



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:08 PM GMT

PDB ID : 3SZ9  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

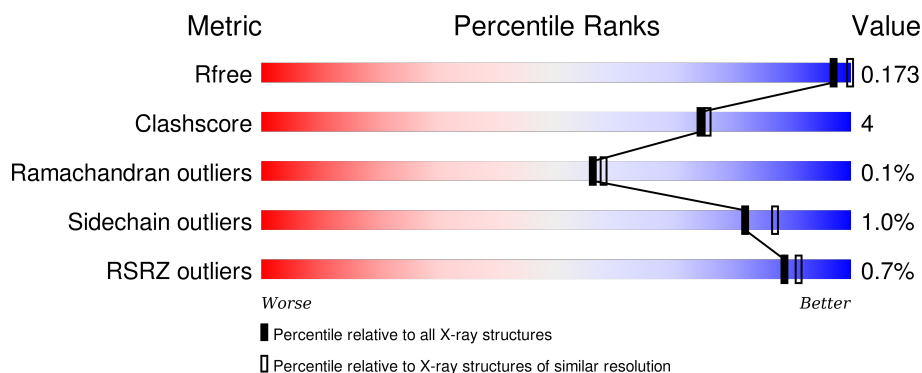
# 1 Overall quality at a glance ⓘ

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))
$R_{free}$	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	<div> <div>89%</div> <div>9%</div> <div>..</div> </div>
1	B	500	<div> <div>92%</div> <div>7%</div> <div>.</div> </div>
1	C	500	<div> <div>88%</div> <div>11%</div> <div>..</div> </div>
1	D	500	<div> <div>2%</div> <div>85%</div> <div>13%</div> <div>.</div> </div>
1	E	500	<div> <div>91%</div> <div>7%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	500	 92% 7%
1	G	500	 91% 7%
1	H	500	 93% 6%

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
3	GAI	B	6801	-	-	-	X
3	GAI	C	6801	-	-	-	X
3	GAI	C	6811	-	-	-	X
3	GAI	D	6801	-	-	-	X
3	GAI	E	6811	-	-	-	X
4	EDO	C	501	-	-	-	X
4	EDO	F	6901	-	-	-	X
4	EDO	F	6921	-	-	-	X
4	EDO	F	6951	-	-	-	X
4	EDO	H	6911	-	-	-	X
4	EDO	H	6921	-	-	-	X
5	I3E	A	8001	-	-	-	X
5	I3E	B	8001	-	-	X	X
5	I3E	C	8001	-	-	-	X
5	I3E	D	8001	-	-	-	X
5	I3E	E	8001	-	-	-	X
5	I3E	F	8001	-	-	-	X
5	I3E	G	8001	-	-	X	X
5	I3E	H	8001	-	-	-	X

## 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 (three-letter code: NA) (formula: Na).

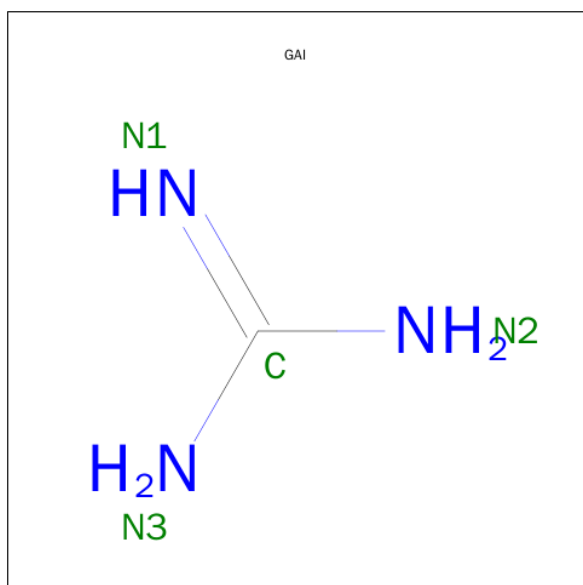
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	Na	0	0
			1	1		
2	D	1	Total	Na	0	0
			1	1		
2	E	1	Total	Na	0	0
			1	1		
2	H	1	Total	Na	0	0
			1	1		
2	B	1	Total	Na	0	0
			1	1		
2	C	1	Total	Na	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Na	0	0
			1	1		
2	F	1	Total	Na	0	0
			1	1		

- Molecule 3 is GUANIDINE (three-letter code: GAI) (formula:  $\text{CH}_5\text{N}_3$ ).



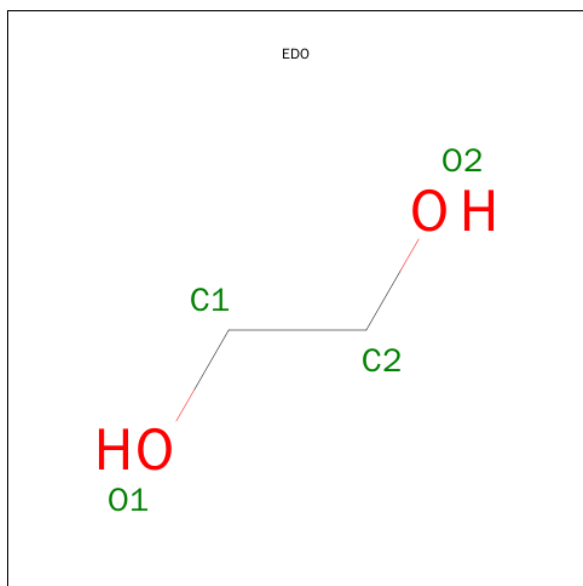
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			4	1	3		
3	A	1	Total	C	N	0	0
			4	1	3		
3	B	1	Total	C	N	0	0
			4	1	3		
3	B	1	Total	C	N	0	0
			4	1	3		
3	C	1	Total	C	N	0	0
			4	1	3		
3	C	1	Total	C	N	0	0
			4	1	3		
3	C	1	Total	C	N	0	0
			4	1	3		
3	C	1	Total	C	N	0	0
			4	1	3		
3	D	1	Total	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 (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



