



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:41 PM UTC

PDB ID : 4KWF / pdb_00004kwf
Title : Crystal Structure Analysis of ALDH2+ALDiB33
Authors : Hurley, T.D.; Kimble-Hill, A.C.
Deposited on : 2013-05-24
Resolution : 2.31 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

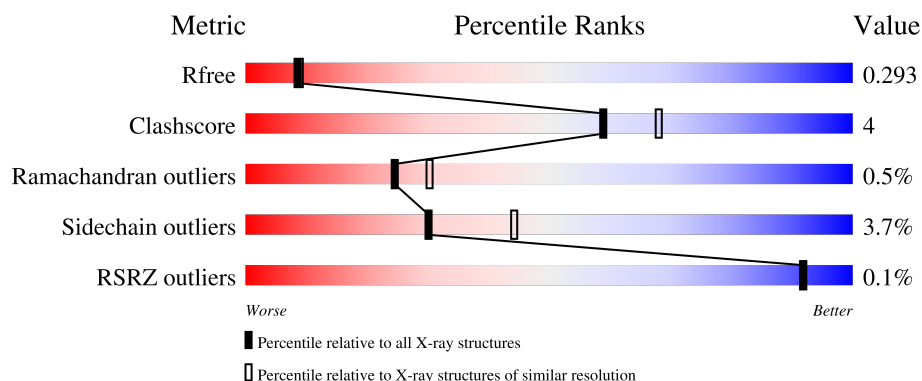
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

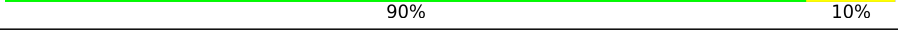
The reported resolution of this entry is 2.31 Å.

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	7754 (2.34-2.30)
Clashscore	190562	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (2.34-2.30)

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	
1	B	494	
1	C	494	
1	D	494	
1	E	494	

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Mol	Chain	Length	Quality of chain
1	F	494	 84% 15% .
1	G	494	 87% 12% .
1	H	494	 90% 9% .

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	3AK	B	601	-	-	X	-

2 Entry composition

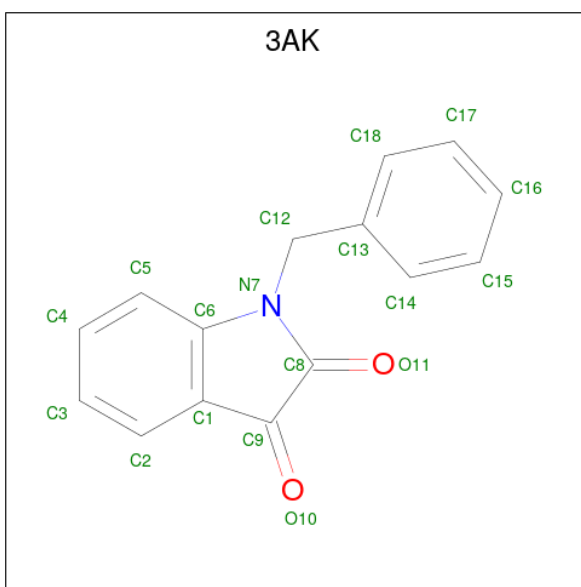
There are 6 unique types of molecules in this entry. The entry contains 30712 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 1-benzyl-1H-indole-2,3-dione (CCD ID: 3AK) (formula: C₁₅H₁₁NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			18	15	1	2		
2	B	1	Total	C	N	O	0	0
			18	15	1	2		
2	E	1	Total	C	N	O	0	0
			18	15	1	2		
2	H	1	Total	C	N	O	0	0
			18	15	1	2		

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

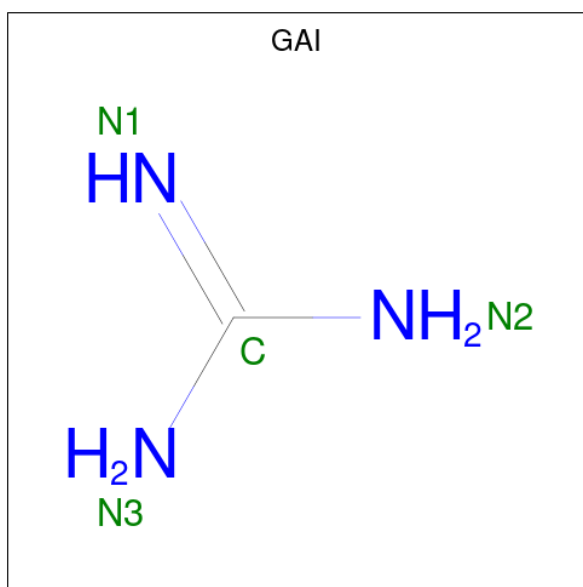
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		
3	B	1	Total	Na	0	0
			1	1		
3	C	1	Total	Na	0	0
			1	1		
3	D	1	Total	Na	0	0
			1	1		
3	E	1	Total	Na	0	0
			1	1		
3	F	1	Total	Na	0	0
			1	1		
3	G	1	Total	Na	0	0
			1	1		
3	H	1	Total	Na	0	0
			1	1		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	E	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	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	24	Total	O	0	0
			24	24		
6	B	15	Total	O	0	0
			15	15		
6	C	17	Total	O	0	0
			17	17		
6	D	31	Total	O	0	0
			31	31		
6	E	20	Total	O	0	0
			20	20		

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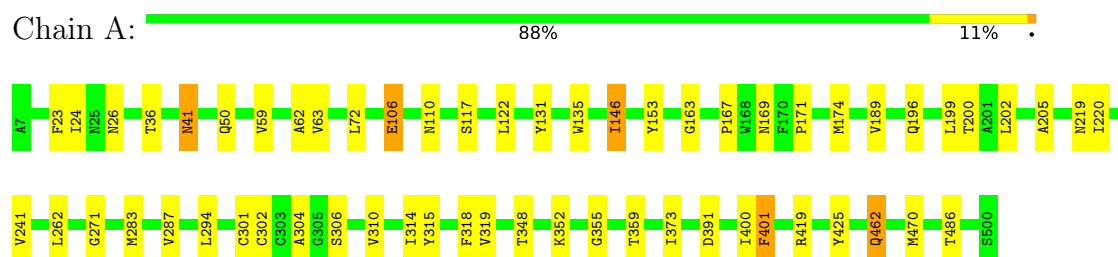
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	20	Total 20	O 20	0	0
6	G	16	Total 16	O 16	0	0
6	H	45	Total 45	O 45	0	0

