



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 12:54 AM UTC

PDB ID : 4KWG / pdb_00004kwg
Title : Crystal Structure Analysis of ALDH2+ALDiB13
Authors : Hurley, T.D.; Kimble-Hill, A.C.
Deposited on : 2013-05-24
Resolution : 2.10 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

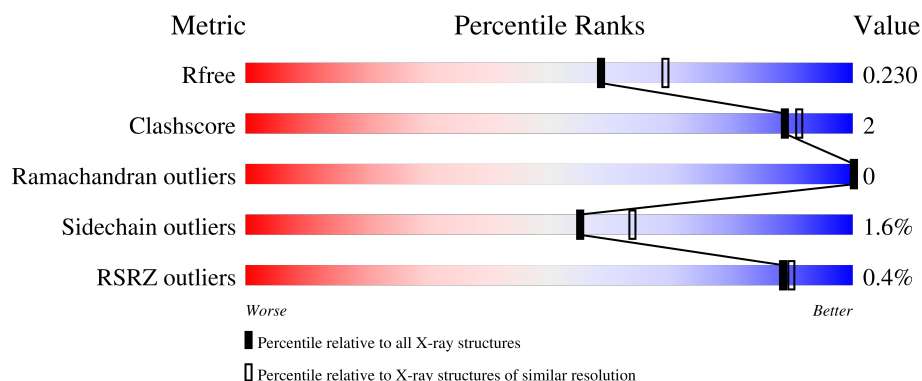
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

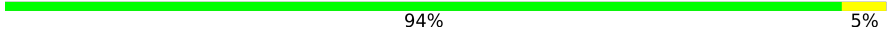
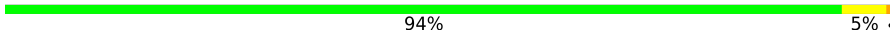
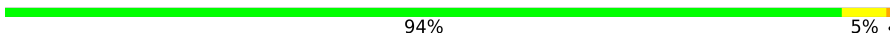
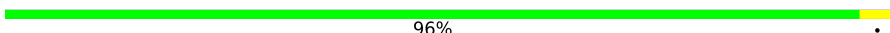
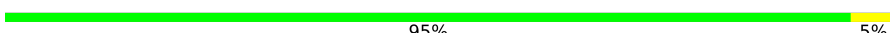
The reported resolution of this entry is 2.10 Å.

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.



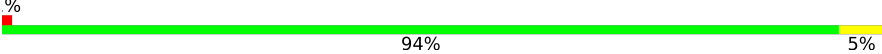
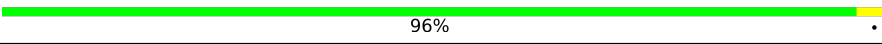
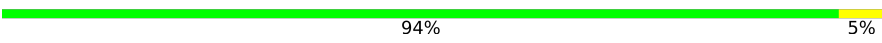
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	494	 94% 5%
1	B	494	 94% 5%
1	C	494	 94% 5%
1	D	494	 96% 5%
1	E	494	 95% 5%

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Mol	Chain	Length	Quality of chain
1	F	494	 94% 5%
1	G	494	 96%
1	H	494	 94% 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	2AK	A	601	-	-	X	-

2 Entry composition

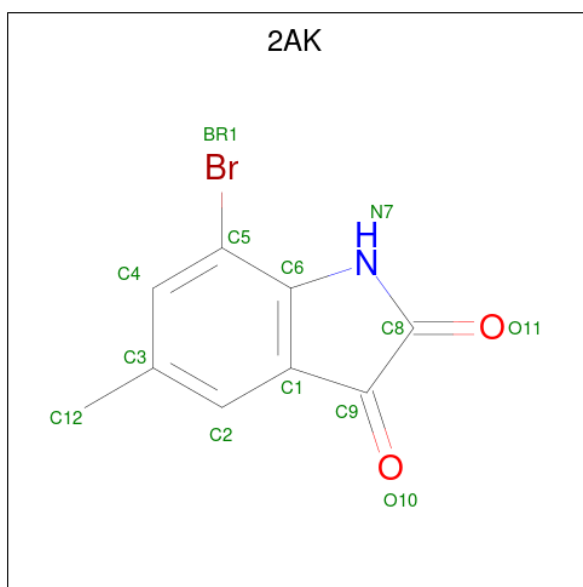
There are 6 unique types of molecules in this entry. The entry contains 31640 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Aldehyde dehydrogenase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	494	Total	C	N	O	S	0	0	0
			3798	2415	648	717	18			
1	B	494	Total	C	N	O	S	0	0	0
			3798	2415	648	717	18			
1	C	494	Total	C	N	O	S	0	0	0
			3798	2415	648	717	18			
1	D	494	Total	C	N	O	S	0	0	0
			3798	2415	648	717	18			
1	E	494	Total	C	N	O	S	0	0	0
			3798	2415	648	717	18			
1	F	494	Total	C	N	O	S	0	0	0
			3798	2415	648	717	18			
1	G	494	Total	C	N	O	S	0	0	0
			3798	2415	648	717	18			
1	H	494	Total	C	N	O	S	0	0	0
			3798	2415	648	717	18			