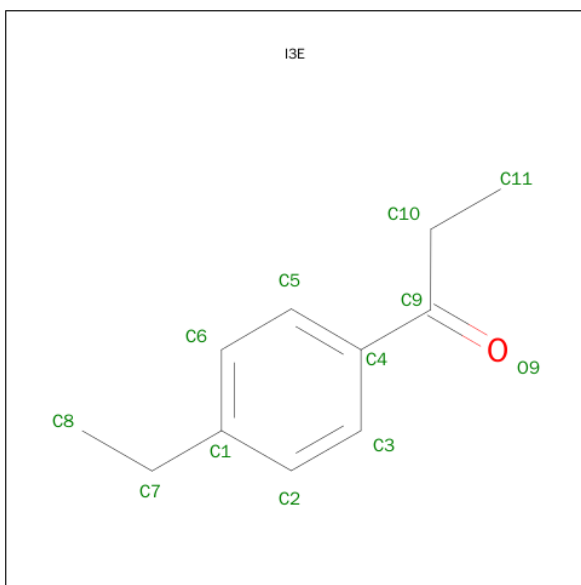
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		

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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	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 (three-letter code: I3E) (formula: C<sub>11</sub>H<sub>14</sub>O).



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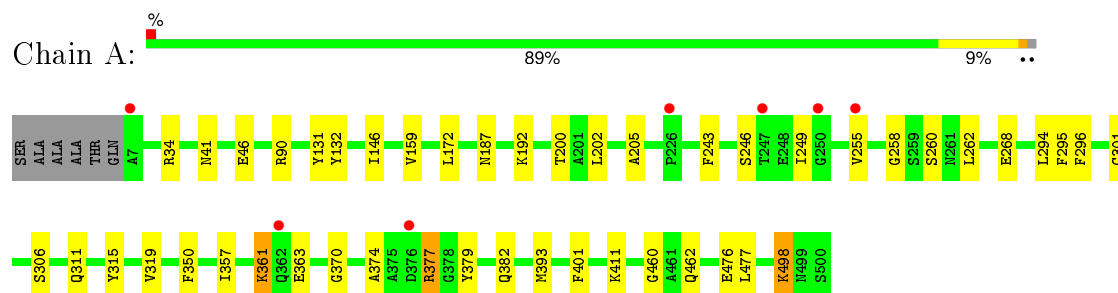
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	361	Total 361	O 361	0	0
6	F	431	Total 431	O 431	0	0
6	G	364	Total 366	O 366	0	2
6	H	285	Total 286	O 286	0	1

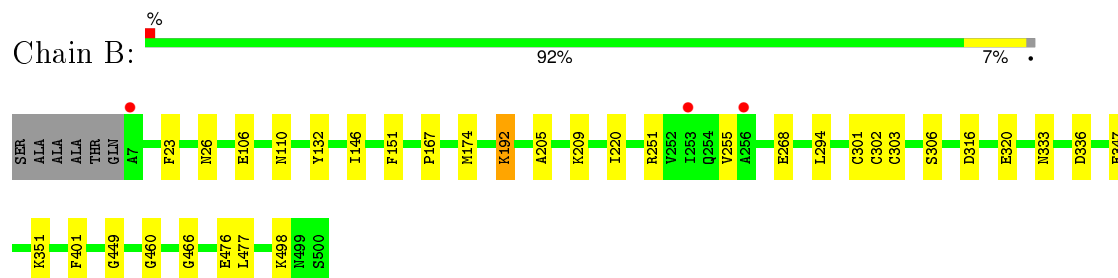
### 3 Residue-property plots [i](#)

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

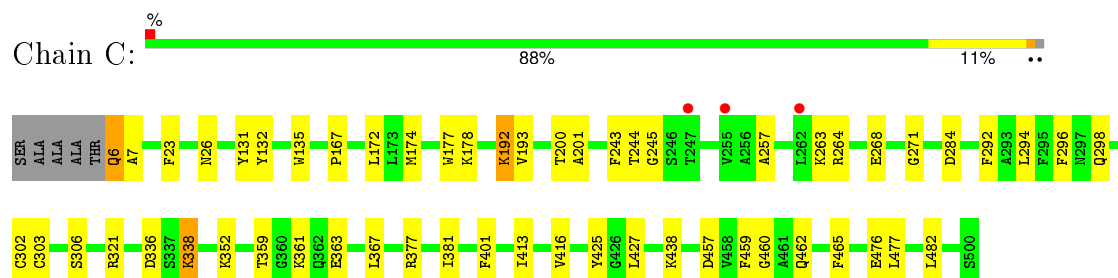
- Molecule 1: Aldehyde dehydrogenase, mitochondrial



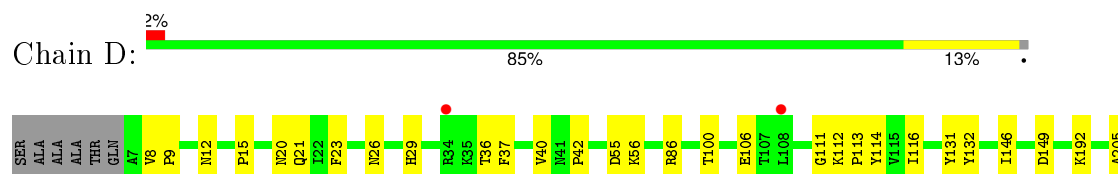
- Molecule 1: Aldehyde dehydrogenase, mitochondrial

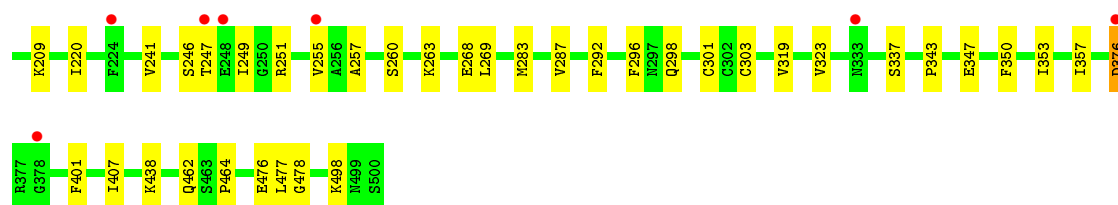


- Molecule 1: Aldehyde dehydrogenase, mitochondrial



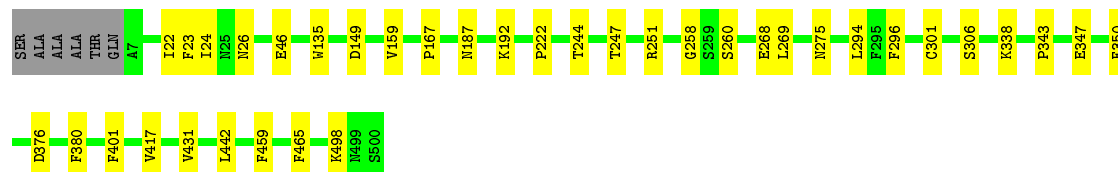
- Molecule 1: Aldehyde dehydrogenase, mitochondrial





