



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 04:40 pm BST

PDB ID : 3L8Q
Title : Structure analysis of the type II cohesin dyad from the adaptor ScaA scaffoldin of *Acetivibrio cellulolyticus*
Authors : Noach, I.; Frolow, F.; Bayer, E.A.
Deposited on : 2010-01-03
Resolution : 1.57 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

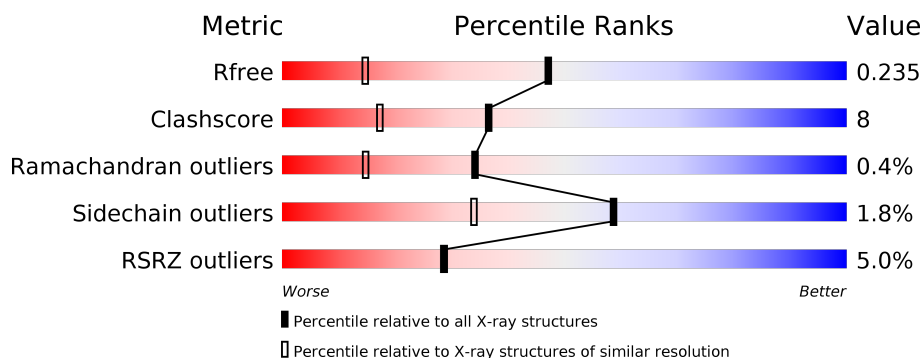
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.57 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5534 (1.60-1.56)
Clashscore	141614	5861 (1.60-1.56)
Ramachandran outliers	138981	5708 (1.60-1.56)
Sidechain outliers	138945	5703 (1.60-1.56)
RSRZ outliers	127900	5431 (1.60-1.56)

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 ≥ 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	350	<div> <div>5%</div> <div> <div></div> <div>84%</div> <div>11%</div> <div>..</div> </div> </div>
1	B	350	<div> <div>5%</div> <div> <div></div> <div>85%</div> <div>12%</div> <div>..</div> </div> </div>
1	C	350	<div> <div>4%</div> <div> <div></div> <div>85%</div> <div>10%</div> <div>..</div> </div> </div>
1	D	350	<div> <div>5%</div> <div> <div></div> <div>84%</div> <div>12%</div> <div>.</div> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EDO	A	359[A]	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12659 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 Cellulosomal scaffoldin adaptor protein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	338	Total	C	N	O	S	0	8	0
			2612	1653	419	531	9			
1	B	341	Total	C	N	O	S	0	3	0
			2610	1650	424	528	8			
1	C	335	Total	C	N	O	S	0	1	0
			2549	1613	411	518	7			
1	D	337	Total	C	N	O	S	0	5	0
			2592	1642	419	524	7			

There are 40 discrepancies between the modelled and reference sequences:

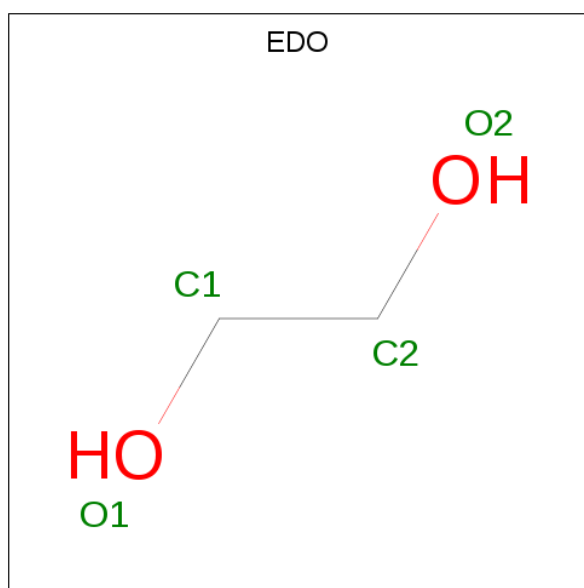
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	EXPRESSION TAG	UNP Q7WYN3
A	170	THR	ILE	SEE REMARK 999	UNP Q7WYN3
A	343	LEU	-	EXPRESSION TAG	UNP Q7WYN3
A	344	GLU	-	EXPRESSION TAG	UNP Q7WYN3
A	345	HIS	-	EXPRESSION TAG	UNP Q7WYN3
A	346	HIS	-	EXPRESSION TAG	UNP Q7WYN3
A	347	HIS	-	EXPRESSION TAG	UNP Q7WYN3
A	348	HIS	-	EXPRESSION TAG	UNP Q7WYN3
A	349	HIS	-	EXPRESSION TAG	UNP Q7WYN3
A	350	HIS	-	EXPRESSION TAG	UNP Q7WYN3
B	1	MET	-	EXPRESSION TAG	UNP Q7WYN3
B	170	THR	ILE	SEE REMARK 999	UNP Q7WYN3
B	343	LEU	-	EXPRESSION TAG	UNP Q7WYN3
B	344	GLU	-	EXPRESSION TAG	UNP Q7WYN3
B	345	HIS	-	EXPRESSION TAG	UNP Q7WYN3
B	346	HIS	-	EXPRESSION TAG	UNP Q7WYN3
B	347	HIS	-	EXPRESSION TAG	UNP Q7WYN3
B	348	HIS	-	EXPRESSION TAG	UNP Q7WYN3
B	349	HIS	-	EXPRESSION TAG	UNP Q7WYN3
B	350	HIS	-	EXPRESSION TAG	UNP Q7WYN3
C	1	MET	-	EXPRESSION TAG	UNP Q7WYN3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	170	THR	ILE	SEE REMARK 999	UNP Q7WYN3
C	343	LEU	-	EXPRESSION TAG	UNP Q7WYN3
C	344	GLU	-	EXPRESSION TAG	UNP Q7WYN3
C	345	HIS	-	EXPRESSION TAG	UNP Q7WYN3
C	346	HIS	-	EXPRESSION TAG	UNP Q7WYN3
C	347	HIS	-	EXPRESSION TAG	UNP Q7WYN3
C	348	HIS	-	EXPRESSION TAG	UNP Q7WYN3
C	349	HIS	-	EXPRESSION TAG	UNP Q7WYN3
C	350	HIS	-	EXPRESSION TAG	UNP Q7WYN3
D	1	MET	-	EXPRESSION TAG	UNP Q7WYN3
D	170	THR	ILE	SEE REMARK 999	UNP Q7WYN3
D	343	LEU	-	EXPRESSION TAG	UNP Q7WYN3
D	344	GLU	-	EXPRESSION TAG	UNP Q7WYN3
D	345	HIS	-	EXPRESSION TAG	UNP Q7WYN3
D	346	HIS	-	EXPRESSION TAG	UNP Q7WYN3
D	347	HIS	-	EXPRESSION TAG	UNP Q7WYN3
D	348	HIS	-	EXPRESSION TAG	UNP Q7WYN3
D	349	HIS	-	EXPRESSION TAG	UNP Q7WYN3
D	350	HIS	-	EXPRESSION TAG	UNP Q7WYN3