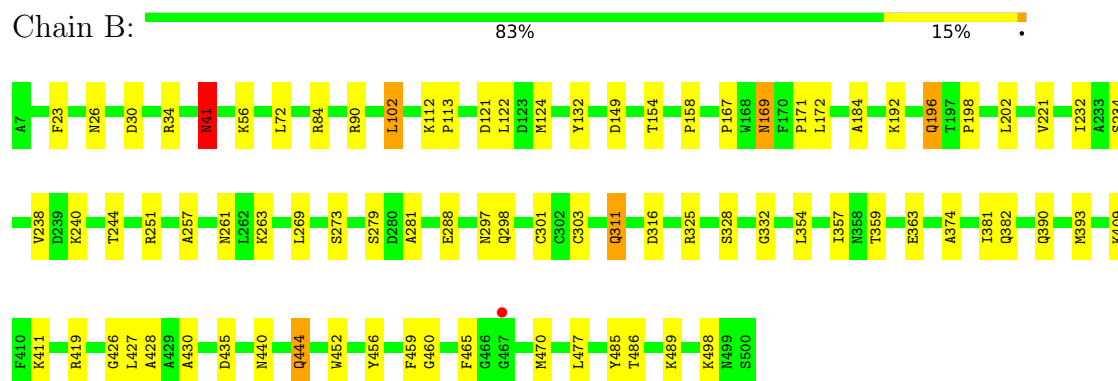
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

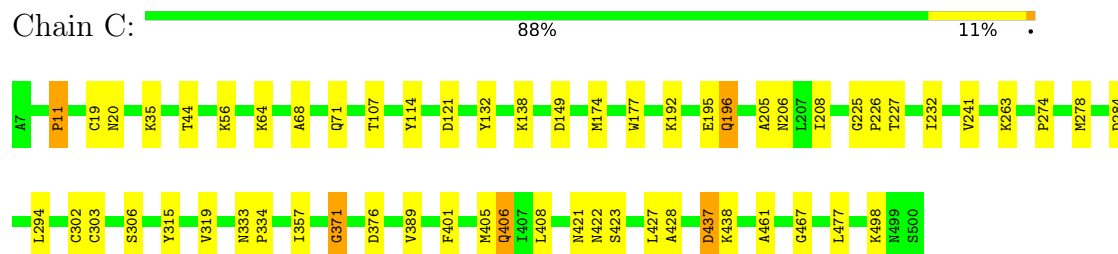
- Molecule 1: Aldehyde dehydrogenase, mitochondrial



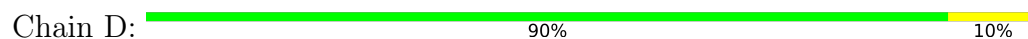
- Molecule 1: Aldehyde dehydrogenase, mitochondrial

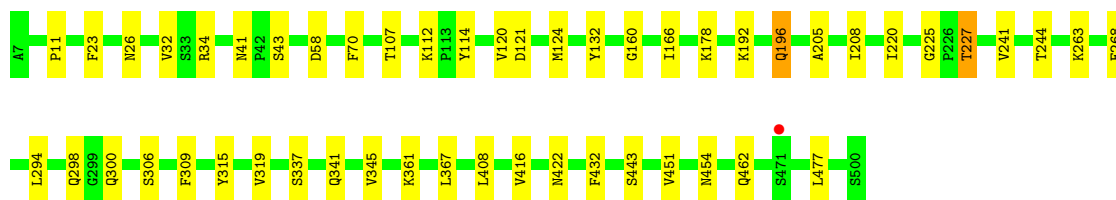


- Molecule 1: Aldehyde dehydrogenase, mitochondrial



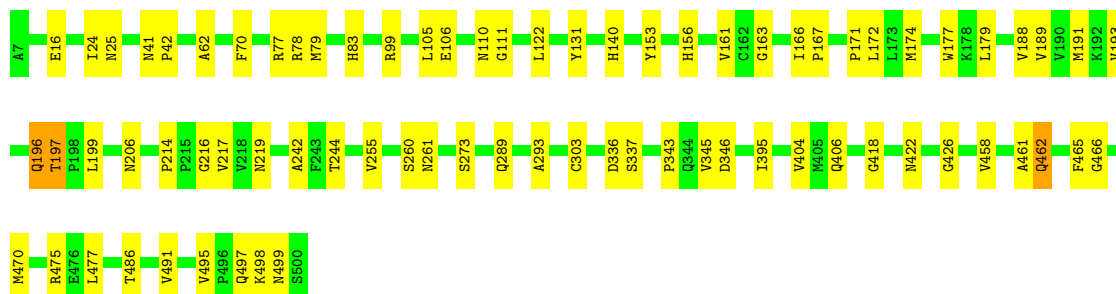
- Molecule 1: Aldehyde dehydrogenase, mitochondrial





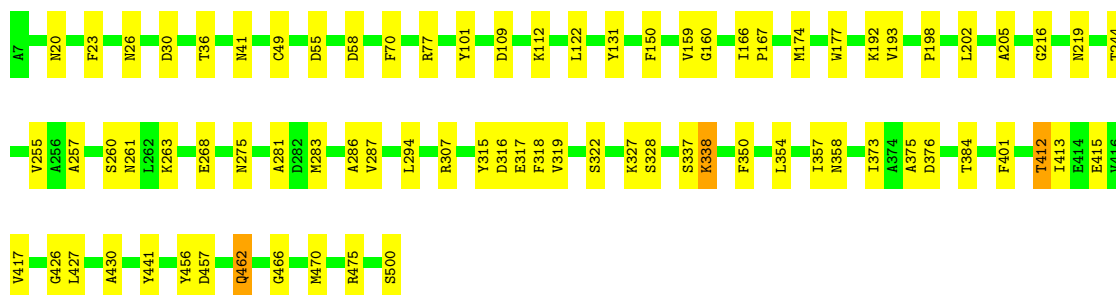
- Molecule 1: Aldehyde dehydrogenase, mitochondrial

Chain E: 85% 15% .



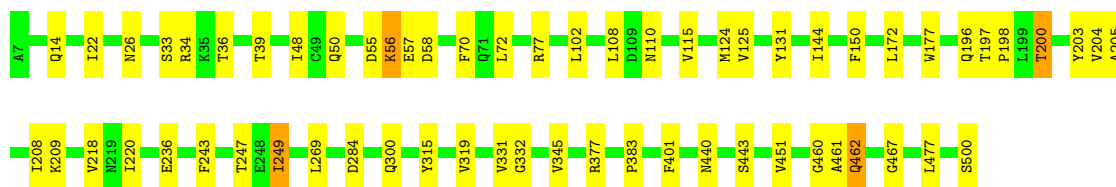
- Molecule 1: Aldehyde dehydrogenase, mitochondrial

Chain F: 84% 15% .



- Molecule 1: Aldehyde dehydrogenase, mitochondrial

Chain G: 87% 12% .



- Molecule 1: Aldehyde dehydrogenase, mitochondrial

Chain H: 90% 9% .