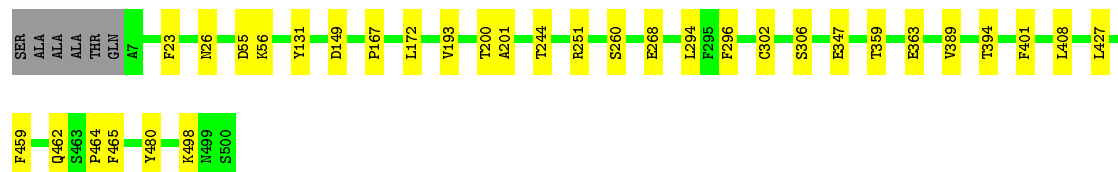
- Molecule 1: Aldehyde dehydrogenase, mitochondrial

Chain E: 91% 7% .



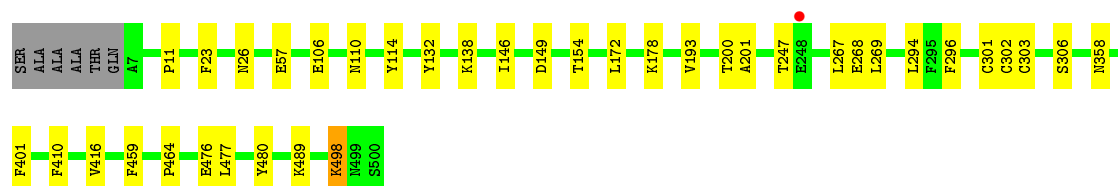
- Molecule 1: Aldehyde dehydrogenase, mitochondrial

Chain F: 92% 7% .



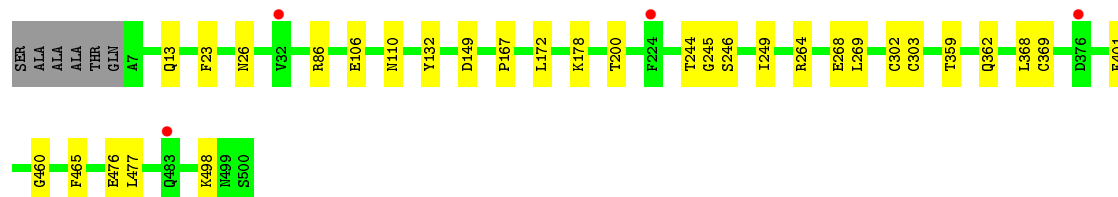
- Molecule 1: Aldehyde dehydrogenase, mitochondrial

Chain G: 91% 7% .



- Molecule 1: Aldehyde dehydrogenase, mitochondrial

Chain H: 93% 6% .



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	140.52Å 151.05Å 177.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.10 49.40 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.6 (50.00-2.10) 99.6 (49.40-2.10)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.60 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.174 , 0.226 0.178 , 0.173	Depositor DCC
$R_{free}$ test set	5387 reflections (2.54%)	DCC
Wilson B-factor (Å <sup>2</sup> )	22.0	Xtriage
Anisotropy	0.430	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 45.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	2 of 217729 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	33400	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage'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.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: NA, EDO, I3E, 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	0.45	0/3912	0.54	0/5307
1	B	0.51	0/3937	0.57	0/5341
1	C	0.50	0/3947	0.59	0/5354
1	D	0.46	0/3912	0.56	0/5307
1	E	0.49	0/3920	0.57	0/5318
1	F	0.52	0/3906	0.59	0/5299
1	G	0.50	0/3920	0.58	0/5318
1	H	0.47	0/3921	0.55	0/5319
All	All	0.49	0/31375	0.57	0/42563

