



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:25 PM UTC

PDB ID : 3SZ9 / pdb_00003sz9
Title : Crystal structure of human ALDH2 modified with the beta-elimination product of Aldi-3; 1-(4-ethylbenzene)prop-2-en-1-one
Authors : Perez-Miller, S.; Hurley, T.D.
Deposited on : 2011-07-18
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

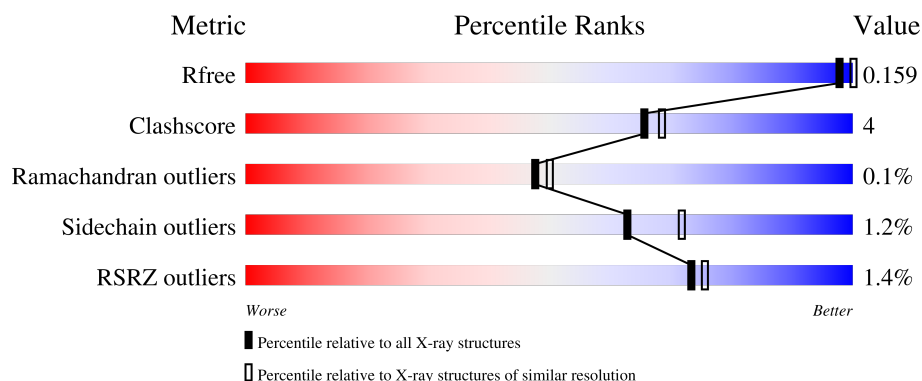
1 Overall quality at a glance

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.



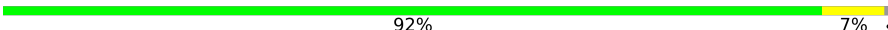
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	500	2% 88% 10% ..
1	B	500	91% 7% .
1	C	500	2% 87% 11% ..
1	D	500	6% 84% 14% .
1	E	500	92% 7% .

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Mol	Chain	Length	Quality of chain
1	F	500	 92% 7% •
1	G	500	 90% 8% •
1	H	500	 91% 7% •

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 33400 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	4	0
			3812	2423	649	720	20			
1	B	494	Total	C	N	O	S	0	7	0
			3825	2430	649	726	20			
1	C	495	Total	C	N	O	S	0	7	0
			3835	2436	652	727	20			
1	D	494	Total	C	N	O	S	0	4	0
			3812	2423	649	720	20			
1	E	494	Total	C	N	O	S	0	5	0
			3816	2425	650	721	20			
1	F	494	Total	C	N	O	S	0	3	0
			3810	2422	649	720	19			
1	G	494	Total	C	N	O	S	0	5	0
			3816	2425	649	722	20			
1	H	494	Total	C	N	O	S	0	5	0
			3817	2426	650	721	20			

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

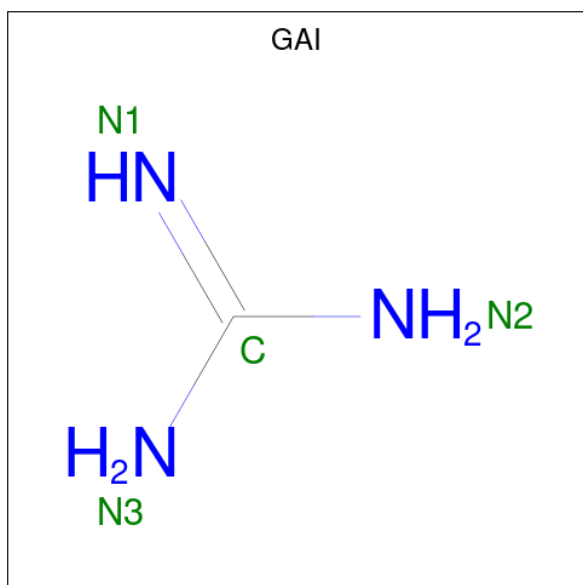
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Na	0	0
			1	1		
2	B	1	Total	Na	0	0
			1	1		
2	C	1	Total	Na	0	0
			1	1		
2	D	1	Total	Na	0	0
			1	1		
2	E	1	Total	Na	0	0
			1	1		
2	F	1	Total	Na	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	Na	0	0
			1	1		
2	H	1	Total	Na	0	0
			1	1		

- Molecule 3 is GUANIDINE (CCD ID: GAI) (formula: CH_5N_3).



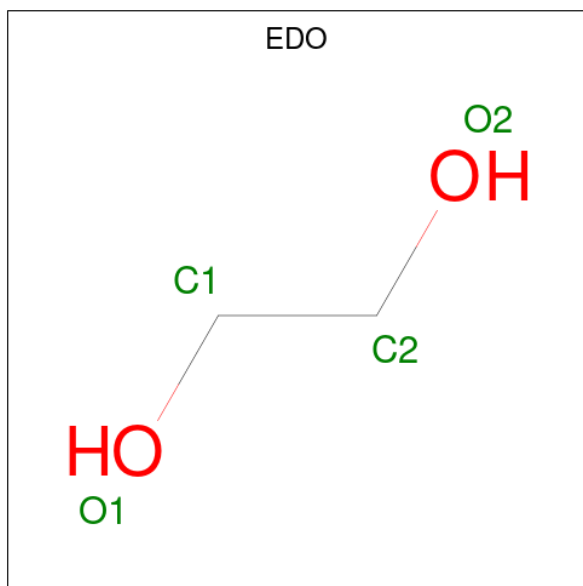
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			4	1	3		
3	A	1	Total	C	N	0	0
			4	1	3		
3	B	1	Total	C	N	0	0
			4	1	3		
3	B	1	Total	C	N	0	0
			4	1	3		
3	C	1	Total	C	N	0	0
			4	1	3		
3	C	1	Total	C	N	0	0
			4	1	3		
3	C	1	Total	C	N	0	0
			4	1	3		
3	C	1	Total	C	N	0	0
			4	1	3		
3	D	1	Total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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	E	1	Total	C	N	0	0
			4	1	3		
3	E	1	Total	C	N	0	0
			4	1	3		
3	F	1	Total	C	N	0	0
			4	1	3		
3	F	1	Total	C	N	0	0
			4	1	3		
3	F	1	Total	C	N	0	0
			4	1	3		
3	G	1	Total	C	N	0	0
			4	1	3		
3	G	1	Total	C	N	0	0
			4	1	3		
3	H	1	Total	C	N	0	0
			4	1	3		
3	H	1	Total	C	N	0	0
			4	1	3		

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



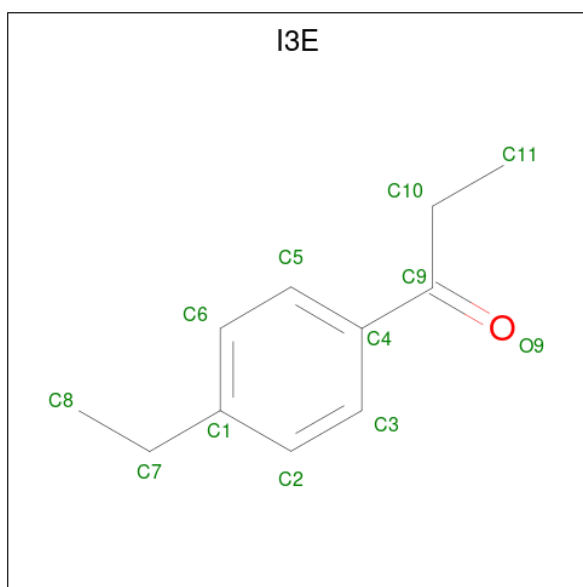
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	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	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	D	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	F	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	F	1	Total	C	O	0	0
			4	2	2		
4	F	1	Total	C	O	0	0
			4	2	2		
4	G	1	Total	C	O	0	0
			4	2	2		
4	H	1	Total	C	O	0	0
			4	2	2		
4	H	1	Total	C	O	0	0
			4	2	2		
4	H	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is 1-(4-ethylphenyl)propan-1-one (CCD ID: I3E) (formula: C₁₁H₁₄O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			12	11	1		
5	B	1	Total	C	O	0	0
			12	11	1		
5	C	1	Total	C	O	0	0
			12	11	1		
5	D	1	Total	C	O	0	0
			12	11	1		
5	E	1	Total	C	O	0	0
			12	11	1		
5	F	1	Total	C	O	0	0
			12	11	1		
5	G	1	Total	C	O	0	0
			12	11	1		
5	H	1	Total	C	O	0	0
			12	11	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	243	Total	O	0	0
			243	243		
6	B	355	Total	O	0	0
			355	355		
6	C	343	Total	O	0	0
			343	343		
6	D	212	Total	O	0	0
			212	212		

