:HA	1:B:142:GLU:OE2	2.04	0.57
1:B:152:VAL:HG21	1:B:163:LEU:CD1	2.34	0.57
1:A:373:PRO:HB3	1:A:378:THR:HG22	1.86	0.56
1:B:339:PHE:HB3	1:B:378:THR:HG21	1.86	0.56
1:A:373:PRO:HG3	1:A:382:LEU:HD12	1.87	0.56
1:B:126:GLY:HA2	1:B:148:HIS:CB	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:TYR:CZ	1:B:226:LEU:HD13	2.41	0.56
1:B:450:ASP:OD1	1:B:451:ARG:HG3	2.07	0.55
1:B:112:SER:HB3	5:B:614:HOH:O	2.06	0.54
1:B:153:ILE:HD12	1:B:275:GLU:HB2	1.92	0.52
1:B:236:HIS:HE1	3:B:505:GOL:H31	1.75	0.52
1:A:257:ALA:HA	1:A:271:PHE:CZ	2.45	0.52
1:A:426:LYS:HG2	1:A:438:PHE:HB2	1.92	0.51
1:A:359:GLY:HA3	1:A:424:ILE:HD11	1.93	0.50
1:B:427:MET:HE2	1:B:437:LEU:HD13	1.93	0.50
1:B:165:ARG:O	1:B:169:ARG:HG2	2.11	0.50
1:B:157:GLU:O	1:B:161:GLU:HG2	2.13	0.49
1:B:145:TYR:CE2	1:B:206:MET:HB3	2.47	0.49
1:A:199:THR:HB	1:A:204:PHE:HB3	1.94	0.49
1:A:164:SER:HB3	1:A:181:TRP:HB2	1.95	0.49
1:B:170:THR:HG22	1:B:171:CYS:SG	2.53	0.49
1:B:430:ASP:OD1	1:B:434:ARG:HD2	2.13	0.48
1:A:102:THR:HG22	1:A:127:LYS:HG2	1.96	0.48
1:B:445:ASP:HB3	3:B:505:GOL:H32	1.95	0.47
1:A:369:MET:HE2	1:A:369:MET:HB2	1.67	0.47
1:A:369:MET:HE3	1:A:417:LEU:HD11	1.96	0.47
1:B:345:GLY:HA3	1:B:365:LYS:O	2.15	0.47
1:B:135:TRP:N	1:B:142:GLU:OE2	2.37	0.47
1:A:64:ARG:HD3	1:A:221:HIS:HA	1.95	0.46
1:B:386:SER:O	1:B:386:SER:OG	2.29	0.46
1:B:289:ILE:HD11	1:B:426:LYS:C	2.35	0.46
1:B:191:GLN:HB2	1:B:194:SER:HB2	1.98	0.46
1:B:200:LYS:H	1:B:200:LYS:CD	2.24	0.46
1:A:78:VAL:HG21	1:A:271:PHE:CD2	2.51	0.45
1:B:218:TYR:CE1	1:B:226:LEU:HB2	2.51	0.45
1:B:76:HIS:HD1	1:B:271:PHE:HD1	1.64	0.45
1:B:422:TYR:CE2	1:B:452:PRO:HG3	2.51	0.45
1:B:131:ARG:HB3	1:B:132[B]:GLN:OE1	2.15	0.45
1:A:100:ASN:OD1	1:A:100:ASN:N	2.49	0.45
1:B:158:ALA:O	1:B:161:GLU:HG3	2.17	0.44
1:B:434:ARG:HH21	1:B:434:ARG:CG	2.30	0.44
1:A:131:ARG:HE	1:A:144:ASP:HB2	1.83	0.43
1:A:333:VAL:HG23	1:A:335:LYS:HG3	1.99	0.43
1:B:312:HIS:HB3	1:B:325:HIS:HB2	2.01	0.43
1:B:136:ILE:H	1:B:136:ILE:HG13	1.68	0.43
1:A:128:ILE:HD11	1:A:212:ILE:HD11	2.01	0.43
1:B:340:THR:HB	1:B:372:THR:HB	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:LEU:O	1:B:167:VAL:HG23	2.19	0.43
1:B:256:ASN:O	1:B:260:HIS:HB3	2.18	0.42
1:A:404:VAL:HG23	1:A:411:VAL:HG13	2.00	0.42
1:A:294:GLU:HG2	1:A:314:ILE:HG12	2.01	0.42
1:B:344:ARG:NH2	1:B:368:HIS:CD2	2.87	0.42
1:B:114:ARG:HD3	1:B:284:LYS:H	1.83	0.42
1:B:153:ILE:HD11	1:B:275:GLU:HB2	2.01	0.42
1:B:158:ALA:O	1:B:162:GLN:HG3	2.20	0.41
1:A:303:ARG:NH2	4:A:505:CL:CL	2.90	0.41
1:A:163:LEU:HA	1:A:163:LEU:HD12	1.81	0.41
1:B:189:LEU:HD22	1:B:198:CYS:O	2.21	0.41
1:A:70:PRO:HA	1:A:71:PRO:HD3	1.92	0.41
1:B:450:ASP:C	1:B:451:ARG:HG2	2.40	0.41
1:B:455:ARG:NH2	5:B:607:HOH:O	2.50	0.41
1:A:127:LYS:HG3	1:A:148:HIS:HE1	1.86	0.40
1:A:177:PRO:HA	2:A:502:NAG:H4	2.04	0.40
1:B:278:PRO:HA	1:B:279:PRO:HD3	1.97	0.40
1:B:351:VAL:HG22	1:B:361:GLU:HB2	2.03	0.40
1:A:65:ILE:HA	1:A:216:LYS:O	2.21	0.40
1:A:369:MET:CE	1:A:417:LEU:HD21	2.52	0.40
1:B:114:ARG:NE	1:B:114:ARG:HA	2.36	0.40
1:B:198:CYS:HA	1:B:200:LYS:HZ2	1.85	0.40
1:B:426:LYS:HG2	1:B:438:PHE:HB2	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)
1:A:388:ASN:ND2	3:B:504:GOL:O2[1_546]	1.90	0.30