- Molecule 2 is 7-bromo-5-methyl-1H-indole-2,3-dione (CCD ID: 2AK) (formula: C₉H₆BrNO₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	Br	C	N	O	0	0
			13	1	9	1	2		
2	H	1	Total	Br	C	N	O	0	0
			13	1	9	1	2		

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

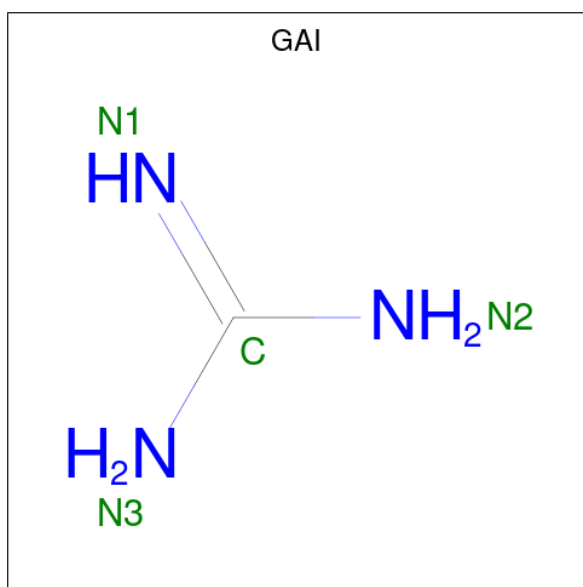
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		
3	B	1	Total	Na	0	0
			1	1		
3	C	1	Total	Na	0	0
			1	1		
3	D	1	Total	Na	0	0
			1	1		
3	E	1	Total	Na	0	0
			1	1		
3	F	1	Total	Na	0	0
			1	1		
3	G	1	Total	Na	0	0
			1	1		
3	H	1	Total	Na	0	0
			1	1		

- 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	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	F	1	Total	C	O	0	0
			4	2	2		
4	F	1	Total	C	O	0	0
			4	2	2		
4	H	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is GUANIDINE (CCD ID: GAI) (formula: CH_5N_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	N	0	0
			4	1	3		
5	B	1	Total	C	N	0	0
			4	1	3		
5	C	1	Total	C	N	0	0
			4	1	3		
5	D	1	Total	C	N	0	0
			4	1	3		
5	F	1	Total	C	N	0	0
			4	1	3		
5	G	1	Total	C	N	0	0
			4	1	3		
5	H	1	Total	C	N	0	0
			4	1	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	133	Total	O	0	0
			133	133		
6	B	121	Total	O	0	0
			121	121		
6	C	138	Total	O	0	0
			138	138		
6	D	189	Total	O	0	0
			189	189		
6	E	149	Total	O	0	0
			149	149		

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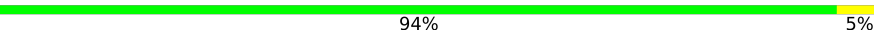
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	117	Total 117	O 117	0	0
6	G	149	Total 149	O 149	0	0
6	H	166	Total 166	O 166	0	0

3 Residue-property plots [i](#)

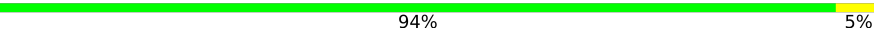
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

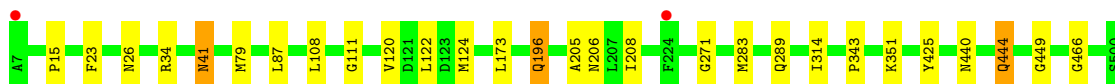
- Molecule 1: Aldehyde dehydrogenase, mitochondrial

Chain A: 

