



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 17, 2024 – 03:20 PM EST

PDB ID : 3SL3  
Title : Crystal structure of the apo form of the catalytic domain of PDE4D2  
Authors : Feil, S.F.  
Deposited on : 2011-06-24  
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

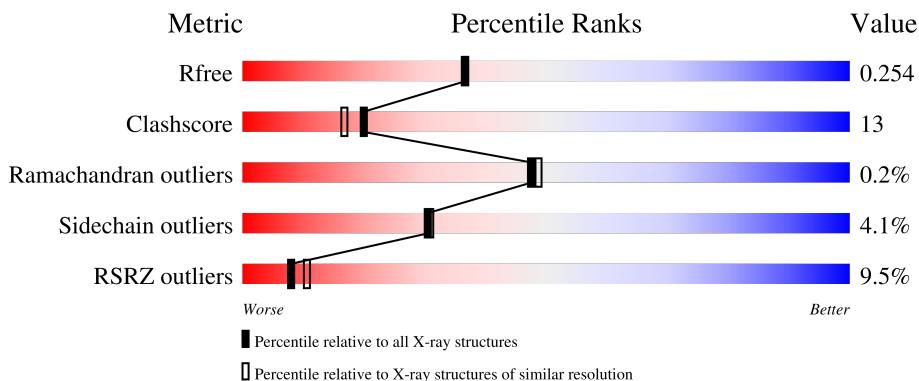
# 1 Overall quality at a glance

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))
$R_{free}$	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (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  $\geq 3$ , 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	361	 9% 73% 15% • 9%
1	B	361	 8% 63% 24% • 11%
1	C	361	 11% 67% 19% • 10%
1	D	361	 6% 72% 17% • 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EDO	A	11	-	-	X	-
2	EDO	A	19	-	-	X	-
2	EDO	A	21	-	-	X	-
2	EDO	B	1	-	-	X	-
2	EDO	B	5	-	-	X	-
2	EDO	C	1	-	-	X	-
2	EDO	C	13	-	-	X	-
2	EDO	C	18	-	-	X	-
2	EDO	D	10	-	-	X	-
2	EDO	D	23	-	-	X	-
5	PO4	A	16	-	-	X	-

## 2 Entry composition [i](#)

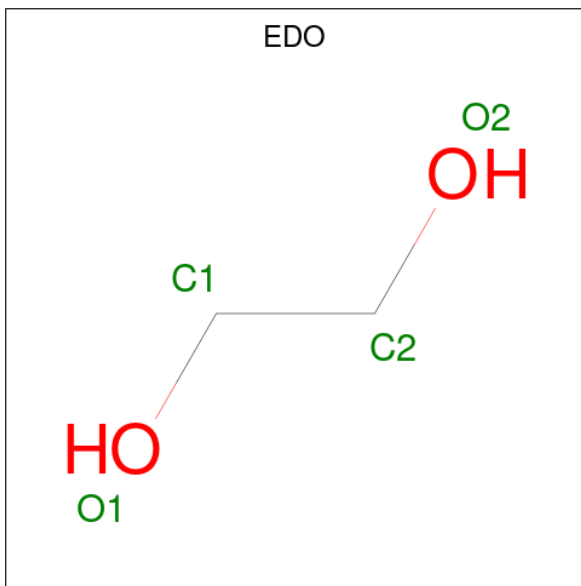
There are 8 unique types of molecules in this entry. The entry contains 11280 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 cAMP-specific 3',5'-cyclic phosphodiesterase 4D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	327	Total 2653	C 1676	N 455	O 508	S 14	0	1	0
1	B	320	Total 2603	C 1649	N 445	O 495	S 14	8	2	0
1	C	324	Total 2641	C 1668	N 451	O 508	S 14	0	2	0
1	D	324	Total 2640	C 1669	N 452	O 505	S 14	0	2	0

- Molecule 2 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
			Total	C	O		
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0

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

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

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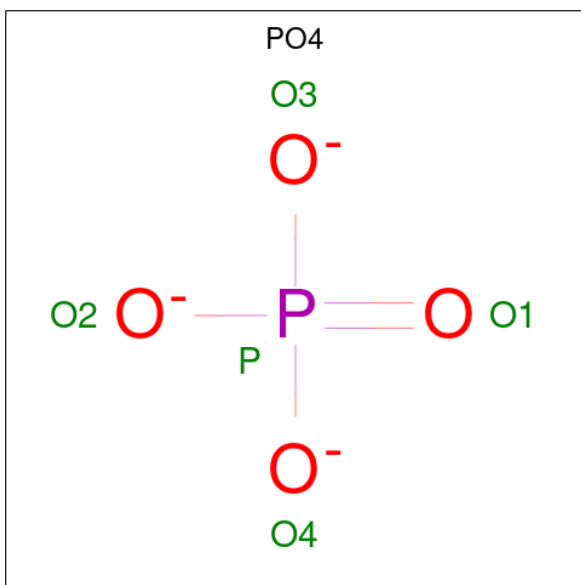
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 7 4 3	0	0
3	B	1	Total C O 7 4 3	0	0
3	D	1	Total C O 7 4 3	0	0
3	D	1	Total C O 7 4 3	0	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Zn 2 2	0	0
4	B	2	Total Zn 2 2	0	0
4	C	2	Total Zn 2 2	0	0
4	D	2	Total Zn 2 2	0	0

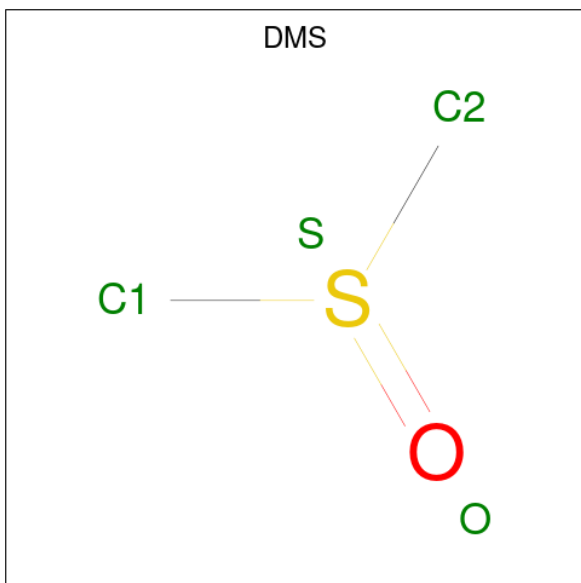
- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).





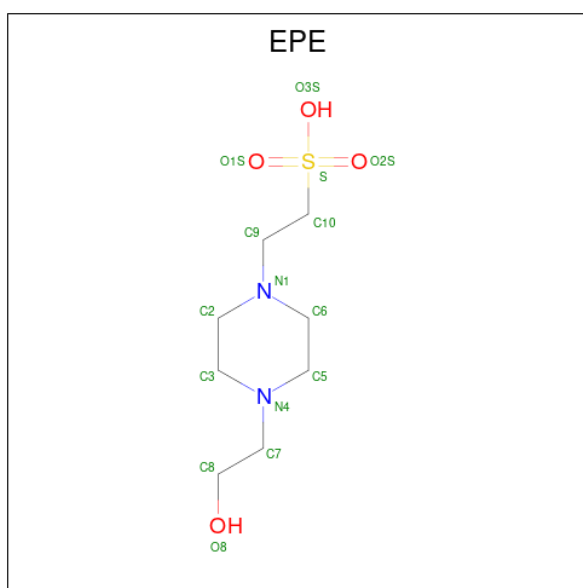
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O P 5 4 1	0	0
5	B	1	Total O P 5 4 1	0	0
5	C	1	Total O P 5 4 1	0	0
5	D	1	Total O P 5 4 1	0	0

- Molecule 6 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C<sub>2</sub>H<sub>6</sub>OS).