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	3812	0	3752	35	0
1	B	3825	0	3754	29	0
1	C	3835	0	3766	40	0
1	D	3812	0	3752	44	0
1	E	3816	0	3754	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3810	0	3751	26	0
1	G	3816	0	3752	32	0
1	H	3817	0	3756	25	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	3	0
5	B	12	0	13	6	0
5	C	12	0	12	5	0
5	D	12	0	12	4	0
5	E	12	0	13	5	0
5	F	12	0	13	5	0
5	G	12	0	13	11	0
5	H	12	0	13	5	0
6	A	243	0	0	3	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	0	0
6	G	366	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	H	286	0	0	2	0
All	All	33400	0	30336	243	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 (243) 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[B]:CYS:SG	5:B:8001:I3E:H3	1.61	1.41
1:G:301[B]:CYS:SG	5:G:8001:I3E:H3	1.58	1.40
1:D:301[B]:CYS:SG	5:D:8001:I3E:H3	1.59	1.39
1:A:301[B]:CYS:SG	5:A:8001:I3E:H3	1.62	1.38
1:E:301[B]:CYS:SG	5:E:8001:I3E:H3	1.65	1.36
1:B:268[B]:GLU:OE1	5:B:8001:I3E:H11	1.20	1.33
1:C:6:GLN:HG3	1:C:7:ALA:H	1.10	1.15
1:G:268[B]:GLU:OE1	5:G:8001:I3E:H11	1.46	1.12
1:A:377:ARG:HH11	1:A:377:ARG:HG3	1.00	1.11
1:A:268[B]:GLU:OE1	5:A:8001:I3E:H11	1.58	1.04
1:H:268[B]:GLU:OE1	5:H:8001:I3E:H11	1.62	0.99
1:G:302[B]:CYS:SG	5:G:8001:I3E:H11A	1.98	0.98
1:E:268[B]:GLU:OE1	5:E:8001:I3E:H11	1.64	0.97
1:G:301[B]:CYS:SG	5:G:8001:I3E:C3	2.53	0.96
1:B:268[B]:GLU:OE1	5:B:8001:I3E:C11	2.12	0.95
1:B:301[B]:CYS:SG	5:B:8001:I3E:C3	2.54	0.95
1:C:6:GLN:CG	1:C:7:ALA:N	2.30	0.95
1:D:301[B]:CYS:SG	5:D:8001:I3E:C3	2.55	0.93
1:C:6:GLN:HG3	1:C:7:ALA:N	1.83	0.93
1:A:377:ARG:NH1	1:A:377:ARG:HG3	1.79	0.93
1:F:268[B]:GLU:OE1	5:F:8001:I3E:H11	1.69	0.91
1:C:303[B]:CYS:SG	1:C:465:PHE:HZ	1.97	0.88
1:H:302[B]:CYS:SG	5:H:8001:I3E:H11A	2.14	0.86
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:E:301[B]:CYS:SG	5:E:8001:I3E:C3	2.61	0.83
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:268[B]:GLU:OE1	5:C:8001:I3E:H11	1.82	0.80
1:G:302[B]:CYS:SG	5:G:8001:I3E:C11	2.71	0.79
1:A:311[B]:GLN:OE1	6:A:2121:HOH:O	1.98	0.78
1:A:301[B]:CYS:SG	5:A:8001:I3E:C3	2.59	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:268[A]:GLU:HG3	1:D:476:GLU:OE1	1.83	0.77
1:C:359:THR:O	1:C:363:GLU:HG3	1.84	0.77
1:G:268[B]:GLU:OE1	5:G:8001:I3E:C11	2.32	0.74
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: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
1:A:377:ARG:NH1	1:A:377:ARG:CG	2.54	0.67
1:D:23:PHE:CZ	1:D:26:ASN:HA	2.32	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:C:302[B]:CYS:SG	5:C:8001:I3E:C11	2.87	0.63
1:E:296:PHE:CE1	5:E:8001:I3E:H8B	2.34	0.62
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:C:178:LYS:NZ	1:C:476:GLU:OE1	2.30	0.59
1:E:135:TRP:CE2	1:G:138:LYS:HD3	2.38	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: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:D:268[B]:GLU:OE2	5:D:8001:I3E:H11	2.05	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:302[B]:CYS:SG	5:B:8001:I3E:H11A	2.44	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: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:B:301[B]:CYS:SG	1:B:303:CYS:SG	3.06	0.54
1:G:302[B]:CYS:HB2	5:G:8001:I3E:C11	2.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:301[B]:CYS:SG	1:G:303:CYS:SG	3.04	0.54
1:E:260:SER:O	1:F:251:ARG:NH2	2.41	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
1:E:159:VAL:HG12	1:E:187:ASN:OD1	2.08	0.52
1:D:131:TYR:CE1	1:D:462:GLN:HG3	2.44	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:B:192:LYS:C	1:B:192:LYS:HD2	2.30	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: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:H:302[B]:CYS:HB2	5:H:8001:I3E:C11	2.41	0.51
1:H:268[B]:GLU:OE1	5:H:8001:I3E:C11	2.48	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:268[B]:GLU:CD	5:G:8001:I3E:H11	2.27	0.50
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: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: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: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:F:268[B]:GLU:CD	5:F:8001:I3E:H11	2.32	0.49
1:A:146:ILE:HG13	1:B:460:GLY:HA3	1.94	0.49
1:H:178:LYS:NZ	1:H:476:GLU:OE2	2.45	0.49
1:E:294:LEU:HD23	1:E:306:SER:HA	1.94	0.49
1:D:8:VAL:CG1	1:D:114:TYR:HE2	2.24	0.49
1:A:131:TYR:CE1	1:A:462:GLN:HG3	2.47	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:353:ILE:O	1:D:357:ILE:HG13	2.13	0.48
1:D:132:TYR:OH	1:D:477:LEU:HA	2.14	0.48
1:F:347:GLU:CG	4:F:6961:EDO:H22	2.44	0.48
1:C:132:TYR:OH	1:C:477:LEU:HA	2.14	0.48
1:G:11:PRO:HB3	1:G:114:TYR:CE1	2.48	0.47
1:A:202:LEU:O	1:A:205:ALA:HB3	2.14	0.47