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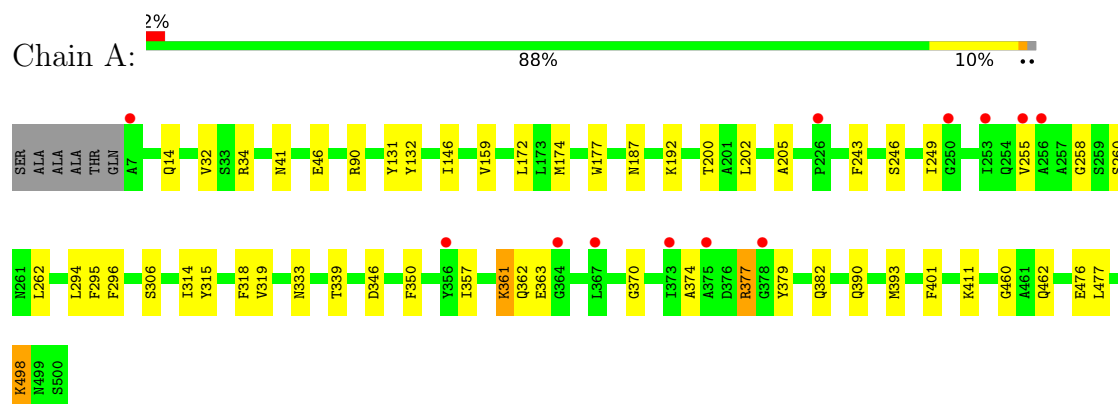
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	361	Total 361	O 361	0	0
6	F	431	Total 431	O 431	0	0
6	G	364	Total 366	O 366	0	2
6	H	285	Total 286	O 286	0	1

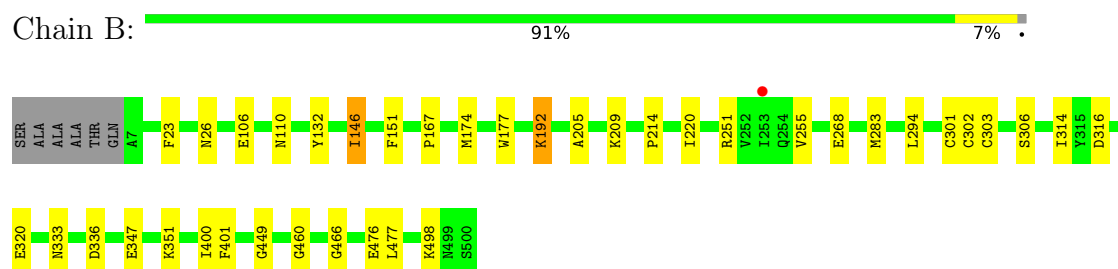
3 Residue-property plots

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.

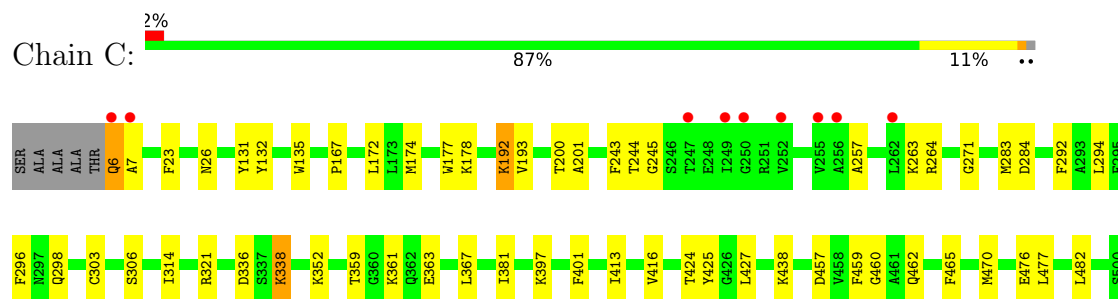
- Molecule 1: Aldehyde dehydrogenase, mitochondrial



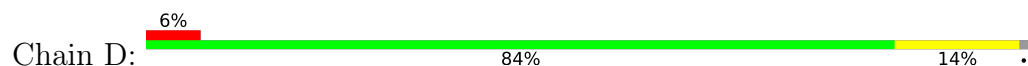
- Molecule 1: Aldehyde dehydrogenase, mitochondrial

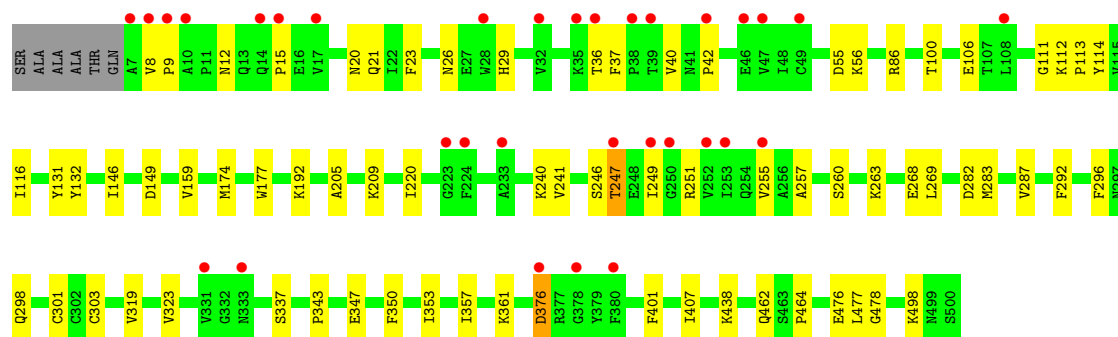


- Molecule 1: Aldehyde dehydrogenase, mitochondrial



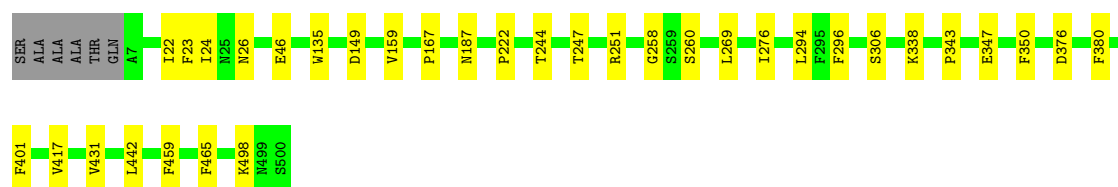
- Molecule 1: Aldehyde dehydrogenase, mitochondrial





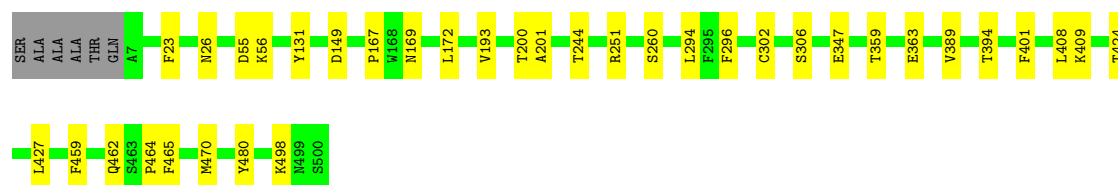
- Molecule 1: Aldehyde dehydrogenase, mitochondrial

Chain E: 92% 7% .