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

- Molecule 7 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C<sub>8</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	112	Total	O	0	0
			112	112		
8	B	97	Total	O	0	0
			97	97		
8	C	84	Total	O	0	0
			84	84		

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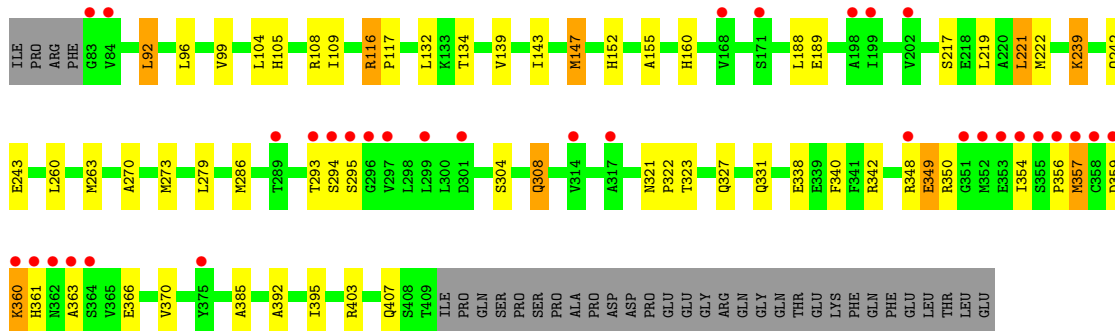
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
8	D	119	Total 119	O 119	0	0

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

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

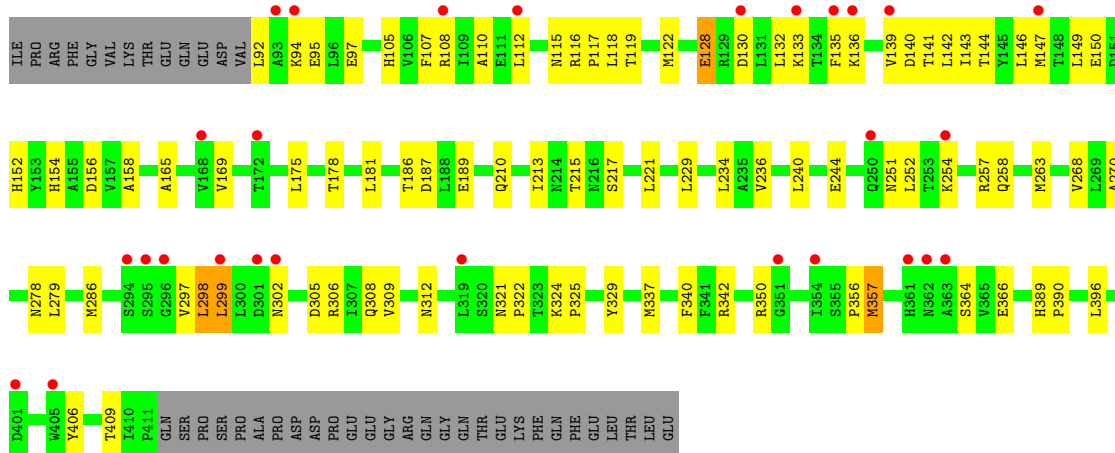
- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D

Chain A: 



- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D

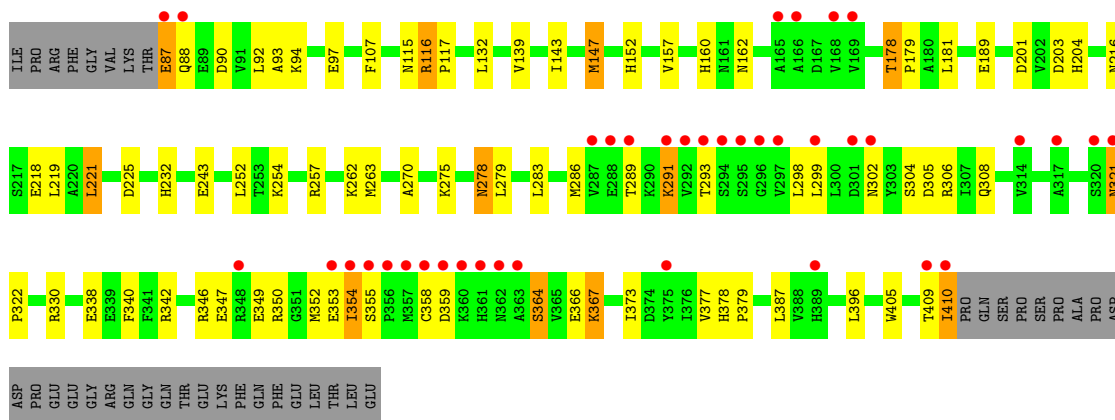
Chain B: 



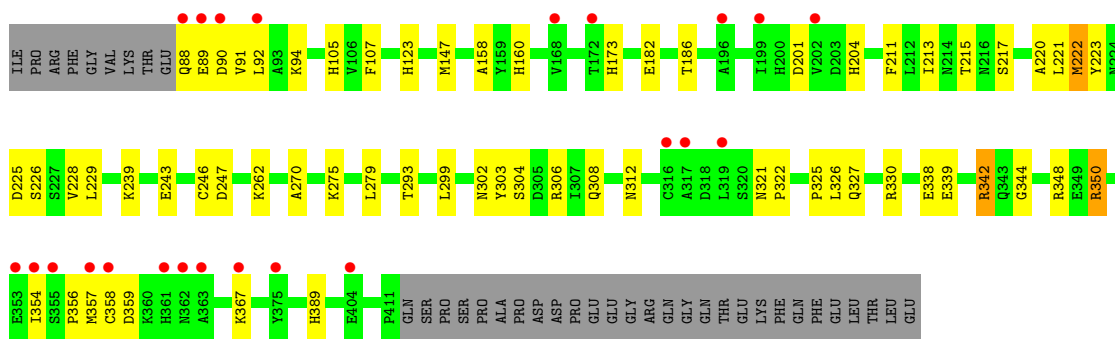
- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D

Chain C: 





● Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.27Å 111.76Å 160.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.88 – 2.10 34.88 – 2.10	Depositor EDS
% Data completeness (in resolution range)	94.3 (34.88-2.10) 99.3 (34.88-2.10)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.63 (at 2.10Å)	Xtrriage
Refinement program	PHENIX 1.5_2	Depositor
R, $R_{free}$	0.205 , 0.252 0.207 , 0.254	Depositor DCC
$R_{free}$ test set	5176 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.2	Xtrriage
Anisotropy	0.169	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 58.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11280	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% of the height of the origin peak. No significant pseudotranslation is detected.*

<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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: DMS, EPE, PO4, ZN, EDO, PEG

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	0.40	0/2707	0.55	0/3676
1	B	0.36	0/2657	0.51	0/3610
1	C	0.36	0/2694	0.50	0/3660
1	D	0.43	0/2695	0.53	0/3662
All	All	0.39	0/10753	0.52	0/14608

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	2653	0	2604	59	0
1	B	2603	0	2565	79	0
1	C	2641	0	2588	66	0
1	D	2640	0	2587	66	0
2	A	68	0	102	23	0
2	B	44	0	66	16	0
2	C	48	0	72	20	0
2	D	80	0	120	24	0
3	A	7	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	7	0	10	2	0
3	D	14	0	20	4	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
5	A	5	0	0	2	0
5	B	5	0	0	0	0
5	C	5	0	0	1	0
5	D	5	0	0	1	0
6	B	8	0	12	2	0
6	C	4	0	6	0	0
6	D	8	0	12	2	0
7	C	15	0	17	1	0
8	A	112	0	0	5	0
8	B	97	0	0	10	0
8	C	84	0	0	3	0
8	D	119	0	0	6	0
All	All	11280	0	10791	273	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 13.

