



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:01 PM GMT

PDB ID : 3SL6  
Title : Crystal structure of the catalytic domain of PDE4D2 with compound 12c  
Authors : Feil, S.F.  
Deposited on : 2011-06-24  
Resolution : 2.44 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

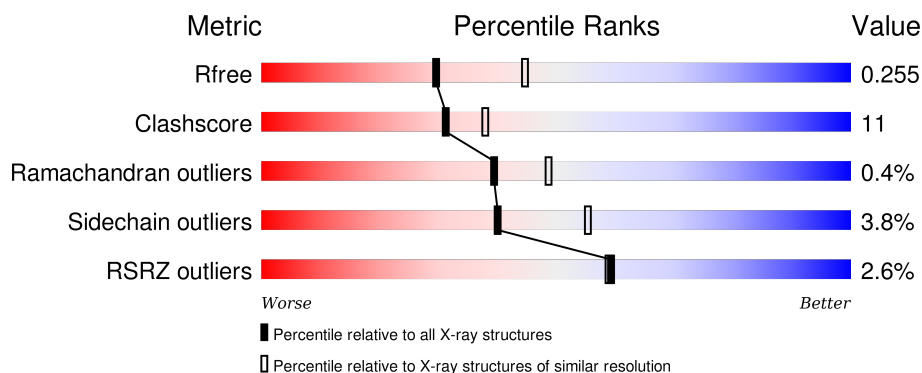
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.44 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	1003 (2.46-2.42)
Clashscore	102246	1071 (2.46-2.42)
Ramachandran outliers	100387	1065 (2.46-2.42)
Sidechain outliers	100360	1065 (2.46-2.42)
RSRZ outliers	91569	1005 (2.46-2.42)

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>3%</div> <div>73%</div> <div>16%</div> <div>9%</div> </div>
1	B	361	<div> <div>3%</div> <div>66%</div> <div>22%</div> <div>10%</div> </div>
1	C	361	<div> <div>3%</div> <div>68%</div> <div>20%</div> <div>10%</div> </div>
1	D	361	<div> <div>%</div> <div>72%</div> <div>17%</div> <div>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
3	EDO	A	442	-	-	-	X
3	EDO	A	8	-	-	-	X
3	EDO	A	9	-	-	-	X
3	EDO	B	4	-	-	-	X
3	EDO	B	5	-	-	X	X
3	EDO	C	440	-	-	-	X
3	EDO	C	8	-	-	-	X
3	EDO	D	10	-	-	-	X
3	EDO	D	11	-	-	X	X
3	EDO	D	3	-	-	X	X
3	EDO	D	4	-	-	-	X
3	EDO	D	440	-	-	-	X
3	EDO	D	8	-	-	-	X
3	EDO	D	9	-	-	-	X
6	EPE	C	2	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11042 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
			2657	1680	455	508	14			
1	B	325	Total	C	N	O	S	0	0	0
			2631	1664	450	503	14			
1	C	325	Total	C	N	O	S	0	0	0
			2631	1663	449	505	14			
1	D	324	Total	C	N	O	S	0	1	0
			2632	1665	451	502	14			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



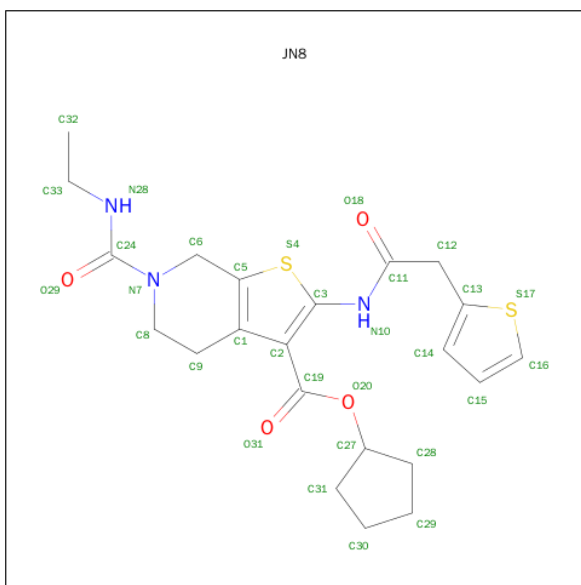
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total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