1:A:41:ASN:C	1:A:41:ASN:OD1	2.53	0.47
1:C:172:LEU:HD21	1:C:200:THR:HB	1.96	0.47
1:C:131:TYR:CE1	1:C:462:GLN:HG3	2.49	0.47
1:C:243:PHE:CZ	1:C:245:GLY:HA3	2.49	0.47
1:C:459:PHE:HE2	1:C:465:PHE:CD1	2.32	0.47
1:A:476:GLU:HG2	6:A:1723:HOH:O	2.14	0.47
1:A:90:ARG:NH1	6:A:2386:HOH:O	2.48	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:C:284:ASP:OD1	1:C:321:ARG:NH1	2.49	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
3:C:502:GAI:N2	6:C:2049:HOH:O	2.36	0.46
1:G:296:PHE:CE1	5:G:8001:I3E:H8B	2.51	0.45
1:E:251:ARG:NH2	1:F:260:SER:O	2.50	0.45
1:C:459:PHE:HE2	1:C:465:PHE:CE1	2.34	0.45
1:D:247:THR:HA	1:D:269:LEU:HD13	1.97	0.45
1:D:86:ARG:HD3	6:D:1113:HOH:O	2.16	0.45
1:B:294:LEU:HD13	1:B:294:LEU:C	2.37	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:F:389:VAL:HB	1:F:408:LEU:HG	1.99	0.45
1:A:498:LYS:HE2	1:A:498:LYS:HB3	1.72	0.45
1:G:23:PHE:CZ	1:G:26:ASN:HA	2.51	0.45
1:E:22:ILE:HG22	1:E:24:ILE:HG13	1.99	0.45
1:C:298:GLN:HA	6:C:1166:HOH:O	2.17	0.45
1:E:459:PHE:HE2	1:E:465:PHE:CD1	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:192:LYS:HD2	1:C:192:LYS:C	2.37	0.45
1:A:363:GLU:CD	1:A:393:MET:HB3	2.38	0.45
1:C:460:GLY:HA3	1:D:146:ILE:HG13	1.98	0.44
1:G:178:LYS:NZ	1:G:476:GLU:OE1	2.49	0.44
1:F:302[B]:CYS:SG	5:F:8001:I3E:H11A	2.57	0.44
1:H:23:PHE:CZ	1:H:26:ASN:HA	2.51	0.44
1:C:294:LEU:HD23	1:C:306:SER:HA	1.99	0.44
1:B:151:PHE:CG	4:C:501:EDO:H22	2.53	0.44
1:G:302[B]:CYS:CB	5:G:8001:I3E:C11	2.95	0.44
1:D:319:VAL:HG22	1:D:407:ILE:HD12	1.98	0.44
1:D:111:GLY:O	1:D:343:PRO:HD2	2.18	0.44
1:C:413:ILE:HD12	1:C:438:LYS:HG2	2.00	0.44
1:H:149:ASP:HA	1:H:498:LYS:HB2	1.98	0.44
1:C:268[B]:GLU:CD	5:C:8001:I3E:H11	2.37	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:C:192:LYS:NZ	6:C:2496:HOH:O	2.51	0.44
1:D:376:ASP:N	1:D:376:ASP:OD1	2.47	0.43
1:E:347:GLU:O	1:E:350:PHE:HB3	2.18	0.43
1:C:167:PRO:HD3	1:C:244:THR:HB	2.00	0.43
1:A:294:LEU:HD23	1:A:306:SER:HA	2.01	0.43
1:D:438:LYS:NZ	6:D:1091:HOH:O	2.42	0.43
1:B:498:LYS:HE2	1:B:498:LYS:HB3	1.75	0.43
1:A:132:TYR:OH	1:A:477:LEU:HA	2.18	0.43
1:H:303[B]:CYS:SG	1:H:465:PHE:HE1	2.39	0.43
1:G:267:LEU:HB3	1:G:269:LEU:HD21	2.01	0.43
1:G:146:ILE:HG13	1:H:460:GLY:HA3	2.00	0.43
1:C:174:MET:HE1	1:C:177:TRP:CZ3	2.53	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:H:476:GLU:HG2	6:H:1055:HOH:O	2.18	0.43
1:G:132:TYR:OH	1:G:477:LEU:HA	2.18	0.43
1:A:295:PHE:O	1:A:296:PHE:C	2.58	0.43
1:A:411:LYS:HB2	1:A:411:LYS:HE2	1.73	0.43
1:E:23:PHE:CZ	1:E:26:ASN:HA	2.54	0.43
1:B:132:TYR:OH	1:B:477:LEU:HA	2.19	0.43
1:H:268[B]:GLU:CD	5:H:8001:I3E:H11	2.36	0.42
1:F:302[A]:CYS:SG	1:F:427:LEU:HD21	2.59	0.42
1:C:457:ASP:HB3	5:C:8001:I3E:H8A	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:172:LEU:HD21	1:G:200:THR:HB	2.01	0.42
1:H:106:GLU:O	1:H:110:ASN:HB3	2.19	0.42
1:F:172:LEU:HD21	1:F:200:THR:HB	2.01	0.42
1:B:106:GLU:O	1:B:110:ASN:HB3	2.18	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:D:37:PHE:C	1:D:37:PHE:CD1	2.93	0.42
1:E:149:ASP:HA	1:E:498:LYS:HB2	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:B:347:GLU:HG2	1:B:351:LYS:HD3	2.01	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:G:106:GLU:O	1:G:110:ASN:HB3	2.20	0.41
1:C:135:TRP:CG	1:C:482:LEU:HD11	2.55	0.41
1:H:172:LEU:HD21	1:H:200:THR:HB	2.02	0.41
1:H:86:ARG:HD2	6:H:1561:HOH:O	2.19	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:F:498:LYS:HE2	1:F:498:LYS:HB3	1.88	0.41
1:F:294:LEU:HD23	1:F:306:SER:HA	2.01	0.41
1:B:167:PRO:HD2	1:B:174:MET:HG3	2.03	0.41
1:C:257:ALA:HB1	1:C:263:LYS:HG3	2.03	0.41
1:D:8:VAL:HG11	1:D:114:TYR:HE2	1.76	0.41
1:B:302[A]:CYS:SG	5:B:8001:I3E:O9	2.79	0.41
1:F:296:PHE:CE1	5:F:8001:I3E:H8B	2.55	0.41
1:A:258:GLY:O	1:B:251:ARG:HB3	2.20	0.41
1:E:431:VAL:HG21	1:E:442:LEU:HB3	2.03	0.41
1:B:316:ASP:O	1:B:320[A]:GLU:HG3	2.20	0.41
1:F:55:ASP:OD1	1:F:56:LYS:N	2.46	0.41
1:H:13:GLN:HE21	1:H:13:GLN:HB3	1.67	0.41
1:F:302[B]:CYS:HB2	5:F:8001:I3E:C11	2.50	0.41
1:D:301[B]:CYS:SG	1:D:303:CYS:SG	3.19	0.40
1:A:260:SER:O	1:B:251:ARG:NH1	2.54	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:292:PHE:CE2	1:D:296:PHE:CD2	3.10	0.40
1:E:301[B]:CYS:HG	5:E:8001:I3E:H3	1.70	0.40
1:D:26:ASN:ND2	6:D:1705:HOH:O	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:464:PRO:HG3	1:G:480:TYR:CD1	2.57	0.40
1:A:243:PHE:CZ	1:A:249:ILE:HB	2.56	0.40
1:A:350:PHE:CD1	1:A:379:TYR:HB3	2.56	0.40
1:D:9:PRO:HG3	1:D:100:THR:OG1	2.21	0.40
1:F:251:ARG:HG3	1:F:251:ARG:H	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%)	39	37
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%)	30	24
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%)	56	58