All (273) 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:218:GLU:HB3	2:C:18:EDO:H22	1.27	1.08
1:B:210:GLN:HE22	2:B:1:EDO:H12	1.24	1.03
1:C:152:HIS:HE1	2:C:1:EDO:H22	1.22	0.98
1:B:178:THR:HB	2:B:5:EDO:H12	1.45	0.98
1:D:243:GLU:HB3	2:D:23:EDO:H11	1.50	0.89
1:A:243:GLU:OE2	2:A:19:EDO:H22	1.72	0.88
1:C:115:ASN:HD21	2:C:13:EDO:H21	1.36	0.88
1:D:158:ALA:H	2:D:13:EDO:H11	1.40	0.87
1:B:175:LEU:HD23	2:B:5:EDO:H11	1.55	0.87
1:A:357:MET:HE3	1:A:357:MET:HA	1.55	0.86
1:A:273:MET:H	2:A:11:EDO:C2	1.89	0.84
1:A:273:MET:H	2:A:11:EDO:H22	1.43	0.84
1:B:158:ALA:H	1:B:342:ARG:HH22	1.26	0.83
1:A:242:GLN:HB2	2:A:21:EDO:H22	1.59	0.82
1:D:308:GLN:HE21	1:D:312:ASN:HD22	1.28	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:186:THR:OG1	3:D:11:PEG:H21	1.80	0.80
1:A:132:LEU:HD22	1:A:139:VAL:HG12	1.64	0.80
3:B:17:PEG:H11	1:D:217:SER:HB2	1.63	0.80
1:A:152:HIS:CE1	2:A:19:EDO:H21	2.17	0.79
1:B:143:ILE:O	1:B:147:MET:HG2	1.83	0.79
1:C:152:HIS:CE1	2:C:1:EDO:H22	2.13	0.78
1:B:350:ARG:HB3	8:B:532:HOH:O	1.83	0.77
1:C:218:GLU:CB	2:C:18:EDO:H22	2.11	0.77
1:A:357:MET:HA	1:A:357:MET:CE	2.14	0.76
1:B:186:THR:HB	2:B:16:EDO:H11	1.67	0.76
2:A:6:EDO:H22	8:A:511:HOH:O	1.87	0.74
1:C:243:GLU:OE1	2:C:1:EDO:H21	1.88	0.74
8:A:555:HOH:O	2:C:18:EDO:H21	1.87	0.73
1:B:105:HIS:CE1	1:B:107:PHE:HB2	2.24	0.73
2:A:8:EDO:H12	8:A:548:HOH:O	1.90	0.72
1:A:188:LEU:HD23	2:A:20:EDO:H12	1.72	0.71
1:B:308:GLN:HE21	1:B:312:ASN:HD22	1.39	0.70
1:C:115:ASN:ND2	2:C:13:EDO:H21	2.07	0.69
1:D:262:LYS:HA	3:D:8:PEG:H12	1.74	0.69
1:C:321[A]:ASN:HB2	1:C:322:PRO:HD3	1.74	0.69
1:B:132:LEU:HD22	1:B:139:VAL:HG12	1.75	0.68
1:B:215:THR:HG22	2:D:23:EDO:H22	1.74	0.68
1:B:130:ASP:OD2	1:B:133:LYS:HB2	1.95	0.67
1:D:213:ILE:HG23	1:D:225:ASP:OD2	1.95	0.67
1:C:203:ASP:OD2	1:C:232:HIS:HE1	1.78	0.67
1:D:123:HIS:CD2	2:D:7:EDO:H12	2.30	0.67
1:B:105:HIS:HE1	1:B:107:PHE:HB2	1.60	0.67
1:B:178:THR:HG21	1:B:181:LEU:HD12	1.77	0.66
1:C:115:ASN:HD21	2:C:13:EDO:C2	2.06	0.66
1:B:210:GLN:HE22	2:B:1:EDO:C1	2.03	0.66
1:C:270:ALA:HB1	1:C:279:LEU:HD11	1.78	0.65
1:D:123:HIS:HD2	2:D:7:EDO:H12	1.61	0.65
1:A:403:ARG:NH1	1:A:407:GLN:HG3	2.12	0.64
1:D:367:LYS:O	1:D:367:LYS:HD3	1.96	0.64
1:B:178:THR:HB	2:B:5:EDO:C1	2.24	0.64
1:C:157:VAL:HG22	2:C:10:EDO:H12	1.80	0.64
1:A:217:SER:O	1:A:221:LEU:HD23	1.99	0.63
1:D:308:GLN:HE21	1:D:312:ASN:ND2	1.95	0.63
1:B:144:THR:HG23	1:D:350:ARG:HG3	1.79	0.62
1:A:105[A]:HIS:CD2	1:A:108:ARG:H	2.17	0.62
1:C:302:ASN:O	1:C:306:ARG:HG3	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:MET:HG2	2:A:11:EDO:O1	1.99	0.62
1:B:116:ARG:N	1:B:117:PRO:HD3	2.15	0.61
1:D:389:HIS:HD2	8:D:533:HOH:O	1.83	0.61
1:B:110:ALA:HA	1:B:117:PRO:HG3	1.82	0.61
1:C:275:LYS:HD2	2:C:12:EDO:H11	1.83	0.61
1:C:340:PHE:HE1	2:C:11:EDO:H11	1.66	0.61
1:A:360:LYS:HB2	8:A:522:HOH:O	2.00	0.61
1:D:158:ALA:N	2:D:13:EDO:H11	2.14	0.60
1:D:302:ASN:HB2	2:D:10:EDO:C2	2.31	0.60
1:B:92:LEU:HB2	1:B:112:LEU:HD13	1.84	0.60
1:D:302:ASN:HB2	2:D:10:EDO:H22	1.84	0.60
1:B:178:THR:CG2	1:B:181:LEU:HB2	2.31	0.60
1:C:162:ASN:OD1	2:C:13:EDO:H12	2.02	0.60
1:B:178:THR:CB	2:B:5:EDO:H12	2.27	0.59
1:D:367:LYS:HD3	1:D:367:LYS:C	2.23	0.59
1:C:340:PHE:CE1	2:C:11:EDO:H11	2.37	0.59
1:A:349:GLU:HB3	1:C:147:MET:SD	2.43	0.59
1:C:87:GLU:HG3	1:C:88:GLN:N	2.17	0.59
1:D:275:LYS:HD2	2:D:26:EDO:H22	1.84	0.59
1:A:327:GLN:O	1:A:331:GLN:HG3	2.03	0.59
1:A:340:PHE:CE1	2:A:18:EDO:H21	2.38	0.58
1:B:117:PRO:HD2	1:B:150:GLU:OE2	2.02	0.58
1:B:270:ALA:HB1	1:B:279:LEU:HD11	1.85	0.58
1:B:181:LEU:HD21	1:B:298:LEU:HD12	1.85	0.58
1:D:303:TYR:N	2:D:10:EDO:H21	2.19	0.58
1:D:222:MET:HG2	1:D:223:TYR:CE2	2.37	0.58
1:D:338:GLU:O	1:D:342:ARG:HD2	2.04	0.58
1:B:409:THR:O	1:B:409:THR:HG22	2.04	0.57
2:A:5:EDO:H11	8:A:599:HOH:O	2.04	0.57
1:D:321:ASN:HB2	1:D:322:PRO:HD3	1.86	0.57
1:A:273:MET:H	2:A:11:EDO:H21	1.65	0.57
1:A:348:ARG:C	1:A:350:ARG:H	2.08	0.57
1:B:158:ALA:N	1:B:342:ARG:HH22	2.00	0.57
1:C:232:HIS:HD2	2:C:2:EDO:O1	1.88	0.57
1:B:350:ARG:NH1	2:D:23:EDO:H21	2.20	0.56
1:B:178:THR:HG23	1:B:181:LEU:HB2	1.87	0.56
1:B:278:ASN:HB2	8:B:564:HOH:O	2.04	0.56
8:B:587:HOH:O	1:D:147:MET:HE1	2.06	0.56
1:D:246:CYS:SG	2:D:23:EDO:H12	2.46	0.56
1:C:330:ARG:HD3	1:C:405:TRP:CH2	2.40	0.56
1:D:211:PHE:CE1	1:D:215:THR:HG21	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:GLU:O	1:A:370:VAL:HG23	2.06	0.55
1:B:236:VAL:O	1:B:240:LEU:HG	2.06	0.55
1:B:213:ILE:HG21	2:B:1:EDO:H21	1.87	0.55
1:D:88:GLN:HB3	1:D:91:VAL:HG23	1.88	0.55
1:D:306:ARG:NH2	8:D:604:HOH:O	2.39	0.55
1:B:356:PRO:O	1:B:357:MET:CB	2.55	0.55
1:C:366:GLU:HG2	1:C:409:THR:HB	1.88	0.55
1:A:105[A]:HIS:HD2	1:A:108:ARG:H	1.55	0.55
1:A:321:ASN:HB2	1:A:322:PRO:HD3	1.88	0.55
1:B:251:ASN:HA	8:B:522:HOH:O	2.07	0.55
8:C:475:HOH:O	1:D:221:LEU:HD23	2.07	0.54
1:C:304:SER:O	1:C:308:GLN:HB2	2.06	0.54
1:B:175:LEU:HA	2:B:5:EDO:H11	1.90	0.54
1:A:96:LEU:O	1:A:99:VAL:HG13	2.06	0.54
1:A:152:HIS:NE2	2:A:19:EDO:H21	2.23	0.54
1:B:215:THR:CG2	2:D:23:EDO:H22	2.37	0.54
1:A:273:MET:HB2	2:A:11:EDO:H21	1.90	0.54
1:D:88:GLN:HG3	1:D:90:ASP:H	1.72	0.54
1:B:142:LEU:O	1:B:146:LEU:HG	2.08	0.53
1:A:273:MET:N	2:A:11:EDO:H22	2.18	0.53
1:A:354:ILE:HG21	1:A:359:ASP:HB2	1.91	0.53
1:C:262:LYS:HG3	2:C:6:EDO:H21	1.89	0.53
1:A:270:ALA:HB1	1:A:279:LEU:HD11	1.91	0.52
1:D:173:HIS:HE1	2:D:27:EDO:H22	1.74	0.52
1:D:270:ALA:HB1	1:D:279:LEU:HD11	1.91	0.52
1:A:239:LYS:HE2	1:A:242:GLN:OE1	2.09	0.52
1:B:158:ALA:H	1:B:342:ARG:NH2	2.01	0.52
1:A:143:ILE:O	1:A:147:MET:HG3	2.10	0.52
1:A:370:VAL:HG11	1:A:407:GLN:HE21	1.73	0.52
1:A:338:GLU:O	1:A:342:ARG:HG3	2.10	0.51
1:A:132:LEU:CD2	1:A:139:VAL:HG12	2.37	0.51
1:C:107:PHE:HB2	7:C:4:EPE:H92	1.91	0.51
1:C:278:ASN:ND2	1:C:278:ASN:H	2.08	0.51
1:A:160:HIS:NE2	5:A:16:PO4:O4	2.44	0.51
1:C:321[A]:ASN:CB	1:C:322:PRO:HD3	2.41	0.51
1:B:217:SER:O	1:B:221:LEU:HD23	2.11	0.50
1:D:105[A]:HIS:HE1	1:D:107:PHE:HB2	1.76	0.50
1:B:122:MET:SD	1:B:169:VAL:HG11	2.51	0.50
1:B:175:LEU:CD2	2:B:5:EDO:H11	2.37	0.50
1:C:218:GLU:H	2:C:18:EDO:C2	2.25	0.50
1:B:107:PHE:O	1:B:110:ALA:HB3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:ASN:C	1:B:117:PRO:HD3	2.31	0.50