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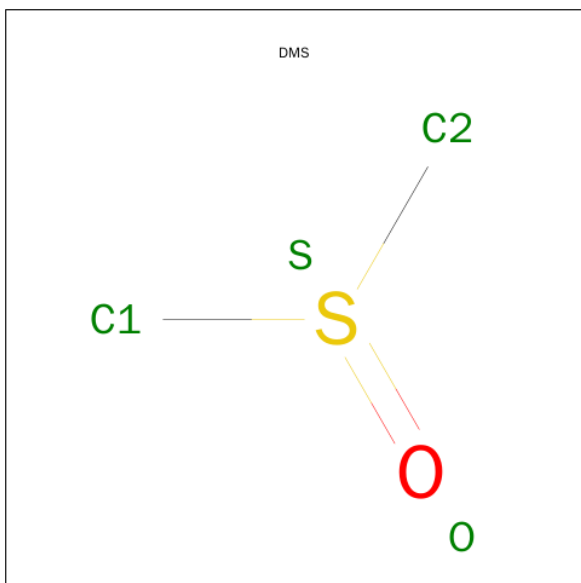
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0
3	D	1	Total 4	C 2	O 2	0	0
3	D	1	Total 4	C 2	O 2	0	0
3	D	1	Total 4	C 2	O 2	0	0
3	D	1	Total 4	C 2	O 2	0	0
3	D	1	Total 4	C 2	O 2	0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

- Molecule 4 is CYCLOPENTYL 6-(ETHYLCARBAMOYL)-2-[(THIOPHEN-2-YLACETYL)AMINO]-4,5,6,7-TETRAHYDROTHIENO[2,3-C]PYRIDINE-3-CARBOXYLATE (three-letter code: JN8) (formula: C<sub>22</sub>H<sub>27</sub>N<sub>3</sub>O<sub>4</sub>S<sub>2</sub>).



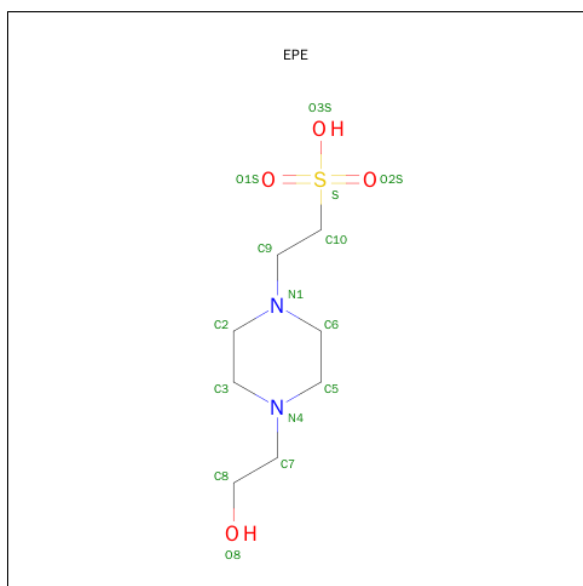
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			31	22	3	4	2		
4	B	1	Total	C	N	O	S	0	0
			31	22	3	4	2		
4	C	1	Total	C	N	O	S	0	0
			31	22	3	4	2		
4	D	1	Total	C	N	O	S	0	0
			31	22	3	4	2		

- Molecule 5 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula:  $C_2H_6OS$ ).



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

- Molecule 6 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).



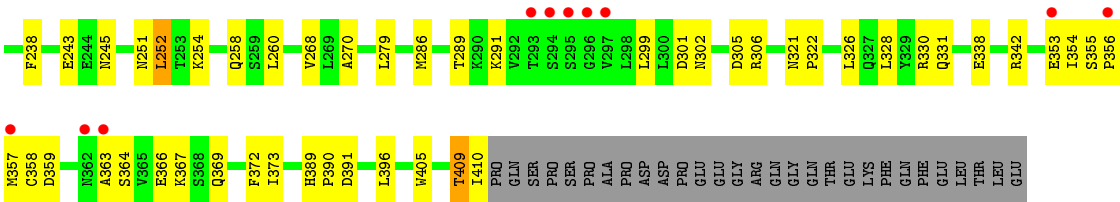
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 7 is water.