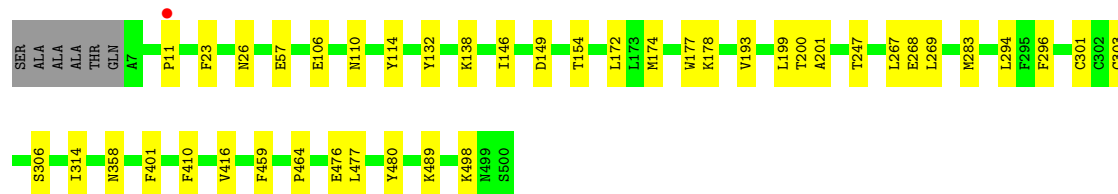
- Molecule 1: Aldehyde dehydrogenase, mitochondrial

Chain F: 92% 7% .



- Molecule 1: Aldehyde dehydrogenase, mitochondrial

Chain G: 90% 8% .



- Molecule 1: Aldehyde dehydrogenase, mitochondrial

Chain H: 91% 7% .



R377	T394	F401	G460	F465	M470	E476	L477	K498	N499	S500
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	140.52Å 151.05Å 177.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.10 50.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.6 (50.00-2.10) 99.6 (50.00-2.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.60 (at 2.10Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.174 , 0.226 (Not available) , 0.159	Depositor DCC
R_{free} test set	5387 reflections (2.47%)	wwPDB-VP
Wilson B-factor (Å ²)	22.0	Xtrriage
Anisotropy	0.430	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 37.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	33400	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 57.15 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.4684e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: GAI, NA, EDO, I3E

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	0.55	0/3912	0.79	0/5307
1	B	0.60	0/3937	0.82	2/5341 (0.0%)
1	C	0.61	0/3947	0.82	0/5354
1	D	0.57	0/3912	0.83	2/5307 (0.0%)
1	E	0.60	0/3920	0.79	1/5318 (0.0%)
1	F	0.63	0/3906	0.80	1/5299 (0.0%)
1	G	0.60	0/3920	0.82	1/5318 (0.0%)
1	H	0.56	0/3921	0.79	1/5319 (0.0%)
All	All	0.59	0/31375	0.81	8/42563 (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	B	400	ILE	N-CA-C	-6.34	106.36	111.81
1	G	199	LEU	N-CA-C	6.03	117.66	111.14
1	F	169	ASN	N-CA-C	5.81	117.70	111.36
1	H	345	VAL	N-CA-C	5.36	116.14	110.72
1	B	214	PRO	O-C-N	5.35	123.77	121.31
1	E	276	ILE	N-CA-C	5.28	115.69	107.99
1	D	112	LYS	CA-C-N	5.09	125.38	119.93
1	D	112	LYS	C-N-CA	5.09	125.38	119.93