1:A:293:THR:C	1:A:295:SER:H	2.16	0.49
1:C:355:SER:O	1:C:358:CYS:HB2	2.12	0.49
2:A:21:EDO:H12	1:C:216:ASN:O	2.11	0.49
1:A:239:LYS:HG3	2:A:21:EDO:O2	2.13	0.49
1:C:275:LYS:HZ2	2:C:12:EDO:H22	1.77	0.49
1:B:340:PHE:CD1	2:B:7:EDO:H12	2.48	0.49
1:C:225:ASP:OD2	3:D:8:PEG:H11	2.12	0.49
1:C:181:LEU:HD21	1:C:298:LEU:HD12	1.95	0.49
1:C:302:ASN:ND2	1:C:305:ASP:H	2.11	0.49
1:D:105[A]:HIS:CE1	1:D:107:PHE:HB2	2.48	0.49
1:B:299:LEU:O	2:B:3:EDO:H21	2.13	0.48
1:C:354:ILE:HD12	1:C:359:ASP:HB2	1.94	0.48
1:A:294:SER:O	1:A:295:SER:HB2	2.13	0.48
1:A:357:MET:HE2	1:A:363:ALA:HB2	1.96	0.48
1:C:321[B]:ASN:HB2	1:C:322:PRO:HD3	1.94	0.48
1:B:116:ARG:N	1:B:117:PRO:CD	2.76	0.48
1:A:273:MET:CB	2:A:11:EDO:H21	2.42	0.48
1:C:116:ARG:N	1:C:117:PRO:CD	2.76	0.48
8:B:591:HOH:O	1:D:350:ARG:HD3	2.13	0.48
1:B:178:THR:CG2	1:B:181:LEU:HD12	2.42	0.48
1:A:116:ARG:HE	1:A:147:MET:CE	2.26	0.48
1:A:323:THR:HB	1:A:395:ILE:HG23	1.96	0.48
2:A:12:EDO:H12	8:C:474:HOH:O	2.14	0.48
1:B:305:ASP:O	1:B:309:VAL:HG23	2.13	0.48
1:D:389:HIS:CD2	8:D:533:HOH:O	2.64	0.48
1:B:254:LYS:HE3	1:B:254:LYS:HA	1.95	0.47
1:B:234:LEU:HD21	1:B:268:VAL:HB	1.96	0.47
8:B:502:HOH:O	2:D:1:EDO:H12	2.14	0.47
1:C:283:LEU:HD11	1:C:387:LEU:HD22	1.96	0.47
1:D:222:MET:HG2	1:D:223:TYR:CD2	2.50	0.47
1:C:93:ALA:O	1:C:97:GLU:HG3	2.14	0.47
1:C:321[A]:ASN:HB2	1:C:322:PRO:CD	2.41	0.47
1:B:94:LYS:O	1:B:97:GLU:HB2	2.14	0.47
1:B:215:THR:CB	2:D:23:EDO:H22	2.44	0.47
1:D:182:GLU:OE2	6:D:6:DMS:H13	2.14	0.47
1:B:116:ARG:HD2	1:B:119:THR:OG1	2.15	0.47
1:D:88:GLN:N	8:D:614:HOH:O	2.48	0.47
1:B:321:ASN:HB2	1:B:322:PRO:HD3	1.96	0.47
1:C:243:GLU:CD	2:C:1:EDO:H21	2.35	0.47
1:D:160:HIS:NE2	5:D:19:PO4:P	2.88	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:MET:CE	1:A:308:GLN:OE1	2.63	0.46
1:B:244:GLU:OE2	1:C:254:LYS:HE2	2.15	0.46
1:D:182:GLU:HB2	6:D:6:DMS:H11	1.98	0.46
1:C:257:ARG:HD3	8:C:478:HOH:O	2.15	0.46
1:D:88:GLN:NE2	1:D:89:GLU:HG2	2.31	0.46
1:B:135:PHE:O	1:B:136:LYS:HB2	2.16	0.46
1:B:140:ASP:OD2	1:B:141:THR:N	2.47	0.46
1:C:373:ILE:HA	1:C:377:VAL:HB	1.97	0.46
1:C:293:THR:HG22	1:C:299:LEU:HB2	1.97	0.46
1:D:339:GLU:HG3	2:D:13:EDO:H22	1.96	0.46
1:B:132:LEU:HD21	1:B:142:LEU:HD22	1.98	0.46
1:D:356:PRO:O	1:D:357:MET:HB2	2.16	0.46
1:D:94:LYS:HD2	1:D:94:LYS:HA	1.69	0.45
1:A:147:MET:SD	1:C:349:GLU:HB3	2.56	0.45
1:A:360:LYS:O	1:A:361:HIS:CB	2.65	0.45
1:B:118:LEU:HD21	1:B:149:LEU:HD23	1.99	0.45
1:B:210:GLN:NE2	2:B:1:EDO:H12	2.09	0.45
1:A:188:LEU:HD11	1:A:260:LEU:HB2	1.98	0.45
1:B:366:GLU:HG2	1:B:409:THR:HG22	1.98	0.45
1:B:92:LEU:HD23	1:B:95:GLU:HG2	1.99	0.45
1:B:297:VAL:HA	8:B:547:HOH:O	2.16	0.45
1:B:154:HIS:HB3	1:B:156:ASP:OD1	2.17	0.44
1:C:221:LEU:HD13	1:C:221:LEU:O	2.16	0.44
1:C:409:THR:C	1:C:410:ILE:HG12	2.38	0.44
1:B:337:MET:HB3	2:B:13:EDO:H21	1.99	0.44
1:B:324:LYS:HB3	1:B:325:PRO:HD2	1.99	0.44
1:D:229:LEU:HD23	1:D:229:LEU:HA	1.87	0.44
1:D:262:LYS:CA	3:D:8:PEG:H12	2.45	0.44
1:A:92:LEU:HD22	1:A:96:LEU:CD1	2.47	0.44
1:D:302:ASN:HB2	2:D:10:EDO:H21	1.98	0.43
1:C:330:ARG:HD3	1:C:405:TRP:CZ3	2.53	0.43
1:D:344:GLY:HA3	1:D:358:CYS:O	2.18	0.43
1:A:155:ALA:H	2:A:9:EDO:C1	2.31	0.43
1:C:291:LYS:HD2	1:C:291:LYS:HA	1.85	0.43
1:B:152:HIS:CD2	1:B:240:LEU:HD21	2.54	0.43
1:D:173:HIS:CE1	2:D:27:EDO:H22	2.51	0.43
1:D:222:MET:O	1:D:222:MET:HG3	2.18	0.43
1:A:116:ARG:HE	1:A:147:MET:HE1	1.83	0.43
1:B:128:GLU:OE1	1:B:128:GLU:HA	2.19	0.43
1:C:289:THR:O	1:C:289:THR:HG22	2.18	0.43
1:A:104:LEU:HD11	1:A:109:ILE:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:19:EDO:O1	1:C:350:ARG:NH1	2.41	0.43
1:C:378:HIS:HB3	1:C:379:PRO:HD3	1.99	0.43
1:B:154:HIS:N	1:B:154:HIS:CD2	2.87	0.43
1:B:165:ALA:O	1:B:169:VAL:HG23	2.18	0.43
1:A:104:LEU:HD11	1:A:109:ILE:CD1	2.49	0.43
1:B:302:ASN:O	1:B:306:ARG:HG3	2.19	0.43
1:C:201:ASP:O	1:C:204:HIS:HB2	2.19	0.43
1:C:178:THR:HA	1:C:179:PRO:HD3	1.89	0.42
1:A:160:HIS:NE2	5:A:16:PO4:P	2.93	0.42
1:D:326:LEU:O	1:D:330:ARG:HG3	2.19	0.42
1:A:293:THR:C	1:A:295:SER:N	2.72	0.42
1:B:389:HIS:HA	1:B:390:PRO:HA	1.78	0.42
1:D:275:LYS:HE2	8:D:532:HOH:O	2.19	0.42
1:B:254:LYS:HG3	1:B:258:GLN:OE1	2.19	0.42
1:B:189:GLU:HG2	1:B:263:MET:SD	2.60	0.42
1:D:348:ARG:NE	1:D:354:ILE:HD11	2.34	0.42
6:B:15:DMS:C1	8:B:577:HOH:O	2.68	0.42
1:D:220:ALA:HA	1:D:228:VAL:HG21	2.01	0.42
1:D:226:SER:HB2	8:D:534:HOH:O	2.18	0.42
1:B:175:LEU:HD23	2:B:5:EDO:C1	2.39	0.42
1:D:247:ASP:OD1	2:D:12:EDO:H21	2.20	0.42
1:D:293:THR:HG22	1:D:299:LEU:HD23	2.01	0.41
1:A:239:LYS:HE3	1:D:239:LYS:NZ	2.35	0.41
1:B:329:TYR:CE2	1:B:406:TYR:CE2	3.08	0.41
1:B:356:PRO:O	1:B:357:MET:HB2	2.19	0.41
1:C:286:MET:HE1	1:C:308:GLN:HB3	2.02	0.41
2:A:21:EDO:C1	1:C:216:ASN:O	2.68	0.41
1:C:347:GLU:O	1:C:352:MET:HB2	2.20	0.41
6:B:15:DMS:H12	8:B:577:HOH:O	2.20	0.41
1:D:321:ASN:HB2	2:D:24:EDO:H11	2.03	0.41
1:D:201:ASP:O	1:D:204:HIS:HB2	2.20	0.41
1:D:325:PRO:HB3	2:D:14:EDO:H11	2.01	0.41
1:D:354:ILE:HG21	1:D:359:ASP:HB2	2.01	0.41
1:A:116:ARG:N	1:A:117:PRO:CD	2.84	0.41
1:A:385:ALA:HA	1:A:392:ALA:HB3	2.03	0.41
1:C:364:SER:OG	1:C:367:LYS:HD2	2.21	0.41
1:D:325:PRO:HB3	2:D:14:EDO:H21	2.03	0.41
1:C:338[B]:GLU:O	1:C:342:ARG:HG3	2.20	0.41
1:B:132:LEU:HD21	1:B:142:LEU:CD2	2.51	0.41
2:B:16:EDO:H12	8:B:582:HOH:O	2.20	0.41
1:C:143:ILE:O	1:C:147:MET:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:HIS:NE2	5:C:16:PO4:P	2.94	0.41
1:C:302:ASN:HD22	1:C:304:SER:HB3	1.86	0.41
1:A:189:GLU:HG2	1:A:263:MET:SD	2.61	0.41
1:A:348:ARG:C	1:A:350:ARG:N	2.72	0.41
1:D:304:SER:H	2:D:10:EDO:H21	1.86	0.41
1:A:134:THR:O	2:A:7:EDO:H21	2.21	0.40
3:B:17:PEG:C1	1:D:217:SER:HB2	2.42	0.40
1:C:143:ILE:O	1:C:147:MET:CG	2.69	0.40
1:C:189:GLU:HG2	1:C:263:MET:SD	2.61	0.40
1:B:229:LEU:HD23	1:B:229:LEU:HA	1.95	0.40
1:C:352:MET:HG2	2:C:7:EDO:H21	2.03	0.40
1:A:239:LYS:HE3	1:D:239:LYS:HZ1	1.87	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	326/361 (90%)	314 (96%)	10 (3%)	2 (1%)	25	21
1	B	320/361 (89%)	300 (94%)	20 (6%)	0	100	100
1	C	324/361 (90%)	307 (95%)	17 (5%)	0	100	100
1	D	324/361 (90%)	317 (98%)	7 (2%)	0	100	100
All	All	1294/1444 (90%)	1238 (96%)	54 (4%)	2 (0%)	47	49

