



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:01 PM GMT

PDB ID : 3SL8  
Title : Crystal structure of the catalytic domain of PDE4D2 with compound 10o  
Authors : Feil, S.F.  
Deposited on : 2011-06-24  
Resolution : 2.60 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

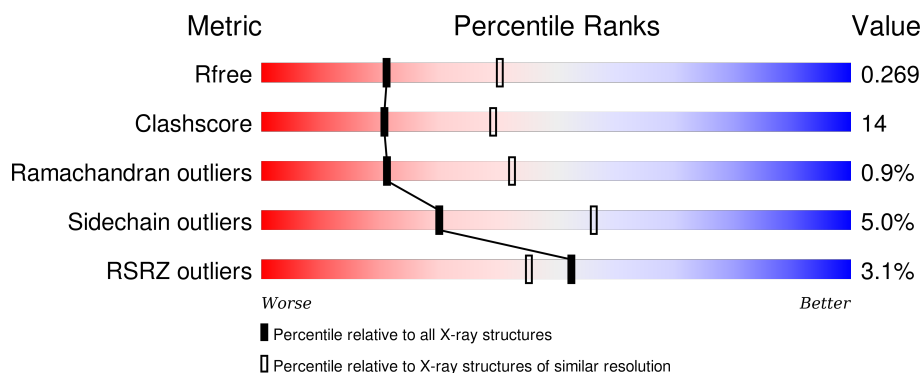
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	361	<div> <div>4%</div> <div>63% 25% 9%</div> </div>
1	B	361	<div> <div>2%</div> <div>59% 28% 10%</div> </div>
1	C	361	<div> <div>4%</div> <div>62% 25% 10%</div> </div>
1	D	361	<div> <div>2%</div> <div>66% 21% 10%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EDO	A	13	-	-	X	-
2	EDO	A	15	-	-	-	X
2	EDO	A	5	-	-	-	X
2	EDO	B	6	-	-	-	X
2	EDO	B	8	-	-	X	X
2	EDO	C	2	-	-	-	X
2	EDO	D	13	-	-	X	X
2	EDO	D	15	-	-	-	X
2	EDO	D	4	-	-	-	X
2	EDO	D	7	-	-	X	X
2	EDO	D	8	-	-	-	X
2	EDO	D	9	-	-	-	X
4	PEG	A	12	-	-	-	X
4	PEG	D	5	-	-	-	X
5	JN7	A	18	-	-	X	-
7	DMS	C	7	-	-	-	X
7	DMS	D	14	-	-	-	X

## 2 Entry composition [i](#)

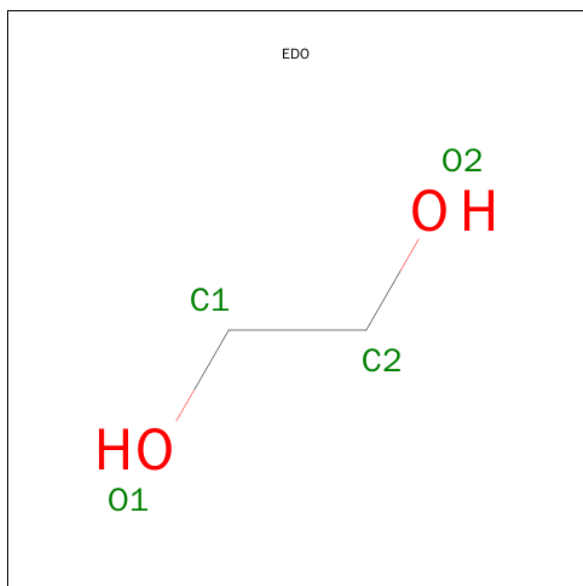
There are 8 unique types of molecules in this entry. The entry contains 11046 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
1	A	327	Total	C	N	O	S	0	1	0
			2653	1679	453	507	14			
1	B	324	Total	C	N	O	S	0	1	0
			2628	1663	448	503	14			
1	C	324	Total	C	N	O	S	0	0	0
			2623	1657	448	504	14			
1	D	324	Total	C	N	O	S	0	0	0
			2622	1659	448	501	14			

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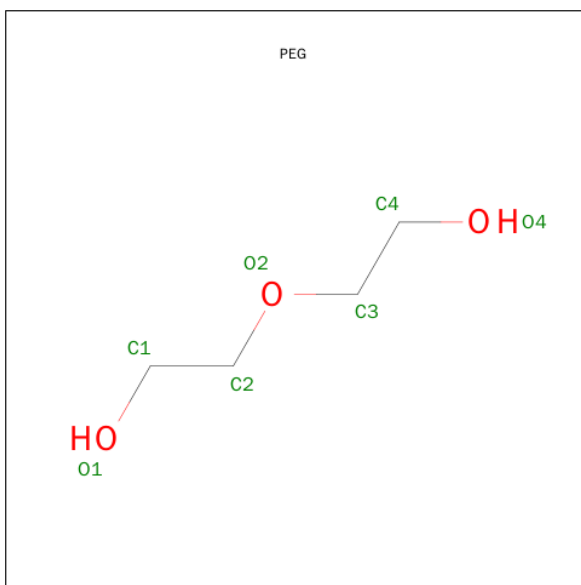
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

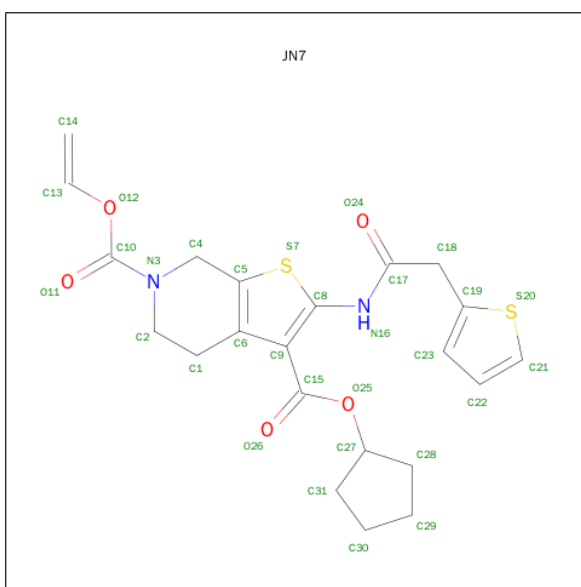
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Zn	0	0
			2	2		
3	A	2	Total	Zn	0	0
			2	2		
3	D	2	Total	Zn	0	0
			2	2		
3	C	2	Total	Zn	0	0
			2	2		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



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

- Molecule 5 is 3-CYCLOPENTYL 6-ETHENYL 2-[(THIOPHEN-2-YLACETYL)AMINO]-4,7-DIHYDROTHIENO[2,3-C]PYRIDINE-3,6(5H)-DICARBOXYLATE (three-letter code: JN7) (formula:  $C_{22}H_{24}N_2O_5S_2$ ).



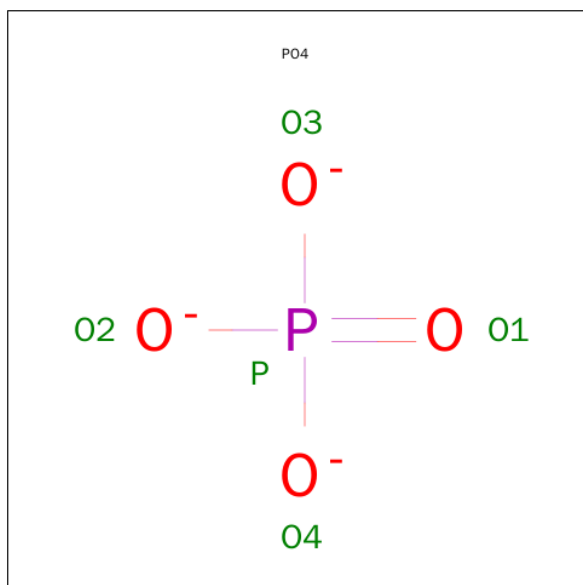
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			31	22	2	5	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	S	0	0
			31	22	2	5	2		
5	C	1	Total	C	N	O	S	0	0
			31	22	2	5	2		
5	D	1	Total	C	N	O	S	0	0
			31	22	2	5	2		

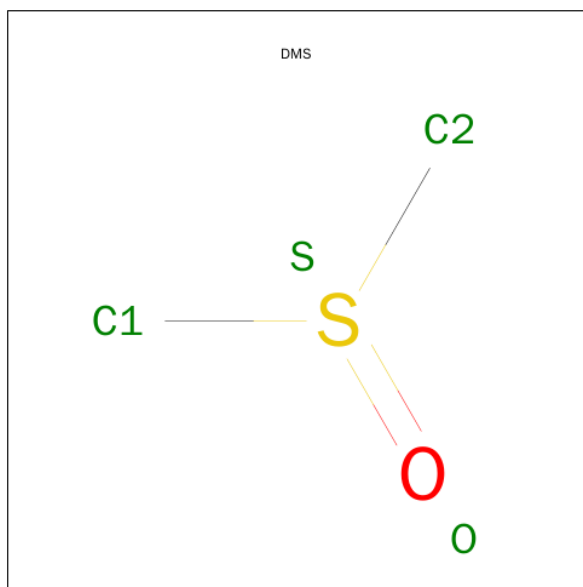
- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

- Molecule 7 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C<sub>2</sub>H<sub>6</sub>OS).