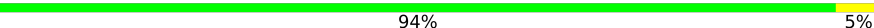


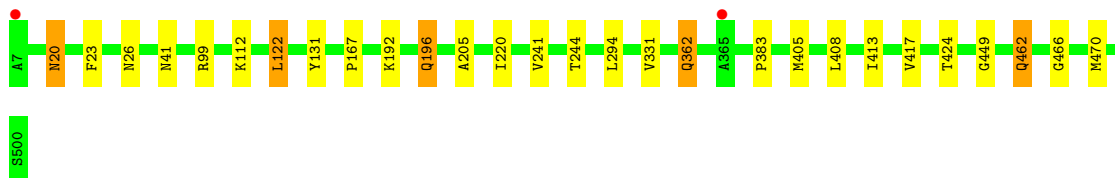
- Molecule 1: Aldehyde dehydrogenase, mitochondrial

Chain B: 

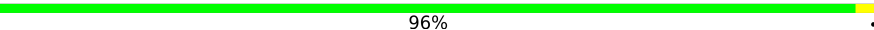


- Molecule 1: Aldehyde dehydrogenase, mitochondrial

Chain C: 

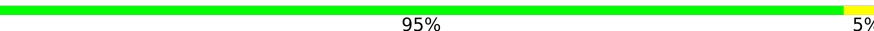


- Molecule 1: Aldehyde dehydrogenase, mitochondrial

Chain D: 

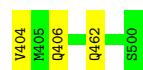


- Molecule 1: Aldehyde dehydrogenase, mitochondrial

Chain E: 



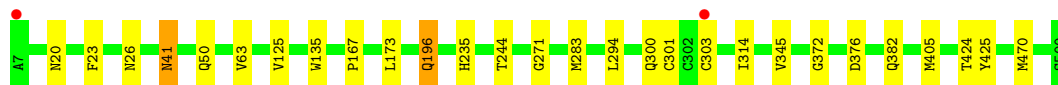
- Molecule 1: Aldehyde dehydrogenase, mitochondrial



- Molecule 1: Aldehyde dehydrogenase, mitochondrial



- Molecule 1: Aldehyde dehydrogenase, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	101.51Å 176.19Å 101.55Å 90.00° 94.92° 90.00°	Depositor
Resolution (Å)	40.39 – 2.10 40.39 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.7 (40.39-2.10) 98.7 (40.39-2.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.73 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.193 , 0.229 0.194 , 0.230	Depositor DCC
R_{free} test set	10373 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	21.5	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 24.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.076 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	31640	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 2AK, EDO, NA, GAI

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	0.43	0/3882	0.72	0/5267
1	B	0.43	0/3882	0.70	0/5267
1	C	0.42	0/3882	0.71	0/5267
1	D	0.43	0/3882	0.70	0/5267
1	E	0.42	0/3882	0.70	0/5267
1	F	0.42	0/3882	0.70	0/5267
1	G	0.42	0/3882	0.70	0/5267
1	H	0.42	0/3882	0.70	0/5267
All	All	0.43	0/31056	0.70	0/42136

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3798	0	3745	20	0
1	B	3798	0	3745	15	0
1	C	3798	0	3745	16	0
1	D	3798	0	3745	13	0
1	E	3798	0	3745	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3798	0	3745	12	0
1	G	3798	0	3745	11	0
1	H	3798	0	3745	18	0
2	A	13	0	6	4	0
2	H	13	0	6	3	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	8	0	12	0	0
4	B	8	0	12	0	0
4	E	4	0	6	0	0
4	F	8	0	12	0	0
4	H	4	0	6	0	0
5	A	4	0	4	0	0
5	B	4	0	4	0	0
5	C	4	0	4	0	0
5	D	4	0	4	0	0
5	F	4	0	4	0	0
5	G	4	0	4	0	0
5	H	4	0	4	0	0
6	A	133	0	0	1	0
6	B	121	0	0	1	0
6	C	138	0	0	0	0
6	D	189	0	0	0	0
6	E	149	0	0	0	0
6	F	117	0	0	0	0
6	G	149	0	0	0	0
6	H	166	0	0	0	0
All	All	31640	0	30048	113	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 2.