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	349	GLU
1	A	356	PRO

### 5.3.2 Protein sidechains [i](#)

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	299/329 (91%)	288 (96%)	11 (4%)	34	35
1	B	294/329 (89%)	283 (96%)	11 (4%)	34	35
1	C	298/329 (91%)	275 (92%)	23 (8%)	13	9
1	D	298/329 (91%)	293 (98%)	5 (2%)	60	67
All	All	1189/1316 (90%)	1139 (96%)	50 (4%)	30	30

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

Mol	Chain	Res	Type
1	A	92	LEU
1	A	116	ARG
1	A	147	MET
1	A	219	LEU
1	A	221	LEU
1	A	222	MET
1	A	239	LYS
1	A	304	SER
1	A	308	GLN
1	A	357	MET
1	A	360	LYS
1	B	108	ARG
1	B	128	GLU
1	B	187	ASP
1	B	252	LEU
1	B	257	ARG
1	B	286	MET
1	B	298	LEU
1	B	299	LEU
1	B	357	MET
1	B	364	SER
1	B	396	LEU
1	C	87	GLU
1	C	90	ASP

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Mol	Chain	Res	Type
1	C	92	LEU
1	C	94	LYS
1	C	116	ARG
1	C	132	LEU
1	C	139	VAL
1	C	147	MET
1	C	178	THR
1	C	219	LEU
1	C	221	LEU
1	C	252	LEU
1	C	278	ASN
1	C	291	LYS
1	C	321[A]	ASN
1	C	321[B]	ASN
1	C	346	ARG
1	C	353	GLU
1	C	354	ILE
1	C	364	SER
1	C	367	LYS
1	C	396	LEU
1	C	410	ILE
1	D	92	LEU
1	D	222	MET
1	D	327	GLN
1	D	342	ARG
1	D	350	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	HIS
1	A	216	ASN
1	A	245	ASN
1	A	258	GLN
1	A	302	ASN
1	A	312	ASN
1	A	321	ASN
1	A	407	GLN
1	B	210	GLN
1	B	245	ASN
1	B	250	GLN
1	B	308	GLN