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	416/468 (89%)	396 (95%)	19 (5%)	1 (0%)	47	46
1	B	406/468 (87%)	384 (95%)	21 (5%)	1 (0%)	47	46
All	All	822/936 (88%)	780 (95%)	40 (5%)	2 (0%)	47	46

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	307	LEU
1	B	307	LEU

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	366/411 (89%)	352 (96%)	14 (4%)	33	31
1	B	366/411 (89%)	353 (96%)	13 (4%)	35	33
All	All	732/822 (89%)	705 (96%)	27 (4%)	34	32

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	SER
1	A	100	ASN
1	A	114	ARG
1	A	132	GLN
1	A	144	ASP
1	A	146	GLN
1	A	189	LEU
1	A	194	SER
1	A	197	GLU
1	A	349	ARG
1	A	369	MET
1	A	407	THR
1	A	448	SER
1	A	451	ARG

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Mol	Chain	Res	Type
1	B	57	LYS
1	B	58	HIS
1	B	66	THR
1	B	136	ILE
1	B	163	LEU
1	B	174	PHE
1	B	197	GLU
1	B	200	LYS
1	B	246	ARG
1	B	309	LEU
1	B	333	VAL
1	B	386	SER
1	B	416	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	148	HIS
1	B	368	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 2 are monoatomic - leaving 9 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	GOL	B	505	-	5,5,5	0.66	0	5,5,5	1.05	0
2	NAG	B	501	1	14,14,15	0.39	0	17,19,21	0.56	0
3	GOL	A	504	-	5,5,5	1.22	1 (20%)	5,5,5	0.69	0
3	GOL	B	504	-	5,5,5	0.89	0	5,5,5	0.99	0
2	NAG	A	503	1	14,14,15	0.31	0	17,19,21	0.45	0
2	NAG	A	501	1	14,14,15	0.43	0	17,19,21	1.48	2 (11%)
2	NAG	A	502	1	14,14,15	0.78	1 (7%)	17,19,21	1.31	2 (11%)
2	NAG	B	503	1	14,14,15	0.39	0	17,19,21	0.38	0
2	NAG	B	502	1	14,14,15	0.32	0	17,19,21	0.42	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
3	GOL	B	505	-	-	0/4/4/4	-
2	NAG	B	501	1	-	0/6/23/26	0/1/1/1
3	GOL	A	504	-	-	0/4/4/4	-
3	GOL	B	504	-	-	2/4/4/4	-
2	NAG	A	503	1	-	0/6/23/26	0/1/1/1
2	NAG	A	501	1	-	3/6/23/26	0/1/1/1
2	NAG	A	502	1	-	1/6/23/26	0/1/1/1
2	NAG	B	503	1	-	0/6/23/26	0/1/1/1
2	NAG	B	502	1	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	502	NAG	C1-C2	2.56	1.56	1.52
3	A	504	GOL	O2-C2	-2.21	1.36	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	502	NAG	C2-N2-C7	4.26	128.97	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	NAG	C1-O5-C5	-4.18	106.52	112.19
2	A	501	NAG	C2-N2-C7	2.76	126.84	122.90
2	A	502	NAG	C1-C2-N2	2.57	114.87	110.49