C301	C302	C303	P343	I381	V389	M405	L408	F432	N454	V458	F459	Q462	S463	P464	F465	T486	E487	V488	Q497	K498	M499	S500
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	102.29Å 177.09Å 102.55Å 90.00° 94.39° 90.00°	Depositor
Resolution (Å)	49.12 – 2.31 49.12 – 2.31	Depositor EDS
% Data completeness (in resolution range)	99.0 (49.12-2.31) 98.7 (49.12-2.31)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 2.32Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.239 , 0.296 0.238 , 0.293	Depositor DCC
R_{free} test set	8016 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	46.6	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 22.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.38$	Xtriage
Estimated twinning fraction	0.277 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	30712	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% 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: 3AK, NA, GAI, 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	0.57	0/3882	0.84	1/5267 (0.0%)
1	B	0.54	0/3882	0.82	2/5267 (0.0%)
1	C	0.57	0/3882	0.82	1/5267 (0.0%)
1	D	0.62	0/3882	0.82	0/5267
1	E	0.57	0/3882	0.83	3/5267 (0.1%)
1	F	0.54	0/3882	0.82	0/5267
1	G	0.56	0/3882	0.81	1/5267 (0.0%)
1	H	0.63	0/3882	0.84	0/5267
All	All	0.57	0/31056	0.82	8/42136 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	273	SER	N-CA-C	6.35	118.63	109.48
1	A	189	VAL	N-CA-C	5.77	116.31	107.77
1	C	467	GLY	N-CA-C	5.46	119.06	110.71
1	B	332	GLY	N-CA-C	5.45	117.54	110.45
1	E	217	VAL	N-CA-C	-5.36	105.49	110.53
1	E	345	VAL	N-CA-C	5.32	116.09	110.72
1	G	467	GLY	N-CA-C	5.30	119.79	112.37
1	B	169	ASN	N-CA-C	5.05	117.52	111.71

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	3798	0	3745	35	0
1	B	3798	0	3745	44	0
1	C	3798	0	3745	26	0
1	D	3798	0	3745	27	0
1	E	3798	0	3745	43	0
1	F	3798	0	3745	35	0
1	G	3798	0	3745	38	0
1	H	3798	0	3745	32	0
2	A	18	0	11	3	0
2	B	18	0	11	9	0
2	E	18	0	11	4	0
2	H	18	0	11	5	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	1	0
4	C	8	0	12	0	0
4	E	8	0	12	0	0
4	F	4	0	6	0	0
4	H	4	0	6	0	0
5	A	4	0	4	0	0
5	B	4	0	4	1	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	24	0	0	0	0
6	B	15	0	0	0	0
6	C	17	0	0	0	0
6	D	31	0	0	0	0
6	E	20	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	20	0	0	0	0
6	G	16	0	0	0	0
6	H	45	0	0	0	0
All	All	30712	0	30080	265	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 4.