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

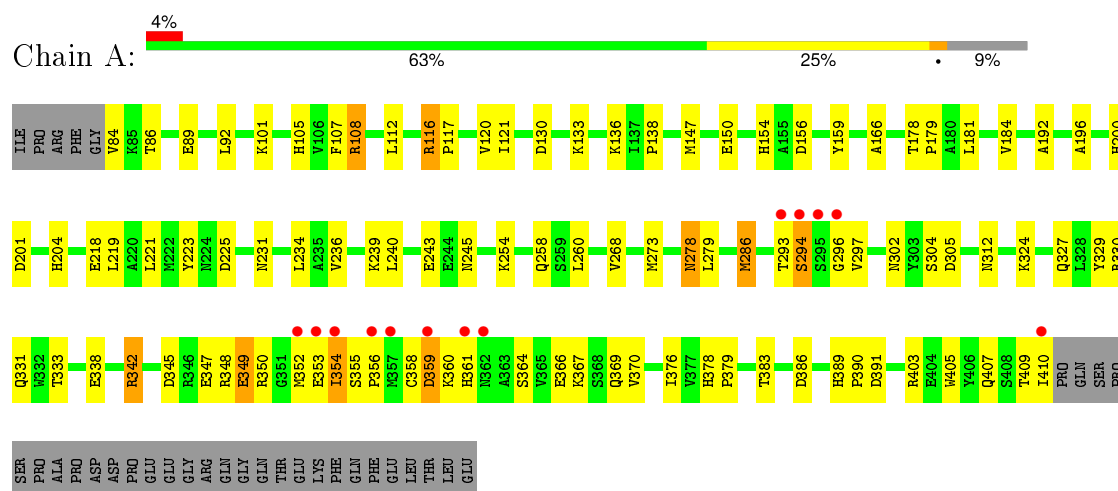
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	72	Total	O	0	0
			72	72		
8	B	46	Total	O	0	0
			46	46		
8	C	39	Total	O	0	0
			39	39		
8	D	79	Total	O	0	0
			79	79		

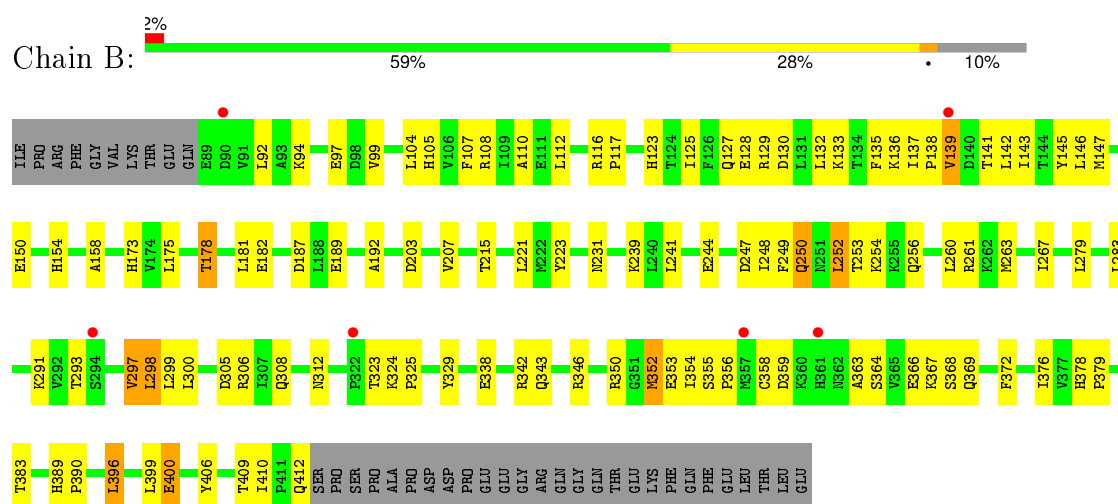
### 3 Residue-property plots

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.

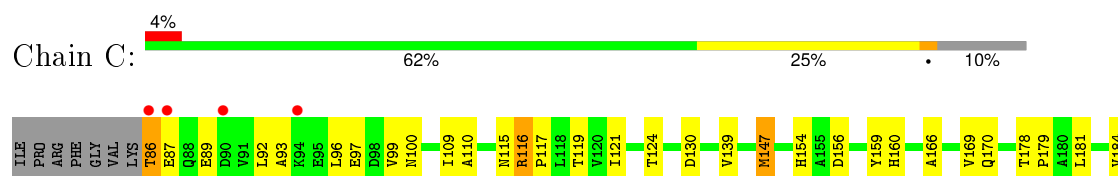
- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D

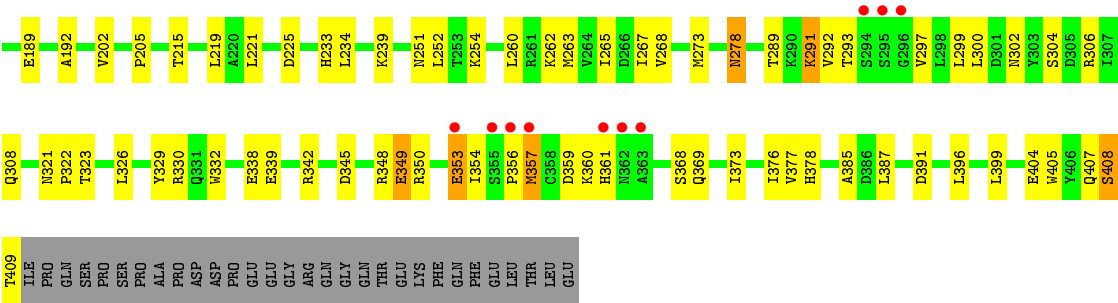


- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D

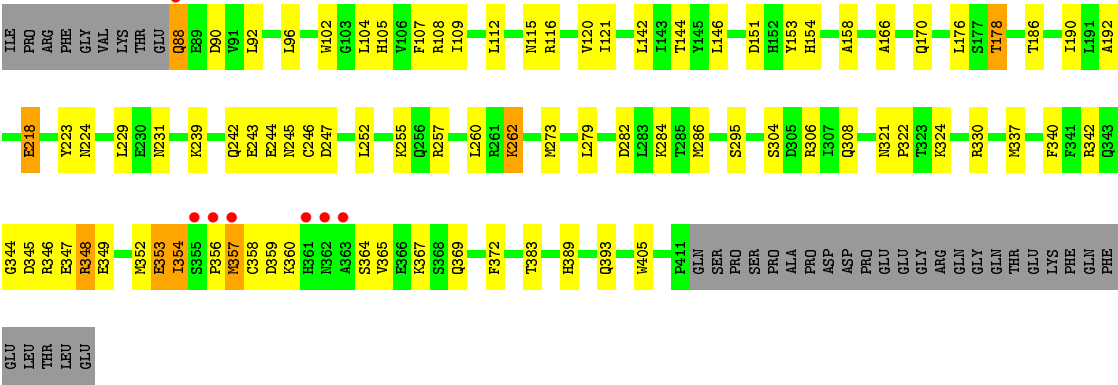


- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D





● 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, $\alpha$ , $\beta$ , $\gamma$	99.14Å 111.65Å 161.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.76 – 2.60 19.76 – 2.60	Depositor EDS
% Data completeness (in resolution range)	95.8 (19.76-2.60) 95.8 (19.76-2.60)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.32 (at 2.59Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, $R_{free}$	0.196 , 0.273 0.195 , 0.269	Depositor DCC
$R_{free}$ test set	2672 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	40.7	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 61.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 53414 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	11046	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% 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, 0.375 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: ZN, JN7, PO4, EDO, DMS, 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	0.43	0/2709	0.59	0/3678
1	B	0.40	0/2685	0.55	0/3648
1	C	0.39	0/2676	0.55	0/3635
1	D	0.45	0/2676	0.59	0/3636
All	All	0.42	0/10746	0.57	0/14597

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	2619	74	0
1	B	2628	0	2584	87	0
1	C	2623	0	2573	87	0
1	D	2622	0	2578	64	0
2	A	52	0	78	9	0
2	B	8	0	12	6	0
2	C	12	0	18	4	0
2	D	48	0	72	15	0
3	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	7	0	10	2	0
4	D	7	0	10	3	0
5	A	31	0	24	11	0
5	B	31	0	24	5	0
5	C	31	0	24	8	0
5	D	31	0	24	3	0
6	B	5	0	0	0	0
6	C	5	0	0	0	0
7	C	4	0	6	1	0
7	D	4	0	6	1	0
8	A	72	0	0	3	0
8	B	46	0	0	3	0
8	C	39	0	0	0	0
8	D	79	0	0	3	0
All	All	11046	0	10662	309	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 14.