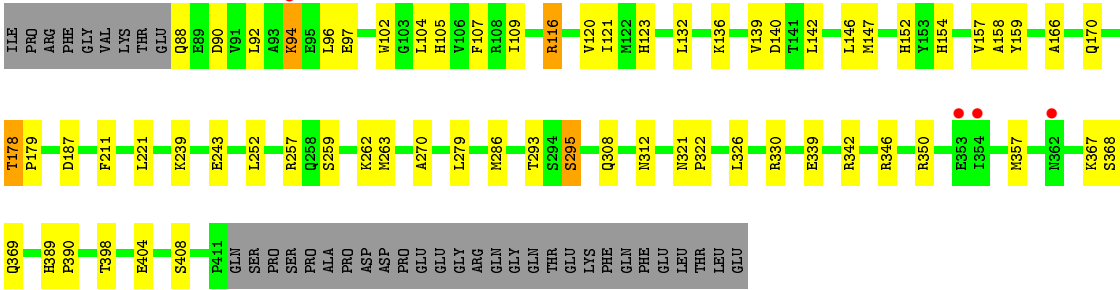
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	64	Total	O	0	0
			64	64		
7	B	47	Total	O	0	0
			47	47		
7	C	36	Total	O	0	0
			36	36		
7	D	73	Total	O	0	0
			73	73		







● 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, $\alpha$ , $\beta$ , $\gamma$	99.54Å 111.20Å 160.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	65.19 – 2.44 67.36 – 2.44	Depositor EDS
% Data completeness (in resolution range)	99.0 (65.19-2.44) 99.5 (67.36-2.44)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.23 (at 2.45Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, $R_{free}$	0.198 , 0.256 0.201 , 0.255	Depositor DCC
$R_{free}$ test set	3382 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	40.9	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 46.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 66836 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	11042	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% 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: EPE, ZN, JN8, DMS, EDO

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	0.42	0/2711	0.55	0/3682
1	B	0.39	0/2685	0.53	0/3648
1	C	0.37	0/2684	0.52	0/3646
1	D	0.44	0/2687	0.56	0/3651
All	All	0.40	0/10767	0.54	0/14627

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	2657	0	2612	43	0
1	B	2631	0	2586	76	0
1	C	2631	0	2584	50	0
1	D	2632	0	2584	61	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	36	0	54	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	12	0	18	4	0
3	C	28	0	42	8	0
3	D	44	0	66	20	0
4	A	31	0	27	3	0
4	B	31	0	27	2	0
4	C	31	0	27	2	0
4	D	31	0	27	4	0
5	B	4	0	6	0	0
6	C	15	0	17	3	0
7	A	64	0	0	2	0
7	B	47	0	0	2	0
7	C	36	0	0	0	0
7	D	73	0	0	5	0
All	All	11042	0	10677	232	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 11.