All (265) 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:301:CYS:SG	2:B:601:3AK:O10	2.26	0.93
1:A:205:ALA:HB2	1:A:220:ILE:HD12	1.60	0.84
1:E:303:CYS:SG	2:E:601:3AK:O10	2.43	0.77
1:G:48:ILE:HG21	1:G:108:LEU:HD21	1.69	0.75
1:E:216:GLY:HA2	1:E:219:ASN:HD21	1.54	0.71
1:F:166:ILE:HD11	1:F:193:VAL:HG12	1.71	0.71
1:G:110:ASN:HD22	1:G:197:THR:HG21	1.56	0.70
1:B:102:LEU:HD22	1:B:172:LEU:HD11	1.73	0.69
1:A:41:ASN:C	1:A:41:ASN:HD22	2.00	0.69
1:C:205:ALA:HA	1:C:208:ILE:HD12	1.74	0.69
1:B:196:GLN:H	1:B:196:GLN:HE21	1.39	0.69
1:D:132:TYR:OH	1:D:477:LEU:HA	1.93	0.68
1:A:294:LEU:HD12	1:A:306:SER:HA	1.75	0.68
1:B:311:GLN:NE2	1:B:411:LYS:O	2.27	0.68
1:H:196:GLN:HE21	1:H:196:GLN:H	1.39	0.68
1:C:19:CYS:SG	1:C:206:ASN:ND2	2.66	0.67
1:H:41:ASN:C	1:H:41:ASN:HD22	2.03	0.67
1:E:255:VAL:HG13	1:F:255:VAL:HG13	1.77	0.67
1:B:427:LEU:HD21	2:B:601:3AK:C16	2.25	0.66
1:D:120:VAL:HG12	1:D:124:MET:HE2	1.76	0.66
1:B:427:LEU:HD21	2:B:601:3AK:C15	2.26	0.66
1:E:174:MET:HE1	1:E:177:TRP:CE3	2.29	0.66
1:G:205:ALA:HB2	1:G:220:ILE:HD12	1.78	0.65
1:B:132:TYR:OH	1:B:477:LEU:HA	1.97	0.65
1:F:23:PHE:CZ	1:F:26:ASN:HA	2.32	0.65
1:B:149:ASP:HA	1:B:498:LYS:HB2	1.79	0.65
1:E:465:PHE:CE2	2:E:601:3AK:H12	2.33	0.64
1:F:287:VAL:HG22	1:F:318:PHE:CD1	2.32	0.64
1:B:440:ASN:O	1:B:444:GLN:HB2	1.97	0.64
1:H:23:PHE:CZ	1:H:26:ASN:HA	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:205:ALA:HB2	1:D:220:ILE:HD12	1.80	0.62
1:H:175:GLN:HG3	1:H:191:MET:SD	2.40	0.61
1:E:465:PHE:CD2	2:E:601:3AK:H12	2.36	0.61
1:D:241:VAL:HG23	1:D:263:LYS:HD3	1.82	0.61
1:A:301:CYS:HB3	2:A:601:3AK:O10	2.01	0.61
1:F:77:ARG:NE	1:G:500:SER:OG	2.32	0.61
1:C:294:LEU:HD12	1:C:306:SER:HA	1.83	0.60
1:A:470:MET:HE2	1:B:261:ASN:HB2	1.84	0.60
1:E:106:GLU:OE1	1:E:171:PRO:HD2	2.01	0.59
1:F:315:TYR:O	1:F:319:VAL:HG23	2.03	0.59
1:E:131:TYR:CE1	1:E:462:GLN:HG3	2.36	0.59
1:D:294:LEU:HD13	1:D:294:LEU:C	2.28	0.58
1:D:196:GLN:H	1:D:196:GLN:HE21	1.51	0.58
1:C:315:TYR:O	1:C:319:VAL:HG23	2.02	0.58
1:E:404:VAL:HG12	1:E:406:GLN:HE22	1.68	0.58
1:G:102:LEU:HD21	1:G:203:TYR:HD2	1.69	0.57
1:D:443:SER:HA	1:D:451:VAL:HG11	1.87	0.56
1:C:132:TYR:OH	1:C:477:LEU:HA	2.06	0.56
1:B:269:LEU:HD12	1:B:470:MET:O	2.05	0.56
1:H:106:GLU:OE1	1:H:171:PRO:HD2	2.06	0.56
1:C:149:ASP:HA	1:C:498:LYS:HB2	1.87	0.55
1:C:461:ALA:HA	1:C:477:LEU:HD22	1.88	0.55
1:D:244:THR:HG23	1:D:268:GLU:HB2	1.89	0.55
1:G:131:TYR:CE1	1:G:462:GLN:HG3	2.42	0.55
1:H:465:PHE:CE2	2:H:601:3AK:H12	2.42	0.55
1:B:112:LYS:HA	1:B:298:GLN:OE1	2.07	0.55
1:H:196:GLN:H	1:H:196:GLN:NE2	2.04	0.55
1:A:36:THR:HB	1:A:50:GLN:HG3	1.90	0.54
1:A:153:TYR:HH	4:A:603:EDO:HO1	1.55	0.53
1:C:68:ALA:HA	1:C:71:GLN:HG2	1.89	0.53
1:D:120:VAL:HG12	1:D:124:MET:CE	2.38	0.53
1:B:459:PHE:CZ	2:B:601:3AK:C2	2.92	0.53
1:C:278:MET:HE2	1:C:438:LYS:HD3	1.91	0.53
1:B:169:ASN:O	1:B:297:ASN:ND2	2.40	0.53
1:E:174:MET:HE1	1:E:177:TRP:CZ3	2.44	0.53
1:F:373:ILE:HG22	1:F:375:ALA:O	2.09	0.52
1:A:41:ASN:C	1:A:41:ASN:ND2	2.65	0.52
1:B:301:CYS:SG	2:B:601:3AK:C9	2.97	0.52
1:G:208:ILE:HD13	1:G:218:VAL:HG11	1.92	0.52
1:E:166:ILE:HD11	1:E:193:VAL:HG12	1.92	0.52
1:A:310:VAL:HG21	1:A:318:PHE:CD2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:465:PHE:CD2	2:H:601:3AK:H12	2.44	0.52
1:B:84:ARG:NH1	1:B:184:ALA:O	2.43	0.51
1:D:23:PHE:CZ	1:D:26:ASN:HA	2.45	0.51
1:C:196:GLN:HE21	1:C:196:GLN:H	1.59	0.51
1:F:281:ALA:HB1	1:F:286:ALA:HB2	1.93	0.51
1:B:41:ASN:C	1:B:41:ASN:HD22	2.18	0.51
1:D:294:LEU:HD23	1:D:306:SER:HA	1.93	0.51
1:G:110:ASN:HD22	1:G:197:THR:CG2	2.23	0.51
1:A:301:CYS:HB2	1:A:304:ALA:HB2	1.93	0.50
1:F:167:PRO:HD3	1:F:244:THR:HB	1.93	0.50
1:B:301:CYS:HG	2:B:601:3AK:C9	2.24	0.50
1:G:462:GLN:H	1:G:462:GLN:HE21	1.59	0.50
1:E:346:ASP:C	1:E:346:ASP:OD1	2.54	0.50
1:H:11:PRO:HB3	1:H:114:TYR:CZ	2.47	0.50
1:B:303:CYS:HB2	1:B:428:ALA:HB3	1.93	0.49
1:G:462:GLN:HB3	1:H:144:ILE:CG2	2.41	0.49
1:A:23:PHE:CZ	1:A:26:ASN:HA	2.46	0.49
1:B:23:PHE:CZ	1:B:26:ASN:HA	2.48	0.49
1:G:22:ILE:HD13	1:G:58:ASP:OD1	2.13	0.49
1:H:294:LEU:HD13	1:H:405:MET:HA	1.95	0.49
1:G:462:GLN:H	1:G:462:GLN:NE2	2.10	0.49
1:F:294:LEU:HD13	1:F:294:LEU:C	2.38	0.49
1:D:205:ALA:HA	1:D:208:ILE:HD12	1.95	0.49
1:D:432:PHE:CD2	1:D:454:ASN:HA	2.48	0.49
1:E:111:GLY:O	1:E:343:PRO:HD2	2.13	0.48
1:E:336:ASP:OD1	1:E:337:SER:N	2.46	0.48
1:E:497:GLN:HE21	1:E:499:ASN:HD21	1.60	0.48
1:C:174:MET:HE1	1:C:177:TRP:CZ3	2.48	0.48
1:D:300:GLN:HE22	1:D:345:VAL:H	1.61	0.48
1:E:395:ILE:HD12	1:E:406:GLN:HE21	1.79	0.48
1:D:32:VAL:HG23	1:D:58:ASP:OD1	2.13	0.48
1:H:11:PRO:HB3	1:H:114:TYR:CE1	2.48	0.48
1:C:389:VAL:HB	1:C:408:LEU:HG	1.96	0.48
1:F:101:TYR:CD1	1:F:101:TYR:C	2.91	0.48
1:B:390:GLN:HB2	1:B:393:MET:HE3	1.96	0.48
1:B:192:LYS:HB2	1:B:232:ILE:CD1	2.44	0.48
1:C:357:ILE:HG21	1:C:371:GLY:O	2.13	0.48
1:E:174:MET:HE2	1:E:174:MET:HA	1.96	0.47
1:E:495:VAL:HG12	1:G:440:ASN:HD22	1.79	0.47
1:G:110:ASN:ND2	1:G:197:THR:HG21	2.26	0.47
1:C:437:ASP:N	1:C:437:ASP:OD2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:ILE:CG1	1:B:460:GLY:HA3	2.45	0.47
1:F:430:ALA:HB2	1:F:456:TYR:CD1	2.50	0.47
1:F:216:GLY:O	1:F:219:ASN:ND2	2.47	0.47
1:F:466:GLY:HA3	1:F:475:ARG:HD3	1.97	0.47
1:A:205:ALA:HB2	1:A:220:ILE:CD1	2.40	0.47
1:G:36:THR:OG1	1:G:50:GLN:NE2	2.47	0.47
1:A:355:GLY:O	1:A:359:THR:HG23	2.14	0.47
1:E:466:GLY:HA3	1:E:475:ARG:HD3	1.97	0.47
1:F:281:ALA:HB1	1:F:286:ALA:CB	2.45	0.47
1:G:460:GLY:O	1:G:462:GLN:N	2.48	0.47
1:A:315:TYR:O	1:A:319:VAL:HG23	2.15	0.46
1:H:174:MET:HE1	2:H:601:3AK:C18	2.44	0.46
1:D:225:GLY:C	1:D:227:THR:H	2.23	0.46
1:E:24:ILE:HG23	1:E:62:ALA:HA	1.96	0.46
1:D:70:PHE:CE1	1:D:160:GLY:HA2	2.50	0.46
1:A:23:PHE:O	1:A:24:ILE:HG13	2.15	0.46
1:B:167:PRO:HG3	1:B:244:THR:HG22	1.97	0.46
1:C:107:THR:OG1	1:C:114:TYR:HA	2.15	0.46
1:F:287:VAL:HG22	1:F:318:PHE:CE1	2.51	0.46
1:E:41:ASN:HD22	1:E:42:PRO:HD2	1.81	0.46
1:E:79:MET:HE3	1:E:83:HIS:HD2	1.81	0.46
1:G:26:ASN:HB3	1:G:209:LYS:HE2	1.97	0.46
1:A:202:LEU:O	1:A:205:ALA:HB3	2.15	0.46
2:A:601:3AK:O11	2:A:601:3AK:C13	2.64	0.46
1:E:465:PHE:CE2	2:E:601:3AK:C15	2.98	0.46