All (309) 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:273:MET:HE2	5:C:1:JN7:H14	1.48	0.94
1:A:105:HIS:HD2	1:A:108:ARG:H	1.17	0.92
1:A:338:GLU:O	1:A:342:ARG:HG2	1.69	0.92
1:C:273:MET:CE	5:C:1:JN7:H14	2.03	0.87
1:B:137:ILE:HG21	1:B:142:LEU:HD13	1.56	0.85
1:B:352:MET:HG2	2:B:6:EDO:H12	1.61	0.81
5:A:18:JN7:H1A	5:A:18:JN7:H27	1.63	0.81
1:C:302:ASN:O	1:C:306:ARG:HG3	1.80	0.81
1:C:265:ILE:HD13	1:D:224:ASN:HB3	1.63	0.78
5:A:18:JN7:C1	5:A:18:JN7:H27	2.14	0.78
1:D:243:GLU:HB3	2:D:7:EDO:H22	1.67	0.77
1:A:105:HIS:CD2	1:A:108:ARG:H	2.03	0.75
1:B:355:SER:HB2	1:B:358:CYS:HB2	1.68	0.75
1:A:278:ASN:ND2	1:A:278:ASN:H	1.85	0.75
1:A:364:SER:HB3	1:A:367:LYS:HD2	1.68	0.75
1:B:178:THR:HG22	1:B:181:LEU:HD12	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:ASN:H	1:A:278:ASN:HD22	1.34	0.72
1:D:345:ASP:O	1:D:349:GLU:HB2	1.89	0.72
1:D:369:GLN:OE1	5:D:1:JN7:H22	1.89	0.72
1:A:403:ARG:NH1	1:A:407:GLN:HG3	2.05	0.72
1:D:282:ASP:HB3	1:D:308:GLN:NE2	2.06	0.71
1:D:273:MET:HG3	5:D:1:JN7:H4A	1.70	0.71
1:A:147:MET:SD	1:C:349:GLU:HB3	2.31	0.70
1:C:353:GLU:CD	1:C:353:GLU:H	1.92	0.70
1:A:366:GLU:HG2	1:A:409:THR:CG2	2.21	0.70
1:C:321:ASN:HB2	1:C:322:PRO:HD3	1.73	0.70
1:B:372:PHE:HE2	5:B:1:JN7:H23	1.57	0.70
1:B:389:HIS:CD2	1:B:390:PRO:HA	2.26	0.70
1:A:121:ILE:HD12	1:A:166:ALA:HB1	1.74	0.69
1:A:192:ALA:HB2	1:A:260:LEU:HD12	1.74	0.69
1:A:178:THR:HG22	1:A:181:LEU:HD12	1.75	0.69
1:B:369:GLN:OE1	5:B:1:JN7:H22	1.93	0.68
1:B:253:THR:OG1	1:B:256:GLN:HG3	1.94	0.68
1:C:189:GLU:OE2	1:C:306:ARG:NH1	2.26	0.68
1:B:105:HIS:CE1	1:B:107:PHE:HB2	2.29	0.68
2:A:13:EDO:H22	1:C:350:ARG:HD3	1.75	0.67
1:A:225:ASP:CG	1:B:261:ARG:HH21	1.98	0.67
1:D:244:GLU:HB3	2:D:7:EDO:O1	1.95	0.67
1:C:192:ALA:HB2	1:C:260:LEU:HD12	1.78	0.66
2:A:13:EDO:C2	1:C:350:ARG:HD3	2.26	0.66
1:A:376:ILE:HD11	5:A:18:JN7:C13	2.25	0.66
1:C:181:LEU:O	1:C:184:VAL:HG23	1.97	0.65
1:B:182:GLU:O	1:B:297:VAL:HG21	1.96	0.65
1:D:96:LEU:HD11	1:D:120:VAL:CG1	2.27	0.64
1:A:409:THR:O	1:A:410:ILE:HG13	1.97	0.64
1:C:369:GLN:O	1:C:373:ILE:HG13	1.98	0.63
1:B:215:THR:HG22	2:D:7:EDO:H11	1.80	0.62
1:A:366:GLU:HG2	1:A:409:THR:HG21	1.80	0.62
1:D:246:CYS:SG	2:D:7:EDO:H21	2.40	0.62
1:B:178:THR:CG2	1:B:181:LEU:HD12	2.30	0.61
1:D:245:ASN:HA	2:D:13:EDO:H21	1.81	0.61
1:B:158:ALA:CB	2:B:8:EDO:H22	2.31	0.61
1:A:333:THR:HA	5:A:18:JN7:H22	1.81	0.61
5:A:18:JN7:C6	5:A:18:JN7:H27	2.31	0.61
1:D:356:PRO:O	1:D:357:MET:HB3	2.01	0.60
1:B:352:MET:CG	2:B:6:EDO:H12	2.31	0.60
1:B:141:THR:HG21	1:B:250:GLN:HE22	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:263:MET:O	1:C:267:ILE:HG13	2.02	0.59
1:C:376:ILE:HG12	5:C:1:JN7:H14A	1.84	0.59
1:B:355:SER:HB2	1:B:358:CYS:CB	2.32	0.59
1:C:262:LYS:NZ	2:C:3:EDO:H12	2.17	0.59
1:A:329:TYR:HE1	5:A:18:JN7:H21	1.67	0.59
1:C:262:LYS:HZ2	2:C:3:EDO:H12	1.68	0.59
1:C:110:ALA:HA	1:C:117:PRO:HG3	1.84	0.59
1:C:116:ARG:N	1:C:117:PRO:HD3	2.18	0.59
1:D:342:ARG:O	1:D:346:ARG:HG2	2.03	0.58
1:A:355:SER:HB2	1:A:358:CYS:HB2	1.86	0.58
1:A:364:SER:CB	1:A:367:LYS:HD2	2.33	0.57
1:C:93:ALA:O	1:C:97:GLU:HG3	2.03	0.57
1:C:99:VAL:HG12	1:C:100:ASN:OD1	2.04	0.57
1:A:218:GLU:HG3	1:C:239:LYS:HE2	1.86	0.57
1:D:96:LEU:HD11	1:D:120:VAL:HG11	1.86	0.57
1:C:323:THR:HG22	1:C:399:LEU:HD13	1.87	0.57
1:C:304:SER:O	1:C:308:GLN:HG3	2.03	0.57
1:D:344:GLY:HA3	1:D:358:CYS:O	2.04	0.57
1:C:369:GLN:OE1	5:C:1:JN7:H22	2.05	0.57
1:D:239:LYS:NZ	1:D:242:GLN:OE1	2.37	0.56
1:C:300:LEU:HB3	1:C:306:ARG:HG2	1.87	0.56
1:C:289:THR:O	1:C:289:THR:HG22	2.06	0.56
1:C:192:ALA:HB2	1:C:260:LEU:CD1	2.36	0.55
1:C:322:PRO:HB3	1:C:329:TYR:CZ	2.41	0.55
1:C:368:SER:HB3	5:C:1:JN7:H31	1.89	0.55
5:A:18:JN7:C27	5:A:18:JN7:H1A	2.36	0.55
1:A:409:THR:HG22	1:A:409:THR:O	2.07	0.55
1:B:125:ILE:O	1:B:128:GLU:HB3	2.07	0.55
1:A:234:LEU:HD21	1:A:268:VAL:HB	1.88	0.54
1:C:338:GLU:HG2	1:C:342:ARG:HD2	1.89	0.54
1:B:346:ARG:HD2	8:D:459:HOH:O	2.08	0.54
1:A:286:MET:HE1	1:A:305:ASP:HB3	1.89	0.54
1:D:356:PRO:O	1:D:357:MET:CB	2.55	0.54
1:B:366:GLU:HG2	1:B:409:THR:HG22	1.90	0.54
1:A:327:GLN:O	1:A:331:GLN:HG3	2.08	0.54
1:A:383:THR:O	1:A:386:ASP:HB2	2.08	0.54
1:B:367:LYS:HG3	1:B:410:ILE:HD13	1.88	0.54
1:B:323:THR:HG22	1:B:399:LEU:HB2	1.90	0.53
2:A:13:EDO:H12	1:C:215:THR:HB	1.91	0.53
1:C:251:ASN:O	2:C:440:EDO:H21	2.09	0.53
1:A:330:ARG:HD3	1:A:405:TRP:CH2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:HIS:CD2	1:B:154:HIS:N	2.76	0.53
1:A:345:ASP:O	1:A:349:GLU:HG3	2.09	0.53
1:B:263:MET:O	1:B:267:ILE:HG13	2.09	0.52
1:C:154:HIS:HB3	1:C:156:ASP:OD1	2.09	0.52
1:D:245:ASN:ND2	2:D:13:EDO:O1	2.38	0.52
1:A:138:PRO:HA	4:A:12:PEG:H41	1.92	0.52