All (232) 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:D:152:HIS:HE1	3:D:3:EDO:H22	1.14	1.10
1:D:140:ASP:HB3	7:D:484:HOH:O	1.53	1.05
1:D:116:ARG:HG2	1:D:116:ARG:HH11	1.20	1.04
1:B:182:GLU:O	1:B:297:VAL:HG21	1.63	0.98
1:D:116:ARG:HE	1:D:147:MET:HG2	1.28	0.96
1:D:152:HIS:CE1	3:D:3:EDO:H22	2.01	0.93
1:D:187:ASP:HB2	3:D:4:EDO:H12	1.52	0.92
1:B:105:HIS:CE1	1:B:107:PHE:HB2	2.07	0.89
1:A:132:LEU:HD22	1:A:139:VAL:HG12	1.58	0.83
1:B:158:ALA:H	1:B:342:ARG:HH22	1.25	0.83
1:D:157:VAL:HA	3:D:11:EDO:H22	1.61	0.82
1:D:152:HIS:HE1	3:D:3:EDO:C2	1.90	0.82
1:D:88:GLN:HG3	1:D:90:ASP:H	1.46	0.80
1:A:105[A]:HIS:HD2	1:A:108:ARG:H	1.26	0.80
1:B:105:HIS:HE1	1:B:107:PHE:HB2	1.45	0.78
7:A:474:HOH:O	1:B:222:MET:HG2	1.83	0.78
1:D:116:ARG:CG	1:D:116:ARG:HH11	1.99	0.75
1:A:96:LEU:O	1:A:99:VAL:HG22	1.90	0.72
1:B:362:ASN:N	1:B:362:ASN:HD22	1.85	0.72
1:D:326:LEU:H	3:D:10:EDO:H22	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:116:ARG:NH1	1:D:116:ARG:HG2	1.95	0.72
1:B:270:ALA:HB1	1:B:279:LEU:HD11	1.72	0.71
1:D:179:PRO:HG2	3:D:7:EDO:H11	1.72	0.70
1:B:132:LEU:HD21	1:B:142:LEU:HD22	1.72	0.70
1:C:225:ASP:OD2	3:D:9:EDO:H12	1.94	0.68
1:B:158:ALA:N	1:B:342:ARG:HH22	1.91	0.67
1:B:158:ALA:H	1:B:342:ARG:NH2	1.94	0.66
1:D:158:ALA:H	3:D:11:EDO:H12	1.60	0.66
1:D:339:GLU:HA	3:D:11:EDO:H11	1.77	0.65
1:D:398:THR:HG23	3:D:10:EDO:H11	1.79	0.64
1:C:364:SER:HB2	1:C:367:LYS:HE3	1.78	0.64
1:A:225:ASP:OD1	1:B:261:ARG:NH2	2.30	0.64
1:A:243:GLU:OE1	3:A:442:EDO:H21	1.98	0.63
1:A:152:HIS:HE1	3:A:442:EDO:H22	1.64	0.63
1:C:369:GLN:OE1	4:C:441:JN8:H15	1.99	0.63
1:D:105[A]:HIS:HE1	1:D:107:PHE:HB2	1.63	0.63
1:B:354:ILE:HG22	1:B:355:SER:N	2.14	0.62
1:D:105[A]:HIS:CE1	1:D:107:PHE:HB2	2.33	0.62
1:B:178:THR:CG2	1:B:181:LEU:HD12	2.28	0.62
1:D:96:LEU:HD11	1:D:120:VAL:HG13	1.81	0.62
1:D:321:ASN:HB2	1:D:322:PRO:HD3	1.82	0.61
1:C:286:MET:HE1	1:C:305:ASP:HA	1.82	0.61
1:B:302:ASN:O	1:B:306:ARG:HG3	2.01	0.61
3:C:8:EDO:H21	1:D:221:LEU:O	2.01	0.60
1:B:355:SER:O	1:B:357:MET:N	2.33	0.60
1:B:178:THR:HG21	1:B:181:LEU:HD12	1.82	0.60
1:B:126:PHE:HA	1:B:131:LEU:HD12	1.83	0.59
1:B:129:ARG:HE	1:B:173:HIS:CE1	2.19	0.59
1:C:409:THR:O	1:C:410:ILE:HG13	2.01	0.59
1:B:354:ILE:HG22	1:B:355:SER:H	1.66	0.59
1:D:178:THR:OG1	3:D:440:EDO:H21	2.02	0.58
1:C:326:LEU:HD21	1:C:405:TRP:CE2	2.38	0.58
1:C:330:ARG:HD3	1:C:405:TRP:CH2	2.39	0.58
1:A:132:LEU:CD2	1:A:139:VAL:HG12	2.33	0.58
1:D:243:GLU:OE1	3:D:3:EDO:H21	2.03	0.57
1:B:109:ILE:O	1:B:113:SER:HB2	2.04	0.57
1:D:123:HIS:HD2	3:D:5:EDO:H21	1.69	0.57
1:A:348:ARG:C	1:A:350:ARG:H	2.07	0.56
1:D:142:LEU:O	1:D:146:LEU:HG	2.04	0.56