All (113) 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:D:120:VAL:HG12	1:D:124:MET:HE2	1.59	0.84
1:H:196:GLN:H	1:H:196:GLN:HE21	1.33	0.74
1:C:424:THR:HB	1:C:470:MET:HE3	1.77	0.67
1:F:284:ASP:OD2	1:F:321:ARG:NH1	2.27	0.66
1:A:205:ALA:HB2	1:A:220:ILE:HD12	1.77	0.66
1:D:196:GLN:H	1:D:196:GLN:HE21	1.42	0.65
1:B:41:ASN:HD22	1:B:41:ASN:C	2.03	0.65
1:E:205:ALA:HB2	1:E:220:ILE:HD12	1.80	0.64
1:H:41:ASN:C	1:H:41:ASN:HD22	2.08	0.61
1:C:196:GLN:HE21	1:C:196:GLN:H	1.49	0.61
1:B:120:VAL:HG12	1:B:124:MET:HE2	1.84	0.60
1:H:301:CYS:HB3	2:H:601:2AK:O11	2.01	0.60
1:D:241:VAL:HG23	1:D:263:LYS:HD3	1.84	0.59
1:B:196:GLN:HE21	1:B:196:GLN:H	1.52	0.58
1:A:41:ASN:C	1:A:41:ASN:HD22	2.12	0.58
1:E:404:VAL:HG12	1:E:406:GLN:HE22	1.68	0.58
1:B:440:ASN:O	1:B:444:GLN:HB2	2.05	0.57
1:A:390:GLN:HG2	1:A:393:MET:HE3	1.87	0.57
1:C:205:ALA:HB2	1:C:220:ILE:HD12	1.87	0.57
1:A:196:GLN:HE21	1:A:196:GLN:H	1.53	0.56
1:A:301:CYS:HB3	2:A:601:2AK:O10	2.04	0.56
1:E:196:GLN:HE21	1:E:196:GLN:H	1.51	0.56
1:G:67:ARG:HD2	1:G:237:ASP:OD2	2.05	0.56
1:F:196:GLN:HE21	1:F:196:GLN:H	1.54	0.55
1:A:36:THR:HB	1:A:50:GLN:HG3	1.88	0.54
1:G:196:GLN:HE21	1:G:196:GLN:H	1.55	0.53
1:A:303:CYS:SG	2:A:601:2AK:C9	2.97	0.53
1:H:283:MET:HE1	1:H:314:ILE:HB	1.91	0.52
1:H:424:THR:HB	1:H:470:MET:HE3	1.90	0.52
1:E:255:VAL:HG13	1:F:255:VAL:HG13	1.91	0.52
1:E:41:ASN:C	1:E:41:ASN:HD22	2.18	0.52
1:B:205:ALA:HA	1:B:208:ILE:HD12	1.92	0.52
1:H:303:CYS:SG	2:H:601:2AK:O11	2.66	0.52
1:E:294:LEU:HD22	1:E:405:MET:HB2	1.92	0.51
1:F:300:GLN:HE22	1:F:345:VAL:H	1.58	0.51
1:D:120:VAL:CG1	1:D:124:MET:HE2	2.35	0.51
1:E:79:MET:HE1	1:E:87:LEU:HD12	1.92	0.51
1:F:41:ASN:HD22	1:F:41:ASN:C	2.19	0.51
1:F:404:VAL:HG12	1:F:406:GLN:HE22	1.75	0.51
1:C:20:ASN:N	1:C:20:ASN:HD22	2.09	0.50
1:A:23:PHE:CZ	1:A:26:ASN:HA	2.47	0.50
1:E:294:LEU:HD22	1:E:405:MET:CB	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:300:GLN:HE22	1:H:345:VAL:H	1.60	0.49
1:D:300:GLN:HE22	1:D:345:VAL:H	1.60	0.49
1:C:167:PRO:HD3	1:C:244:THR:HB	1.94	0.48
1:D:193:VAL:HG11	1:D:201:ALA:CB	2.42	0.48
1:D:23:PHE:CZ	1:D:26:ASN:HA	2.48	0.48
1:F:23:PHE:CZ	1:F:26:ASN:HA	2.49	0.47
1:D:205:ALA:HB2	1:D:220:ILE:HD12	1.97	0.47
1:E:19:CYS:SG	1:E:206:ASN:ND2	2.88	0.47
1:F:55:ASP:CG	1:F:56:LYS:H	2.23	0.46
1:D:377:ARG:NH2	1:H:376:ASP:OD1	2.47	0.46
1:C:331:VAL:HG21	1:C:383:PRO:HD3	1.97	0.46
1:H:167:PRO:HD3	1:H:244:THR:HB	1.97	0.46
1:E:23:PHE:CZ	1:E:26:ASN:HA	2.51	0.46
1:B:79:MET:HE1	1:B:87:LEU:HD12	1.98	0.46
1:B:289:GLN:NE2	6:B:710:HOH:O	2.35	0.46
1:C:413:ILE:O	1:C:417:VAL:HG23	2.15	0.46
1:E:15:PRO:HD2	1:E:108:LEU:HD22	1.98	0.46
1:E:63:VAL:HG11	1:E:235:HIS:CE1	2.51	0.46
1:C:20:ASN:HD22	1:C:20:ASN:H	1.63	0.46
1:G:41:ASN:C	1:G:41:ASN:HD22	2.24	0.45
1:G:331:VAL:HG21	1:G:383:PRO:HD3	1.99	0.45
1:H:23:PHE:CZ	1:H:26:ASN:HA	2.51	0.45
1:G:247:THR:HA	1:G:269:LEU:HD13	1.97	0.45
1:A:294:LEU:HD12	1:A:306:SER:HA	1.98	0.45
1:D:41:ASN:C	1:D:41:ASN:HD22	2.24	0.44