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	3812	0	3752	39	0
1	B	3825	0	3754	27	0
1	C	3835	0	3766	40	0
1	D	3812	0	3752	46	0
1	E	3816	0	3754	19	0
1	F	3810	0	3751	24	0
1	G	3816	0	3752	27	0
1	H	3817	0	3756	23	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	8	0	8	0	0
3	B	8	0	8	0	0
3	C	16	0	16	1	0
3	D	4	0	4	0	0
3	E	8	0	8	0	0
3	F	12	0	12	0	0
3	G	8	0	8	0	0
3	H	8	0	8	0	0
4	A	8	0	12	0	0
4	B	4	0	6	0	0
4	C	20	0	30	1	0
4	D	4	0	6	0	0
4	E	8	0	12	0	0
4	F	24	0	36	2	0
4	G	4	0	6	0	0
4	H	12	0	18	1	0
5	A	12	0	12	0	0
5	B	12	0	13	1	0
5	C	12	0	12	2	0
5	D	12	0	12	1	0
5	E	12	0	13	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	12	0	13	1	0
5	G	12	0	13	2	0
5	H	12	0	13	0	0
6	A	243	0	0	2	0
6	B	355	0	0	0	0
6	C	343	0	0	4	0
6	D	212	0	0	3	0
6	E	361	0	0	1	0
6	F	431	0	0	1	0
6	G	366	0	0	1	0
6	H	286	0	0	2	0
All	All	33400	0	30336	234	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 (234) 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:C:6:GLN:HG3	1:C:7:ALA:H	1.10	1.15
1:A:377:ARG:HG3	1:A:377:ARG:HH11	1.00	1.11
1:C:6:GLN:CG	1:C:7:ALA:N	2.30	0.95
1:C:6:GLN:HG3	1:C:7:ALA:N	1.83	0.93
1:A:377:ARG:HG3	1:A:377:ARG:NH1	1.79	0.93
1:C:303[B]:CYS:SG	1:C:465:PHE:HZ	1.97	0.88
1:D:12:ASN:O	1:D:15:PRO:HD3	1.77	0.84
1:C:303[B]:CYS:SG	1:C:465:PHE:CZ	2.71	0.84
1:D:241:VAL:HG23	1:D:263:LYS:HD3	1.61	0.82
1:H:303[B]:CYS:SG	1:H:465:PHE:CZ	2.73	0.81
1:C:359:THR:O	1:C:363:GLU:HG3	1.84	0.77
1:D:268[A]:GLU:HG3	1:D:476:GLU:OE1	1.83	0.77
1:A:377:ARG:HH11	1:A:377:ARG:CG	1.89	0.74
1:H:303[B]:CYS:SG	1:H:465:PHE:HZ	2.11	0.73
1:D:8:VAL:HG11	1:D:114:TYR:CE2	2.26	0.70
1:C:336:ASP:OD1	1:C:338:LYS:HG3	1.92	0.69
1:D:283:MET:O	1:D:287:VAL:HG23	1.93	0.69
1:E:46:GLU:HG3	6:E:2242:HOH:O	1.93	0.68
1:F:424:THR:HB	1:F:470:MET:HE3	1.76	0.67
1:C:174:MET:HE1	1:C:177:TRP:CZ3	2.29	0.67
1:C:296:PHE:CE1	5:C:8001:I3E:H8B	2.29	0.67
1:H:303[B]:CYS:SG	1:H:465:PHE:CE1	2.87	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:ARG:NH1	1:A:377:ARG:CG	2.54	0.67
1:C:178:LYS:NZ	1:C:476:GLU:OE1	2.30	0.64
1:D:23:PHE:CZ	1:D:26:ASN:HA	2.32	0.64
1:G:174:MET:HE1	1:G:177:TRP:CE3	2.33	0.64
1:A:357:ILE:O	1:A:361:LYS:HD3	1.99	0.63
1:D:246:SER:OG	1:D:249:ILE:HG12	1.97	0.63
1:E:296:PHE:CE1	5:E:8001:I3E:H8B	2.34	0.62
1:C:174:MET:HE1	1:C:177:TRP:CE3	2.35	0.61
1:B:205:ALA:HB2	1:B:220:ILE:HD12	1.82	0.61
1:D:21:GLN:HB3	1:D:29:HIS:O	2.02	0.59
1:E:135:TRP:CE2	1:G:138:LYS:HD3	2.38	0.58
1:C:424:THR:HB	1:C:470:MET:HE3	1.86	0.58
1:D:8:VAL:CG1	1:D:114:TYR:CE2	2.86	0.58
1:F:23:PHE:CZ	1:F:26:ASN:HA	2.38	0.58
1:D:319:VAL:O	1:D:323:VAL:HG23	2.04	0.57
1:A:174:MET:HE1	1:A:177:TRP:CE3	2.39	0.57
1:D:347:GLU:O	1:D:350:PHE:HB3	2.05	0.57
1:D:296:PHE:CE1	5:D:8001:I3E:H8B	2.40	0.57
1:C:23:PHE:CZ	1:C:26:ASN:HA	2.40	0.57
1:D:149:ASP:HA	1:D:498:LYS:HB2	1.86	0.56
1:B:192:LYS:HD2	1:B:192:LYS:C	2.30	0.56
1:G:268[A]:GLU:HG3	1:G:476:GLU:OE2	2.05	0.56
1:H:246:SER:OG	1:H:249:ILE:HG12	2.06	0.56
1:A:262:LEU:HD21	1:B:251:ARG:HG2	1.88	0.55
1:B:333:ASN:HB3	1:B:336[B]:ASP:OD2	2.07	0.55
1:H:245:GLY:O	1:H:269:LEU:HA	2.06	0.55
1:H:251:ARG:NH1	1:H:470:MET:HE1	2.22	0.55
1:C:271:GLY:HA2	1:C:425:TYR:CG	2.42	0.54
1:F:363:GLU:OE1	1:F:394:THR:N	2.38	0.54
1:C:303[B]:CYS:SG	1:C:427:LEU:HG	2.47	0.54
1:A:159:VAL:HG12	1:A:187:ASN:OD1	2.07	0.54
1:A:390:GLN:HG2	1:A:393:MET:HE3	1.90	0.54
1:E:260:SER:O	1:F:251:ARG:NH2	2.41	0.54
1:G:301[B]:CYS:SG	1:G:303:CYS:SG	3.04	0.54
1:D:257:ALA:HB1	1:D:263:LYS:HG3	1.89	0.53
1:A:172:LEU:HD21	1:A:200:THR:HB	1.91	0.53
1:D:55:ASP:OD1	1:D:56:LYS:N	2.35	0.53
1:A:460:GLY:HA3	1:B:146:ILE:HG13	1.91	0.53
1:F:459:PHE:HE2	1:F:465:PHE:CD1	2.26	0.53
1:B:268[A]:GLU:HG3	1:B:476:GLU:OE1	2.09	0.53
1:D:40:VAL:O	1:D:42:PRO:HD3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:131:TYR:CE1	1:D:462:GLN:HG3	2.44	0.52
1:E:159:VAL:HG12	1:E:187:ASN:OD1	2.08	0.52
1:A:41:ASN:OD1	1:A:41:ASN:C	2.53	0.52
1:C:303[B]:CYS:SG	1:C:465:PHE:CE1	3.02	0.52
1:G:358:ASN:ND2	6:G:2210:HOH:O	2.42	0.52
1:G:294:LEU:HD23	1:G:306:SER:HA	1.91	0.52
1:A:255:VAL:HG13	1:B:255:VAL:HG13	1.92	0.52
1:G:174:MET:HE1	1:G:177:TRP:CZ3	2.45	0.52
1:B:174:MET:HE2	1:B:174:MET:HA	1.92	0.51
1:B:301[B]:CYS:SG	1:B:303:CYS:SG	3.06	0.51
1:F:347:GLU:HG3	4:F:6961:EDO:H22	1.93	0.51
1:G:459:PHE:CD1	5:G:8001:I3E:H7A	2.45	0.51
1:C:361:LYS:HD3	1:C:367:LEU:HD22	1.93	0.51
1:E:258:GLY:O	1:F:251:ARG:HB3	2.10	0.51
1:C:6:GLN:HG2	1:C:7:ALA:N	2.22	0.51
1:G:247:THR:HA	1:G:269:LEU:HD13	1.93	0.50
1:G:11:PRO:HB3	1:G:114:TYR:CZ	2.46	0.50
1:G:283:MET:HE1	1:G:314:ILE:HB	1.93	0.50
1:G:149:ASP:HA	1:G:498:LYS:HB2	1.93	0.50
1:H:359:THR:HA	1:H:362:GLN:HG2	1.94	0.50
1:B:294:LEU:C	1:B:294:LEU:HD13	2.37	0.50
1:A:374:ALA:HB2	1:A:382:GLN:HG3	1.93	0.50
1:D:205:ALA:HB2	1:D:220:ILE:HD12	1.92	0.50
1:A:363:GLU:CD	1:A:393:MET:HB3	2.38	0.49
1:C:192:LYS:C	1:C:192:LYS:HD2	2.37	0.49
1:C:264:ARG:HG2	6:C:2500:HOH:O	2.12	0.49
1:E:247:THR:HA	1:E:269:LEU:HD13	1.94	0.49
1:A:146:ILE:HG13	1:B:460:GLY:HA3	1.94	0.49
1:E:294:LEU:HD23	1:E:306:SER:HA	1.94	0.49
1:A:131:TYR:CE1	1:A:462:GLN:HG3	2.47	0.49
1:D:8:VAL:CG1	1:D:114:TYR:HE2	2.24	0.49
1:C:283:MET:HE1	1:C:314:ILE:HB	1.95	0.49
1:H:368:LEU:O	1:H:369:CYS:HB3	2.13	0.49
1:A:246:SER:OG	1:A:249:ILE:HG12	2.13	0.49
1:B:23:PHE:CZ	1:B:26:ASN:HA	2.47	0.49
1:D:113:PRO:HB2	1:D:116:ILE:HG12	1.95	0.49
1:D:26:ASN:O	1:D:209:LYS:HD2	2.13	0.49
1:B:449:GLY:HA3	1:B:466:GLY:O	2.13	0.48
1:D:257:ALA:CB	1:D:263:LYS:HG3	2.42	0.48
1:D:251:ARG:O	1:D:255:VAL:HG23	2.13	0.48
1:E:22:ILE:HG12	1:E:222:PRO:HD2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:246:SER:HG	1:D:249:ILE:HG12	1.78	0.48