1:A:106:GLU:O	1:A:110:ASN:HB3	2.15	0.46
1:H:301:CYS:HB3	2:H:601:3AK:O10	2.16	0.46
1:D:11:PRO:HB3	1:D:114:TYR:CZ	2.51	0.46
1:E:105:LEU:HD11	1:E:199:LEU:HD13	1.98	0.46
1:H:432:PHE:HA	1:H:454:ASN:OD1	2.15	0.46
1:A:135:TRP:CD1	1:C:138:LYS:HE3	2.51	0.46
1:B:374:ALA:HB2	1:B:382:GLN:N	2.31	0.45
1:B:409:LYS:O	1:B:419:ARG:NH2	2.46	0.45
1:E:163:GLY:O	1:E:242:ALA:N	2.43	0.45
1:E:167:PRO:HD3	1:E:244:THR:HB	1.98	0.45
1:G:443:SER:HA	1:G:451:VAL:HG11	1.97	0.45
1:D:309:PHE:CD2	1:D:416:VAL:HG23	2.52	0.45
1:A:294:LEU:CD1	1:A:306:SER:HA	2.43	0.45
1:D:408:LEU:N	1:D:408:LEU:HD12	2.32	0.45
1:F:70:PHE:CZ	1:F:160:GLY:HA2	2.52	0.45
1:H:238:VAL:O	1:H:263:LYS:HE3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:238:VAL:O	1:B:263:LYS:HE3	2.17	0.45
1:D:107:THR:HG23	1:D:112:LYS:O	2.17	0.45
1:E:418:GLY:O	1:E:422:ASN:HB2	2.16	0.45
1:F:412:THR:OG1	1:F:415:GLU:HB2	2.16	0.45
1:A:302:CYS:HB2	2:A:601:3AK:O11	2.17	0.44
1:E:79:MET:HE3	1:E:83:HIS:CD2	2.52	0.44
1:E:261:ASN:HB2	1:F:470:MET:HE2	1.99	0.44
1:C:107:THR:HG23	1:C:334:PRO:HB2	1.98	0.44
1:E:196:GLN:H	1:E:196:GLN:HE21	1.65	0.44
1:A:283:MET:HE1	1:A:314:ILE:HB	1.99	0.44
1:F:174:MET:HE1	1:F:177:TRP:CE3	2.53	0.44
1:H:298:GLN:O	1:H:300:GLN:HG3	2.18	0.44
1:A:163:GLY:O	1:A:241:VAL:HA	2.17	0.44
1:B:354:LEU:HA	1:B:357:ILE:HD12	1.99	0.44
1:A:196:GLN:H	1:A:196:GLN:NE2	2.16	0.44
1:D:432:PHE:CE2	1:D:454:ASN:HA	2.53	0.44
1:G:461:ALA:HA	1:G:477:LEU:HD22	1.98	0.44
1:A:131:TYR:CE1	1:A:462:GLN:HG3	2.52	0.43
1:B:459:PHE:CE1	2:B:601:3AK:C3	3.00	0.43
1:F:413:ILE:HG12	1:F:441:TYR:CE2	2.53	0.43
1:F:441:TYR:CD2	1:F:441:TYR:C	2.96	0.43
1:A:391:ASP:OD2	1:A:419:ARG:HD2	2.17	0.43
1:H:14:GLN:HE21	1:H:14:GLN:HB2	1.64	0.43
1:B:257:ALA:HB1	1:B:263:LYS:HG3	2.00	0.43
1:B:465:PHE:CE2	2:B:601:3AK:H13	2.54	0.43
1:H:41:ASN:C	1:H:41:ASN:ND2	2.75	0.43
1:D:166:ILE:HG22	1:D:178:LYS:HD2	1.99	0.43
1:F:350:PHE:CZ	1:F:354:LEU:HD11	2.53	0.43
1:C:192:LYS:HB2	1:C:232:ILE:CD1	2.49	0.43
1:G:243:PHE:CZ	1:G:249:ILE:HB	2.53	0.43
1:H:156:HIS:CD2	1:H:488:VAL:HG22	2.53	0.43
1:C:406:GLN:HE21	1:C:406:GLN:HB2	1.67	0.43
1:B:430:ALA:HA	1:B:452:TRP:O	2.19	0.43
1:D:315:TYR:O	1:D:319:VAL:HG23	2.19	0.43
1:G:55:ASP:O	1:G:56:LYS:C	2.62	0.43
1:H:106:GLU:O	1:H:110:ASN:HB3	2.19	0.43
1:E:153:TYR:CZ	1:E:491:VAL:HB	2.54	0.43
1:G:300:GLN:HE22	1:G:345:VAL:HB	1.84	0.43
1:E:161:VAL:HA	1:E:188:VAL:HG23	2.01	0.43
1:B:288:GLU:OE1	1:B:325:ARG:NH2	2.52	0.42
1:A:62:ALA:O	1:A:219:ASN:ND2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:41:ASN:C	1:D:41:ASN:HD22	2.27	0.42
1:E:461:ALA:HA	1:E:477:LEU:HD22	2.00	0.42
1:C:11:PRO:HB3	1:C:114:TYR:CE1	2.53	0.42
1:E:167:PRO:HD2	1:E:174:MET:HG3	2.01	0.42
1:G:150:PHE:CE2	1:H:458:VAL:HG21	2.54	0.42
1:B:154:THR:HA	1:B:489:LYS:O	2.19	0.42
1:B:192:LYS:HB2	1:B:232:ILE:HD11	2.01	0.42
1:C:274:PRO:HD2	1:C:428:ALA:O	2.19	0.42
1:G:144:ILE:HG23	1:H:462:GLN:HB3	2.02	0.42
1:G:177:TRP:NE1	1:G:477:LEU:HD21	2.35	0.42
1:A:167:PRO:HD2	1:A:174:MET:HG3	2.01	0.42
1:C:241:VAL:HG23	1:C:263:LYS:HD3	2.00	0.42
1:E:140:HIS:O	1:E:156:HIS:CE1	2.72	0.42
1:F:257:ALA:HB1	1:F:263:LYS:HG3	2.01	0.42
1:E:110:ASN:HB2	1:E:197:THR:HG21	2.01	0.42
1:G:200:THR:O	1:G:204:VAL:HG23	2.19	0.42
1:G:331:VAL:HG12	1:G:332:GLY:N	2.35	0.42
1:H:63:VAL:HG11	1:H:235:HIS:CE1	2.54	0.42
1:B:113:PRO:HD3	1:B:298:GLN:OE1	2.20	0.42
1:H:111:GLY:O	1:H:343:PRO:HD2	2.20	0.42
1:A:271:GLY:HA2	1:A:425:TYR:HB3	2.01	0.42
1:C:302:CYS:HB3	1:C:427:LEU:CD2	2.49	0.42
1:E:70:PHE:CD1	1:E:77:ARG:HD3	2.55	0.42
1:E:470:MET:HE2	1:F:261:ASN:HB2	2.02	0.42
1:G:70:PHE:CD2	1:G:70:PHE:O	2.73	0.42
1:G:460:GLY:C	1:G:462:GLN:N	2.78	0.41
1:C:225:GLY:C	1:C:227:THR:H	2.28	0.41
1:E:179:LEU:HD21	1:E:191:MET:HE3	2.02	0.41
1:F:109:ASP:OD2	1:F:198:PRO:HD2	2.20	0.41
1:H:303:CYS:SG	2:H:601:3AK:O10	2.72	0.41
1:G:33:SER:O	1:G:34:ARG:HB2	2.20	0.41
1:C:421:ASN:O	1:C:423:SER:N	2.54	0.41
1:F:283:MET:O	1:F:287:VAL:HG23	2.20	0.41
1:B:279:SER:C	1:B:281:ALA:H	2.28	0.41
1:E:289:GLN:O	1:E:293:ALA:N	2.45	0.41
1:F:131:TYR:CZ	1:F:462:GLN:HA	2.55	0.41
1:F:202:LEU:O	1:F:205:ALA:HB3	2.21	0.41
1:H:194:ALA:HB1	1:H:196:GLN:NE2	2.36	0.41
1:A:59:VAL:O	1:A:63:VAL:HG23	2.20	0.41
1:F:500:SER:OG	1:G:77:ARG:NE	2.53	0.41
1:G:247:THR:HA	1:G:269:LEU:HD13	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:LEU:O	1:A:200:THR:C	2.64	0.41
1:B:198:PRO:O	1:B:202:LEU:HG	2.21	0.41
1:D:361:LYS:HD3	1:D:367:LEU:HD22	2.03	0.41
1:E:78:ARG:HE	1:H:497:GLN:NE2	2.19	0.41
1:E:458:VAL:HG21	1:F:150:PHE:CE2	2.56	0.41
1:G:48:ILE:CG2	1:G:108:LEU:HD21	2.46	0.41
1:F:337:SER:O	1:F:338:LYS:HB2	2.19	0.41
1:A:400:ILE:O	1:A:401:PHE:CB	2.69	0.41
1:B:381:ILE:HG22	1:B:382:GLN:O	2.21	0.41
1:D:298:GLN:HG3	1:D:341:GLN:HG3	2.02	0.41
1:F:55:ASP:HB3	1:F:58:ASP:OD2	2.21	0.40
1:F:244:THR:HG23	1:F:268:GLU:O	2.21	0.40
1:G:150:PHE:CZ	1:H:458:VAL:HG21	2.57	0.40
1:G:315:TYR:CE1	1:G:319:VAL:HG21	2.56	0.40
1:H:389:VAL:HB	1:H:408:LEU:HG	2.04	0.40
1:H:459:PHE:HE2	1:H:465:PHE:CE2	2.39	0.40
1:B:124:MET:HE1	2:B:601:3AK:H4	2.02	0.40
1:B:240:LYS:HE3	1:B:485:TYR:CE2	2.57	0.40
1:E:99:ARG:HG3	1:E:122:LEU:HD23	2.03	0.40
1:G:102:LEU:HD21	1:G:203:TYR:CD2	2.54	0.40
1:H:149:ASP:HA	1:H:498:LYS:HB2	2.02	0.40
1:A:169:ASN:C	1:A:171:PRO:HD3	2.46	0.40
1:A:283:MET:O	1:A:287:VAL:HG23	2.21	0.40
1:F:456:TYR:HD2	1:F:457:ASP:OD2	2.04	0.40
1:A:262:LEU:HD21	1:B:251:ARG:HG3	2.04	0.40
1:B:158:PRO:O	5:B:603:GAI:N3	2.55	0.40
1:B:430:ALA:HB2	1:B:456:TYR:CE1	2.57	0.40
1:C:205:ALA:O	1:C:208:ILE:HB	2.21	0.40
1:G:55:ASP:O	1:G:57:GLU:N	2.54	0.40
1:G:125:VAL:HG21	1:G:172:LEU:HB3	2.04	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%)	463 (94%)	29 (6%)	0	100	100
1	B	492/494 (100%)	445 (90%)	43 (9%)	4 (1%)	16	19
1	C	492/494 (100%)	457 (93%)	30 (6%)	5 (1%)	12	14
1	D	492/494 (100%)	469 (95%)	22 (4%)	1 (0%)	43	53
1	E	492/494 (100%)	468 (95%)	21 (4%)	3 (1%)	21	25
1	F	492/494 (100%)	451 (92%)	38 (8%)	3 (1%)	21	25
1	G	492/494 (100%)	456 (93%)	33 (7%)	3 (1%)	21	25
1	H	492/494 (100%)	469 (95%)	23 (5%)	0	100	100
All	All	3936/3952 (100%)	3678 (93%)	239 (6%)	19 (0%)	24	30