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Mol	Chain	Res	Type
1	B	327	GLN
1	C	152	HIS
1	C	232	HIS
1	C	245	ASN
1	C	278	ASN
1	C	302	ASN
1	C	308	GLN
1	C	393	GLN
1	D	88	GLN
1	D	123	HIS
1	D	127	GLN
1	D	216	ASN
1	D	245	ASN
1	D	278	ASN
1	D	312	ASN
1	D	361	HIS
1	D	389	HIS
1	D	393	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 82 ligands modelled in this entry, 8 are monoatomic - leaving 74 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	$\# Z  > 2$
2	EDO	C	13	-	3,3,3	0.45	0	2,2,2	0.37	0
2	EDO	D	7	-	3,3,3	0.49	0	2,2,2	0.41	0
2	EDO	A	2	-	3,3,3	0.45	0	2,2,2	0.49	0
2	EDO	C	6	-	3,3,3	0.55	0	2,2,2	0.16	0
2	EDO	D	21	-	3,3,3	0.54	0	2,2,2	0.26	0
2	EDO	C	1	-	3,3,3	0.58	0	2,2,2	0.33	0
2	EDO	A	12	-	3,3,3	0.45	0	2,2,2	0.47	0
2	EDO	B	6	-	3,3,3	0.59	0	2,2,2	0.02	0
2	EDO	D	23	-	3,3,3	0.44	0	2,2,2	0.58	0
2	EDO	A	1	-	3,3,3	0.49	0	2,2,2	0.15	0
2	EDO	C	7	-	3,3,3	0.47	0	2,2,2	0.37	0
2	EDO	B	4	-	3,3,3	0.51	0	2,2,2	0.32	0
2	EDO	D	27	-	3,3,3	0.59	0	2,2,2	0.13	0
2	EDO	D	15	-	3,3,3	0.44	0	2,2,2	0.74	0
2	EDO	B	2	-	3,3,3	0.49	0	2,2,2	0.19	0
2	EDO	B	7	-	3,3,3	0.54	0	2,2,2	0.44	0
2	EDO	A	3	-	3,3,3	0.51	0	2,2,2	0.21	0
2	EDO	D	4	-	3,3,3	0.54	0	2,2,2	0.23	0
7	EPE	C	4	-	15,15,15	0.91	1 (6%)	18,20,20	1.84	6 (33%)
2	EDO	B	13	-	3,3,3	0.54	0	2,2,2	0.11	0
2	EDO	A	20	-	3,3,3	0.46	0	2,2,2	0.45	0
6	DMS	B	15	-	3,3,3	2.66	1 (33%)	3,3,3	0.46	0
6	DMS	C	5	-	3,3,3	2.72	1 (33%)	3,3,3	0.53	0
2	EDO	D	5	-	3,3,3	0.57	0	2,2,2	0.07	0
2	EDO	B	1	-	3,3,3	0.46	0	2,2,2	0.26	0
3	PEG	D	8	-	6,6,6	0.46	0	5,5,5	1.90	2 (40%)
2	EDO	D	22	-	3,3,3	0.48	0	2,2,2	0.41	0
6	DMS	D	25	-	3,3,3	2.74	1 (33%)	3,3,3	0.68	0
2	EDO	C	10	-	3,3,3	0.52	0	2,2,2	0.37	0
5	PO4	D	19	4	4,4,4	1.02	0	6,6,6	0.70	0
2	EDO	A	6	-	3,3,3	0.52	0	2,2,2	0.15	0
2	EDO	D	3	-	3,3,3	0.55	0	2,2,2	0.30	0
2	EDO	A	18	-	3,3,3	0.48	0	2,2,2	0.50	0
2	EDO	D	13	-	3,3,3	0.53	0	2,2,2	0.23	0
2	EDO	D	24	-	3,3,3	0.45	0	2,2,2	0.56	0
3	PEG	D	11	-	6,6,6	0.48	0	5,5,5	1.80	2 (40%)
2	EDO	A	19	-	3,3,3	0.42	0	2,2,2	0.77	0
5	PO4	C	16	4	4,4,4	0.92	0	6,6,6	0.49	0
2	EDO	D	26	-	3,3,3	0.48	0	2,2,2	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PEG	A	13	-	6,6,6	0.60	0	5,5,5	1.42	0
2	EDO	A	8	-	3,3,3	0.52	0	2,2,2	0.29	0
2	EDO	C	18	-	3,3,3	0.55	0	2,2,2	0.39	0
5	PO4	B	10	4	4,4,4	0.91	0	6,6,6	0.89	0
2	EDO	A	10	-	3,3,3	0.42	0	2,2,2	0.44	0
2	EDO	D	10	-	3,3,3	0.54	0	2,2,2	0.24	0
5	PO4	A	16	4	4,4,4	0.92	0	6,6,6	0.79	0
2	EDO	A	7	-	3,3,3	0.56	0	2,2,2	0.31	0
2	EDO	A	11	-	3,3,3	0.50	0	2,2,2	0.28	0
2	EDO	D	16	-	3,3,3	0.49	0	2,2,2	0.47	0
2	EDO	C	3	-	3,3,3	0.48	0	2,2,2	0.35	0
2	EDO	C	8	-	3,3,3	0.39	0	2,2,2	0.57	0
2	EDO	A	5	-	3,3,3	0.53	0	2,2,2	0.27	0
2	EDO	B	3	-	3,3,3	0.48	0	2,2,2	0.18	0
2	EDO	C	11	-	3,3,3	0.60	0	2,2,2	0.34	0
2	EDO	D	14	-	3,3,3	0.53	0	2,2,2	0.27	0
2	EDO	C	12	-	3,3,3	0.46	0	2,2,2	0.36	0
2	EDO	D	9	-	3,3,3	0.55	0	2,2,2	0.20	0
2	EDO	A	9	-	3,3,3	0.58	0	2,2,2	0.15	0
2	EDO	B	12	-	3,3,3	0.48	0	2,2,2	0.39	0
2	EDO	B	11	-	3,3,3	0.42	0	2,2,2	0.51	0
2	EDO	B	16	-	3,3,3	0.50	0	2,2,2	0.09	0
2	EDO	D	20	-	3,3,3	0.47	0	2,2,2	0.37	0
2	EDO	D	12	-	3,3,3	0.56	0	2,2,2	0.39	0
2	EDO	A	21	-	3,3,3	0.53	0	2,2,2	0.13	0
2	EDO	C	9	-	3,3,3	0.53	0	2,2,2	0.13	0
3	PEG	B	17	-	6,6,6	0.55	0	5,5,5	1.60	1 (20%)
2	EDO	D	2	-	3,3,3	0.43	0	2,2,2	0.41	0
2	EDO	A	17	-	3,3,3	0.49	0	2,2,2	0.40	0
2	EDO	B	5	-	3,3,3	0.60	0	2,2,2	0.27	0
6	DMS	B	14	-	3,3,3	2.66	1 (33%)	3,3,3	0.48	0
6	DMS	D	6	-	3,3,3	2.69	1 (33%)	3,3,3	0.62	0
2	EDO	A	4	-	3,3,3	0.39	0	2,2,2	0.66	0
2	EDO	D	1	-	3,3,3	0.54	0	2,2,2	0.11	0
2	EDO	C	2	-	3,3,3	0.58	0	2,2,2	0.10	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	13	-	-	0/1/1/1	-
2	EDO	D	7	-	-	1/1/1/1	-
2	EDO	A	2	-	-	1/1/1/1	-
2	EDO	C	6	-	-	1/1/1/1	-
2	EDO	D	21	-	-	1/1/1/1	-
2	EDO	C	1	-	-	0/1/1/1	-
2	EDO	A	12	-	-	0/1/1/1	-
2	EDO	B	6	-	-	1/1/1/1	-
2	EDO	D	23	-	-	1/1/1/1	-
2	EDO	A	1	-	-	0/1/1/1	-
2	EDO	C	7	-	-	1/1/1/1	-
2	EDO	B	4	-	-	0/1/1/1	-
2	EDO	D	27	-	-	0/1/1/1	-
2	EDO	D	15	-	-	1/1/1/1	-
2	EDO	B	2	-	-	0/1/1/1	-
2	EDO	B	7	-	-	0/1/1/1	-
2	EDO	A	3	-	-	0/1/1/1	-
2	EDO	D	4	-	-	1/1/1/1	-
7	EPE	C	4	-	-	4/9/19/19	0/1/1/1
2	EDO	B	13	-	-	0/1/1/1	-
2	EDO	A	20	-	-	1/1/1/1	-
2	EDO	D	5	-	-	0/1/1/1	-
2	EDO	B	1	-	-	1/1/1/1	-
3	PEG	D	8	-	-	2/4/4/4	-
2	EDO	D	22	-	-	0/1/1/1	-
2	EDO	C	10	-	-	0/1/1/1	-
2	EDO	A	6	-	-	1/1/1/1	-
2	EDO	D	3	-	-	1/1/1/1	-
2	EDO	A	18	-	-	0/1/1/1	-
2	EDO	D	13	-	-	1/1/1/1	-
2	EDO	D	24	-	-	1/1/1/1	-
3	PEG	D	11	-	-	2/4/4/4	-
2	EDO	A	19	-	-	0/1/1/1	-
2	EDO	D	26	-	-	0/1/1/1	-
3	PEG	A	13	-	-	1/4/4/4	-
2	EDO	A	8	-	-	1/1/1/1	-
2	EDO	C	18	-	-	0/1/1/1	-
2	EDO	A	10	-	-	1/1/1/1	-
2	EDO	D	10	-	-	1/1/1/1	-
2	EDO	A	7	-	-	1/1/1/1	-
2	EDO	A	11	-	-	0/1/1/1	-
2	EDO	D	16	-	-	0/1/1/1	-
2	EDO	C	3	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	C	8	-	-	0/1/1/1	-
2	EDO	A	5	-	-	0/1/1/1	-
2	EDO	B	3	-	-	0/1/1/1	-
2	EDO	C	11	-	-	1/1/1/1	-
2	EDO	D	14	-	-	1/1/1/1	-
2	EDO	C	12	-	-	0/1/1/1	-
2	EDO	D	9	-	-	0/1/1/1	-
2	EDO	A	9	-	-	0/1/1/1	-
2	EDO	B	12	-	-	0/1/1/1	-
2	EDO	B	11	-	-	1/1/1/1	-
2	EDO	B	16	-	-	0/1/1/1	-
2	EDO	D	20	-	-	0/1/1/1	-
2	EDO	D	12	-	-	1/1/1/1	-
2	EDO	A	21	-	-	0/1/1/1	-
2	EDO	C	9	-	-	1/1/1/1	-
3	PEG	B	17	-	-	2/4/4/4	-
2	EDO	D	2	-	-	1/1/1/1	-
2	EDO	A	17	-	-	0/1/1/1	-
2	EDO	B	5	-	-	0/1/1/1	-
2	EDO	A	4	-	-	0/1/1/1	-
2	EDO	D	1	-	-	0/1/1/1	-
2	EDO	C	2	-	-	0/1/1/1	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	25	DMS	O-S	4.58	1.81	1.50
6	C	5	DMS	O-S	4.58	1.81	1.50
6	D	6	DMS	O-S	4.51	1.80	1.50
6	B	14	DMS	O-S	4.49	1.80	1.50
6	B	15	DMS	O-S	4.47	1.80	1.50
7	C	4	EPE	C10-S	3.11	1.81	1.77