1:D:132:TYR:OH	1:D:477:LEU:HA	2.14	0.48
1:D:353:ILE:O	1:D:357:ILE:HG13	2.13	0.48
1:C:132:TYR:OH	1:C:477:LEU:HA	2.14	0.48
1:F:347:GLU:CG	4:F:6961:EDO:H22	2.44	0.48
1:A:202:LEU:O	1:A:205:ALA:HB3	2.14	0.47
1:A:295:PHE:O	1:A:296:PHE:C	2.58	0.47
1:G:11:PRO:HB3	1:G:114:TYR:CE1	2.48	0.47
1:C:131:TYR:CE1	1:C:462:GLN:HG3	2.49	0.47
1:C:172:LEU:HD21	1:C:200:THR:HB	1.96	0.47
1:C:243:PHE:CZ	1:C:245:GLY:HA3	2.49	0.47
1:D:174:MET:HE1	1:D:177:TRP:CZ3	2.48	0.47
1:A:90:ARG:NH1	6:A:2386:HOH:O	2.48	0.47
1:A:476:GLU:HG2	6:A:1723:HOH:O	2.14	0.47
1:C:459:PHE:HE2	1:C:465:PHE:CD1	2.32	0.47
1:D:37:PHE:CD1	1:D:37:PHE:C	2.93	0.47
1:A:46:GLU:OE2	1:A:377:ARG:NH2	2.48	0.47
1:A:476:GLU:O	1:A:477:LEU:HB2	2.15	0.47
1:H:167:PRO:HD3	1:H:244:THR:HB	1.96	0.47
1:D:8:VAL:HG12	1:D:9:PRO:O	2.15	0.46
1:A:333:ASN:O	1:A:339:THR:OG1	2.28	0.46
1:C:284:ASP:OD1	1:C:321:ARG:NH1	2.49	0.46
3:C:502:GAI:N2	6:C:2049:HOH:O	2.36	0.46
1:D:464:PRO:HA	1:D:476:GLU:O	2.15	0.46
1:F:131:TYR:CE1	1:F:462:GLN:HG3	2.50	0.46
1:A:174:MET:HE1	1:A:177:TRP:CZ3	2.51	0.45
1:E:251:ARG:NH2	1:F:260:SER:O	2.50	0.45
1:G:296:PHE:CE1	5:G:8001:I3E:H8B	2.51	0.45
1:C:459:PHE:HE2	1:C:465:PHE:CE1	2.34	0.45
1:D:86:ARG:HD3	6:D:1113:HOH:O	2.16	0.45
1:D:247:THR:HA	1:D:269:LEU:HD13	1.97	0.45
1:D:298:GLN:HG2	1:D:343:PRO:O	2.17	0.45
1:E:167:PRO:HD3	1:E:244:THR:HB	1.99	0.45
1:A:498:LYS:HB3	1:A:498:LYS:HE2	1.72	0.45
1:F:389:VAL:HB	1:F:408:LEU:HG	1.99	0.45
1:G:23:PHE:CZ	1:G:26:ASN:HA	2.51	0.45
1:C:298:GLN:HA	6:C:1166:HOH:O	2.17	0.45
1:E:22:ILE:HG22	1:E:24:ILE:HG13	1.99	0.45
1:E:459:PHE:HE2	1:E:465:PHE:CD1	2.35	0.45
1:C:460:GLY:HA3	1:D:146:ILE:HG13	1.98	0.44
1:F:409:LYS:NZ	6:F:2397:HOH:O	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:178:LYS:NZ	1:G:476:GLU:OE1	2.49	0.44
1:H:23:PHE:CZ	1:H:26:ASN:HA	2.51	0.44
1:B:151:PHE:CG	4:C:501:EDO:H22	2.53	0.44
1:C:294:LEU:HD23	1:C:306:SER:HA	1.99	0.44
1:H:283:MET:HE1	1:H:314:ILE:HB	1.99	0.44
1:C:413:ILE:HD12	1:C:438:LYS:HG2	2.00	0.44
1:D:111:GLY:O	1:D:343:PRO:HD2	2.18	0.44
1:D:319:VAL:HG22	1:D:407:ILE:HD12	1.98	0.44
1:H:149:ASP:HA	1:H:498:LYS:HB2	1.98	0.44
1:A:390:GLN:CG	1:A:393:MET:HE3	2.47	0.44
1:E:343:PRO:HD3	1:E:380:PHE:CE2	2.53	0.44
1:C:292:PHE:HE1	1:C:457:ASP:HB2	1.81	0.44
1:F:149:ASP:HA	1:F:498:LYS:HB2	2.00	0.44
1:G:193:VAL:HG11	1:G:201:ALA:HB3	1.99	0.44
1:B:174:MET:HE1	1:B:177:TRP:CE3	2.52	0.44
1:C:192:LYS:NZ	6:C:2496:HOH:O	2.51	0.44
1:D:376:ASP:OD1	1:D:376:ASP:N	2.47	0.43
1:E:347:GLU:O	1:E:350:PHE:HB3	2.18	0.43
1:A:294:LEU:HD23	1:A:306:SER:HA	2.01	0.43
1:A:314:ILE:O	1:A:315:TYR:C	2.62	0.43
1:B:498:LYS:HB3	1:B:498:LYS:HE2	1.75	0.43
1:C:167:PRO:HD3	1:C:244:THR:HB	2.00	0.43
1:D:438:LYS:NZ	6:D:1091:HOH:O	2.42	0.43
1:A:132:TYR:OH	1:A:477:LEU:HA	2.18	0.43
1:G:146:ILE:HG13	1:H:460:GLY:HA3	2.00	0.43
1:G:267:LEU:HB3	1:G:269:LEU:HD21	2.01	0.43
1:H:303[B]:CYS:SG	1:H:465:PHE:HE1	2.39	0.43
1:B:294:LEU:HD23	1:B:306:SER:HA	2.00	0.43
1:F:167:PRO:HD3	1:F:244:THR:HB	1.99	0.43
1:D:12:ASN:OD1	1:D:12:ASN:C	2.62	0.43
1:G:132:TYR:OH	1:G:477:LEU:HA	2.18	0.43
1:H:476:GLU:HG2	6:H:1055:HOH:O	2.18	0.43
1:A:411:LYS:HB2	1:A:411:LYS:HE2	1.73	0.43
1:B:132:TYR:OH	1:B:477:LEU:HA	2.19	0.43
1:E:23:PHE:CZ	1:E:26:ASN:HA	2.54	0.43
1:B:106:GLU:O	1:B:110:ASN:HB3	2.18	0.42
1:C:457:ASP:HB3	5:C:8001:I3E:H8A	2.01	0.42
1:D:282:ASP:C	1:D:282:ASP:OD1	2.62	0.42
1:F:172:LEU:HD21	1:F:200:THR:HB	2.01	0.42
1:F:302[A]:CYS:SG	1:F:427:LEU:HD21	2.59	0.42
1:G:172:LEU:HD21	1:G:200:THR:HB	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:106:GLU:O	1:H:110:ASN:HB3	2.19	0.42
1:A:315:TYR:CE1	1:A:319:VAL:HG21	2.54	0.42
1:F:193:VAL:HG11	1:F:201:ALA:CB	2.49	0.42
1:C:193:VAL:HG11	1:C:201:ALA:CB	2.49	0.42
1:G:154:THR:HA	1:G:489:LYS:O	2.18	0.42
1:E:149:ASP:HA	1:E:498:LYS:HB2	2.01	0.42
1:B:347:GLU:HG2	1:B:351:LYS:HD3	2.01	0.42
1:F:359:THR:O	1:F:363:GLU:HG3	2.19	0.42
1:G:410:PHE:CD1	1:G:416:VAL:HB	2.54	0.42
1:D:174:MET:HE1	1:D:177:TRP:CE3	2.55	0.42
1:E:417:VAL:CG2	1:E:442:LEU:HD23	2.50	0.42
1:H:132:TYR:OH	1:H:477:LEU:HA	2.19	0.42
1:C:135:TRP:CG	1:C:482:LEU:HD11	2.55	0.41
1:G:106:GLU:O	1:G:110:ASN:HB3	2.20	0.41
1:H:86:ARG:HD2	6:H:1561:HOH:O	2.19	0.41
1:H:172:LEU:HD21	1:H:200:THR:HB	2.02	0.41
1:B:26:ASN:HB3	1:B:209:LYS:HG3	2.03	0.41
1:F:464:PRO:HG3	1:F:480:TYR:CD1	2.55	0.41
1:B:167:PRO:HD2	1:B:174:MET:HG3	2.03	0.41
1:F:294:LEU:HD23	1:F:306:SER:HA	2.01	0.41
1:F:498:LYS:HE2	1:F:498:LYS:HB3	1.88	0.41
1:C:257:ALA:HB1	1:C:263:LYS:HG3	2.03	0.41
1:G:294:LEU:C	1:G:294:LEU:HD13	2.46	0.41
1:D:8:VAL:HG11	1:D:114:TYR:HE2	1.76	0.41
1:A:258:GLY:O	1:B:251:ARG:HB3	2.20	0.41
1:B:302[A]:CYS:SG	5:B:8001:I3E:O9	2.79	0.41
1:B:316:ASP:O	1:B:320[A]:GLU:HG3	2.20	0.41
1:E:431:VAL:HG21	1:E:442:LEU:HB3	2.03	0.41
1:F:55:ASP:OD1	1:F:56:LYS:N	2.46	0.41
1:F:296:PHE:CE1	5:F:8001:I3E:H8B	2.55	0.41
1:H:13:GLN:HE21	1:H:13:GLN:HB3	1.67	0.41
1:B:283:MET:HE1	1:B:314:ILE:HB	2.03	0.41
1:H:178:LYS:NZ	1:H:476:GLU:OE2	2.45	0.41
1:A:260:SER:O	1:B:251:ARG:NH1	2.54	0.40
1:A:318:PHE:CD2	1:A:318:PHE:C	2.98	0.40
1:D:301[B]:CYS:SG	1:D:303:CYS:SG	3.19	0.40
1:C:271:GLY:HA2	1:C:425:TYR:CD1	2.56	0.40
1:G:498:LYS:HE2	1:G:498:LYS:HB3	1.85	0.40
1:D:26:ASN:ND2	6:D:1705:HOH:O	2.53	0.40
1:D:292:PHE:CE2	1:D:296:PHE:CD2	3.10	0.40
1:G:464:PRO:HG3	1:G:480:TYR:CD1	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:PHE:CZ	1:A:249:ILE:HB	2.56	0.40
1:A:346:ASP:OD1	1:A:346:ASP:C	2.64	0.40
1:A:350:PHE:CD1	1:A:379:TYR:HB3	2.56	0.40
1:H:363:GLU:CD	1:H:394:THR:H	2.28	0.40
1:D:9:PRO:HG3	1:D:100:THR:OG1	2.21	0.40
1:F:251:ARG:H	1:F:251:ARG:HG3	1.74	0.40
1:H:264:ARG:NH1	4:H:6911:EDO:H21	2.37	0.40