1:C:376:ILE:HG12	5:C:1:JN7:C14	2.40	0.52
1:B:116:ARG:NE	1:B:147:MET:SD	2.79	0.52
1:B:158:ALA:HB3	2:B:8:EDO:H22	1.91	0.52
1:D:347:GLU:HA	1:D:352:MET:HG3	1.91	0.52
1:D:262:LYS:HA	4:D:5:PEG:H12	1.91	0.52
1:B:145:TYR:CD2	1:B:145:TYR:C	2.83	0.52
1:D:337:MET:HG3	1:D:365:VAL:HG22	1.92	0.51
1:B:247:ASP:O	1:B:249:PHE:N	2.43	0.51
1:B:138:PRO:HG2	1:B:250:GLN:OE1	2.10	0.51
1:C:159:TYR:OH	5:C:1:JN7:H18	2.10	0.51
1:C:115:ASN:O	1:C:116:ARG:HD2	2.11	0.51
1:C:356:PRO:O	1:C:357:MET:HB2	2.11	0.51
1:C:179:PRO:HD2	1:C:391:ASP:CG	2.31	0.51
1:C:121:ILE:HD12	1:C:166:ALA:HB1	1.93	0.51
1:B:355:SER:HB2	1:B:358:CYS:SG	2.50	0.51
5:A:18:JN7:H1	5:A:18:JN7:H31A	1.93	0.51
1:D:192:ALA:HB2	1:D:260:LEU:HD12	1.92	0.51
1:B:239:LYS:NZ	1:D:218:GLU:HG3	2.26	0.51
1:A:101:LYS:NZ	8:A:468:HOH:O	2.43	0.50
1:B:372:PHE:CE2	5:B:1:JN7:H23	2.41	0.50
1:B:366:GLU:HG2	1:B:409:THR:CG2	2.42	0.50
1:B:123:HIS:CE1	1:B:127:GLN:HE21	2.29	0.50
1:B:192:ALA:HB2	1:B:260:LEU:HD12	1.94	0.50
1:B:132:LEU:HD22	1:B:139:VAL:HG13	1.94	0.50
1:C:99:VAL:HG21	1:C:124:THR:HG21	1.94	0.50
1:D:142:LEU:O	1:D:146:LEU:HG	2.12	0.50
1:C:86:THR:OG1	1:C:87:GLU:N	2.44	0.49
1:A:273:MET:HE2	5:A:18:JN7:O11	2.12	0.49
1:A:154:HIS:HB3	1:A:156:ASP:OD1	2.12	0.49
1:C:373:ILE:HA	1:C:377:VAL:HB	1.94	0.49
1:B:105:HIS:HE1	1:B:107:PHE:HB2	1.76	0.49
1:D:284:LYS:HG2	2:D:12:EDO:H22	1.93	0.49
1:B:354:ILE:N	1:B:354:ILE:HD12	2.27	0.49
1:A:86:THR:HB	2:A:17:EDO:H21	1.93	0.49
1:B:142:LEU:O	1:B:146:LEU:HG	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:LEU:HD12	8:B:463:HOH:O	2.12	0.49
1:C:234:LEU:HD21	1:C:268:VAL:HB	1.94	0.49
1:B:300:LEU:HB3	1:B:306:ARG:HG2	1.94	0.49
1:A:348:ARG:C	1:A:350:ARG:H	2.16	0.49
1:A:236:VAL:O	1:A:240:LEU:HG	2.13	0.49
1:D:102:TRP:CE2	1:D:324:LYS:HE2	2.48	0.49
1:A:354:ILE:HG21	1:A:359:ASP:OD2	2.13	0.49
1:C:345:ASP:OD1	1:C:348:ARG:NH2	2.47	0.48
1:B:143:ILE:O	1:B:147:MET:HG2	2.14	0.48
1:D:151:ASP:O	2:D:9:EDO:H11	2.13	0.48
1:B:207:VAL:HA	1:B:343:GLN:OE1	2.13	0.48
1:B:247:ASP:O	1:B:247:ASP:OD1	2.31	0.48
1:C:169:VAL:HG12	1:C:170:GLN:N	2.27	0.48
1:D:105:HIS:CE1	1:D:107:PHE:HB2	2.48	0.48
1:D:330:ARG:HD3	1:D:405:TRP:CZ3	2.48	0.48
1:A:184:VAL:HG22	1:A:297:VAL:HG13	1.95	0.48
1:D:247:ASP:H	2:D:13:EDO:C2	2.26	0.48
1:B:137:ILE:CG2	1:B:142:LEU:HD13	2.37	0.48
1:D:186:THR:O	1:D:190:ILE:HG13	2.14	0.48
1:D:354:ILE:HG21	1:D:359:ASP:HB2	1.96	0.48
1:D:108:ARG:O	1:D:112:LEU:HG	2.14	0.48
1:D:229:LEU:HA	1:D:229:LEU:HD23	1.70	0.48
1:D:154:HIS:N	1:D:154:HIS:CD2	2.82	0.47
1:B:291:LYS:HB2	1:B:299:LEU:HD12	1.95	0.47
1:C:353:GLU:N	1:C:353:GLU:CD	2.65	0.47
1:B:129:ARG:HE	1:B:173:HIS:CE1	2.32	0.47
1:C:184:VAL:CG1	1:C:300:LEU:HD12	2.44	0.47
1:D:389:HIS:HD2	8:D:62:HOH:O	1.97	0.47
1:D:96:LEU:HD23	1:D:109:ILE:HD12	1.96	0.47
1:D:262:LYS:NZ	4:D:5:PEG:O2	2.45	0.47
1:B:104:LEU:HD12	8:B:14:HOH:O	2.15	0.47
1:B:359:ASP:O	1:B:363:ALA:HB2	2.15	0.47
1:B:368:SER:HB3	5:B:1:JN7:H31	1.96	0.47
1:B:244:GLU:OE2	1:C:254:LYS:HE2	2.14	0.47
1:D:176:LEU:HD13	1:D:190:ILE:HG23	1.97	0.47
1:A:360:LYS:O	1:A:361:HIS:HB2	2.14	0.47
1:D:245:ASN:CA	2:D:13:EDO:H21	2.45	0.47
1:A:86:THR:HG23	1:A:89:GLU:OE1	2.15	0.46
1:C:116:ARG:HG2	1:C:147:MET:HE1	1.95	0.46
1:A:201:ASP:O	1:A:204:HIS:HB2	2.16	0.46
1:B:132:LEU:HD23	1:B:137:ILE:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:302:ASN:HD22	1:C:304:SER:HB3	1.80	0.46
1:B:376:ILE:HG13	5:B:1:JN7:H13	1.96	0.46
1:B:223:TYR:CE1	1:B:231:ASN:HB3	2.50	0.46
1:B:110:ALA:HA	1:B:117:PRO:HD3	1.97	0.46
1:C:86:THR:HG23	1:C:89:GLU:HG3	1.98	0.46
1:B:108:ARG:NH1	1:B:112:LEU:HD21	2.31	0.46
1:C:116:ARG:CG	1:C:147:MET:HE1	2.45	0.46
1:C:354:ILE:HD11	1:C:359:ASP:HA	1.98	0.46
1:B:158:ALA:HB2	2:B:8:EDO:H22	1.97	0.45
1:B:189:GLU:HG2	1:B:263:MET:SD	2.55	0.45
1:A:117:PRO:HD2	1:A:150:GLU:OE2	2.15	0.45
1:B:298:LEU:HD23	1:B:298:LEU:HA	1.74	0.45
1:B:94:LYS:O	1:B:97:GLU:HG3	2.17	0.45
1:D:88:GLN:CB	1:D:90:ASP:OD1	2.63	0.45
1:D:372:PHE:HE2	5:D:1:JN7:H23	1.80	0.45
1:B:329:TYR:CE2	1:B:406:TYR:CE2	3.05	0.45
1:B:130:ASP:OD2	1:B:133:LYS:HB3	2.16	0.45
1:B:338:GLU:O	1:B:342:ARG:HG2	2.16	0.45
1:B:145:TYR:CE1	1:B:241:LEU:HD23	2.51	0.45
2:A:13:EDO:H12	1:C:215:THR:CB	2.47	0.45
1:C:160:HIS:ND1	1:C:339:GLU:OE2	2.43	0.45
1:D:383:THR:HG23	2:D:12:EDO:H11	1.97	0.45
1:C:385:ALA:C	1:C:387:LEU:H	2.19	0.45
1:A:278:ASN:ND2	1:A:278:ASN:N	2.57	0.45
1:C:119:THR:OG1	1:C:147:MET:HE3	2.17	0.45
1:B:116:ARG:HA	1:B:150:GLU:OE2	2.17	0.45
1:C:291:LYS:HB2	1:C:299:LEU:HB3	1.99	0.45
1:C:273:MET:HE1	5:C:1:JN7:H14	1.91	0.45
1:D:247:ASP:H	2:D:13:EDO:H22	1.81	0.45
1:B:154:HIS:NE2	1:B:203:ASP:OD1	2.34	0.45
1:C:184:VAL:HG11	1:C:300:LEU:HD12	1.99	0.45