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

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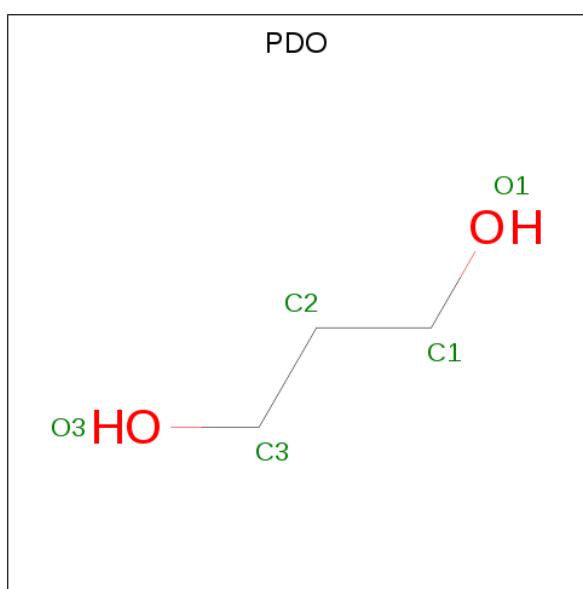
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 12	C 6	O 6	0	1
2	B	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	C	1	Total 4	C 2	O 2	0	0
2	C	1	Total 4	C 2	O 2	0	0
2	C	1	Total 4	C 2	O 2	0	0
2	C	1	Total 4	C 2	O 2	0	0
2	C	1	Total 4	C 2	O 2	0	0
2	C	1	Total 4	C 2	O 2	0	0
2	C	1	Total 4	C 2	O 2	0	0
2	C	1	Total 4	C 2	O 2	0	0
2	D	1	Total 4	C 2	O 2	0	0
2	D	1	Total 4	C 2	O 2	0	0
2	D	1	Total 4	C 2	O 2	0	0

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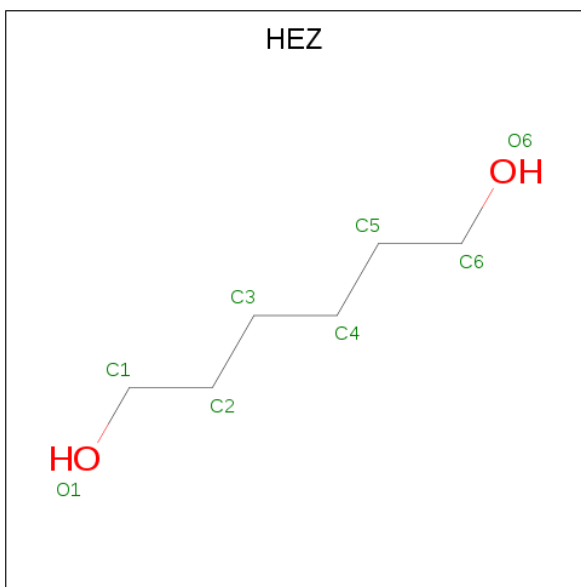
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is 1,3-PROPANDIOL (three-letter code: PDO) (formula: $C_3H_8O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			5	3	2		
3	C	1	Total	C	O	0	0
			5	3	2		

- Molecule 4 is HEXANE-1,6-DIOL (three-letter code: HEZ) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			8	6	2		

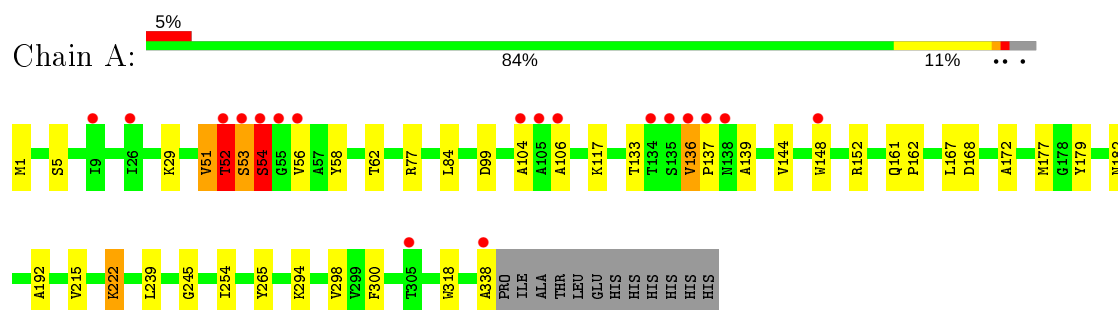
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	530	Total	O	0	1
			531	531		
5	B	548	Total	O	0	2
			550	550		
5	C	547	Total	O	0	2
			549	549		
5	D	531	Total	O	0	1
			532	532		