There are no symmetry-related clashes.

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	496/500 (99%)	467 (94%)	27 (5%)	2 (0%)	30	28
1	B	499/500 (100%)	484 (97%)	15 (3%)	0	100	100
1	C	500/500 (100%)	480 (96%)	20 (4%)	0	100	100
1	D	496/500 (99%)	468 (94%)	25 (5%)	3 (1%)	21	18
1	E	497/500 (99%)	485 (98%)	12 (2%)	0	100	100
1	F	495/500 (99%)	480 (97%)	15 (3%)	0	100	100
1	G	497/500 (99%)	480 (97%)	17 (3%)	0	100	100
1	H	497/500 (99%)	478 (96%)	19 (4%)	0	100	100
All	All	3977/4000 (99%)	3822 (96%)	150 (4%)	5 (0%)	48	50

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	370	GLY
1	D	260	SER
1	D	478	GLY

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Mol	Chain	Res	Type
1	D	20	ASN
1	A	34	ARG

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	403/402 (100%)	395 (98%)	8 (2%)	48	56
1	B	406/402 (101%)	403 (99%)	3 (1%)	76	83
1	C	407/402 (101%)	399 (98%)	8 (2%)	48	56
1	D	403/402 (100%)	393 (98%)	10 (2%)	42	48
1	E	404/402 (100%)	401 (99%)	3 (1%)	76	83
1	F	402/402 (100%)	401 (100%)	1 (0%)	87	93
1	G	404/402 (100%)	402 (100%)	2 (0%)	81	88
1	H	404/402 (100%)	402 (100%)	2 (0%)	81	88
All	All	3233/3216 (100%)	3196 (99%)	37 (1%)	63	74

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	32	VAL
1	A	192	LYS
1	A	361	LYS
1	A	362	GLN
1	A	377	ARG
1	A	401	PHE
1	A	498	LYS
1	B	146	ILE
1	B	192	LYS
1	B	401	PHE
1	C	6	GLN
1	C	192	LYS

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Mol	Chain	Res	Type
1	C	338	LYS
1	C	352	LYS
1	C	381	ILE
1	C	397	LYS
1	C	401	PHE
1	C	416	VAL
1	D	36	THR
1	D	106	GLU
1	D	159	VAL
1	D	192	LYS
1	D	240	LYS
1	D	247	THR
1	D	337	SER
1	D	361	LYS
1	D	376	ASP
1	D	401	PHE
1	E	338	LYS
1	E	376	ASP
1	E	401	PHE
1	F	401	PHE
1	G	57	GLU
1	G	401	PHE
1	H	377	ARG
1	H	401	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	29	HIS
1	A	164	GLN
1	A	254	GLN
1	A	275	ASN
1	A	300	GLN
1	A	390	GLN
1	C	21	GLN
1	C	25	ASN
1	C	275	ASN
1	D	13	GLN
1	D	25	ASN
1	D	26	ASN
1	D	50	GLN