1:B:396:LEU:O	1:B:400:GLU:OE2	2.35	0.45
2:A:13:EDO:H21	1:C:350:ARG:HD3	1.99	0.44
1:A:133:LYS:O	1:A:136:LYS:HD2	2.18	0.44
1:C:348:ARG:HH11	1:C:354:ILE:HD12	1.82	0.44
1:C:278:ASN:H	1:C:278:ASN:ND2	2.15	0.44
1:A:254:LYS:HE3	1:A:258:GLN:CD	2.37	0.44
1:C:181:LEU:C	1:C:184:VAL:HG23	2.37	0.44
1:D:96:LEU:CD2	1:D:109:ILE:HD12	2.46	0.44
1:D:306:ARG:NH2	8:D:47:HOH:O	2.49	0.44
1:C:326:LEU:HD21	1:C:405:TRP:CE2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:156:ASP:N	1:C:156:ASP:OD1	2.45	0.44
1:A:403:ARG:HD3	1:A:403:ARG:C	2.37	0.44
1:D:252:LEU:HB2	1:D:257:ARG:HG3	2.00	0.44
1:D:340:PHE:O	1:D:358:CYS:HB3	2.18	0.44
1:C:225:ASP:OD2	4:D:5:PEG:H11	2.17	0.44
1:A:179:PRO:HD2	1:A:391:ASP:CG	2.38	0.44
1:D:178:THR:OG1	2:D:4:EDO:H22	2.17	0.44
1:C:262:LYS:HG3	2:C:3:EDO:H21	2.00	0.44
1:A:296:GLY:O	1:A:297:VAL:HG23	2.17	0.44
2:A:13:EDO:H21	1:C:350:ARG:HH11	1.83	0.44
1:B:279:LEU:HD22	1:B:312:ASN:ND2	2.33	0.44
1:D:304:SER:O	1:D:308:GLN:HG3	2.18	0.43
1:C:360:LYS:HD2	1:C:361:HIS:CE1	2.53	0.43
1:D:321:ASN:HB2	1:D:322:PRO:HD3	2.00	0.43
1:A:369:GLN:OE1	5:A:18:JN7:H21	2.18	0.43
1:A:389:HIS:HA	1:A:390:PRO:HA	1.62	0.43
1:A:108:ARG:NH2	1:A:112:LEU:HD21	2.34	0.43
1:A:136:LYS:HA	4:A:12:PEG:H12	1.99	0.43
1:B:338:GLU:HG2	2:B:8:EDO:H12	2.00	0.43
1:C:110:ALA:CA	1:C:117:PRO:HG3	2.49	0.43
1:A:245:ASN:ND2	8:A:445:HOH:O	2.50	0.43
1:C:360:LYS:HG3	1:C:361:HIS:ND1	2.33	0.43
1:B:299:LEU:HD13	1:B:299:LEU:O	2.17	0.43
1:A:324:LYS:NZ	8:A:53:HOH:O	2.40	0.43
1:B:355:SER:HB3	1:B:356:PRO:HD2	2.01	0.43
1:C:321:ASN:HD22	1:C:332:TRP:HB3	1.83	0.43
1:B:305:ASP:HA	1:B:308:GLN:HE21	1.84	0.43
1:B:324:LYS:HB3	1:B:325:PRO:HD2	2.00	0.43
1:A:324:LYS:HA	1:A:324:LYS:HD2	1.86	0.43
1:A:223:TYR:CE1	1:A:231:ASN:HB3	2.54	0.42
1:C:329:TYR:OH	1:C:373:ILE:HD11	2.19	0.42
1:A:105:HIS:HD2	1:A:108:ARG:N	2.00	0.42
1:B:116:ARG:HD3	1:B:150:GLU:OE1	2.18	0.42
1:D:353:GLU:O	1:D:354:ILE:C	2.57	0.42
1:C:326:LEU:HD21	1:C:405:TRP:CD2	2.53	0.42
1:A:355:SER:HB2	1:A:358:CYS:SG	2.60	0.42
1:C:348:ARG:HH22	1:C:360:LYS:HE3	1.84	0.42
1:D:104:LEU:HD22	1:D:170:GLN:HG3	2.01	0.42
1:C:407:GLN:O	1:C:409:THR:N	2.46	0.42
1:C:265:ILE:HD13	1:D:224:ASN:CB	2.40	0.42
1:D:348:ARG:HG3	1:D:354:ILE:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:THR:O	1:A:294:SER:O	2.38	0.42
1:A:279:LEU:HD22	1:A:312:ASN:ND2	2.35	0.42
1:B:247:ASP:C	1:B:249:PHE:H	2.23	0.42
1:A:116:ARG:O	1:A:120:VAL:HG22	2.19	0.42
1:D:223:TYR:CE1	1:D:231:ASN:HB3	2.54	0.42
1:A:159:TYR:OH	5:A:18:JN7:H18	2.20	0.41
1:A:378:HIS:N	1:A:379:PRO:CD	2.83	0.41
1:A:243:GLU:OE1	2:A:440:EDO:H11	2.20	0.41
1:B:350:ARG:NH1	2:D:7:EDO:O2	2.53	0.41
1:B:261:ARG:NH1	8:B:463:HOH:O	2.51	0.41
1:B:254:LYS:HB2	1:B:254:LYS:HE3	1.77	0.41
1:C:96:LEU:HD23	1:C:109:ILE:HD13	2.02	0.41
1:A:376:ILE:O	1:A:379:PRO:HD2	2.21	0.41
1:D:158:ALA:H	1:D:342:ARG:HH12	1.69	0.41
1:C:254:LYS:NZ	1:C:254:LYS:HB2	2.35	0.41
1:A:376:ILE:C	1:A:379:PRO:HD2	2.41	0.41
1:B:135:PHE:O	1:B:136:LYS:HB2	2.21	0.41
1:A:225:ASP:OD1	1:B:261:ARG:NH2	2.51	0.41
1:B:250:GLN:HE21	1:B:250:GLN:HB3	1.60	0.41
1:C:116:ARG:NH1	7:C:7:DMS:H23	2.36	0.41
1:B:409:THR:O	1:B:409:THR:HG22	2.20	0.41
1:D:279:LEU:HD23	1:D:279:LEU:HA	1.90	0.41
1:D:115:ASN:HD21	7:D:14:DMS:C1	2.34	0.41
1:A:105:HIS:NE2	1:A:107:PHE:HB2	2.36	0.41
1:D:144:THR:HG22	1:D:246:CYS:SG	2.61	0.41
1:A:350:ARG:C	1:A:352:MET:H	2.24	0.41
1:A:302:ASN:ND2	1:A:304:SER:HB2	2.36	0.41
1:B:378:HIS:HB3	1:B:379:PRO:HD3	2.02	0.41
1:B:175:LEU:HA	1:B:175:LEU:HD23	1.81	0.41
1:D:345:ASP:OD1	1:D:360:LYS:HE2	2.20	0.41
1:A:370:VAL:HG11	1:A:407:GLN:NE2	2.36	0.41
1:D:96:LEU:CD1	1:D:120:VAL:CG1	2.97	0.41
1:C:404:GLU:OE2	1:C:404:GLU:HA	2.21	0.41
1:B:353:GLU:HA	1:B:353:GLU:OE2	2.20	0.41
1:C:202:VAL:O	1:C:233:HIS:ND1	2.51	0.41
1:B:116:ARG:N	1:B:117:PRO:CD	2.84	0.41
1:D:88:GLN:HB2	1:D:90:ASP:OD1	2.21	0.40
1:B:283:LEU:HG	1:B:383:THR:HG22	2.03	0.40
1:C:330:ARG:HD3	1:C:405:TRP:CH2	2.56	0.40
1:D:121:ILE:HD12	1:D:166:ALA:HB1	2.03	0.40
2:A:440:EDO:O1	1:C:350:ARG:NH1	2.42	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:ALA:O	1:A:200:HIS:HB3	2.21	0.40
1:B:389:HIS:HA	1:B:390:PRO:HA	1.84	0.40
1:A:347:GLU:CD	1:A:355:SER:HG	2.24	0.40
1:A:239[B]:LYS:HE3	1:A:239[B]:LYS:HB2	1.85	0.40
1:C:378:HIS:HA	1:C:399:LEU:HD21	2.03	0.40
1:D:153:TYR:O	2:D:9:EDO:H21	2.21	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%)	304 (93%)	19 (6%)	3 (1%)	21	42
1	B	323/361 (90%)	292 (90%)	27 (8%)	4 (1%)	16	33
1	C	322/361 (89%)	299 (93%)	20 (6%)	3 (1%)	21	42
1	D	322/361 (89%)	306 (95%)	14 (4%)	2 (1%)	30	56
All	All	1293/1444 (90%)	1201 (93%)	80 (6%)	12 (1%)	21	42