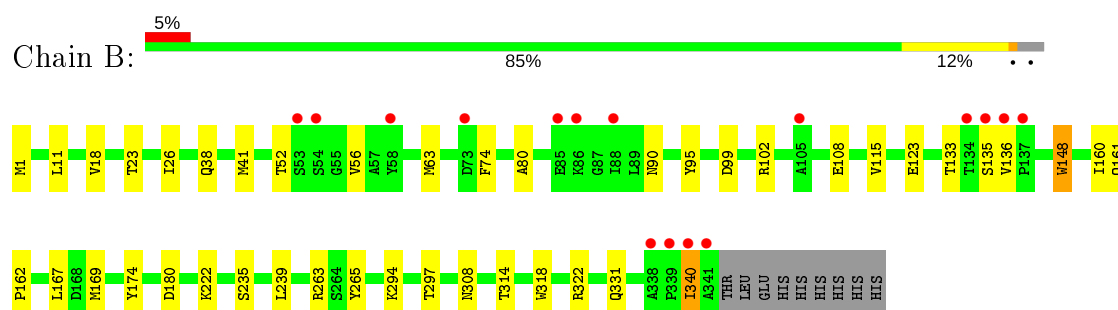
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

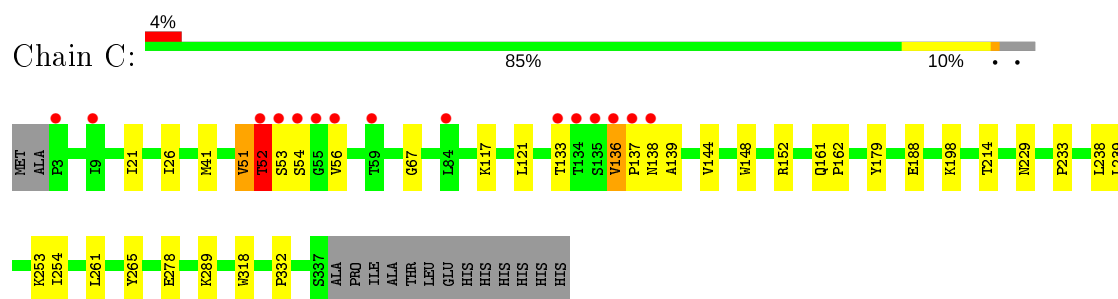
- Molecule 1: Cellulosomal scaffoldin adaptor protein B



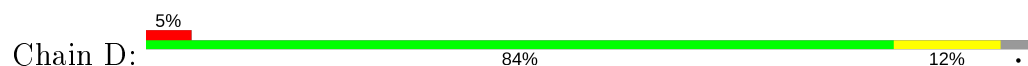
- Molecule 1: Cellulosomal scaffoldin adaptor protein B

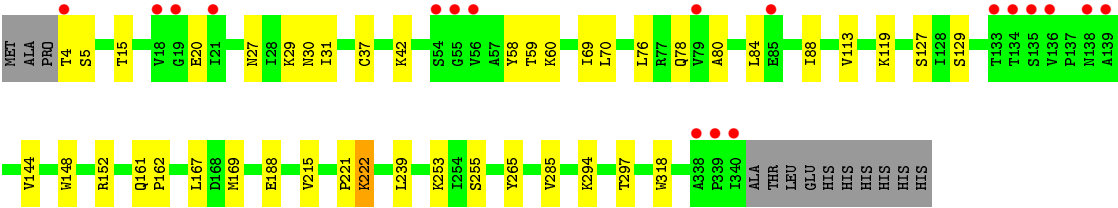


- Molecule 1: Cellulosomal scaffoldin adaptor protein B



- Molecule 1: Cellulosomal scaffoldin adaptor protein B





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	59.23Å 73.91Å 90.79Å 100.25° 94.26° 112.15°	Depositor
Resolution (Å)	29.63 – 1.57 29.63 – 1.57	Depositor EDS
% Data completeness (in resolution range)	97.0 (29.63-1.57) 96.5 (29.63-1.57)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 1.57Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.178 , 0.226 0.190 , 0.235	Depositor DCC
R_{free} test set	9366 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	16.3	Xtriage
Anisotropy	0.410	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 87.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12659	wwPDB-VP
Average B, all atoms (Å ²)	25.0	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 61.99 % 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 1.2054e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: PDO, EDO, HEZ

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	0.50	0/2668	0.66	0/3630
1	B	0.49	0/2655	0.63	0/3616
1	C	0.51	0/2596	0.65	0/3534
1	D	0.48	0/2642	0.64	0/3594
All	All	0.49	0/10561	0.65	0/14374

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	51	VAL	Peptide
1	A	52	THR	Peptide
1	A	53	SER	Peptide
1	C	51	VAL	Peptide

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	2612	0	2615	45	0
1	B	2610	0	2606	33	0
1	C	2549	0	2543	46	0
1	D	2592	0	2599	39	0
2	A	36	0	54	7	0
2	B	20	0	30	0	0
2	C	32	0	48	0	0
2	D	28	0	42	1	0
3	A	5	0	8	0	0
3	C	5	0	8	0	0
4	B	8	0	14	2	0
5	A	531	0	0	15	2
5	B	550	0	0	15	1
5	C	549	0	0	13	2
5	D	532	0	0	12	1
All	All	12659	0	10567	166	3

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 8.