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	56	LYS
1	F	307	ARG
1	F	338	LYS
1	G	56	LYS
1	B	426	GLY
1	C	422	ASN
1	E	214	PRO
1	E	260	SER
1	G	383	PRO
1	D	422	ASN
1	C	56	LYS
1	F	426	GLY
1	B	41	ASN
1	B	171	PRO
1	C	11	PRO
1	C	226	PRO
1	C	371	GLY
1	G	198	PRO
1	E	426	GLY

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%)	387 (97%)	12 (3%)	36	52
1	B	399/399 (100%)	379 (95%)	20 (5%)	22	32
1	C	399/399 (100%)	384 (96%)	15 (4%)	29	43
1	D	399/399 (100%)	391 (98%)	8 (2%)	48	66
1	E	399/399 (100%)	389 (98%)	10 (2%)	42	59
1	F	399/399 (100%)	374 (94%)	25 (6%)	16	22
1	G	399/399 (100%)	386 (97%)	13 (3%)	33	48
1	H	399/399 (100%)	385 (96%)	14 (4%)	32	46
All	All	3192/3192 (100%)	3075 (96%)	117 (4%)	30	44

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	72	LEU
1	A	106	GLU
1	A	117	SER
1	A	122	LEU
1	A	146	ILE
1	A	348	THR
1	A	352	LYS
1	A	373	ILE
1	A	401	PHE
1	A	462	GLN
1	A	486	THR
1	B	30	ASP
1	B	34	ARG
1	B	41	ASN
1	B	72	LEU
1	B	90	ARG
1	B	102	LEU
1	B	121	ASP
1	B	122	LEU
1	B	196	GLN
1	B	221	VAL
1	B	234	SER

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Mol	Chain	Res	Type
1	B	273	SER
1	B	311	GLN
1	B	316	ASP
1	B	328	SER
1	B	359	THR
1	B	363	GLU
1	B	435	ASP
1	B	444	GLN
1	B	486	THR
1	C	20	ASN
1	C	35	LYS
1	C	44	THR
1	C	64	LYS
1	C	121	ASP
1	C	195	GLU
1	C	196	GLN
1	C	284	ASP
1	C	303	CYS
1	C	333	ASN
1	C	376	ASP
1	C	401	PHE
1	C	405	MET
1	C	406	GLN
1	C	437	ASP
1	D	34	ARG
1	D	43	SER
1	D	121	ASP
1	D	192	LYS
1	D	196	GLN
1	D	227	THR
1	D	337	SER
1	D	462	GLN
1	E	16	GLU
1	E	25	ASN
1	E	172	LEU
1	E	189	VAL
1	E	196	GLN
1	E	197	THR
1	E	206	ASN
1	E	462	GLN
1	E	486	THR
1	E	498	LYS