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	294	SER
1	A	349	GLU
1	B	248	ILE
1	D	357	MET
1	C	293	THR
1	B	252	LEU
1	B	293	THR
1	B	352	MET
1	C	408	SER

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Mol	Chain	Res	Type
1	C	349	GLU
1	D	354	ILE
1	A	356	PRO

### 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	300/329 (91%)	288 (96%)	12 (4%)	38	67
1	B	297/329 (90%)	283 (95%)	14 (5%)	32	59
1	C	296/329 (90%)	277 (94%)	19 (6%)	22	43
1	D	296/329 (90%)	282 (95%)	14 (5%)	32	59
All	All	1189/1316 (90%)	1130 (95%)	59 (5%)	30	56

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	VAL
1	A	92	LEU
1	A	108	ARG
1	A	116	ARG
1	A	130	ASP
1	A	219	LEU
1	A	278	ASN
1	A	286	MET
1	A	342	ARG
1	A	353	GLU
1	A	354	ILE
1	A	359	ASP
1	B	92	LEU
1	B	99	VAL
1	B	139	VAL
1	B	178	THR
1	B	187	ASP
1	B	221	LEU

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Mol	Chain	Res	Type
1	B	250	GLN
1	B	252	LEU
1	B	297	VAL
1	B	298	LEU
1	B	364	SER
1	B	396	LEU
1	B	400	GLU
1	B	412	GLN
1	C	86	THR
1	C	92	LEU
1	C	116	ARG
1	C	130	ASP
1	C	139	VAL
1	C	147	MET
1	C	178	THR
1	C	205	PRO
1	C	219	LEU
1	C	221	LEU
1	C	252	LEU
1	C	278	ASN
1	C	291	LYS
1	C	292	VAL
1	C	297	VAL
1	C	353	GLU
1	C	357	MET
1	C	396	LEU
1	C	408	SER
1	D	88	GLN
1	D	92	LEU
1	D	116	ARG
1	D	178	THR
1	D	218	GLU
1	D	255	LYS
1	D	262	LYS
1	D	286	MET
1	D	295	SER
1	D	348	ARG
1	D	353	GLU
1	D	364	SER
1	D	367	LYS
1	D	393	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such



sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	HIS
1	A	245	ASN
1	A	258	GLN
1	A	278	ASN
1	A	312	ASN
1	A	407	GLN
1	B	123	HIS
1	B	245	ASN
1	B	250	GLN
1	B	308	GLN
1	B	389	HIS
1	C	210	GLN
1	C	214	ASN
1	C	245	ASN
1	C	250	GLN
1	C	278	ASN
1	D	123	HIS
1	D	127	GLN
1	D	245	ASN
1	D	250	GLN
1	D	258	GLN
1	D	308	GLN
1	D	389	HIS