All (166) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:VAL:HG13	1:A:137:PRO:CA	1.64	1.27
1:D:60[B]:LYS:NZ	1:D:60[B]:LYS:HB2	1.57	1.18
1:A:136:VAL:CG1	1:A:137:PRO:HA	1.77	1.14
1:D:222[A]:LYS:NZ	5:D:480:HOH:O	1.78	1.09
1:D:20:GLU:OE1	5:D:1711:HOH:O	1.69	1.09
1:A:52:THR:HG23	1:A:54:SER:H	1.27	0.98
1:D:60[B]:LYS:HZ3	1:D:60[B]:LYS:HB2	1.18	0.97
1:C:136:VAL:HG11	1:C:139:ALA:HB2	1.49	0.95
1:A:52:THR:HG23	1:A:54:SER:N	1.84	0.92
1:B:297:THR:HG21	5:B:1515:HOH:O	1.71	0.91
1:B:1:MET:HE2	5:B:2064:HOH:O	1.70	0.91
1:C:136:VAL:HG11	1:C:139:ALA:CB	2.03	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:VAL:HG13	1:A:137:PRO:HA	0.90	0.89
1:B:63[B]:MET:SD	1:B:63[B]:MET:O	2.35	0.84
1:C:133:THR:HG23	1:C:136:VAL:HG23	1.61	0.83
2:A:359[C]:EDO:C1	5:A:520:HOH:O	2.25	0.82
1:D:60[B]:LYS:HZ2	1:D:60[B]:LYS:HB2	1.44	0.81
1:A:136:VAL:HG21	1:A:139:ALA:HB2	1.63	0.80
1:C:133:THR:CG2	1:C:136:VAL:HG23	2.11	0.79
1:D:4:THR:N	1:D:31:ILE:HA	1.98	0.79
1:D:60[B]:LYS:CB	1:D:60[B]:LYS:NZ	2.41	0.78
1:D:188:GLU:OE1	5:D:1457:HOH:O	2.02	0.76
1:B:80:ALA:O	5:B:2007:HOH:O	2.07	0.72
1:C:136:VAL:CG1	1:C:139:ALA:HB2	2.20	0.72
1:A:222[A]:LYS:HE3	1:A:222[A]:LYS:HA	1.72	0.71
1:C:52:THR:HG23	1:C:54:SER:HA	1.71	0.71
1:C:53:SER:N	1:C:54:SER:HA	2.05	0.71
1:D:15:THR:HG22	5:D:1055:HOH:O	1.90	0.70
1:A:117:LYS:NZ	5:A:1772:HOH:O	2.25	0.69
1:A:177[B]:MET:HE3	1:A:192:ALA:HB1	1.75	0.69
1:A:1[A]:MET:HE2	5:A:2041:HOH:O	1.93	0.69
1:B:52:THR:OG1	1:B:56:VAL:HG22	1.93	0.68
1:C:53:SER:HB3	1:C:56:VAL:HG12	1.76	0.67
1:A:179:TYR:O	5:A:1037:HOH:O	2.11	0.67
1:C:179:TYR:O	5:C:1467:HOH:O	2.13	0.66
1:C:136:VAL:HB	1:C:137:PRO:HA	1.77	0.65
1:D:297:THR:HG23	5:D:1168:HOH:O	1.95	0.65
1:D:5:SER:HB3	1:D:29:LYS:O	1.96	0.64
1:C:56:VAL:HG23	5:C:1801:HOH:O	1.98	0.63
1:D:144:VAL:HG13	1:D:152:ARG:HG3	1.79	0.63
1:D:119:LYS:NZ	5:D:547:HOH:O	2.32	0.62
1:B:63[B]:MET:SD	1:B:63[B]:MET:C	2.79	0.61
1:D:127:SER:O	5:D:378:HOH:O	2.16	0.60
1:A:53:SER:N	1:A:56:VAL:HG22	2.16	0.60
1:A:133:THR:O	1:A:136:VAL:HG12	2.01	0.60
1:C:121:LEU:HD22	5:C:1717:HOH:O	2.01	0.60
1:D:80:ALA:O	5:D:1278:HOH:O	2.16	0.60
1:C:136:VAL:HG11	1:C:139:ALA:H	1.67	0.59
1:B:133:THR:HG23	5:B:1827:HOH:O	2.02	0.59
1:A:222[A]:LYS:CE	1:A:222[A]:LYS:HA	2.32	0.59
1:A:51:VAL:O	1:A:52:THR:HB	2.02	0.59
1:A:239:LEU:HA	1:A:265:TYR:CZ	2.38	0.59
1:D:215:VAL:HG22	1:D:294:LYS:HE3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:ALA:HB3	5:A:994:HOH:O	2.02	0.58
1:D:5:SER:HB2	1:D:30:ASN:HB2	1.86	0.57
1:A:168:ASP:HB3	2:A:359[A]:EDO:H12	1.85	0.57
2:A:359[C]:EDO:H11	5:A:520:HOH:O	1.93	0.57
1:C:188:GLU:OE2	5:C:1719:HOH:O	2.17	0.57
1:D:4:THR:N	1:D:31:ILE:HD13	2.20	0.57
1:B:38[B]:GLN:NE2	5:B:1832:HOH:O	2.36	0.57
1:D:76:LEU:HD23	1:D:78:GLN:HE21	1.69	0.57
1:C:53:SER:HB3	1:C:56:VAL:CG1	2.34	0.57
1:B:161:GLN:HB2	1:B:162:PRO:HA	1.87	0.56
1:A:168:ASP:HB3	2:A:359[A]:EDO:C1	2.35	0.56
1:A:136:VAL:HG13	1:A:137:PRO:C	2.23	0.55
1:A:52:THR:HG23	1:A:54:SER:CA	2.36	0.55
1:A:136:VAL:CG1	1:A:137:PRO:CA	2.57	0.55
1:B:18:VAL:HG13	1:B:123:GLU:HG3	1.89	0.55
2:A:359[C]:EDO:H12	5:A:520:HOH:O	1.97	0.54
1:B:180:ASP:O	5:B:1114:HOH:O	2.18	0.54
1:D:70:LEU:HD12	1:D:113:VAL:HG13	1.90	0.54
1:C:133:THR:HG22	1:C:136:VAL:HG23	1.88	0.53
1:A:254:ILE:HG23	5:A:443:HOH:O	2.08	0.53
1:C:161:GLN:HB2	1:C:162:PRO:HA	1.90	0.53
1:C:136:VAL:HG11	1:C:139:ALA:N	2.22	0.53
1:A:52:THR:HG22	5:A:442:HOH:O	2.09	0.53
1:D:167:LEU:HD21	1:D:169[A]:MET:SD	2.48	0.53
1:C:233:PRO:HD3	1:C:261:LEU:HD22	1.92	0.52
1:B:23:THR:CG2	1:B:115:VAL:CG1	2.87	0.52
1:A:177[B]:MET:CE	1:A:192:ALA:HB1	2.38	0.52
1:B:23:THR:HG23	1:B:115:VAL:CG1	2.40	0.52
1:A:53:SER:H	1:A:56:VAL:HG22	1.74	0.52