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	370	GLY
1	D	260	SER
1	D	478	GLY
1	D	20	ASN

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Mol	Chain	Res	Type
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%)	398 (99%)	5 (1%)	78	84
1	B	406/402 (101%)	404 (100%)	2 (0%)	92	95
1	C	407/402 (101%)	399 (98%)	8 (2%)	63	68
1	D	403/402 (100%)	396 (98%)	7 (2%)	68	74
1	E	404/402 (100%)	399 (99%)	5 (1%)	78	84
1	F	402/402 (100%)	401 (100%)	1 (0%)	95	97
1	G	404/402 (100%)	401 (99%)	3 (1%)	88	92
1	H	404/402 (100%)	403 (100%)	1 (0%)	95	97
All	All	3233/3216 (100%)	3201 (99%)	32 (1%)	82	87

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	192	LYS
1	A	361	LYS
1	A	377	ARG
1	A	401	PHE
1	A	498	LYS
1	B	192	LYS
1	B	401	PHE
1	C	6	GLN
1	C	192	LYS
1	C	338	LYS
1	C	352	LYS
1	C	377	ARG
1	C	381	ILE
1	C	401	PHE

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Mol	Chain	Res	Type
1	C	416	VAL
1	D	36	THR
1	D	106	GLU
1	D	112	LYS
1	D	192	LYS
1	D	337	SER
1	D	376	ASP
1	D	401	PHE
1	E	192	LYS
1	E	275	ASN
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	G	498	LYS
1	H	401	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	275	ASN
1	A	300	GLN
1	A	390	GLN
1	B	14	GLN
1	B	26	ASN
1	C	26	ASN
1	C	275	ASN
1	D	13	GLN
1	D	26	ASN
1	D	50	GLN
1	D	275	ASN
1	D	362	GLN
1	E	26	ASN
1	E	50	GLN
1	E	275	ASN
1	F	13	GLN
1	F	26	ASN
1	G	13	GLN
1	G	26	ASN

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Mol	Chain	Res	Type
1	G	275	ASN
1	G	358	ASN
1	H	13	GLN
1	H	26	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 carbohydrates 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	$\# Z  > 2$
3	GAI	A	6801	-	0,3,3	0.00	-	0,3,3	0.00	-
3	GAI	A	6811	-	0,3,3	0.00	-	0,3,3	0.00	-
4	EDO	A	6901	-	3,3,3	0.45	0	2,2,2	0.28	0
4	EDO	A	6921	-	3,3,3	0.37	0	2,2,2	0.69	0
5	I3E	A	8001	1	12,12,12	0.55	0	15,15,15	1.09	2 (13%)
3	GAI	B	6801	-	0,3,3	0.00	-	0,3,3	0.00	-
3	GAI	B	6811	-	0,3,3	0.00	-	0,3,3	0.00	-
4	EDO	B	6911	-	3,3,3	0.45	0	2,2,2	0.55	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	I3E	B	8001	1	12,12,12	0.54	0	15,15,15	1.16	2 (13%)
4	EDO	C	501	-	3,3,3	0.51	0	2,2,2	0.40	0
3	GAI	C	502	-	0,3,3	0.00	-	0,3,3	0.00	-
3	GAI	C	6801	-	0,3,3	0.00	-	0,3,3	0.00	-
3	GAI	C	6811	-	0,3,3	0.00	-	0,3,3	0.00	-
3	GAI	C	6821	-	0,3,3	0.00	-	0,3,3	0.00	-
4	EDO	C	6901	-	3,3,3	0.37	0	2,2,2	0.57	0
4	EDO	C	6911	-	3,3,3	0.40	0	2,2,2	0.59	0
4	EDO	C	6921	-	3,3,3	0.33	0	2,2,2	0.67	0
4	EDO	C	6961	-	3,3,3	0.41	0	2,2,2	0.42	0
5	I3E	C	8001	1	12,12,12	0.57	0	15,15,15	1.38	2 (13%)
3	GAI	D	6801	-	0,3,3	0.00	-	0,3,3	0.00	-
4	EDO	D	6901	-	3,3,3	0.45	0	2,2,2	0.28	0
5	I3E	D	8001	1	12,12,12	0.63	0	15,15,15	0.93	1 (6%)
3	GAI	E	6801	-	0,3,3	0.00	-	0,3,3	0.00	-
3	GAI	E	6811	-	0,3,3	0.00	-	0,3,3	0.00	-
4	EDO	E	6901	-	3,3,3	0.42	0	2,2,2	0.36	0