### 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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 48 ligands modelled in this entry, 8 are monoatomic - leaving 40 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	A	1	-	3,3,3	0.53	0	2,2,2	0.37	0
2	EDO	A	11	-	3,3,3	0.42	0	2,2,2	0.56	0
4	PEG	A	12	-	6,6,6	0.58	0	5,5,5	1.43	1 (20%)
2	EDO	A	13	-	3,3,3	0.52	0	2,2,2	0.46	0
2	EDO	A	14	-	3,3,3	0.55	0	2,2,2	0.20	0
2	EDO	A	15	-	3,3,3	0.55	0	2,2,2	0.34	0
2	EDO	A	16	-	3,3,3	0.40	0	2,2,2	0.76	0
2	EDO	A	17	-	3,3,3	0.55	0	2,2,2	0.25	0
5	JN7	A	18	-	31,34,34	4.20	15 (48%)	21,47,47	2.50	7 (33%)
2	EDO	A	440	-	3,3,3	0.40	0	2,2,2	0.55	0
2	EDO	A	5	-	3,3,3	0.49	0	2,2,2	0.35	0
2	EDO	A	6	-	3,3,3	0.54	0	2,2,2	0.31	0
2	EDO	A	7	-	3,3,3	0.55	0	2,2,2	0.43	0
2	EDO	A	8	-	3,3,3	0.49	0	2,2,2	0.53	0
2	EDO	A	9	-	3,3,3	0.58	0	2,2,2	0.08	0
5	JN7	B	1	-	31,34,34	4.09	14 (45%)	21,47,47	2.05	6 (28%)
6	PO4	B	4	3	4,4,4	0.38	0	6,6,6	0.27	0
2	EDO	B	6	-	3,3,3	0.58	0	2,2,2	0.27	0
2	EDO	B	8	-	3,3,3	0.56	0	2,2,2	0.18	0
5	JN7	C	1	-	31,34,34	4.10	16 (51%)	21,47,47	2.07	5 (23%)
2	EDO	C	2	-	3,3,3	0.63	0	2,2,2	0.18	0
2	EDO	C	3	-	3,3,3	0.50	0	2,2,2	0.43	0
2	EDO	C	440	-	3,3,3	0.46	0	2,2,2	0.49	0
6	PO4	C	6	-	4,4,4	0.50	0	6,6,6	0.29	0
7	DMS	C	7	-	3,3,3	2.69	1 (33%)	3,3,3	0.77	0
5	JN7	D	1	-	31,34,34	4.11	16 (51%)	21,47,47	2.16	5 (23%)
2	EDO	D	10	-	3,3,3	0.49	0	2,2,2	0.51	0
2	EDO	D	11	-	3,3,3	0.56	0	2,2,2	0.48	0
2	EDO	D	12	-	3,3,3	0.57	0	2,2,2	0.34	0
2	EDO	D	13	-	3,3,3	0.61	0	2,2,2	0.30	0
7	DMS	D	14	-	3,3,3	2.67	1 (33%)	3,3,3	0.66	0
2	EDO	D	15	-	3,3,3	0.49	0	2,2,2	0.49	0
2	EDO	D	2	-	3,3,3	0.54	0	2,2,2	0.35	0
2	EDO	D	3	-	3,3,3	0.62	0	2,2,2	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	EDO	D	4	-	3,3,3	0.45	0	2,2,2	0.54	0
2	EDO	D	441	-	3,3,3	0.56	0	2,2,2	0.21	0
4	PEG	D	5	-	6,6,6	0.40	0	5,5,5	1.78	2 (40%)
2	EDO	D	7	-	3,3,3	0.45	0	2,2,2	0.52	0
2	EDO	D	8	-	3,3,3	0.58	0	2,2,2	0.30	0
2	EDO	D	9	-	3,3,3	0.58	0	2,2,2	0.26	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	A	1	-	-	0/1/1/1	0/0/0/0
2	EDO	A	11	-	-	0/1/1/1	0/0/0/0
4	PEG	A	12	-	-	0/4/4/4	0/0/0/0
2	EDO	A	13	-	-	0/1/1/1	0/0/0/0
2	EDO	A	14	-	-	0/1/1/1	0/0/0/0
2	EDO	A	15	-	-	0/1/1/1	0/0/0/0
2	EDO	A	16	-	-	0/1/1/1	0/0/0/0
2	EDO	A	17	-	-	0/1/1/1	0/0/0/0
5	JN7	A	18	-	-	2/18/39/39	0/4/4/4
2	EDO	A	440	-	-	0/1/1/1	0/0/0/0
2	EDO	A	5	-	-	0/1/1/1	0/0/0/0
2	EDO	A	6	-	-	0/1/1/1	0/0/0/0
2	EDO	A	7	-	-	0/1/1/1	0/0/0/0
2	EDO	A	8	-	-	0/1/1/1	0/0/0/0
2	EDO	A	9	-	-	0/1/1/1	0/0/0/0
5	JN7	B	1	-	-	0/18/39/39	0/4/4/4
6	PO4	B	4	3	-	0/0/0/0	0/0/0/0
2	EDO	B	6	-	-	0/1/1/1	0/0/0/0
2	EDO	B	8	-	-	0/1/1/1	0/0/0/0
5	JN7	C	1	-	-	0/18/39/39	0/4/4/4
2	EDO	C	2	-	-	0/1/1/1	0/0/0/0
2	EDO	C	3	-	-	0/1/1/1	0/0/0/0
2	EDO	C	440	-	-	0/1/1/1	0/0/0/0
6	PO4	C	6	-	-	0/0/0/0	0/0/0/0
7	DMS	C	7	-	-	0/0/0/0	0/0/0/0
5	JN7	D	1	-	-	2/18/39/39	0/4/4/4
2	EDO	D	10	-	-	0/1/1/1	0/0/0/0
2	EDO	D	11	-	-	0/1/1/1	0/0/0/0
2	EDO	D	12	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	D	13	-	-	0/1/1/1	0/0/0/0
7	DMS	D	14	-	-	0/0/0/0	0/0/0/0
2	EDO	D	15	-	-	0/1/1/1	0/0/0/0
2	EDO	D	2	-	-	0/1/1/1	0/0/0/0
2	EDO	D	3	-	-	0/1/1/1	0/0/0/0
2	EDO	D	4	-	-	0/1/1/1	0/0/0/0
2	EDO	D	441	-	-	0/1/1/1	0/0/0/0
4	PEG	D	5	-	-	0/4/4/4	0/0/0/0
2	EDO	D	7	-	-	0/1/1/1	0/0/0/0
2	EDO	D	8	-	-	0/1/1/1	0/0/0/0
2	EDO	D	9	-	-	0/1/1/1	0/0/0/0

All (63) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1	JN7	O12-C10	-7.43	1.27	1.37
5	B	1	JN7	O12-C10	-7.27	1.27	1.37
5	A	18	JN7	O12-C10	-7.25	1.28	1.37
5	C	1	JN7	C5-S7	-7.14	1.60	1.74
5	A	18	JN7	C5-S7	-7.09	1.60	1.74
5	D	1	JN7	O12-C10	-6.94	1.28	1.37
5	B	1	JN7	C5-S7	-6.65	1.61	1.74
5	D	1	JN7	C5-S7	-6.40	1.62	1.74
5	B	1	JN7	O25-C15	-3.82	1.26	1.34
5	D	1	JN7	O25-C15	-3.75	1.26	1.34
5	C	1	JN7	O25-C15	-3.71	1.26	1.34
5	B	1	JN7	O25-C27	-3.62	1.37	1.46
5	C	1	JN7	O25-C27	-3.51	1.37	1.46
5	D	1	JN7	O25-C27	-3.46	1.37	1.46
5	A	18	JN7	O25-C15	-3.04	1.28	1.34
5	A	18	JN7	O25-C27	-2.90	1.39	1.46
5	D	1	JN7	C18-C19	-2.36	1.49	1.51
5	C	1	JN7	C8-S7	-2.36	1.68	1.72
5	B	1	JN7	C1-C6	2.01	1.54	1.51
5	C	1	JN7	C2-C1	2.10	1.55	1.51
5	D	1	JN7	C1-C6	2.21	1.55	1.51
5	A	18	JN7	C1-C6	2.25	1.55	1.51
5	C	1	JN7	C1-C6	2.26	1.55	1.51
5	A	18	JN7	C2-C1	2.37	1.55	1.51
5	B	1	JN7	C23-C19	2.48	1.54	1.39
5	D	1	JN7	C23-C19	2.52	1.54	1.39
5	D	1	JN7	C2-C1	2.54	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	1	JN7	C22-C21	2.58	1.53	1.35
5	B	1	JN7	C22-C21	2.66	1.53	1.35
5	C	1	JN7	C22-C21	2.67	1.53	1.35
5	A	18	JN7	C23-C19	2.69	1.55	1.39
5	C	1	JN7	C23-C19	2.71	1.55	1.39
5	A	18	JN7	C22-C21	2.72	1.54	1.35
5	D	1	JN7	C9-C8	3.21	1.48	1.41
5	B	1	JN7	C17-N16	3.36	1.43	1.35
5	C	1	JN7	O11-C10	3.41	1.26	1.21
5	D	1	JN7	C17-N16	3.43	1.43	1.35
5	C	1	JN7	C17-N16	3.47	1.44	1.35
5	C	1	JN7	C9-C8	3.62	1.49	1.41
5	B	1	JN7	O11-C10	3.75	1.27	1.21
5	A	18	JN7	O11-C10	3.84	1.27	1.21
5	A	18	JN7	C17-N16	3.88	1.45	1.35
5	D	1	JN7	O11-C10	3.89	1.27	1.21
5	A	18	JN7	C9-C8	3.96	1.50	1.41
5	B	1	JN7	C9-C8	4.01	1.50	1.41
7	D	14	DMS	O-S	4.47	1.80	1.50
7	C	7	DMS	O-S	4.49	1.81	1.50
5	C	1	JN7	C10-N3	4.88	1.44	1.35
5	A	18	JN7	C14-C13	5.02	1.50	1.31
5	C	1	JN7	C14-C13	5.08	1.50	1.31
5	B	1	JN7	C14-C13	5.11	1.50	1.31
5	D	1	JN7	C14-C13	5.26	1.51	1.31
5	D	1	JN7	C10-N3	5.27	1.45	1.35
5	A	18	JN7	C10-N3	5.55	1.45	1.35
5	B	1	JN7	C10-N3	5.57	1.45	1.35
5	C	1	JN7	C22-C23	7.30	1.63	1.39
5	D	1	JN7	C22-C23	7.40	1.64	1.39
5	B	1	JN7	C22-C23	7.47	1.64	1.39
5	A	18	JN7	C22-C23	7.66	1.65	1.39
5	B	1	JN7	C9-C6	14.31	1.69	1.39
5	C	1	JN7	C9-C6	14.43	1.69	1.39
5	D	1	JN7	C9-C6	14.68	1.70	1.39
5	A	18	JN7	C9-C6	15.14	1.71	1.39