1:C:136:VAL:HG12	1:C:138:ASN:N	2.26	0.51
1:D:42:LYS:HD3	1:D:88:ILE:HD11	1.91	0.51
1:B:11:LEU:HD12	5:B:2038:HOH:O	2.11	0.51
1:C:188:GLU:CD	5:C:1719:HOH:O	2.48	0.51
1:A:161:GLN:HB2	1:A:162:PRO:HA	1.92	0.51
1:A:58:TYR:O	1:A:84:LEU:HD11	2.11	0.50
1:C:53:SER:N	1:C:54:SER:CA	2.74	0.50
1:D:255:SER:OG	5:D:1067:HOH:O	2.19	0.50
1:A:177[B]:MET:HG3	1:A:300:PHE:CZ	2.46	0.50
1:D:58:TYR:O	1:D:84:LEU:CD1	2.60	0.50
1:B:26:ILE:HD11	1:B:41:MET:HE1	1.94	0.50
1:D:58:TYR:O	1:D:84:LEU:HD13	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:VAL:HG12	5:C:864:HOH:O	2.10	0.50
1:C:254:ILE:HG22	5:C:1204:HOH:O	2.11	0.50
1:B:331:GLN:O	5:B:1078:HOH:O	2.20	0.49
1:C:188:GLU:OE1	5:C:1719:HOH:O	2.20	0.49
1:D:239:LEU:HA	1:D:265:TYR:CZ	2.48	0.49
1:D:215:VAL:CG2	1:D:294:LYS:HE3	2.42	0.49
1:B:308:ASN:HA	5:B:1403:HOH:O	2.13	0.49
1:D:161:GLN:HB2	1:D:162:PRO:HA	1.94	0.48
1:D:76:LEU:CD2	1:D:78:GLN:HE21	2.26	0.48
1:A:182:ASN:HB3	5:A:880:HOH:O	2.14	0.48
1:C:198:LYS:HB3	1:C:198:LYS:NZ	2.29	0.48
1:B:239:LEU:HA	1:B:265:TYR:CZ	2.49	0.47
1:B:340:ILE:H	1:B:340:ILE:HD13	1.79	0.47
1:B:26:ILE:HD11	1:B:41:MET:CE	2.43	0.47
1:A:62:THR:HG23	5:A:894:HOH:O	2.15	0.47
1:A:215:VAL:HG22	1:A:294:LYS:HE3	1.96	0.47
1:A:136:VAL:HG22	1:A:137:PRO:O	2.15	0.47
1:C:144:VAL:HG11	5:C:1430:HOH:O	2.15	0.47
1:C:138:ASN:HB2	1:C:152:ARG:NH1	2.29	0.47
1:C:21:ILE:HG21	1:C:117:LYS:HD3	1.97	0.46
1:C:136:VAL:CG1	1:C:139:ALA:H	2.28	0.46
1:C:239:LEU:HA	1:C:265:TYR:CZ	2.50	0.46
1:C:253:LYS:NZ	5:C:422:HOH:O	2.49	0.46
1:B:160:ILE:HG22	5:B:741:HOH:O	2.15	0.46
1:B:99:ASP:HB2	5:B:2094:HOH:O	2.14	0.46
1:C:52:THR:HG23	1:C:54:SER:OG	2.16	0.46
1:B:263:ARG:HH22	4:B:356:HEZ:H62	1.80	0.46
1:A:245:GLY:HA2	5:A:1755:HOH:O	2.16	0.46
1:C:51:VAL:O	1:C:52:THR:HB	2.15	0.46
1:A:172:ALA:HA	2:A:359[A]:EDO:C2	2.46	0.45
1:B:108:GLU:HA	5:B:992:HOH:O	2.17	0.45
1:C:52:THR:HG22	5:C:1602:HOH:O	2.16	0.45
1:D:69:ILE:HG22	5:D:1224:HOH:O	2.17	0.45
1:C:144:VAL:HG13	1:C:152:ARG:HG2	1.98	0.45
1:A:172:ALA:HA	2:A:359[A]:EDO:H21	1.97	0.45
1:D:37:CYS:SG	1:D:113:VAL:HG11	2.56	0.45
1:D:60[B]:LYS:CB	1:D:60[B]:LYS:HZ3	2.05	0.45
1:C:144:VAL:HG11	1:C:152:ARG:HE	1.82	0.45
1:A:298[B]:VAL:O	1:A:298[B]:VAL:HG23	2.15	0.45
1:C:26:ILE:HD11	1:C:41:MET:CE	2.47	0.44
1:D:144:VAL:HG13	1:D:152:ARG:CG	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:THR:HG23	1:A:54:SER:HA	1.99	0.44
1:C:53:SER:O	1:C:53:SER:OG	2.31	0.44
1:D:27:ASN:HD22	2:D:352:EDO:H22	1.83	0.44
1:D:129:SER:OG	1:D:162:PRO:HB3	2.18	0.44
1:B:74:PHE:HB2	1:B:95:TYR:CD1	2.52	0.44
1:D:253:LYS:NZ	5:D:1536:HOH:O	2.44	0.44
1:B:169:MET:HE2	5:B:834:HOH:O	2.18	0.43
1:D:60[B]:LYS:CB	1:D:60[B]:LYS:HZ2	2.19	0.43
1:C:289:LYS:NZ	5:C:1302:HOH:O	2.28	0.43
1:B:235:SER:HB2	4:B:356:HEZ:H11	2.00	0.43
1:A:5:SER:HA	1:A:29:LYS:O	2.19	0.43
1:B:102:ARG:HG2	1:B:148:TRP:CG	2.54	0.43
1:C:238:LEU:HD22	1:C:278:GLU:HB3	2.01	0.43
1:A:104:ALA:HB1	5:A:994:HOH:O	2.19	0.42
1:D:221:PRO:HG3	1:D:285:VAL:HG12	2.01	0.42
1:B:174:TYR:HE1	5:B:783:HOH:O	2.02	0.42
1:C:179:TYR:CZ	1:C:332:PRO:HB2	2.54	0.42
1:C:53:SER:H	1:C:54:SER:CA	2.33	0.42
1:C:229:ASN:OD1	1:C:254:ILE:HG12	2.19	0.42
1:A:254:ILE:CG2	5:A:443:HOH:O	2.67	0.42
1:A:222[B]:LYS:HE2	1:A:222[B]:LYS:HA	2.01	0.42
1:A:338:ALA:HB3	5:A:848:HOH:O	2.19	0.42
1:A:52:THR:OG1	1:A:54:SER:HA	2.20	0.42
1:B:294:LYS:HA	5:B:2050:HOH:O	2.20	0.41
1:C:67:GLY:O	5:C:1930:HOH:O	2.22	0.41
1:A:144:VAL:HG13	1:A:152:ARG:HG3	2.02	0.41
1:B:314:THR:HG23	1:B:322:ARG:HG3	2.02	0.41
1:C:214:THR:HG22	5:D:1388:HOH:O	2.19	0.41
1:D:5:SER:CB	1:D:30:ASN:HB2	2.49	0.41
1:C:53:SER:H	1:C:54:SER:HA	1.83	0.41
1:B:135:SER:O	1:B:136:VAL:C	2.58	0.41