1:F:138:LYS:HD3	1:H:135:TRP:CE2	2.52	0.44
1:B:23:PHE:CZ	1:B:26:ASN:HA	2.53	0.44
1:F:167:PRO:HD3	1:F:244:THR:HB	1.99	0.44
1:A:391:ASP:OD2	1:A:419:ARG:HD2	2.17	0.44
1:A:409:LYS:O	1:A:419:ARG:NH1	2.44	0.44
1:D:355:GLY:HA2	1:H:50:GLN:HE22	1.83	0.44
1:E:167:PRO:HD3	1:E:244:THR:HB	2.00	0.44
1:C:449:GLY:HA3	1:C:466:GLY:O	2.17	0.43
1:A:167:PRO:HD3	1:A:244:THR:HB	1.99	0.43
1:H:294:LEU:HD22	1:H:405:MET:HB2	1.99	0.43
1:C:408:LEU:HD12	1:C:408:LEU:N	2.34	0.43
1:H:303:CYS:SG	2:H:601:2AK:C8	3.07	0.43
1:C:131:TYR:CE1	1:C:462:GLN:HG3	2.54	0.43
1:A:391:ASP:OD2	1:A:419:ARG:CD	2.67	0.43
1:G:208:ILE:HD13	1:G:218:VAL:HG11	2.01	0.43
1:A:300:GLN:HE22	1:A:345:VAL:H	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:449:GLY:HA3	1:B:466:GLY:O	2.19	0.42
1:C:99:ARG:HG3	1:C:122:LEU:HD22	2.00	0.42
1:C:294:LEU:HD13	1:C:405:MET:HA	2.01	0.42
1:B:283:MET:HE1	1:B:314:ILE:HB	2.02	0.42
1:C:23:PHE:CZ	1:C:26:ASN:HA	2.54	0.42
1:A:26:ASN:ND2	6:A:705:HOH:O	2.52	0.42
1:G:167:PRO:HD3	1:G:244:THR:HB	2.01	0.42
1:A:247:THR:HA	1:A:269:LEU:HD13	2.01	0.42
1:F:174:MET:HE1	1:F:177:TRP:CE3	2.55	0.42
1:B:15:PRO:HG2	1:B:108:LEU:HD22	2.02	0.42
1:B:124:MET:HE3	1:B:173:LEU:HD22	2.02	0.42
1:C:41:ASN:C	1:C:41:ASN:HD22	2.27	0.42
1:H:63:VAL:HG11	1:H:235:HIS:CE1	2.55	0.41
1:H:271:GLY:HA2	1:H:425:TYR:HB3	2.03	0.41
1:B:111:GLY:O	1:B:343:PRO:HD2	2.21	0.41
1:F:192:LYS:HB2	1:F:232:ILE:HD12	2.02	0.41
1:G:417:VAL:HG23	1:G:442:LEU:HD23	2.02	0.41
1:H:372:GLY:H	1:H:382:GLN:HE21	1.67	0.41
1:B:196:GLN:H	1:B:196:GLN:NE2	2.18	0.41
1:H:125:VAL:HG22	1:H:173:LEU:HA	2.01	0.41
1:A:301:CYS:SG	2:A:601:2AK:C8	3.09	0.41
1:A:111:GLY:O	1:A:343:PRO:HD2	2.21	0.41
1:B:271:GLY:HA2	1:B:425:TYR:HB3	2.03	0.41
1:C:362:GLN:NE2	1:G:36:THR:O	2.54	0.41
1:A:303:CYS:SG	2:A:601:2AK:O10	2.79	0.41
1:G:417:VAL:CG2	1:G:442:LEU:HD23	2.51	0.40
1:A:149:ASP:HA	1:A:498:LYS:HB2	2.03	0.40
1:D:462:GLN:NE2	1:D:462:GLN:H	2.20	0.40
1:G:276:ILE:HG23	1:G:416:VAL:HG21	2.04	0.40
1:D:124:MET:HE3	1:D:173:LEU:HD22	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	492/494 (100%)	479 (97%)	13 (3%)	0	100	100
1	B	492/494 (100%)	479 (97%)	13 (3%)	0	100	100
1	C	492/494 (100%)	476 (97%)	16 (3%)	0	100	100
1	D	492/494 (100%)	479 (97%)	13 (3%)	0	100	100
1	E	492/494 (100%)	480 (98%)	12 (2%)	0	100	100
1	F	492/494 (100%)	478 (97%)	14 (3%)	0	100	100
1	G	492/494 (100%)	478 (97%)	14 (3%)	0	100	100
1	H	492/494 (100%)	478 (97%)	14 (3%)	0	100	100
All	All	3936/3952 (100%)	3827 (97%)	109 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	399/399 (100%)	395 (99%)	4 (1%)	68	76
1	B	399/399 (100%)	392 (98%)	7 (2%)	51	60
1	C	399/399 (100%)	391 (98%)	8 (2%)	48	56
1	D	399/399 (100%)	395 (99%)	4 (1%)	68	76
1	E	399/399 (100%)	392 (98%)	7 (2%)	51	60
1	F	399/399 (100%)	388 (97%)	11 (3%)	38	43
1	G	399/399 (100%)	393 (98%)	6 (2%)	57	65
1	H	399/399 (100%)	396 (99%)	3 (1%)	73	81
All	All	3192/3192 (100%)	3142 (98%)	50 (2%)	55	64