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1	JN7	C22-C21-S20	-5.57	107.06	113.23
5	D	1	JN7	C22-C21-S20	-5.54	107.10	113.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	1	JN7	C9-C6-C5	-4.66	108.76	113.61
5	A	18	JN7	O25-C15-O26	-4.57	115.89	123.53
5	C	1	JN7	C22-C21-S20	-4.54	108.21	113.23
5	C	1	JN7	C9-C6-C5	-4.39	109.04	113.61
5	A	18	JN7	C9-C6-C5	-4.39	109.05	113.61
5	A	18	JN7	C22-C21-S20	-4.14	108.64	113.23
5	B	1	JN7	C9-C6-C5	-4.12	109.32	113.61
5	D	1	JN7	O24-C17-N16	-3.37	117.70	123.72
5	D	1	JN7	O11-C10-N3	-3.08	118.46	124.32
5	C	1	JN7	O24-C17-N16	-3.01	118.34	123.72
5	B	1	JN7	O11-C10-N3	-3.01	118.59	124.32
5	C	1	JN7	O11-C10-N3	-2.54	119.50	124.32
5	B	1	JN7	O25-C15-O26	-2.38	119.55	123.53
5	B	1	JN7	C6-C9-C15	-2.05	121.18	126.02
4	A	12	PEG	O2-C3-C4	2.04	119.84	110.43
4	D	5	PEG	O2-C2-C1	2.11	120.14	110.43
5	D	1	JN7	C27-O25-C15	2.19	121.66	117.67
5	A	18	JN7	O25-C27-C28	2.22	118.48	105.90
5	A	18	JN7	O25-C27-C31	2.23	118.51	105.90
4	D	5	PEG	C3-O2-C2	2.24	122.92	113.31
5	B	1	JN7	C27-O25-C15	2.25	121.78	117.67
5	C	1	JN7	C27-O25-C15	4.00	124.96	117.67
5	A	18	JN7	C27-O25-C15	4.13	125.21	117.67
5	A	18	JN7	O25-C15-C9	5.42	126.19	113.03

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	1	JN7	O11-C10-N3-C4
5	D	1	JN7	O11-C10-N3-C2
5	A	18	JN7	C27-O25-C15-C9
5	A	18	JN7	C27-O25-C15-O26

There are no ring outliers.

20 monomers are involved in 68 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	12	PEG	2	0
2	A	13	EDO	6	0
2	A	17	EDO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	18	JN7	11	0
2	A	440	EDO	2	0
5	B	1	JN7	5	0
2	B	6	EDO	2	0
2	B	8	EDO	4	0
5	C	1	JN7	8	0
2	C	3	EDO	3	0
2	C	440	EDO	1	0
7	C	7	DMS	1	0
5	D	1	JN7	3	0
2	D	12	EDO	2	0
2	D	13	EDO	5	0
7	D	14	DMS	1	0
2	D	4	EDO	1	0
4	D	5	PEG	3	0
2	D	7	EDO	5	0
2	D	9	EDO	2	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	327/361 (90%)	-0.24	13 (3%) 42 34	21, 37, 74, 99	0
1	B	324/361 (89%)	-0.08	6 (1%) 70 64	24, 48, 67, 85	0
1	C	324/361 (89%)	-0.18	14 (4%) 39 31	26, 44, 72, 88	0
1	D	324/361 (89%)	-0.32	7 (2%) 65 59	21, 34, 62, 85	0
All	All	1299/1444 (89%)	-0.20	40 (3%) 52 45	21, 41, 69, 99	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	86	THR	4.5
1	D	362	ASN	4.4
1	C	353	GLU	4.3
1	A	357	MET	4.0
1	C	362	ASN	4.0
1	C	356	PRO	3.9
1	B	90	ASP	3.9
1	A	295	SER	3.8
1	C	295	SER	3.6
1	D	356	PRO	3.6
1	A	353	GLU	3.5
1	A	293	THR	3.4
1	C	361	HIS	3.3
1	A	361	HIS	3.2
1	A	362	ASN	3.2
1	A	294	SER	3.2
1	C	87	GLU	3.1
1	A	296	GLY	3.0
1	C	296	GLY	2.9
1	A	356	PRO	2.8
1	B	294	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	361	HIS	2.7
1	C	294	SER	2.7
1	C	357	MET	2.6
1	A	354	ILE	2.5
1	D	357	MET	2.5
1	B	361	HIS	2.4
1	C	363	ALA	2.4
1	A	410	ILE	2.3
1	D	88	GLN	2.3
1	C	94	LYS	2.3
1	A	359	ASP	2.2
1	C	90	ASP	2.1
1	B	357	MET	2.1
1	B	322	PRO	2.1
1	D	363	ALA	2.1
1	B	139	VAL	2.1
1	D	355	SER	2.1
1	A	352	MET	2.1
1	C	355	SER	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
2	EDO	D	13	4/4	0.89	0.43	17.16	38,40,41,44	0
7	DMS	D	14	4/4	0.93	0.30	11.39	35,47,51,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	EDO	D	7	4/4	0.97	0.32	10.27	36,37,37,41	0
4	PEG	D	5	7/7	0.83	0.29	7.09	36,39,47,48	0
2	EDO	D	9	4/4	0.87	0.23	6.95	36,41,41,46	0
7	DMS	C	7	4/4	0.88	0.26	6.91	43,45,51,64	0
2	EDO	B	6	4/4	0.88	0.35	6.71	39,40,41,49	0
4	PEG	A	12	7/7	0.92	0.36	6.19	37,39,46,47	0
2	EDO	B	8	4/4	0.91	0.38	4.38	40,46,51,57	0
2	EDO	D	8	4/4	0.90	0.24	4.09	31,36,37,38	0
2	EDO	C	2	4/4	0.91	0.24	3.60	39,40,44,45	0
2	EDO	A	15	4/4	0.80	0.29	3.42	47,47,48,56	0
2	EDO	D	15	4/4	0.88	0.32	3.06	48,49,49,51	0
2	EDO	A	5	4/4	0.94	0.20	2.83	44,47,48,54	0
2	EDO	D	4	4/4	0.97	0.17	2.81	27,33,36,44	0
2	EDO	C	3	4/4	0.91	0.20	2.00	43,45,48,49	0
2	EDO	A	6	4/4	0.94	0.17	1.99	27,30,31,34	0
2	EDO	D	12	4/4	0.84	0.27	1.71	48,51,54,55	0
2	EDO	A	11	4/4	0.94	0.16	1.42	25,27,31,33	0
5	JN7	A	18	31/31	0.84	0.29	1.37	47,66,86,91	0
2	EDO	A	13	4/4	0.95	0.18	1.28	27,33,33,38	0
2	EDO	C	440	4/4	0.95	0.22	1.19	43,45,46,46	0
6	PO4	B	4	5/5	0.95	0.14	0.96	36,41,43,45	2
5	JN7	C	1	31/31	0.91	0.20	0.84	36,48,61,66	0
2	EDO	A	7	4/4	0.90	0.21	0.72	44,49,53,54	0
2	EDO	D	11	4/4	0.89	0.16	0.68	43,43,44,51	0
5	JN7	D	1	31/31	0.90	0.18	0.58	32,53,68,69	0
5	JN7	B	1	31/31	0.87	0.21	0.48	38,52,61,66	0
2	EDO	A	440	4/4	0.96	0.15	0.00	32,35,37,45	0
2	EDO	A	8	4/4	0.95	0.13	-0.23	27,35,41,43	0
2	EDO	A	14	4/4	0.93	0.18	-0.27	50,52,57,59	0
3	ZN	C	5	1/1	0.99	0.10	-0.94	38,38,38,38	0
3	ZN	B	3	1/1	0.99	0.10	-0.99	39,39,39,39	0
3	ZN	D	440	1/1	0.99	0.11	-1.19	29,29,29,29	0
3	ZN	A	3	1/1	1.00	0.10	-1.53	34,34,34,34	0
3	ZN	C	4	1/1	0.98	0.07	-1.83	65,65,65,65	0
3	ZN	D	6	1/1	0.99	0.08	-3.28	59,59,59,59	0
6	PO4	C	6	5/5	0.98	0.07	-4.23	43,45,48,51	0
3	ZN	A	4	1/1	0.99	0.05	-5.30	58,58,58,58	0
3	ZN	B	2	1/1	0.99	0.03	-6.59	64,64,64,64	0
2	EDO	A	17	4/4	0.94	0.35	-	44,52,54,63	0
2	EDO	D	441	4/4	0.89	0.24	-	44,44,44,46	0
2	EDO	A	16	4/4	0.90	0.30	-	40,41,42,49	0
2	EDO	D	2	4/4	0.85	0.24	-	38,42,50,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	EDO	A	9	4/4	0.88	0.24	-	34,37,42,44	0
2	EDO	A	1	4/4	0.93	0.19	-	40,44,47,49	0
2	EDO	D	10	4/4	0.91	0.38	-	35,40,44,54	0
2	EDO	D	3	4/4	0.90	0.23	-	36,37,42,50	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.