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1673:HOH:O	5:D:1999:HOH:O[1_454]	1.80	0.40
5:A:1875:HOH:O	5:C:1856:HOH:O[1_454]	1.94	0.26
5:B:1132:HOH:O	5:C:1738:HOH:O[1_565]	2.13	0.07

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	343/350 (98%)	333 (97%)	7 (2%)	3 (1%)	17	4
1	B	342/350 (98%)	336 (98%)	6 (2%)	0	100	100
1	C	334/350 (95%)	328 (98%)	4 (1%)	2 (1%)	25	8
1	D	340/350 (97%)	337 (99%)	3 (1%)	0	100	100
All	All	1359/1400 (97%)	1334 (98%)	20 (2%)	5 (0%)	34	15

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	THR
1	C	52	THR
1	A	54	SER
1	A	136	VAL
1	C	136	VAL

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	296/299 (99%)	287 (97%)	9 (3%)	41	15
1	B	293/299 (98%)	287 (98%)	6 (2%)	55	29
1	C	288/299 (96%)	285 (99%)	3 (1%)	76	59
1	D	293/299 (98%)	288 (98%)	5 (2%)	60	36
All	All	1170/1196 (98%)	1147 (98%)	23 (2%)	59	29

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	THR
1	A	54	SER
1	A	77	ARG
1	A	99	ASP
1	A	148	TRP
1	A	167	LEU
1	A	222[A]	LYS
1	A	222[B]	LYS
1	A	318	TRP
1	B	90	ASN
1	B	148	TRP
1	B	167	LEU
1	B	222	LYS
1	B	318	TRP
1	B	340	ILE
1	C	52	THR
1	C	148	TRP
1	C	318	TRP
1	D	59	THR
1	D	148	TRP
1	D	222[A]	LYS
1	D	222[B]	LYS
1	D	318	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	154	GLN
1	C	30	ASN
1	C	78	GLN
1	D	78	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

32 ligands are modelled in this entry.