1:D:308:GLN:HE21	1:D:312:ASN:ND2	2.03	0.56
1:D:321:ASN:H	1:D:321:ASN:ND2	2.03	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:ARG:NH1	7:B:22:HOH:O	2.39	0.56
1:B:323:THR:HB	1:B:395:ILE:HG23	1.88	0.56
1:A:178:THR:OG1	3:A:5:EDO:H12	2.06	0.55
1:A:278:ASN:H	1:A:278:ASN:ND2	2.04	0.55
1:A:273:MET:HE2	4:A:440:JN8:HN28	1.71	0.55
1:A:302:ASN:HD22	1:A:304:SER:HB2	1.71	0.55
1:B:369:GLN:OE1	4:B:440:JN8:H15	2.07	0.54
1:B:366:GLU:HG2	1:B:409:THR:HG22	1.88	0.54
1:C:364:SER:CB	1:C:367:LYS:HE3	2.38	0.53
1:B:178:THR:HG23	1:B:181:LEU:HB2	1.89	0.53
1:C:291:LYS:HB2	1:C:299:LEU:HB3	1.90	0.53
1:A:105[A]:HIS:CD2	1:A:108:ARG:H	2.17	0.53
1:D:342:ARG:HD3	7:D:480:HOH:O	2.08	0.53
1:B:99:VAL:HG13	1:B:100:ASN:OD1	2.09	0.53
1:D:346:ARG:HH21	1:D:350:ARG:HH22	1.56	0.53
1:B:362:ASN:N	1:B:362:ASN:ND2	2.56	0.52
1:B:384:TRP:O	1:B:388:VAL:HG22	2.09	0.52
1:C:354:ILE:O	1:C:354:ILE:HG12	2.09	0.52
1:C:243:GLU:OE1	3:C:3:EDO:H12	2.08	0.52
1:C:302:ASN:O	1:C:306:ARG:HG3	2.09	0.52
1:A:105[A]:HIS:NE2	1:A:107:PHE:HB2	2.23	0.52
1:B:143:ILE:O	1:B:147:MET:HG2	2.09	0.52
1:B:366:GLU:HG2	1:B:409:THR:CG2	2.39	0.52
1:C:152:HIS:HE1	3:C:3:EDO:H11	1.75	0.52
1:B:354:ILE:C	1:B:356:PRO:HD3	2.30	0.52
1:C:372:PHE:HE2	4:C:441:JN8:H14	1.75	0.52
1:A:302:ASN:ND2	1:A:304:SER:HB2	2.25	0.51
1:A:104:LEU:HD11	1:A:109:ILE:HD11	1.92	0.51
1:A:192:ALA:HB2	1:A:260:LEU:HD12	1.91	0.51
1:A:225:ASP:CG	1:B:261:ARG:HH21	2.13	0.51
1:C:270:ALA:HB1	1:C:279:LEU:HD11	1.93	0.51
1:B:305:ASP:O	1:B:309:VAL:HG23	2.11	0.50
1:B:92:LEU:HD21	1:B:109:ILE:HG23	1.93	0.50
1:B:355:SER:C	1:B:357:MET:H	2.15	0.50
1:D:123:HIS:CD2	3:D:5:EDO:H21	2.47	0.50
1:A:265:ILE:HD13	1:B:224:ASN:O	2.12	0.50
1:B:342:ARG:NH2	7:B:466:HOH:O	2.45	0.50
1:A:366:GLU:HG2	1:A:409:THR:CG2	2.41	0.50
1:B:182:GLU:HG2	3:B:5:EDO:H11	1.93	0.49
1:B:163:ILE:HG22	1:B:332:TRP:HH2	1.78	0.49
1:A:270:ALA:HB1	1:A:279:LEU:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:291:LYS:O	1:C:299:LEU:HB3	2.11	0.49
4:D:15:JN8:O18	4:D:15:JN8:S4	2.70	0.49
1:B:412:GLN:O	1:B:412:GLN:HG2	2.13	0.49
4:A:440:JN8:H32A	4:A:440:JN8:O29	2.13	0.49
1:C:369:GLN:O	1:C:373:ILE:HG13	2.13	0.49
1:A:366:GLU:HG2	1:A:409:THR:HB	1.95	0.49
1:D:132:LEU:HD22	1:D:139:VAL:HG12	1.95	0.49
1:B:182:GLU:HA	3:B:5:EDO:H11	1.94	0.48
1:B:109:ILE:O	1:B:113:SER:CB	2.62	0.48
1:B:182:GLU:HA	3:B:5:EDO:C1	2.44	0.48
1:B:189:GLU:HG2	1:B:263:MET:SD	2.54	0.48
1:A:323:THR:HG22	1:A:399:LEU:HB2	1.95	0.48
1:B:182:GLU:HA	3:B:5:EDO:C2	2.44	0.48
1:B:389:HIS:CD2	1:B:390:PRO:HA	2.49	0.48
1:D:158:ALA:H	3:D:11:EDO:C1	2.27	0.48
1:A:223:TYR:CE1	1:A:231:ASN:HB3	2.49	0.48