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	4	EPE	C5-N4-C3	4.61	119.20	108.83
7	C	4	EPE	C7-N4-C3	2.71	118.17	111.23
3	D	8	PEG	O2-C2-C1	2.65	121.70	110.07
7	C	4	EPE	C7-N4-C5	2.34	117.21	111.23
7	C	4	EPE	O2S-S-C10	2.22	109.59	106.92
3	D	8	PEG	C3-O2-C2	2.16	122.65	113.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	4	EPE	O1S-S-C10	2.13	109.47	106.92
3	D	11	PEG	C3-O2-C2	2.11	122.43	113.29
3	D	11	PEG	O2-C2-C1	2.08	119.21	110.07
3	B	17	PEG	O2-C3-C4	2.04	119.03	110.07
7	C	4	EPE	O3S-S-C10	2.04	109.07	105.77

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	4	EPE	C8-C7-N4-C3
3	D	11	PEG	O2-C3-C4-O4
2	D	14	EDO	O1-C1-C2-O2
2	D	15	EDO	O1-C1-C2-O2
3	D	8	PEG	O1-C1-C2-O2
2	A	2	EDO	O1-C1-C2-O2
2	A	8	EDO	O1-C1-C2-O2
2	A	20	EDO	O1-C1-C2-O2
2	B	1	EDO	O1-C1-C2-O2
2	B	11	EDO	O1-C1-C2-O2
2	C	6	EDO	O1-C1-C2-O2
2	D	3	EDO	O1-C1-C2-O2
2	D	7	EDO	O1-C1-C2-O2
2	D	10	EDO	O1-C1-C2-O2
3	B	17	PEG	O1-C1-C2-O2
2	D	13	EDO	O1-C1-C2-O2
2	D	24	EDO	O1-C1-C2-O2
7	C	4	EPE	C9-C10-S-O3S
2	C	11	EDO	O1-C1-C2-O2
2	D	2	EDO	O1-C1-C2-O2
3	B	17	PEG	C1-C2-O2-C3
2	A	10	EDO	O1-C1-C2-O2
2	C	7	EDO	O1-C1-C2-O2
2	D	12	EDO	O1-C1-C2-O2
7	C	4	EPE	C9-C10-S-O1S
7	C	4	EPE	C9-C10-S-O2S
3	D	8	PEG	O2-C3-C4-O4
3	A	13	PEG	C4-C3-O2-C2
2	A	7	EDO	O1-C1-C2-O2
2	B	6	EDO	O1-C1-C2-O2
3	D	11	PEG	C1-C2-O2-C3
2	D	4	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	D	21	EDO	O1-C1-C2-O2
2	A	6	EDO	O1-C1-C2-O2
2	D	23	EDO	O1-C1-C2-O2
2	C	9	EDO	O1-C1-C2-O2

There are no ring outliers.

45 monomers are involved in 98 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	13	EDO	4	0
2	D	7	EDO	2	0
2	C	6	EDO	1	0
2	C	1	EDO	4	0
2	A	12	EDO	1	0
2	D	23	EDO	6	0
2	C	7	EDO	1	0
2	D	27	EDO	2	0
2	B	7	EDO	1	0
7	C	4	EPE	1	0
2	B	13	EDO	1	0
2	A	20	EDO	1	0
6	B	15	DMS	2	0
2	B	1	EDO	4	0
3	D	8	PEG	3	0
2	C	10	EDO	1	0
5	D	19	PO4	1	0
2	A	6	EDO	1	0
2	A	18	EDO	1	0
2	D	13	EDO	3	0
2	D	24	EDO	1	0
3	D	11	PEG	1	0
2	A	19	EDO	4	0
5	C	16	PO4	1	0
2	D	26	EDO	1	0
2	A	8	EDO	1	0
2	C	18	EDO	4	0
2	D	10	EDO	5	0
5	A	16	PO4	2	0
2	A	7	EDO	1	0
2	A	11	EDO	7	0
2	A	5	EDO	1	0
2	B	3	EDO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	11	EDO	2	0
2	D	14	EDO	2	0
2	C	12	EDO	2	0
2	A	9	EDO	1	0
2	B	16	EDO	2	0
2	D	12	EDO	1	0
2	A	21	EDO	4	0
3	B	17	PEG	2	0
2	B	5	EDO	7	0
6	D	6	DMS	2	0
2	D	1	EDO	1	0
2	C	2	EDO	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 [i](#)

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	327/361 (90%)	0.49	33 (10%) <b>7</b> <b>9</b>	16, 31, 67, 95	0
1	B	320/361 (88%)	0.47	28 (8%) <b>10</b> <b>12</b>	19, 42, 61, 78	0
1	C	324/361 (89%)	0.51	39 (12%) <b>4</b> <b>5</b>	20, 38, 69, 87	0
1	D	324/361 (89%)	0.34	23 (7%) <b>16</b> <b>20</b>	15, 29, 60, 86	0
All	All	1295/1444 (89%)	0.45	123 (9%) <b>8</b> <b>10</b>	15, 35, 64, 95	0