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	$\# Z > 2$
2	EDO	C	352	-	3,3,3	0.27	0	2,2,2	0.19	0
2	EDO	D	355	-	3,3,3	0.36	0	2,2,2	0.31	0
2	EDO	A	353	-	3,3,3	0.44	0	2,2,2	0.27	0
2	EDO	D	354	-	3,3,3	0.57	0	2,2,2	0.16	0
2	EDO	D	351	-	3,3,3	0.42	0	2,2,2	0.36	0
2	EDO	A	359[A]	-	3,3,3	0.42	0	2,2,2	0.14	0
2	EDO	C	354	-	3,3,3	0.53	0	2,2,2	0.20	0
2	EDO	A	351	-	3,3,3	0.46	0	2,2,2	0.21	0
2	EDO	A	359[C]	-	3,3,3	0.30	0	2,2,2	0.25	0
2	EDO	B	354	-	3,3,3	0.55	0	2,2,2	0.17	0
2	EDO	A	359[B]	-	3,3,3	0.31	0	2,2,2	0.25	0
2	EDO	A	352	-	3,3,3	0.45	0	2,2,2	0.37	0
3	PDO	C	359	-	4,4,4	0.61	0	3,3,3	0.25	0
2	EDO	B	355	-	3,3,3	0.49	0	2,2,2	0.23	0
4	HEZ	B	356	-	7,7,7	0.31	0	6,6,6	0.48	0
2	EDO	A	354	-	3,3,3	0.42	0	2,2,2	0.35	0
2	EDO	B	352	-	3,3,3	0.67	0	2,2,2	0.11	0
2	EDO	D	356	-	3,3,3	0.53	0	2,2,2	0.11	0
2	EDO	A	356	-	3,3,3	0.44	0	2,2,2	0.26	0
2	EDO	C	356	-	3,3,3	0.45	0	2,2,2	0.06	0
2	EDO	C	357	-	3,3,3	0.66	0	2,2,2	0.10	0
2	EDO	C	358	-	3,3,3	0.45	0	2,2,2	0.34	0
3	PDO	A	357	-	4,4,4	0.38	0	3,3,3	0.26	0
2	EDO	C	351	-	3,3,3	0.45	0	2,2,2	0.30	0
2	EDO	C	355	-	3,3,3	0.45	0	2,2,2	0.19	0
2	EDO	C	353	-	3,3,3	0.49	0	2,2,2	0.24	0
2	EDO	D	352	-	3,3,3	0.50	0	2,2,2	0.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	B	351	-	3,3,3	0.48	0	2,2,2	0.42	0
2	EDO	D	357	-	3,3,3	0.54	0	2,2,2	0.16	0
2	EDO	A	355	-	3,3,3	0.75	0	2,2,2	0.31	0
2	EDO	B	353	-	3,3,3	0.44	0	2,2,2	0.45	0
2	EDO	D	353	-	3,3,3	0.35	0	2,2,2	0.37	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	EDO	C	352	-	-	1/1/1/1	-
2	EDO	D	355	-	-	0/1/1/1	-
2	EDO	A	353	-	-	1/1/1/1	-
2	EDO	D	354	-	-	0/1/1/1	-
2	EDO	D	351	-	-	0/1/1/1	-
2	EDO	A	359[A]	-	-	1/1/1/1	-
2	EDO	C	354	-	-	0/1/1/1	-
2	EDO	A	351	-	-	0/1/1/1	-
2	EDO	A	359[C]	-	-	0/1/1/1	-
2	EDO	B	354	-	-	1/1/1/1	-
2	EDO	A	359[B]	-	-	0/1/1/1	-
2	EDO	A	352	-	-	1/1/1/1	-
3	PDO	C	359	-	-	2/2/2/2	-
2	EDO	B	355	-	-	1/1/1/1	-
4	HEZ	B	356	-	-	1/5/5/5	-
2	EDO	A	354	-	-	0/1/1/1	-
2	EDO	B	352	-	-	0/1/1/1	-
2	EDO	D	356	-	-	0/1/1/1	-
2	EDO	A	356	-	-	0/1/1/1	-
2	EDO	C	356	-	-	0/1/1/1	-
2	EDO	C	357	-	-	1/1/1/1	-
2	EDO	C	358	-	-	1/1/1/1	-
3	PDO	A	357	-	-	1/2/2/2	-
2	EDO	C	351	-	-	0/1/1/1	-
2	EDO	C	355	-	-	0/1/1/1	-
2	EDO	C	353	-	-	0/1/1/1	-
2	EDO	D	352	-	-	1/1/1/1	-
2	EDO	B	351	-	-	1/1/1/1	-
2	EDO	D	357	-	-	1/1/1/1	-
2	EDO	A	355	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	B	353	-	-	0/1/1/1	-
2	EDO	D	353	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	359	PDO	O1-C1-C2-C3
3	C	359	PDO	C1-C2-C3-O3
2	C	357	EDO	O1-C1-C2-O2
2	B	351	EDO	O1-C1-C2-O2
4	B	356	HEZ	C1-C2-C3-C4
3	A	357	PDO	C1-C2-C3-O3
2	C	352	EDO	O1-C1-C2-O2
2	A	353	EDO	O1-C1-C2-O2
2	D	357	EDO	O1-C1-C2-O2
2	A	352	EDO	O1-C1-C2-O2
2	D	352	EDO	O1-C1-C2-O2
2	A	359[A]	EDO	O1-C1-C2-O2
2	B	355	EDO	O1-C1-C2-O2
2	D	353	EDO	O1-C1-C2-O2
2	B	354	EDO	O1-C1-C2-O2
2	C	358	EDO	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	359[A]	EDO	4	0
2	A	359[C]	EDO	3	0
4	B	356	HEZ	2	0
2	D	352	EDO	1	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 ⓘ