1:A:364:SER:HB2	1:A:367:LYS:HB2	1.96	0.48
1:D:152:HIS:CE1	3:D:3:EDO:C2	2.80	0.47
4:B:440:JN8:S4	4:B:440:JN8:O18	2.72	0.47
1:B:409:THR:HG22	1:B:409:THR:O	2.13	0.47
1:C:356:PRO:O	1:C:357:MET:HB2	2.14	0.47
1:B:122:MET:HB2	1:B:146:LEU:HD13	1.97	0.47
1:D:321:ASN:H	1:D:321:ASN:HD22	1.62	0.47
1:C:359:ASP:O	1:C:363:ALA:HB2	2.14	0.47
1:A:152:HIS:CE1	3:A:442:EDO:H22	2.48	0.47
1:D:159:TYR:HB3	1:D:339:GLU:OE1	2.14	0.47
1:D:262:LYS:HB2	3:D:9:EDO:H21	1.95	0.47
4:A:440:JN8:C32	4:A:440:JN8:O29	2.61	0.47
1:B:346:ARG:O	1:B:350:ARG:HG3	2.15	0.47
1:C:234:LEU:HD21	1:C:268:VAL:HB	1.96	0.47
1:B:150:GLU:HG3	1:B:162:ASN:HB2	1.96	0.47
1:C:104:LEU:HD11	1:C:109:ILE:HD11	1.97	0.47
1:D:104:LEU:HD11	1:D:109:ILE:HD11	1.96	0.46
1:D:326:LEU:O	1:D:330:ARG:HG3	2.14	0.46
1:B:88:GLN:OE1	1:B:88:GLN:HA	2.15	0.46
1:B:254:LYS:HB2	1:B:254:LYS:HE3	1.62	0.46
1:C:96:LEU:HD23	1:C:109:ILE:HD13	1.96	0.46
1:D:408:SER:HB3	7:D:464:HOH:O	2.16	0.46
1:A:330:ARG:HD3	1:A:405:TRP:CH2	2.51	0.46
1:C:331:GLN:HE22	6:C:2:EPE:H101	1.81	0.46
1:C:99:VAL:HG13	1:C:100:ASN:OD1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:116:ARG:N	1:C:117:PRO:CD	2.79	0.46
1:B:154:HIS:CD2	1:B:154:HIS:N	2.83	0.46
1:D:252:LEU:HB2	1:D:257:ARG:HG3	1.98	0.45
1:C:192:ALA:HB2	1:C:260:LEU:HD12	1.98	0.45
1:D:94:LYS:O	1:D:97:GLU:HB2	2.16	0.45
4:D:15:JN8:O29	4:D:15:JN8:H32A	2.16	0.45
1:A:286:MET:SD	1:A:308:GLN:OE1	2.74	0.45
1:C:328:LEU:HD23	6:C:2:EPE:O3S	2.17	0.45
1:C:160:HIS:HD2	1:C:201:ASP:OD2	2.00	0.45
1:D:369:GLN:OE1	4:D:15:JN8:H15	2.17	0.45
1:D:259:SER:O	1:D:263:MET:HG3	2.17	0.45
1:C:178:THR:OG1	3:C:440:EDO:H11	2.17	0.45
1:A:360:LYS:HE2	1:A:360:LYS:HB3	1.69	0.45
1:A:218:GLU:OE2	3:A:2:EDO:H22	2.16	0.45
1:A:348:ARG:C	1:A:350:ARG:N	2.70	0.45
1:C:179:PRO:HD2	1:C:391:ASP:CG	2.37	0.45
1:B:154:HIS:HB2	1:B:157:VAL:HG23	1.99	0.45
1:C:254:LYS:H	3:C:7:EDO:H22	1.82	0.45
1:A:170:GLN:O	1:A:173:HIS:HB3	2.17	0.44
1:B:135:PHE:O	1:B:136:LYS:HB2	2.18	0.44
1:B:354:ILE:CG2	1:B:355:SER:N	2.80	0.44
1:D:104:LEU:HD22	1:D:170:GLN:HG3	1.99	0.44
1:A:116:ARG:N	1:A:117:PRO:CD	2.80	0.44
1:C:364:SER:HB2	1:C:367:LYS:HB2	2.00	0.44
1:B:354:ILE:CG2	1:B:355:SER:H	2.30	0.44
1:C:238:PHE:HD2	3:C:8:EDO:H12	1.82	0.44
1:A:348:ARG:O	1:A:350:ARG:N	2.51	0.44
1:C:366:GLU:CD	1:C:366:GLU:H	2.19	0.44
1:B:304:SER:O	1:B:307:ILE:HG22	2.18	0.44
1:B:347:GLU:HG2	1:B:352:MET:HE1	2.00	0.44
1:B:260:LEU:O	1:B:264:VAL:HG23	2.17	0.44
6:C:2:EPE:H31	6:C:2:EPE:H81	1.81	0.43
1:C:321:ASN:HB2	1:C:322:PRO:HD3	1.99	0.43
1:A:105[A]:HIS:HD2	1:A:108:ARG:N	2.04	0.43
1:C:251:ASN:O	3:C:4:EDO:H12	2.18	0.43
1:D:293:THR:O	1:D:295:SER:O	2.36	0.43