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Mol	Chain	Res	Type
1	F	20	ASN
1	F	30	ASP
1	F	36	THR
1	F	41	ASN
1	F	49	CYS
1	F	112	LYS
1	F	122	LEU
1	F	159	VAL
1	F	192	LYS
1	F	260	SER
1	F	275	ASN
1	F	316	ASP
1	F	317	GLU
1	F	322	SER
1	F	327	LYS
1	F	328	SER
1	F	357	ILE
1	F	358	ASN
1	F	376	ASP
1	F	384	THR
1	F	401	PHE
1	F	412	THR
1	F	417	VAL
1	F	427	LEU
1	F	462	GLN
1	G	14	GLN
1	G	39	THR
1	G	72	LEU
1	G	115	VAL
1	G	124	MET
1	G	196	GLN
1	G	200	THR
1	G	236	GLU
1	G	249	ILE
1	G	284	ASP
1	G	377	ARG
1	G	401	PHE
1	G	462	GLN
1	H	13	GLN
1	H	14	GLN
1	H	20	ASN
1	H	41	ASN

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Mol	Chain	Res	Type
1	H	112	LYS
1	H	117	SER
1	H	159	VAL
1	H	174	MET
1	H	192	LYS
1	H	196	GLN
1	H	220	ILE
1	H	381	ILE
1	H	463	SER
1	H	486	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (84) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	41	ASN
1	A	175	GLN
1	A	196	GLN
1	A	349	GLN
1	A	362	GLN
1	A	406	GLN
1	A	462	GLN
1	B	20	ASN
1	B	26	ASN
1	B	41	ASN
1	B	196	GLN
1	B	444	GLN
1	C	13	GLN
1	C	14	GLN
1	C	20	ASN
1	C	26	ASN
1	C	41	ASN
1	C	83	HIS
1	C	89	ASN
1	C	164	GLN
1	C	196	GLN
1	C	206	ASN
1	C	333	ASN
1	C	349	GLN
1	C	362	GLN
1	C	462	GLN
1	D	26	ASN

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Mol	Chain	Res	Type
1	D	41	ASN
1	D	175	GLN
1	D	196	GLN
1	D	289	GLN
1	D	300	GLN
1	D	462	GLN
1	E	13	GLN
1	E	14	GLN
1	E	26	ASN
1	E	41	ASN
1	E	83	HIS
1	E	110	ASN
1	E	175	GLN
1	E	196	GLN
1	E	219	ASN
1	E	289	GLN
1	E	390	GLN
1	E	406	GLN
1	E	462	GLN
1	E	497	GLN
1	F	20	ASN
1	F	26	ASN
1	F	41	ASN
1	F	156	HIS
1	F	164	GLN
1	F	175	GLN
1	F	196	GLN
1	F	206	ASN
1	F	254	GLN
1	F	344	GLN
1	F	358	ASN
1	F	462	GLN
1	G	26	ASN
1	G	41	ASN
1	G	50	GLN
1	G	110	ASN
1	G	196	GLN
1	G	206	ASN
1	G	275	ASN
1	G	300	GLN
1	G	440	ASN
1	G	444	GLN

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Mol	Chain	Res	Type
1	G	447	GLN
1	G	462	GLN
1	H	13	GLN
1	H	14	GLN
1	H	20	ASN
1	H	26	ASN
1	H	41	ASN
1	H	50	GLN
1	H	164	GLN
1	H	175	GLN
1	H	196	GLN
1	H	298	GLN
1	H	300	GLN
1	H	497	GLN

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 27 ligands modelled in this entry, 8 are monoatomic - leaving 19 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GAI	B	603	-	3,3,3	1.02	0	3,3,3	1.10	0
5	GAI	A	605	-	3,3,3	0.99	0	3,3,3	1.11	0
5	GAI	F	603	-	3,3,3	0.96	0	3,3,3	1.08	0
4	EDO	C	602	-	3,3,3	0.36	0	2,2,2	0.32	0
4	EDO	E	603	-	3,3,3	0.33	0	2,2,2	0.38	0
2	3AK	A	601	-	20,20,20	2.47	4 (20%)	28,28,28	2.56	7 (25%)
2	3AK	E	601	-	20,20,20	2.47	4 (20%)	28,28,28	2.49	9 (32%)
4	EDO	A	603	-	3,3,3	0.29	0	2,2,2	0.66	0
4	EDO	H	603	-	3,3,3	0.33	0	2,2,2	0.47	0
4	EDO	F	602	-	3,3,3	0.34	0	2,2,2	0.36	0
5	GAI	D	602	-	3,3,3	0.89	0	3,3,3	0.99	0
4	EDO	C	603	-	3,3,3	0.41	0	2,2,2	0.18	0
5	GAI	H	604	-	3,3,3	1.02	0	3,3,3	1.13	0
5	GAI	G	602	-	3,3,3	0.98	0	3,3,3	0.89	0
2	3AK	H	601	-	20,20,20	2.41	4 (20%)	28,28,28	2.54	9 (32%)
4	EDO	A	604	-	3,3,3	0.31	0	2,2,2	0.40	0
2	3AK	B	601	-	20,20,20	2.35	5 (25%)	28,28,28	2.54	9 (32%)
5	GAI	C	604	-	3,3,3	1.06	0	3,3,3	1.07	0
4	EDO	E	604	-	3,3,3	0.35	0	2,2,2	0.33	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	3AK	H	601	-	-	2/4/20/20	0/3/3/3
4	EDO	F	602	-	-	0/1/1/1	-
4	EDO	H	603	-	-	1/1/1/1	-
4	EDO	C	602	-	-	1/1/1/1	-
4	EDO	A	604	-	-	1/1/1/1	-
2	3AK	B	601	-	-	2/4/20/20	0/3/3/3
4	EDO	C	603	-	-	1/1/1/1	-
4	EDO	E	603	-	-	1/1/1/1	-
2	3AK	A	601	-	-	2/4/20/20	0/3/3/3
2	3AK	E	601	-	-	2/4/20/20	0/3/3/3
4	EDO	A	603	-	-	0/1/1/1	-
4	EDO	E	604	-	-	0/1/1/1	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	601	3AK	C1-C6	7.15	1.50	1.41
2	H	601	3AK	C1-C6	7.04	1.50	1.41
2	A	601	3AK	C1-C6	7.04	1.50	1.41
2	A	601	3AK	C8-C9	-6.86	1.45	1.55
2	H	601	3AK	C8-C9	-6.58	1.45	1.55
2	B	601	3AK	C8-C9	-6.55	1.45	1.55
2	E	601	3AK	C8-C9	-6.55	1.45	1.55
2	B	601	3AK	C1-C6	6.38	1.49	1.41
2	E	601	3AK	O11-C8	3.13	1.29	1.23
2	E	601	3AK	O10-C9	2.98	1.29	1.23
2	B	601	3AK	O10-C9	2.91	1.29	1.23
2	H	601	3AK	O11-C8	2.76	1.28	1.23
2	B	601	3AK	O11-C8	2.69	1.28	1.23
2	A	601	3AK	O11-C8	2.61	1.28	1.23
2	A	601	3AK	O10-C9	2.48	1.28	1.23
2	H	601	3AK	O10-C9	2.14	1.27	1.23
2	B	601	3AK	C6-N7	-2.08	1.35	1.39