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	338/350 (96%)	0.21	18 (5%) 26 26	6, 13, 24, 39	0
1	B	341/350 (97%)	0.39	16 (4%) 31 31	8, 15, 28, 56	0
1	C	335/350 (95%)	0.21	15 (4%) 33 33	7, 14, 28, 45	0
1	D	337/350 (96%)	0.32	18 (5%) 26 26	7, 14, 32, 56	0
All	All	1351/1400 (96%)	0.28	67 (4%) 28 29	6, 14, 28, 56	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	136	VAL	15.7
1	B	340	ILE	10.9
1	B	135	SER	10.6
1	D	340	ILE	9.9
1	C	53	SER	7.8
1	A	136	VAL	7.2
1	B	339	PRO	7.1
1	C	136	VAL	6.8
1	A	338	ALA	6.3
1	B	341	ALA	6.2
1	C	134	THR	5.8
1	A	135	SER	5.1
1	D	56	VAL	4.7
1	D	4	THR	4.6
1	A	54	SER	4.6
1	D	136	VAL	4.6
1	D	339	PRO	4.5
1	C	137	PRO	4.3
1	D	134	THR	4.3
1	B	54	SER	4.1
1	C	54	SER	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	135	SER	3.8
1	C	133	THR	3.8
1	D	138	ASN	3.7
1	B	73	ASP	3.7
1	A	53	SER	3.6
1	D	19	GLY	3.5
1	C	56	VAL	3.5
1	A	137	PRO	3.4
1	B	85	GLU	3.3
1	C	55	GLY	3.3
1	B	137	PRO	3.3
1	D	21	ILE	3.2
1	A	56	VAL	3.2
1	D	55	GLY	3.1
1	D	338	ALA	3.0
1	D	54	SER	2.9
1	A	305	THR	2.8
1	A	138	ASN	2.8
1	B	86	LYS	2.7
1	A	52	THR	2.5
1	D	85	GLU	2.5
1	B	53	SER	2.4
1	D	79	VAL	2.4
1	A	148	TRP	2.4
1	B	338	ALA	2.4
1	A	9	ILE	2.4
1	C	9	ILE	2.4
1	C	84	LEU	2.4
1	C	59	THR	2.3
1	A	26	ILE	2.3
1	D	133	THR	2.3
1	C	138	ASN	2.3
1	A	55	GLY	2.3
1	D	139	ALA	2.3
1	B	58	TYR	2.3
1	C	52	THR	2.2
1	A	106	ALA	2.2
1	B	105	ALA	2.2
1	D	18	VAL	2.2
1	A	105	ALA	2.2
1	A	104	ALA	2.1
1	D	135	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	134	THR	2.1
1	B	134	THR	2.1
1	B	88	ILE	2.1
1	C	3	PRO	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. 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(\AA^2)	Q<0.9
2	EDO	C	353	4/4	0.48	0.21	44,45,46,47	0
2	EDO	C	357	4/4	0.62	0.14	34,35,39,40	0
3	PDO	A	357	5/5	0.65	0.34	48,49,51,51	0
2	EDO	C	354	4/4	0.66	0.19	45,45,47,53	0
2	EDO	D	356	4/4	0.73	0.16	45,47,48,50	0
3	PDO	C	359	5/5	0.73	0.20	25,30,35,35	0
2	EDO	B	355	4/4	0.76	0.19	44,48,48,49	0
2	EDO	B	352	4/4	0.76	0.17	24,27,30,30	0
2	EDO	A	355	4/4	0.78	0.21	29,29,30,33	0
2	EDO	B	354	4/4	0.80	0.10	31,36,36,37	0
2	EDO	B	351	4/4	0.81	0.17	45,46,46,47	0
2	EDO	D	352	4/4	0.81	0.17	33,35,35,41	0
2	EDO	A	359[B]	4/4	0.83	0.34	8,9,10,14	4
2	EDO	A	359[C]	4/4	0.83	0.34	16,18,20,21	4
2	EDO	A	359[A]	4/4	0.83	0.34	9,24,30,34	4
4	HEZ	B	356	8/8	0.83	0.14	28,30,33,37	0
2	EDO	C	358	4/4	0.84	0.23	31,33,34,38	0
2	EDO	A	356	4/4	0.85	0.12	29,31,31,34	0
2	EDO	A	353	4/4	0.85	0.22	35,36,36,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	EDO	A	352	4/4	0.86	0.12	28,31,34,38	0
2	EDO	C	356	4/4	0.89	0.18	26,26,28,37	0
2	EDO	D	357	4/4	0.89	0.15	33,37,38,40	0
2	EDO	D	354	4/4	0.89	0.13	34,35,35,36	0
2	EDO	D	353	4/4	0.90	0.21	30,31,33,36	0
2	EDO	C	352	4/4	0.91	0.18	20,20,22,27	0
2	EDO	A	351	4/4	0.94	0.10	22,29,30,32	0
2	EDO	D	355	4/4	0.95	0.14	29,35,38,38	0
2	EDO	C	351	4/4	0.95	0.13	25,25,27,27	0
2	EDO	D	351	4/4	0.97	0.13	17,22,24,24	0
2	EDO	B	353	4/4	0.97	0.11	17,18,18,22	0
2	EDO	C	355	4/4	0.97	0.07	16,17,19,21	0
2	EDO	A	354	4/4	0.98	0.10	18,19,22,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.