1:D:367:LYS:C	1:D:367:LYS:HD3	2.38	0.43
1:A:292:VAL:HG11	1:A:296:GLY:HA2	2.00	0.43
1:B:145:TYR:CE1	1:B:241:LEU:HD23	2.53	0.43
1:A:189:GLU:HG2	1:A:263:MET:SD	2.58	0.43
1:C:389:HIS:CE1	1:C:390:PRO:HB3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:LYS:HB2	1:A:89:GLU:HB2	2.01	0.43
1:D:211:PHE:CD1	1:D:211:PHE:C	2.92	0.43
1:C:142:LEU:O	1:C:146:LEU:HG	2.18	0.43
1:D:104:LEU:HD11	1:D:109:ILE:CD1	2.49	0.43
1:C:355:SER:O	1:C:358:CYS:HB2	2.19	0.42
1:A:370:VAL:HG11	1:A:407:GLN:HE21	1.84	0.42
1:D:308:GLN:HE21	1:D:312:ASN:HD22	1.64	0.42
1:C:143:ILE:O	1:C:147:MET:HG3	2.20	0.42
1:A:204:HIS:HA	1:A:205:PRO:HD3	1.85	0.42
1:D:286:MET:CE	1:D:308:GLN:OE1	2.67	0.42
1:D:404:GLU:HG2	7:D:487:HOH:O	2.18	0.42
1:B:354:ILE:HB	1:B:356:PRO:HD3	2.01	0.42
1:D:270:ALA:HB1	1:D:279:LEU:HD11	2.02	0.42
1:B:128:GLU:HG3	1:B:129:ARG:N	2.32	0.42
7:A:474:HOH:O	1:B:222:MET:CG	2.56	0.42
1:C:135:PHE:HB3	1:C:252:LEU:HD21	2.01	0.42
1:B:154:HIS:HB3	1:B:156:ASP:OD1	2.19	0.42
1:C:254:LYS:HB3	3:C:7:EDO:H22	2.02	0.42
1:B:178:THR:CG2	1:B:181:LEU:HB2	2.49	0.42
1:D:132:LEU:CD2	1:D:139:VAL:HG12	2.50	0.42
1:A:138:PRO:HB2	1:A:141:THR:OG1	2.19	0.42
1:B:116:ARG:N	1:B:117:PRO:CD	2.83	0.41
1:B:144:THR:HG22	1:B:246:CYS:SG	2.60	0.41
1:B:175:LEU:HA	1:B:175:LEU:HD23	1.85	0.41
1:C:204:HIS:HA	1:C:205:PRO:HD3	1.94	0.41
1:D:121:ILE:HD12	1:D:166:ALA:HB1	2.02	0.41
1:B:349:GLU:HB3	1:D:147:MET:SD	2.60	0.41
1:A:279:LEU:HD23	1:A:279:LEU:HA	1.88	0.41
1:C:181:LEU:O	1:C:184:VAL:HG23	2.21	0.41
1:C:279:LEU:HD23	1:C:279:LEU:HA	1.86	0.41
1:C:221:LEU:HD13	1:C:221:LEU:O	2.20	0.41
1:D:102:TRP:HB2	3:D:8:EDO:H11	2.03	0.41
1:B:389:HIS:HA	1:B:390:PRO:HA	1.74	0.41
1:B:260:LEU:O	1:B:260:LEU:HG	2.21	0.41
1:D:187:ASP:HB2	3:D:4:EDO:C1	2.38	0.41
1:B:142:LEU:O	1:B:146:LEU:HG	2.20	0.41
1:C:252:LEU:HD23	1:C:252:LEU:N	2.36	0.41
1:C:338:GLU:O	1:C:342:ARG:HG3	2.20	0.41
1:D:154:HIS:N	1:D:154:HIS:CD2	2.87	0.41
1:B:253:THR:OG1	1:B:256:GLN:HB2	2.21	0.41
1:A:178:THR:HA	1:A:179:PRO:HD3	1.96	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:389:HIS:HA	1:D:390:PRO:HA	1.82	0.40
1:B:181:LEU:O	1:B:184:VAL:HG23	2.21	0.40
1:C:204:HIS:ND1	1:C:205:PRO:HD2	2.36	0.40
1:D:239:LYS:HG3	7:D:490:HOH:O	2.21	0.40
1:B:132:LEU:HD21	1:B:142:LEU:CD2	2.45	0.40
1:C:326:LEU:HD21	1:C:405:TRP:CD2	2.55	0.40
1:D:368:SER:HB3	4:D:15:JN8:H29A	2.04	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%)	312 (96%)	12 (4%)	2 (1%)	30	36
1	B	323/361 (90%)	300 (93%)	21 (6%)	2 (1%)	30	36
1	C	323/361 (90%)	305 (94%)	17 (5%)	1 (0%)	46	56
1	D	323/361 (90%)	313 (97%)	10 (3%)	0	100	100
All	All	1295/1444 (90%)	1230 (95%)	60 (5%)	5 (0%)	39	49