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Mol	Chain	Res	Type
1	D	175	GLN
1	D	254	GLN
1	D	362	GLN
1	D	406	GLN
1	D	447	GLN
1	E	50	GLN
1	E	275	ASN
1	E	349	GLN
1	F	29	HIS
1	F	275	ASN
1	F	390	GLN
1	G	13	GLN
1	G	275	ASN
1	G	358	ASN
1	G	483	GLN
1	H	13	GLN
1	H	50	GLN
1	H	206	ASN
1	H	275	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 55 ligands modelled in this entry, 8 are monoatomic - leaving 47 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	C	6921	-	3,3,3	0.28	0	2,2,2	0.61	0
4	EDO	C	6901	-	3,3,3	0.32	0	2,2,2	0.51	0
5	I3E	H	8001	1	12,12,12	0.43	0	15,15,15	1.18	1 (6%)
4	EDO	A	6921	-	3,3,3	0.32	0	2,2,2	0.63	0
4	EDO	F	6911	-	3,3,3	0.38	0	2,2,2	0.43	0
3	GAI	F	6821	-	3,3,3	0.85	0	3,3,3	1.30	0
4	EDO	C	6961	-	3,3,3	0.36	0	2,2,2	0.38	0
4	EDO	H	6911	-	3,3,3	0.42	0	2,2,2	0.03	0
4	EDO	D	6901	-	3,3,3	0.40	0	2,2,2	0.25	0
3	GAI	F	6801	-	3,3,3	0.63	0	3,3,3	0.63	0
4	EDO	C	501	-	3,3,3	0.46	0	2,2,2	0.36	0
5	I3E	G	8001	1	12,12,12	0.75	1 (8%)	15,15,15	1.39	2 (13%)
5	I3E	B	8001	1	12,12,12	0.58	0	15,15,15	1.22	2 (13%)
4	EDO	B	6911	-	3,3,3	0.40	0	2,2,2	0.50	0
4	EDO	F	6921	-	3,3,3	0.34	0	2,2,2	0.63	0
5	I3E	E	8001	1	12,12,12	0.74	1 (8%)	15,15,15	1.21	3 (20%)
5	I3E	F	8001	1	12,12,12	0.82	1 (8%)	15,15,15	1.13	1 (6%)
3	GAI	G	6801	-	3,3,3	0.94	0	3,3,3	0.90	0
4	EDO	F	6901	-	3,3,3	0.33	0	2,2,2	0.23	0
4	EDO	A	6901	-	3,3,3	0.40	0	2,2,2	0.25	0
4	EDO	H	6921	-	3,3,3	0.31	0	2,2,2	0.59	0
3	GAI	C	6811	-	3,3,3	0.91	0	3,3,3	1.02	0
3	GAI	D	6801	-	3,3,3	0.91	0	3,3,3	0.95	0
4	EDO	E	6921	-	3,3,3	0.31	0	2,2,2	0.68	0
5	I3E	C	8001	1	12,12,12	0.63	0	15,15,15	1.46	3 (20%)
5	I3E	D	8001	1	12,12,12	0.69	1 (8%)	15,15,15	0.97	1 (6%)
3	GAI	G	6811	-	3,3,3	1.01	0	3,3,3	0.86	0
3	GAI	E	6811	-	3,3,3	1.07	0	3,3,3	0.58	0
3	GAI	F	6811	-	3,3,3	0.95	0	3,3,3	1.00	0
3	GAI	C	6801	-	3,3,3	0.81	0	3,3,3	0.96	0
3	GAI	C	6821	-	3,3,3	0.99	0	3,3,3	1.21	0
3	GAI	H	6801	-	3,3,3	0.60	0	3,3,3	0.73	0
4	EDO	F	6961	-	3,3,3	0.38	0	2,2,2	0.22	0
3	GAI	H	6811	-	3,3,3	1.08	0	3,3,3	0.95	0
3	GAI	A	6801	-	3,3,3	0.83	0	3,3,3	1.12	0
3	GAI	E	6801	-	3,3,3	0.64	0	3,3,3	0.72	0
3	GAI	A	6811	-	3,3,3	1.09	0	3,3,3	1.24	0
5	I3E	A	8001	1	12,12,12	0.60	0	15,15,15	1.13	2 (13%)
4	EDO	C	6911	-	3,3,3	0.35	0	2,2,2	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GAI	B	6801	-	3,3,3	0.81	0	3,3,3	0.85	0
4	EDO	F	501	-	3,3,3	0.38	0	2,2,2	0.47	0
3	GAI	C	502	-	3,3,3	0.95	0	3,3,3	1.12	0
4	EDO	G	6921	-	3,3,3	0.30	0	2,2,2	0.57	0
4	EDO	H	6901	-	3,3,3	0.37	0	2,2,2	0.06	0
3	GAI	B	6811	-	3,3,3	0.78	0	3,3,3	0.99	0
4	EDO	F	6951	-	3,3,3	0.45	0	2,2,2	0.39	0
4	EDO	E	6901	-	3,3,3	0.36	0	2,2,2	0.32	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	C	6921	-	-	1/1/1/1	-
4	EDO	C	6901	-	-	0/1/1/1	-
5	I3E	H	8001	1	-	1/8/8/8	0/1/1/1
4	EDO	A	6921	-	-	1/1/1/1	-
4	EDO	F	6911	-	-	0/1/1/1	-
4	EDO	C	6961	-	-	0/1/1/1	-
4	EDO	H	6911	-	-	1/1/1/1	-
4	EDO	D	6901	-	-	0/1/1/1	-
4	EDO	C	501	-	-	1/1/1/1	-
5	I3E	B	8001	1	-	4/8/8/8	0/1/1/1
4	EDO	B	6911	-	-	0/1/1/1	-
4	EDO	F	6921	-	-	1/1/1/1	-
5	I3E	E	8001	1	-	5/8/8/8	0/1/1/1
5	I3E	F	8001	1	-	4/8/8/8	0/1/1/1
5	I3E	D	8001	1	-	6/8/8/8	0/1/1/1
4	EDO	F	6901	-	-	0/1/1/1	-
4	EDO	A	6901	-	-	1/1/1/1	-
4	EDO	H	6921	-	-	1/1/1/1	-
5	I3E	G	8001	1	-	4/8/8/8	0/1/1/1
4	EDO	E	6921	-	-	1/1/1/1	-
5	I3E	C	8001	1	-	4/8/8/8	0/1/1/1
4	EDO	F	6961	-	-	0/1/1/1	-
5	I3E	A	8001	1	-	4/8/8/8	0/1/1/1
4	EDO	C	6911	-	-	0/1/1/1	-
4	EDO	F	501	-	-	0/1/1/1	-
4	EDO	G	6921	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	H	6901	-	-	1/1/1/1	-
4	EDO	F	6951	-	-	0/1/1/1	-
4	EDO	E	6901	-	-	1/1/1/1	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	8001	I3E	C10-C9	-2.57	1.47	1.50
5	E	8001	I3E	C10-C9	-2.31	1.47	1.50
5	G	8001	I3E	C10-C9	-2.28	1.47	1.50
5	D	8001	I3E	C10-C9	-2.12	1.47	1.50

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	8001	I3E	C10-C9-C4	3.22	122.78	119.00
5	G	8001	I3E	C11-C10-C9	3.11	118.50	113.91
5	E	8001	I3E	C10-C9-C4	2.87	122.38	119.00
5	F	8001	I3E	C10-C9-C4	2.85	122.34	119.00
5	B	8001	I3E	C10-C9-C4	2.58	122.03	119.00
5	G	8001	I3E	C10-C9-C4	2.54	121.98	119.00
5	C	8001	I3E	C11-C10-C9	2.51	117.62	113.91
5	A	8001	I3E	C11-C10-C9	2.41	117.46	113.91
5	H	8001	I3E	C10-C9-C4	2.32	121.73	119.00
5	A	8001	I3E	C10-C9-C4	2.24	121.63	119.00
5	B	8001	I3E	C11-C10-C9	2.20	117.16	113.91
5	E	8001	I3E	C11-C10-C9	2.20	117.16	113.91
5	D	8001	I3E	C11-C10-C9	2.16	117.10	113.91
5	C	8001	I3E	O9-C9-C4	-2.08	117.95	120.73
5	E	8001	I3E	O9-C9-C10	-2.01	117.34	120.73

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	F	8001	I3E	C5-C4-C9-O9
5	F	8001	I3E	C3-C4-C9-O9
5	D	8001	I3E	C3-C4-C9-O9
5	D	8001	I3E	C5-C4-C9-O9
5	F	8001	I3E	C5-C4-C9-C10
5	C	8001	I3E	C5-C4-C9-O9

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Mol	Chain	Res	Type	Atoms
5	E	8001	I3E	C5-C4-C9-O9
5	F	8001	I3E	C3-C4-C9-C10
5	E	8001	I3E	C3-C4-C9-O9
5	D	8001	I3E	C3-C4-C9-C10
5	D	8001	I3E	C5-C4-C9-C10
5	C	8001	I3E	C3-C4-C9-O9
5	G	8001	I3E	C5-C4-C9-O9
5	B	8001	I3E	C5-C4-C9-O9
5	B	8001	I3E	C3-C4-C9-O9
5	G	8001	I3E	C3-C4-C9-O9
5	C	8001	I3E	C5-C4-C9-C10
5	E	8001	I3E	C5-C4-C9-C10
5	E	8001	I3E	C3-C4-C9-C10
4	G	6921	EDO	O1-C1-C2-O2
5	C	8001	I3E	C3-C4-C9-C10
5	B	8001	I3E	C5-C4-C9-C10
5	B	8001	I3E	C3-C4-C9-C10
5	G	8001	I3E	C5-C4-C9-C10
5	G	8001	I3E	C3-C4-C9-C10
4	H	6901	EDO	O1-C1-C2-O2
5	A	8001	I3E	C5-C4-C9-O9
5	A	8001	I3E	C3-C4-C9-O9
4	F	6921	EDO	O1-C1-C2-O2
4	H	6921	EDO	O1-C1-C2-O2
5	D	8001	I3E	C11-C10-C9-C4
5	A	8001	I3E	C3-C4-C9-C10
4	C	501	EDO	O1-C1-C2-O2
4	E	6901	EDO	O1-C1-C2-O2
5	A	8001	I3E	C5-C4-C9-C10
4	C	6921	EDO	O1-C1-C2-O2
4	A	6921	EDO	O1-C1-C2-O2
4	E	6921	EDO	O1-C1-C2-O2
5	D	8001	I3E	C11-C10-C9-O9
4	A	6901	EDO	O1-C1-C2-O2
5	H	8001	I3E	C2-C1-C7-C8
5	E	8001	I3E	C2-C1-C7-C8
4	H	6911	EDO	O1-C1-C2-O2

There are no ring outliers.