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	196	GLN
1	A	336	ASP
1	A	462	GLN
1	B	34	ARG
1	B	41	ASN
1	B	122	LEU
1	B	196	GLN
1	B	206	ASN
1	B	351	LYS
1	B	444	GLN
1	C	20	ASN
1	C	112	LYS
1	C	122	LEU
1	C	192	LYS
1	C	196	GLN
1	C	241	VAL
1	C	362	GLN
1	C	462	GLN
1	D	14	GLN
1	D	34	ARG
1	D	196	GLN
1	D	462	GLN
1	E	16	GLU
1	E	46	GLU
1	E	112	LYS
1	E	189	VAL
1	E	192	LYS
1	E	196	GLN
1	E	462	GLN
1	F	16	GLU
1	F	20	ASN
1	F	30	ASP
1	F	34	ARG
1	F	117	SER
1	F	122	LEU
1	F	192	LYS
1	F	196	GLN
1	F	311	GLN
1	F	358	ASN
1	F	462	GLN
1	G	124	MET
1	G	196	GLN

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Mol	Chain	Res	Type
1	G	236	GLU
1	G	361	LYS
1	G	417	VAL
1	G	462	GLN
1	H	20	ASN
1	H	41	ASN
1	H	196	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	A	26	ASN
1	A	41	ASN
1	A	196	GLN
1	A	275	ASN
1	A	300	GLN
1	A	462	GLN
1	B	26	ASN
1	B	41	ASN
1	B	50	GLN
1	B	196	GLN
1	B	362	GLN
1	C	13	GLN
1	C	20	ASN
1	C	25	ASN
1	C	41	ASN
1	C	196	GLN
1	C	289	GLN
1	C	300	GLN
1	C	333	ASN
1	C	358	ASN
1	C	462	GLN
1	D	13	GLN
1	D	41	ASN
1	D	175	GLN
1	D	196	GLN
1	D	275	ASN
1	D	300	GLN
1	D	358	ASN
1	D	462	GLN
1	E	13	GLN