4	EDO	E	6921	-	3,3,3	0.36	0	2,2,2	0.75	0
5	I3E	E	8001	1	12,12,12	0.67	1 (8%)	15,15,15	1.17	2 (13%)
4	EDO	F	501	-	3,3,3	0.43	0	2,2,2	0.52	0
3	GAI	F	6801	-	0,3,3	0.00	-	0,3,3	0.00	-
3	GAI	F	6811	-	0,3,3	0.00	-	0,3,3	0.00	-
3	GAI	F	6821	-	0,3,3	0.00	-	0,3,3	0.00	-
4	EDO	F	6901	-	3,3,3	0.38	0	2,2,2	0.27	0
4	EDO	F	6911	-	3,3,3	0.43	0	2,2,2	0.47	0
4	EDO	F	6921	-	3,3,3	0.39	0	2,2,2	0.69	0
4	EDO	F	6951	-	3,3,3	0.51	0	2,2,2	0.43	0
4	EDO	F	6961	-	3,3,3	0.43	0	2,2,2	0.25	0
5	I3E	F	8001	1	12,12,12	0.75	1 (8%)	15,15,15	1.09	1 (6%)
3	GAI	G	6801	-	0,3,3	0.00	-	0,3,3	0.00	-
3	GAI	G	6811	-	0,3,3	0.00	-	0,3,3	0.00	-
4	EDO	G	6921	-	3,3,3	0.35	0	2,2,2	0.62	0
5	I3E	G	8001	1	12,12,12	0.69	1 (8%)	15,15,15	1.33	2 (13%)
3	GAI	H	6801	-	0,3,3	0.00	-	0,3,3	0.00	-
3	GAI	H	6811	-	0,3,3	0.00	-	0,3,3	0.00	-
4	EDO	H	6901	-	3,3,3	0.42	0	2,2,2	0.04	0
4	EDO	H	6911	-	3,3,3	0.47	0	2,2,2	0.04	0
4	EDO	H	6921	-	3,3,3	0.36	0	2,2,2	0.65	0
5	I3E	H	8001	1	12,12,12	0.42	0	15,15,15	1.11	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GAI	A	6801	-	-	0/0/0/0	0/0/0/0
3	GAI	A	6811	-	-	0/0/0/0	0/0/0/0
4	EDO	A	6901	-	-	0/1/1/1	0/0/0/0
4	EDO	A	6921	-	-	0/1/1/1	0/0/0/0
5	I3E	A	8001	1	-	0/8/8/8	0/1/1/1
3	GAI	B	6801	-	-	0/0/0/0	0/0/0/0
3	GAI	B	6811	-	-	0/0/0/0	0/0/0/0
4	EDO	B	6911	-	-	0/1/1/1	0/0/0/0
5	I3E	B	8001	1	-	0/8/8/8	0/1/1/1
4	EDO	C	501	-	-	0/1/1/1	0/0/0/0
3	GAI	C	502	-	-	0/0/0/0	0/0/0/0
3	GAI	C	6801	-	-	0/0/0/0	0/0/0/0
3	GAI	C	6811	-	-	0/0/0/0	0/0/0/0
3	GAI	C	6821	-	-	0/0/0/0	0/0/0/0
4	EDO	C	6901	-	-	0/1/1/1	0/0/0/0
4	EDO	C	6911	-	-	0/1/1/1	0/0/0/0
4	EDO	C	6921	-	-	0/1/1/1	0/0/0/0
4	EDO	C	6961	-	-	0/1/1/1	0/0/0/0
5	I3E	C	8001	1	-	0/8/8/8	0/1/1/1
3	GAI	D	6801	-	-	0/0/0/0	0/0/0/0
4	EDO	D	6901	-	-	0/1/1/1	0/0/0/0
5	I3E	D	8001	1	-	0/8/8/8	0/1/1/1
3	GAI	E	6801	-	-	0/0/0/0	0/0/0/0
3	GAI	E	6811	-	-	0/0/0/0	0/0/0/0
4	EDO	E	6901	-	-	0/1/1/1	0/0/0/0
4	EDO	E	6921	-	-	0/1/1/1	0/0/0/0
5	I3E	E	8001	1	-	0/8/8/8	0/1/1/1
4	EDO	F	501	-	-	0/1/1/1	0/0/0/0
3	GAI	F	6801	-	-	0/0/0/0	0/0/0/0
3	GAI	F	6811	-	-	0/0/0/0	0/0/0/0
3	GAI	F	6821	-	-	0/0/0/0	0/0/0/0
4	EDO	F	6901	-	-	0/1/1/1	0/0/0/0
4	EDO	F	6911	-	-	0/1/1/1	0/0/0/0
4	EDO	F	6921	-	-	0/1/1/1	0/0/0/0
4	EDO	F	6951	-	-	0/1/1/1	0/0/0/0
4	EDO	F	6961	-	-	0/1/1/1	0/0/0/0
5	I3E	F	8001	1	-	0/8/8/8	0/1/1/1
3	GAI	G	6801	-	-	0/0/0/0	0/0/0/0
3	GAI	G	6811	-	-	0/0/0/0	0/0/0/0
4	EDO	G	6921	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	I3E	G	8001	1	-	0/8/8/8	0/1/1/1
3	GAI	H	6801	-	-	0/0/0/0	0/0/0/0
3	GAI	H	6811	-	-	0/0/0/0	0/0/0/0
4	EDO	H	6901	-	-	0/1/1/1	0/0/0/0
4	EDO	H	6911	-	-	0/1/1/1	0/0/0/0
4	EDO	H	6921	-	-	0/1/1/1	0/0/0/0
5	I3E	H	8001	1	-	0/8/8/8	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	8001	I3E	C10-C9	-2.29	1.47	1.50
5	E	8001	I3E	C10-C9	-2.05	1.47	1.50
5	G	8001	I3E	C10-C9	-2.02	1.47	1.50