10 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	6911	EDO	1	0
4	C	501	EDO	1	0
5	G	8001	I3E	2	0
5	B	8001	I3E	1	0
5	E	8001	I3E	1	0
5	F	8001	I3E	1	0
5	C	8001	I3E	2	0
5	D	8001	I3E	1	0
4	F	6961	EDO	2	0
3	C	502	GAI	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	494/500 (98%)	0.15	12 (2%) 59 62	11, 31, 51, 63	4 (0%)
1	B	494/500 (98%)	-0.35	1 (0%) 91 92	10, 22, 40, 60	7 (1%)
1	C	495/500 (99%)	-0.38	9 (1%) 67 70	11, 21, 39, 65	8 (1%)
1	D	494/500 (98%)	0.41	32 (6%) 25 26	12, 32, 54, 72	4 (0%)
1	E	494/500 (98%)	-0.44	0 100 100	10, 21, 35, 49	5 (1%)
1	F	494/500 (98%)	-0.63	0 100 100	11, 18, 29, 47	3 (0%)
1	G	494/500 (98%)	-0.50	1 (0%) 91 92	11, 21, 35, 52	5 (1%)
1	H	494/500 (98%)	-0.07	1 (0%) 91 92	11, 27, 45, 60	5 (1%)
All	All	3953/4000 (98%)	-0.23	56 (1%) 73 75	10, 23, 45, 72	41 (1%)

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	378	GLY	4.1
1	D	47	VAL	4.0
1	C	252	VAL	3.4
1	A	255	VAL	3.3
1	H	7	ALA	3.0
1	D	247	THR	2.9
1	D	224	PHE	2.8
1	C	247	THR	2.8
1	D	8	VAL	2.8
1	A	7	ALA	2.8
1	D	10	ALA	2.8
1	D	333	ASN	2.7
1	A	356	TYR	2.7
1	A	250	GLY	2.7
1	A	256	ALA	2.7
1	D	36	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	252	VAL	2.7
1	D	253	ILE	2.7
1	D	7	ALA	2.6
1	D	32	VAL	2.6
1	D	380	PHE	2.5
1	D	223	GLY	2.5
1	D	249	ILE	2.5
1	D	331	VAL	2.5
1	A	367	LEU	2.5
1	D	35	LYS	2.5
1	D	38	PRO	2.4
1	C	6	GLN	2.4
1	A	226	PRO	2.4
1	C	249	ILE	2.3
1	D	14	GLN	2.3
1	D	108	LEU	2.3
1	D	255	VAL	2.3
1	D	250	GLY	2.3
1	A	253	ILE	2.2
1	C	262	LEU	2.2
1	B	253	ILE	2.2
1	A	378	GLY	2.2
1	C	250	GLY	2.2
1	D	233	ALA	2.2
1	D	15	PRO	2.1
1	D	39	THR	2.2
1	D	376	ASP	2.2
1	D	46	GLU	2.1
1	G	11	PRO	2.1
1	A	375	ALA	2.1
1	D	9	PRO	2.1
1	D	42	PRO	2.1
1	C	255	VAL	2.1
1	C	256	ALA	2.1
1	A	364	GLY	2.1
1	A	373	ILE	2.1
1	D	17	VAL	2.1
1	C	7	ALA	2.0
1	D	28	TRP	2.0
1	D	49	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
4	EDO	C	501	4/4	0.79	0.15	35,36,37,40	0
5	I3E	B	8001	12/12	0.80	0.21	30,32,34,35	12
5	I3E	C	8001	12/12	0.82	0.25	31,33,36,40	12
5	I3E	F	8001	12/12	0.82	0.22	27,32,36,39	12
5	I3E	D	8001	12/12	0.83	0.23	33,35,37,37	12
5	I3E	G	8001	12/12	0.84	0.24	24,27,35,35	12
5	I3E	A	8001	12/12	0.86	0.22	27,30,36,38	12
5	I3E	E	8001	12/12	0.86	0.20	27,29,33,35	12
4	EDO	C	6961	4/4	0.86	0.12	40,42,44,45	0
4	EDO	E	6921	4/4	0.86	0.14	43,43,45,48	0
5	I3E	H	8001	12/12	0.86	0.24	33,35,39,40	12
3	GAI	F	6821	4/4	0.88	0.10	41,42,43,43	0
4	EDO	F	6961	4/4	0.88	0.13	41,42,42,44	0
3	GAI	C	6801	4/4	0.88	0.12	35,36,37,37	0
3	GAI	C	6821	4/4	0.88	0.11	40,41,41,41	0
4	EDO	D	6901	4/4	0.88	0.10	29,33,35,38	0
4	EDO	A	6921	4/4	0.89	0.14	46,47,47,50	0
4	EDO	F	6951	4/4	0.89	0.14	24,32,34,37	0
3	GAI	A	6811	4/4	0.89	0.11	37,40,41,42	0
4	EDO	G	6921	4/4	0.89	0.14	49,52,52,52	0
3	GAI	C	6811	4/4	0.90	0.10	34,34,35,35	0
3	GAI	D	6801	4/4	0.90	0.12	44,44,44,45	0
4	EDO	F	6921	4/4	0.90	0.09	29,31,37,44	0
4	EDO	H	6921	4/4	0.90	0.13	49,49,51,56	0
4	EDO	F	6901	4/4	0.91	0.10	23,29,30,33	0
3	GAI	A	6801	4/4	0.91	0.09	30,30,32,32	0
4	EDO	H	6911	4/4	0.91	0.12	36,36,37,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GAI	E	6811	4/4	0.91	0.09	28,31,31,32	0
3	GAI	B	6811	4/4	0.92	0.12	25,28,28,28	0
3	GAI	H	6801	4/4	0.92	0.09	28,28,28,29	0
3	GAI	H	6811	4/4	0.92	0.10	39,39,39,41	0
3	GAI	C	502	4/4	0.92	0.10	36,37,38,39	0
2	NA	H	601	1/1	0.92	0.07	31,31,31,31	0
4	EDO	C	6921	4/4	0.92	0.08	36,38,40,45	0
3	GAI	B	6801	4/4	0.92	0.10	32,34,35,35	0
3	GAI	F	6801	4/4	0.92	0.09	21,21,24,24	0
4	EDO	F	501	4/4	0.93	0.08	24,27,28,32	0
4	EDO	A	6901	4/4	0.93	0.08	27,29,30,34	0
3	GAI	G	6811	4/4	0.94	0.12	32,32,33,36	0
4	EDO	H	6901	4/4	0.94	0.09	18,22,24,27	0
2	NA	E	601	1/1	0.94	0.06	33,33,33,33	0
4	EDO	B	6911	4/4	0.94	0.08	26,30,34,34	0
4	EDO	E	6901	4/4	0.94	0.08	21,28,29,29	0
3	GAI	F	6811	4/4	0.94	0.10	30,31,32,34	0
3	GAI	E	6801	4/4	0.95	0.08	27,27,29,29	0
4	EDO	C	6901	4/4	0.95	0.07	29,32,33,37	0
2	NA	D	601	1/1	0.95	0.07	36,36,36,36	0
4	EDO	C	6911	4/4	0.95	0.05	30,31,32,32	0
4	EDO	F	6911	4/4	0.95	0.07	27,29,30,33	0
3	GAI	G	6801	4/4	0.95	0.11	28,28,29,31	0
2	NA	A	601	1/1	0.95	0.06	34,34,34,34	0
2	NA	G	601	1/1	0.96	0.05	26,26,26,26	0
2	NA	F	601	1/1	0.97	0.04	23,23,23,23	0
2	NA	B	601	1/1	0.98	0.03	29,29,29,29	0
2	NA	C	601	1/1	0.98	0.04	22,22,22,22	0

6.5 Other polymers ⓘ

There are no such residues in this entry.