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Mol	Chain	Res	Type
1	E	26	ASN
1	E	41	ASN
1	E	83	HIS
1	E	196	GLN
1	E	206	ASN
1	E	219	ASN
1	E	275	ASN
1	E	390	GLN
1	E	406	GLN
1	E	462	GLN
1	E	497	GLN
1	F	13	GLN
1	F	20	ASN
1	F	25	ASN
1	F	26	ASN
1	F	41	ASN
1	F	50	GLN
1	F	175	GLN
1	F	196	GLN
1	F	300	GLN
1	F	311	GLN
1	F	406	GLN
1	F	462	GLN
1	G	13	GLN
1	G	20	ASN
1	G	26	ASN
1	G	41	ASN
1	G	50	GLN
1	G	83	HIS
1	G	196	GLN
1	G	447	GLN
1	G	462	GLN
1	H	13	GLN
1	H	20	ASN
1	H	26	ASN
1	H	41	ASN
1	H	50	GLN
1	H	196	GLN
1	H	300	GLN
1	H	349	GLN
1	H	382	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 25 ligands modelled in this entry, 8 are monoatomic - leaving 17 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	$\# Z > 2$
4	EDO	E	602	-	3,3,3	0.32	0	2,2,2	0.49	0
4	EDO	A	604	-	3,3,3	0.34	0	2,2,2	0.35	0
5	GAI	A	605	-	3,3,3	1.02	0	3,3,3	1.15	0
4	EDO	B	603	-	3,3,3	0.35	0	2,2,2	0.32	0
4	EDO	F	603	-	3,3,3	0.34	0	2,2,2	0.37	0
2	2AK	A	601	-	14,14,14	2.96	5 (35%)	20,21,21	3.19	11 (55%)
2	2AK	H	601	-	14,14,14	2.88	5 (35%)	20,21,21	3.38	10 (50%)
4	EDO	B	602	-	3,3,3	0.33	0	2,2,2	0.40	0
5	GAI	B	604	-	3,3,3	0.97	0	3,3,3	1.11	0
5	GAI	C	602	-	3,3,3	1.04	0	3,3,3	1.13	0
5	GAI	F	604	-	3,3,3	0.98	0	3,3,3	1.09	0
5	GAI	G	602	-	3,3,3	1.00	0	3,3,3	1.19	0
4	EDO	H	603	-	3,3,3	0.31	0	2,2,2	0.43	0
5	GAI	H	604	-	3,3,3	1.00	0	3,3,3	1.19	0
4	EDO	F	602	-	3,3,3	0.32	0	2,2,2	0.46	0
4	EDO	A	603	-	3,3,3	0.35	0	2,2,2	0.31	0
5	GAI	D	602	-	3,3,3	0.99	0	3,3,3	0.98	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
4	EDO	E	602	-	-	0/1/1/1	-
4	EDO	A	604	-	-	0/1/1/1	-
4	EDO	B	603	-	-	1/1/1/1	-
4	EDO	F	603	-	-	0/1/1/1	-
2	2AK	A	601	-	-	-	0/2/2/2
2	2AK	H	601	-	-	-	0/2/2/2
4	EDO	B	602	-	-	0/1/1/1	-
4	EDO	H	603	-	-	0/1/1/1	-
4	EDO	F	602	-	-	0/1/1/1	-
4	EDO	A	603	-	-	0/1/1/1	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	2AK	C8-C9	-7.04	1.46	1.56
2	H	601	2AK	C8-C9	-6.33	1.47	1.56
2	H	601	2AK	C1-C6	5.95	1.49	1.41
2	A	601	2AK	C1-C6	5.90	1.49	1.41
2	A	601	2AK	C6-C5	4.41	1.48	1.39
2	H	601	2AK	C6-C5	4.32	1.47	1.39
2	H	601	2AK	O10-C9	2.69	1.28	1.23
2	A	601	2AK	O11-C8	2.67	1.28	1.23
2	H	601	2AK	O11-C8	2.59	1.28	1.23
2	A	601	2AK	O10-C9	2.44	1.28	1.23