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	3AK	C9-C8-N7	8.65	112.35	106.18
2	B	601	3AK	C9-C8-N7	8.13	111.98	106.18
2	H	601	3AK	C9-C8-N7	7.89	111.81	106.18
2	E	601	3AK	C9-C8-N7	7.88	111.80	106.18
2	A	601	3AK	O11-C8-C9	-5.38	122.24	126.57
2	H	601	3AK	C6-C1-C9	-5.37	102.91	107.78
2	B	601	3AK	O11-C8-C9	-5.29	122.32	126.57
2	H	601	3AK	C5-C6-C1	-5.19	116.15	121.95
2	A	601	3AK	C6-C1-C9	-5.10	103.15	107.78
2	E	601	3AK	O11-C8-C9	-5.04	122.52	126.57
2	E	601	3AK	C5-C6-C1	-4.86	116.52	121.95
2	B	601	3AK	C6-C1-C9	-4.49	103.71	107.78
2	E	601	3AK	C6-C1-C9	-4.45	103.74	107.78
2	A	601	3AK	C5-C6-C1	-4.35	117.09	121.95
2	B	601	3AK	C5-C6-C1	-4.32	117.13	121.95
2	H	601	3AK	O11-C8-C9	-4.30	123.11	126.57
2	H	601	3AK	C2-C1-C6	3.03	122.74	119.24
2	B	601	3AK	C12-N7-C8	2.83	127.88	123.57
2	E	601	3AK	C13-C12-N7	-2.80	108.90	113.46
2	B	601	3AK	C6-N7-C8	-2.67	108.67	110.73
2	A	601	3AK	C2-C1-C9	2.58	134.70	129.70
2	B	601	3AK	O10-C9-C8	2.53	125.66	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	3AK	C2-C1-C6	2.53	122.15	119.24
2	E	601	3AK	O10-C9-C8	2.52	125.65	123.70
2	E	601	3AK	C2-C1-C9	2.48	134.50	129.70
2	B	601	3AK	C2-C1-C9	2.43	134.42	129.70
2	H	601	3AK	C2-C1-C9	2.40	134.35	129.70
2	H	601	3AK	C6-N7-C8	-2.37	108.90	110.73
2	A	601	3AK	C6-N7-C8	-2.35	108.92	110.73
2	B	601	3AK	C2-C1-C6	2.29	121.87	119.24
2	H	601	3AK	O10-C9-C8	2.26	125.45	123.70
2	E	601	3AK	C6-N7-C8	-2.22	109.02	110.73
2	E	601	3AK	C2-C1-C6	2.18	121.75	119.24
2	H	601	3AK	C3-C4-C5	2.09	122.81	120.24

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	3AK	C13-C12-N7-C8
2	A	601	3AK	C13-C12-N7-C6
2	B	601	3AK	C13-C12-N7-C6
2	B	601	3AK	C13-C12-N7-C8
2	H	601	3AK	C13-C12-N7-C8
2	H	601	3AK	C13-C12-N7-C6
2	E	601	3AK	C13-C12-N7-C8
2	E	601	3AK	C13-C12-N7-C6
4	C	603	EDO	O1-C1-C2-O2
4	E	603	EDO	O1-C1-C2-O2
4	A	604	EDO	O1-C1-C2-O2
4	C	602	EDO	O1-C1-C2-O2
4	H	603	EDO	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	603	GAI	1	0
2	A	601	3AK	3	0
2	E	601	3AK	4	0
4	A	603	EDO	1	0
2	H	601	3AK	5	0
2	B	601	3AK	9	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.96	0 100 100	29, 49, 73, 111	0
1	B	494/494 (100%)	-0.88	1 (0%) 91 91	28, 63, 88, 102	0
1	C	494/494 (100%)	-0.93	0 100 100	30, 52, 74, 87	0
1	D	494/494 (100%)	-0.99	1 (0%) 91 91	27, 42, 63, 79	0
1	E	494/494 (100%)	-0.98	0 100 100	29, 48, 76, 106	0
1	F	494/494 (100%)	-0.88	0 100 100	26, 63, 89, 111	0
1	G	494/494 (100%)	-0.95	0 100 100	29, 54, 76, 90	0
1	H	494/494 (100%)	-1.02	0 100 100	27, 42, 65, 88	0
All	All	3952/3952 (100%)	-0.95	2 (0%) 92 92	26, 50, 82, 111	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	471	SER	2.2
1	B	467	GLY	2.1

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(Å ²)	Q<0.9
3	NA	C	601	1/1	0.93	0.10	88,88,88,88	0
3	NA	H	602	1/1	0.95	0.08	65,65,65,65	0
3	NA	D	601	1/1	0.96	0.08	64,64,64,64	0
3	NA	A	602	1/1	0.96	0.10	91,91,91,91	0
5	GAI	A	605	4/4	0.96	0.08	69,72,73,76	0
4	EDO	E	604	4/4	0.97	0.08	75,78,78,80	0
3	NA	F	601	1/1	0.97	0.06	84,84,84,84	0
5	GAI	B	603	4/4	0.97	0.06	93,93,94,95	0
5	GAI	C	604	4/4	0.97	0.09	74,75,75,75	0
5	GAI	D	602	4/4	0.97	0.09	74,77,79,79	0
5	GAI	H	604	4/4	0.97	0.07	70,75,75,77	0
4	EDO	C	603	4/4	0.98	0.06	60,65,67,68	0
4	EDO	E	603	4/4	0.98	0.07	81,86,88,89	0
2	3AK	A	601	18/18	0.98	0.04	42,50,59,59	0
4	EDO	F	602	4/4	0.98	0.09	80,82,82,83	0
4	EDO	H	603	4/4	0.98	0.05	71,71,72,73	0
3	NA	E	602	1/1	0.98	0.08	73,73,73,73	0
3	NA	B	602	1/1	0.98	0.07	93,93,93,93	0
2	3AK	E	601	18/18	0.98	0.04	43,46,49,50	0
4	EDO	A	603	4/4	0.98	0.06	68,71,72,75	0
5	GAI	F	603	4/4	0.98	0.10	73,74,74,75	0
5	GAI	G	602	4/4	0.98	0.06	66,66,69,71	0
4	EDO	A	604	4/4	0.98	0.07	65,67,67,69	0
2	3AK	B	601	18/18	0.99	0.05	46,51,56,57	0
2	3AK	H	601	18/18	0.99	0.04	47,54,63,64	0
3	NA	G	601	1/1	0.99	0.06	83,83,83,83	0
4	EDO	C	602	4/4	0.99	0.09	63,64,64,65	0

6.5 Other polymers [i](#)

There are no such residues in this entry.