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	NAG	C3-C2-N2-C7
2	A	501	NAG	C8-C7-N2-C2
2	A	501	NAG	O7-C7-N2-C2
2	A	502	NAG	C1-C2-N2-C7
3	B	504	GOL	O1-C1-C2-C3
3	B	504	GOL	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	505	GOL	3	0
3	B	504	GOL	0	1
2	A	502	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, 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	418/468 (89%)	0.67	36 (8%)	10	15	30, 52, 97, 154	0
1	B	409/468 (87%)	0.73	49 (11%)	4	6	30, 54, 110, 177	0
All	All	827/936 (88%)	0.70	85 (10%)	6	9	30, 53, 107, 177	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	194	SER	7.4
1	A	179	GLY	7.3
1	A	388	ASN	6.1
1	B	388	ASN	6.1
1	B	195	ASN	6.1
1	A	221	HIS	5.8
1	A	220	HIS	5.1
1	B	196	HIS	5.0
1	B	193	GLU	5.0
1	B	432	ARG	4.9
1	B	431	THR	4.7
1	A	177	PRO	4.5
1	B	411	VAL	4.5
1	B	389	GLU	4.5
1	A	135	TRP	4.5
1	B	191	GLN	4.3
1	A	180	PRO	4.3
1	A	178	GLY	4.2
1	A	389	GLU	4.1
1	B	135	TRP	4.1
1	B	179	GLY	4.0
1	B	410	CYS	3.9
1	B	181	TRP	3.9
1	B	168	ASN	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	225	HIS	3.7
1	A	467	ALA	3.4
1	B	221	HIS	3.4
1	B	390	CYS	3.4
1	A	225	HIS	3.2
1	B	50	SER	3.2
1	B	262	HIS	3.1
1	B	408	ASN	3.0
1	B	409	GLY	2.9
1	B	166	LEU	2.9
1	A	219	PRO	2.9
1	A	416	LYS	2.8
1	B	197	GLU	2.7
1	B	169	ARG	2.7
1	B	157	GLU	2.7
1	B	163	LEU	2.7
1	A	174	PHE	2.7
1	A	350	GLY	2.6
1	B	198	CYS	2.6
1	B	407	THR	2.6
1	A	165	ARG	2.6
1	B	148	HIS	2.6
1	A	290	GLY	2.6
1	B	53	HIS	2.6
1	A	146	GLN	2.6
1	A	349	ARG	2.5
1	B	265	ILE	2.5
1	A	224	ASP	2.4
1	B	173	GLY	2.4
1	B	180	PRO	2.4
1	B	350	GLY	2.4
1	A	390	CYS	2.4
1	B	254	LEU	2.4
1	B	51	GLN	2.4
1	A	161	GLU	2.3
1	B	165	ARG	2.3
1	A	195	ASN	2.3
1	A	318	ASN	2.3
1	B	161	GLU	2.3
1	A	252	PRO	2.2
1	A	317	ASP	2.2
1	A	407	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	434	ARG	2.2
1	A	168	ASN	2.2
1	A	438	PHE	2.2
1	B	271	PHE	2.2
1	A	223	LEU	2.2
1	A	222	SER	2.2
1	A	159	VAL	2.1
1	A	194	SER	2.1
1	A	394	GLY	2.1
1	B	162	GLN	2.1
1	B	220	HIS	2.1
1	B	284	LYS	2.1
1	A	172	PRO	2.1
1	B	70	PRO	2.1
1	B	272	ARG	2.1
1	B	167	VAL	2.0
1	B	189	LEU	2.0
1	A	406	HIS	2.0
1	B	192	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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors(Å^2)	Q<0.9
2	NAG	B	502	14/15	0.55	0.39	107,121,132,134	0
2	NAG	A	502	14/15	0.72	0.43	74,98,106,108	0
3	GOL	B	505	6/6	0.83	0.18	51,59,65,68	0
3	GOL	A	504	6/6	0.85	0.28	41,59,61,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	A	501	14/15	0.85	0.24	71,80,86,87	0
3	GOL	B	504	6/6	0.87	0.20	52,58,64,77	0
2	NAG	B	501	14/15	0.89	0.28	64,72,79,81	0
2	NAG	A	503	14/15	0.91	0.25	61,70,77,78	0
2	NAG	B	503	14/15	0.95	0.16	57,60,71,75	0
4	CL	A	505	1/1	0.98	0.19	31,31,31,31	0
4	CL	B	506	1/1	0.98	0.06	35,35,35,35	0

6.5 Other polymers (i)

There are no such residues in this entry.