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	8001	I3E	C11-C10-C9	2.01	117.10	113.91
5	E	8001	I3E	C11-C10-C9	2.05	117.16	113.91
5	B	8001	I3E	C11-C10-C9	2.05	117.16	113.91
5	A	8001	I3E	C11-C10-C9	2.24	117.46	113.91
5	A	8001	I3E	C10-C9-C4	2.28	121.63	118.86
5	C	8001	I3E	C11-C10-C9	2.34	117.62	113.91
5	H	8001	I3E	C10-C9-C4	2.36	121.73	118.86
5	G	8001	I3E	C10-C9-C4	2.57	121.98	118.86
5	B	8001	I3E	C10-C9-C4	2.61	122.03	118.86
5	F	8001	I3E	C10-C9-C4	2.87	122.34	118.86
5	E	8001	I3E	C10-C9-C4	2.90	122.38	118.86
5	G	8001	I3E	C11-C10-C9	2.90	118.50	113.91
5	C	8001	I3E	C10-C9-C4	3.23	122.78	118.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 49 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	8001	I3E	3	0
5	B	8001	I3E	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	501	EDO	1	0
3	C	502	GAI	1	0
5	C	8001	I3E	5	0
5	D	8001	I3E	4	0
5	E	8001	I3E	5	0
4	F	6961	EDO	2	0
5	F	8001	I3E	5	0
5	G	8001	I3E	11	0
4	H	6911	EDO	1	0
5	H	8001	I3E	5	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	494/500 (98%)	-0.12	7 (1%) 78 82	11, 31, 51, 63	0
1	B	494/500 (98%)	-0.50	3 (0%) 90 92	12, 22, 40, 60	0
1	C	495/500 (99%)	-0.51	3 (0%) 90 92	11, 21, 39, 65	1 (0%)
1	D	494/500 (98%)	-0.04	9 (1%) 71 76	12, 32, 54, 72	0
1	E	494/500 (98%)	-0.63	0 100 100	10, 22, 35, 49	0
1	F	494/500 (98%)	-0.68	0 100 100	11, 18, 29, 47	0
1	G	494/500 (98%)	-0.64	1 (0%) 95 96	11, 21, 35, 52	0
1	H	494/500 (98%)	-0.30	4 (0%) 87 90	11, 27, 45, 60	0
All	All	3953/4000 (98%)	-0.43	27 (0%) 89 91	10, 23, 45, 72	1 (0%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	226	PRO	3.4
1	D	224	PHE	3.2
1	A	250	GLY	3.2
1	H	376	ASP	3.1
1	A	255	VAL	3.0
1	D	248	GLU	3.0
1	C	255	VAL	2.9
1	B	253	ILE	2.8
1	D	333	ASN	2.7
1	D	34	ARG	2.7
1	D	376	ASP	2.5
1	D	247	THR	2.5
1	A	376	ASP	2.4
1	H	224	PHE	2.4
1	A	7	ALA	2.3
1	D	255	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	362	GLN	2.3
1	C	262	LEU	2.3
1	A	247	THR	2.2
1	B	7	ALA	2.2
1	H	32	VAL	2.2
1	B	256	ALA	2.1
1	G	248	GLU	2.1
1	H	483[A]	GLN	2.1
1	D	378	GLY	2.1
1	C	247	THR	2.0
1	D	108	LEU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	I3E	E	8001	12/12	0.86	0.31	13.95	27,29,33,35	12
5	I3E	B	8001	12/12	0.81	0.38	10.86	30,32,34,35	12
5	I3E	H	8001	12/12	0.88	0.34	10.45	33,35,39,40	12
5	I3E	G	8001	12/12	0.83	0.43	10.33	24,27,35,35	12
5	I3E	F	8001	12/12	0.83	0.33	10.20	27,32,36,39	12
5	I3E	C	8001	12/12	0.81	0.39	9.03	31,33,36,40	12
4	EDO	F	6951	4/4	0.93	0.21	7.85	24,32,34,37	0
5	I3E	A	8001	12/12	0.84	0.33	6.91	27,30,36,38	12
4	EDO	C	501	4/4	0.76	0.20	6.86	35,36,37,40	0
4	EDO	H	6921	4/4	0.87	0.17	6.51	49,49,51,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	I3E	D	8001	12/12	0.82	0.33	5.20	33,35,37,37	12
3	GAI	C	6801	4/4	0.84	0.16	4.43	35,36,37,37	0
4	EDO	F	6921	4/4	0.88	0.13	3.37	29,31,37,44	0
3	GAI	E	6811	4/4	0.94	0.12	3.31	28,31,31,32	0
3	GAI	D	6801	4/4	0.91	0.14	3.08	44,44,44,45	0
3	GAI	B	6801	4/4	0.94	0.14	2.42	32,34,35,35	0
4	EDO	H	6911	4/4	0.90	0.13	2.39	36,36,37,39	0
4	EDO	F	6901	4/4	0.91	0.13	2.29	23,29,30,33	0
3	GAI	C	6811	4/4	0.91	0.13	2.02	34,34,35,35	0
3	GAI	G	6801	4/4	0.97	0.13	1.96	28,28,29,31	0
3	GAI	H	6811	4/4	0.95	0.13	1.93	39,39,39,41	0
3	GAI	A	6811	4/4	0.94	0.15	1.90	37,40,41,42	0
3	GAI	F	6801	4/4	0.93	0.12	1.87	21,21,24,24	0
4	EDO	F	6961	4/4	0.89	0.14	1.83	41,42,42,44	0
3	GAI	G	6811	4/4	0.95	0.12	1.72	32,32,33,36	0
2	NA	G	601	1/1	0.96	0.10	1.61	26,26,26,26	0
3	GAI	E	6801	4/4	0.96	0.10	1.57	27,27,29,29	0
3	GAI	F	6821	4/4	0.87	0.15	1.50	41,42,43,43	0
3	GAI	C	502	4/4	0.92	0.15	1.45	36,37,38,39	0
4	EDO	B	6911	4/4	0.95	0.19	1.45	26,30,34,34	0
3	GAI	B	6811	4/4	0.94	0.13	1.23	25,28,28,28	0
3	GAI	F	6811	4/4	0.92	0.12	0.97	30,31,32,34	0
3	GAI	A	6801	4/4	0.91	0.11	0.93	30,30,32,32	0
4	EDO	F	501	4/4	0.95	0.10	0.82	24,27,28,32	0
4	EDO	C	6961	4/4	0.91	0.12	0.54	40,42,44,45	0
3	GAI	C	6821	4/4	0.91	0.13	0.53	40,41,41,41	0
4	EDO	D	6901	4/4	0.92	0.10	0.52	29,33,35,38	0
2	NA	A	601	1/1	0.95	0.14	0.41	34,34,34,34	0
4	EDO	F	6911	4/4	0.94	0.11	0.38	27,29,30,33	0
3	GAI	H	6801	4/4	0.96	0.10	0.20	28,28,28,29	0
4	EDO	C	6901	4/4	0.95	0.09	-0.01	29,32,33,37	0
4	EDO	A	6901	4/4	0.96	0.08	-0.57	27,29,30,34	0
4	EDO	H	6901	4/4	0.96	0.08	-0.70	18,22,24,27	0
2	NA	F	601	1/1	0.98	0.07	-0.73	23,23,23,23	0
4	EDO	C	6911	4/4	0.96	0.07	-1.17	30,31,32,32	0
2	NA	H	601	1/1	0.94	0.07	-1.68	31,31,31,31	0
4	EDO	E	6901	4/4	0.97	0.06	-1.78	21,28,29,29	0
2	NA	E	601	1/1	0.96	0.06	-2.61	33,33,33,33	0
2	NA	D	601	1/1	0.97	0.07	-2.64	36,36,36,36	0
2	NA	B	601	1/1	0.96	0.04	-3.66	29,29,29,29	0
2	NA	C	601	1/1	0.98	0.05	-5.89	22,22,22,22	0
4	EDO	C	6921	4/4	0.93	0.11	-	36,38,40,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	EDO	E	6921	4/4	0.92	0.11	-	43,43,45,48	0
4	EDO	A	6921	4/4	0.95	0.10	-	46,47,47,50	0
4	EDO	G	6921	4/4	0.92	0.16	-	49,52,52,52	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.