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	296	GLY	7.2
1	D	362	ASN	6.9
1	D	363	ALA	6.4
1	A	357	MET	6.0
1	A	354	ILE	5.9
1	C	294	SER	5.8
1	A	295	SER	5.6
1	D	361	HIS	5.3
1	C	362	ASN	5.2
1	A	359	ASP	5.1
1	A	293	THR	5.1
1	C	357	MET	5.1
1	D	89	GLU	5.1
1	C	363	ALA	4.6
1	A	363	ALA	4.6
1	B	108	ARG	4.6
1	C	295	SER	4.6
1	A	362	ASN	4.6
1	C	356	PRO	4.5
1	C	361	HIS	4.4
1	A	353	GLU	4.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	297	VAL	4.2
1	B	363	ALA	4.2
1	B	139	VAL	4.2
1	B	295	SER	4.1
1	C	354	ILE	4.0
1	D	354	ILE	4.0
1	C	410	ILE	4.0
1	C	353	GLU	4.0
1	C	292	VAL	4.0
1	A	294	SER	3.9
1	B	112	LEU	3.9
1	B	354	ILE	3.9
1	B	94	LYS	3.9
1	C	409	THR	3.9
1	C	302	ASN	3.8
1	A	352	MET	3.8
1	C	293	THR	3.8
1	B	294	SER	3.8
1	C	297	VAL	3.7
1	A	299	LEU	3.7
1	D	353	GLU	3.7
1	A	351	GLY	3.6
1	C	296	GLY	3.6
1	A	361	HIS	3.6
1	A	168	VAL	3.5
1	B	296	GLY	3.5
1	A	356	PRO	3.4
1	A	84	VAL	3.4
1	B	361	HIS	3.4
1	C	87	GLU	3.3
1	A	83	GLY	3.2
1	D	168	VAL	3.1
1	A	289	THR	3.1
1	A	358	CYS	3.1
1	D	357	MET	2.9
1	C	289	THR	2.9
1	B	362	ASN	2.9
1	A	364	SER	2.8
1	D	375	TYR	2.8
1	C	301	ASP	2.8
1	A	355	SER	2.8
1	D	202	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	367	LYS	2.8
1	A	360	LYS	2.7
1	C	360	LYS	2.7
1	D	358	CYS	2.7
1	C	291	LYS	2.7
1	C	165	ALA	2.7
1	B	136	LYS	2.7
1	C	355	SER	2.7
1	B	168	VAL	2.7
1	C	359	ASP	2.7
1	C	168	VAL	2.6
1	D	88	GLN	2.6
1	C	287	VAL	2.6
1	D	317	ALA	2.6
1	D	90	ASP	2.6
1	B	250	GLN	2.6
1	C	375	TYR	2.6
1	C	317	ALA	2.6
1	B	301	ASP	2.5
1	B	351	GLY	2.4
1	C	166	ALA	2.4
1	C	314	VAL	2.4
1	B	133	LYS	2.4
1	C	288	GLU	2.4
1	B	254	LYS	2.4
1	B	93	ALA	2.3
1	A	375	TYR	2.3
1	D	404	GLU	2.3
1	C	88	GLN	2.3
1	C	299	LEU	2.3
1	A	202	VAL	2.3
1	A	301	ASP	2.2
1	D	199	ILE	2.2
1	A	317	ALA	2.2
1	A	348	ARG	2.2
1	C	321[A]	ASN	2.2
1	B	130	ASP	2.2
1	B	405	TRP	2.2
1	C	358	CYS	2.2
1	B	299	LEU	2.2
1	C	320	SER	2.2
1	A	198	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	319	LEU	2.2
1	B	401	ASP	2.2
1	D	92	LEU	2.1
1	D	316	CYS	2.1
1	D	355	SER	2.1
1	C	389	HIS	2.1
1	B	302	ASN	2.1
1	B	172	THR	2.1
1	B	135	PHE	2.1
1	C	348	ARG	2.0
1	A	171	SER	2.0
1	D	319	LEU	2.0
1	D	196	ALA	2.0
1	B	147	MET	2.0
1	A	199	ILE	2.0
1	D	172	THR	2.0
1	A	314	VAL	2.0
1	C	169	VAL	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 monosaccharides 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, 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	B-factors(Å <sup>2</sup> )	Q<0.9
2	EDO	B	6	4/4	0.64	0.31	48,51,53,59	0
2	EDO	A	6	4/4	0.69	0.30	33,42,46,48	0
2	EDO	D	16	4/4	0.70	0.30	40,46,52,55	0
2	EDO	C	11	4/4	0.75	0.30	25,41,42,52	0
2	EDO	D	27	4/4	0.75	0.24	46,47,47,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	EDO	B	5	4/4	0.75	0.20	42,44,45,50	0
2	EDO	B	16	4/4	0.76	0.37	49,52,56,68	0
2	EDO	D	12	4/4	0.77	0.21	26,36,36,38	0
2	EDO	C	18	4/4	0.77	0.26	23,32,37,42	0
3	PEG	A	13	7/7	0.77	0.21	39,43,52,54	0
2	EDO	B	12	4/4	0.78	0.25	50,55,56,66	0
2	EDO	A	9	4/4	0.81	0.19	35,36,39,45	0
2	EDO	D	14	4/4	0.81	0.35	41,45,49,52	0
3	PEG	D	8	7/7	0.81	0.19	20,32,40,41	0
2	EDO	C	1	4/4	0.82	0.15	29,36,41,46	0
2	EDO	D	1	4/4	0.83	0.19	33,34,36,38	0
2	EDO	D	3	4/4	0.83	0.11	26,32,35,36	0
2	EDO	B	13	4/4	0.83	0.33	51,52,53,56	0
3	PEG	B	17	7/7	0.83	0.27	42,48,52,52	0
2	EDO	A	5	4/4	0.83	0.16	34,42,47,49	0
2	EDO	B	3	4/4	0.84	0.31	47,53,54,56	0
2	EDO	D	22	4/4	0.85	0.15	46,47,48,59	0
2	EDO	D	4	4/4	0.85	0.16	39,40,40,47	0
2	EDO	C	12	4/4	0.85	0.16	49,53,55,58	0
2	EDO	D	10	4/4	0.85	0.39	43,44,48,49	0
2	EDO	D	15	4/4	0.86	0.20	33,39,40,42	0
2	EDO	C	9	4/4	0.86	0.20	40,45,53,53	0
2	EDO	C	8	4/4	0.86	0.19	42,46,47,58	0
2	EDO	D	24	4/4	0.87	0.25	39,41,47,51	0
2	EDO	C	6	4/4	0.87	0.13	41,44,46,48	0
2	EDO	D	21	4/4	0.87	0.20	35,40,42,48	0
2	EDO	D	13	4/4	0.87	0.26	34,35,42,45	0
2	EDO	C	7	4/4	0.88	0.31	40,43,46,48	0
2	EDO	D	20	4/4	0.88	0.37	54,56,57,63	0
3	PEG	D	11	7/7	0.88	0.37	22,37,43,45	0
2	EDO	A	19	4/4	0.89	0.17	29,32,37,38	0
2	EDO	C	13	4/4	0.89	0.21	40,41,50,53	0
2	EDO	C	3	4/4	0.89	0.18	36,37,38,47	0
2	EDO	A	20	4/4	0.89	0.23	31,39,39,48	0
2	EDO	A	7	4/4	0.89	0.14	28,34,37,44	0
2	EDO	B	2	4/4	0.89	0.11	51,52,53,54	0
2	EDO	A	11	4/4	0.89	0.33	33,42,42,50	0
2	EDO	D	26	4/4	0.90	0.11	40,45,46,51	0
2	EDO	A	21	4/4	0.90	0.21	30,31,37,41	0
2	EDO	A	1	4/4	0.90	0.13	27,29,32,37	0
2	EDO	A	3	4/4	0.90	0.16	30,36,38,41	0
2	EDO	A	10	4/4	0.90	0.20	40,43,46,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	DMS	B	14	4/4	0.90	0.22	47,48,60,70	0
2	EDO	B	7	4/4	0.91	0.28	27,37,39,44	0
2	EDO	D	5	4/4	0.91	0.10	31,33,34,40	0
2	EDO	C	2	4/4	0.91	0.20	25,38,38,52	0
2	EDO	D	7	4/4	0.91	0.13	39,46,48,49	0
5	PO4	B	10	5/5	0.91	0.21	25,31,34,35	2
5	PO4	C	16	5/5	0.91	0.24	26,28,35,37	2
2	EDO	B	1	4/4	0.91	0.39	34,40,41,45	0
6	DMS	D	6	4/4	0.91	0.23	40,40,46,65	0
6	DMS	D	25	4/4	0.91	0.18	36,37,46,58	0
2	EDO	A	18	4/4	0.92	0.31	36,36,45,48	0
2	EDO	A	4	4/4	0.93	0.15	27,31,32,34	0
2	EDO	A	2	4/4	0.93	0.10	24,27,35,43	0
2	EDO	B	11	4/4	0.93	0.13	28,32,47,48	0
7	EPE	C	4	15/15	0.93	0.27	37,58,74,78	0
2	EDO	A	12	4/4	0.94	0.10	40,41,44,55	0
5	PO4	D	19	5/5	0.94	0.26	26,28,29,33	3
2	EDO	B	4	4/4	0.94	0.12	38,43,45,51	0
2	EDO	A	17	4/4	0.94	0.07	43,44,47,52	0
2	EDO	A	8	4/4	0.94	0.10	29,34,36,46	0
2	EDO	C	10	4/4	0.94	0.14	35,41,42,46	0
6	DMS	B	15	4/4	0.95	0.27	45,51,52,67	0
6	DMS	C	5	4/4	0.95	0.16	49,52,53,74	0
2	EDO	D	9	4/4	0.95	0.13	27,28,30,30	0
2	EDO	D	23	4/4	0.95	0.22	22,22,24,28	0
2	EDO	D	2	4/4	0.95	0.15	28,29,29,35	0
5	PO4	A	16	5/5	0.97	0.16	23,24,29,30	2
4	ZN	B	8	1/1	0.98	0.10	38,38,38,38	1
4	ZN	C	14	1/1	0.98	0.05	43,43,43,43	0
4	ZN	D	17	1/1	0.99	0.09	34,34,34,34	1
4	ZN	D	18	1/1	0.99	0.14	26,26,26,26	0
4	ZN	B	9	1/1	0.99	0.10	30,30,30,30	0
4	ZN	A	14	1/1	0.99	0.12	28,28,28,28	1
4	ZN	A	15	1/1	1.00	0.13	25,25,25,25	0
4	ZN	C	15	1/1	1.00	0.13	30,30,30,30	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.