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	601	2AK	C9-C8-N7	9.71	112.10	106.03
2	A	601	2AK	C9-C8-N7	8.82	111.54	106.03
2	H	601	2AK	C6-N7-C8	-6.38	107.97	110.85
2	A	601	2AK	C6-N7-C8	-6.26	108.02	110.85
2	H	601	2AK	O10-C9-C8	4.63	127.64	123.78
2	A	601	2AK	O10-C9-C8	4.09	127.19	123.78
2	H	601	2AK	C2-C3-C4	3.81	122.34	118.11
2	A	601	2AK	C1-C6-C5	-3.34	115.23	120.55
2	A	601	2AK	C2-C3-C4	3.18	121.64	118.11
2	H	601	2AK	BR1-C5-C4	3.07	123.88	118.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	601	2AK	C1-C6-N7	3.06	112.05	108.13
2	A	601	2AK	C1-C6-N7	2.91	111.86	108.13
2	H	601	2AK	C2-C1-C9	2.77	135.38	129.46
2	H	601	2AK	C1-C6-C5	-2.59	116.42	120.55
2	A	601	2AK	C2-C1-C6	2.57	122.81	119.51
2	H	601	2AK	O11-C8-N7	-2.46	122.39	126.30
2	A	601	2AK	O11-C8-C9	-2.45	123.69	125.88
2	A	601	2AK	C2-C1-C9	2.36	134.51	129.46
2	A	601	2AK	BR1-C5-C4	2.26	122.39	118.28
2	H	601	2AK	BR1-C5-C6	-2.15	116.72	119.58
2	A	601	2AK	C1-C9-C8	2.04	105.89	105.00

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	603	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	2AK	4	0
2	H	601	2AK	3	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	494/494 (100%)	0.10	1 (0%) 91 92	13, 22, 31, 39	0
1	B	494/494 (100%)	0.16	2 (0%) 88 90	14, 23, 33, 45	0
1	C	494/494 (100%)	0.12	2 (0%) 88 90	14, 21, 32, 40	0
1	D	494/494 (100%)	-0.07	1 (0%) 91 92	13, 18, 26, 34	0
1	E	494/494 (100%)	0.06	2 (0%) 88 90	13, 20, 30, 46	0
1	F	494/494 (100%)	0.16	5 (1%) 79 81	13, 22, 32, 43	0
1	G	494/494 (100%)	-0.00	1 (0%) 91 92	12, 20, 30, 38	0
1	H	494/494 (100%)	-0.06	2 (0%) 88 90	13, 19, 27, 39	0
All	All	3952/3952 (100%)	0.06	16 (0%) 88 90	12, 20, 31, 46	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	7	ALA	4.5
1	B	7	ALA	3.2
1	F	7	ALA	2.8
1	G	7	ALA	2.7
1	H	7	ALA	2.7
1	F	376	ASP	2.6
1	D	7	ALA	2.4
1	B	224	PHE	2.3
1	A	27	GLU	2.3
1	F	331	VAL	2.2
1	C	7	ALA	2.2
1	F	224	PHE	2.2
1	C	365	ALA	2.2
1	E	373	ILE	2.1
1	F	245	GLY	2.0
1	H	303	CYS	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
3	NA	F	601	1/1	0.44	0.30	59,59,59,59	0
5	GAI	H	604	4/4	0.60	0.23	48,48,49,49	0
3	NA	C	601	1/1	0.72	0.19	58,58,58,58	0
5	GAI	F	604	4/4	0.73	0.20	44,44,44,44	0
3	NA	D	601	1/1	0.76	0.17	40,40,40,40	0
4	EDO	B	602	4/4	0.77	0.15	35,35,36,37	0
3	NA	A	602	1/1	0.80	0.11	39,39,39,39	0
4	EDO	E	602	4/4	0.80	0.14	37,38,38,38	0
4	EDO	F	602	4/4	0.81	0.20	36,36,36,38	0
5	GAI	C	602	4/4	0.81	0.16	37,38,39,39	0
4	EDO	B	603	4/4	0.81	0.16	37,38,39,40	0
3	NA	B	601	1/1	0.81	0.16	44,44,44,44	0
5	GAI	G	602	4/4	0.82	0.15	42,43,43,43	0
5	GAI	B	604	4/4	0.82	0.19	46,46,47,47	0
4	EDO	H	603	4/4	0.83	0.14	38,39,39,39	0
2	2AK	H	601	13/13	0.83	0.19	51,53,54,62	0
4	EDO	F	603	4/4	0.83	0.19	38,38,38,38	0
2	2AK	A	601	13/13	0.85	0.18	52,52,53,58	0
4	EDO	A	603	4/4	0.86	0.12	41,41,42,43	0
3	NA	E	601	1/1	0.86	0.09	33,33,33,33	0
4	EDO	A	604	4/4	0.87	0.12	34,34,34,34	0
3	NA	H	602	1/1	0.87	0.10	29,29,29,29	0
5	GAI	A	605	4/4	0.88	0.12	32,33,33,33	0
3	NA	G	601	1/1	0.92	0.06	35,35,35,35	0
5	GAI	D	602	4/4	0.94	0.08	27,27,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.