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	356	PRO
1	A	294	SER
1	A	349	GLU
1	C	353	GLU
1	B	355	SER

### 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%)	290 (97%)	10 (3%)	45	61
1	B	297/329 (90%)	284 (96%)	13 (4%)	35	49
1	C	297/329 (90%)	282 (95%)	15 (5%)	29	41
1	D	297/329 (90%)	290 (98%)	7 (2%)	57	72
All	All	1191/1316 (90%)	1146 (96%)	45 (4%)	40	55

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	VAL
1	A	92	LEU
1	A	99	VAL
1	A	222	MET
1	A	239	LYS
1	A	278	ASN
1	A	284	LYS
1	A	293	THR
1	A	304	SER
1	A	308	GLN
1	B	92	LEU
1	B	128	GLU
1	B	221	LEU
1	B	252	LEU
1	B	259	SER
1	B	297	VAL
1	B	298	LEU
1	B	299	LEU
1	B	346	ARG
1	B	356	PRO
1	B	362	ASN
1	B	396	LEU
1	B	403	ARG
1	C	86	THR

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Mol	Chain	Res	Type
1	C	90	ASP
1	C	92	LEU
1	C	116	ARG
1	C	132	LEU
1	C	139	VAL
1	C	147	MET
1	C	178	THR
1	C	245	ASN
1	C	252	LEU
1	C	258	GLN
1	C	289	THR
1	C	301	ASP
1	C	396	LEU
1	C	409	THR
1	D	92	LEU
1	D	94	LYS
1	D	116	ARG
1	D	136	LYS
1	D	178	THR
1	D	295	SER
1	D	357	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	HIS
1	A	224	ASN
1	A	245	ASN
1	A	258	GLN
1	A	278	ASN
1	A	302	ASN
1	A	331	GLN
1	A	361	HIS
1	A	407	GLN
1	B	231	ASN
1	B	245	ASN
1	B	308	GLN
1	B	327	GLN
1	B	362	ASN
1	B	389	HIS
1	C	245	ASN
1	C	258	GLN

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Mol	Chain	Res	Type
1	C	308	GLN
1	C	331	GLN
1	C	393	GLN
1	D	123	HIS
1	D	127	GLN
1	D	152	HIS
1	D	245	ASN
1	D	278	ASN
1	D	312	ASN
1	D	321	ASN
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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 44 ligands modelled in this entry, 8 are monoatomic - leaving 36 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	EDO	A	2	-	3,3,3	0.52	0	2,2,2	0.30	0
3	EDO	A	4	-	3,3,3	0.53	0	2,2,2	0.33	0
4	JN8	A	440	-	31,34,34	2.05	8 (25%)	25,47,47	1.63	3 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	EDO	A	441	-	3,3,3	0.44	0	2,2,2	0.51	0
3	EDO	A	442	-	3,3,3	0.61	0	2,2,2	0.34	0
3	EDO	A	5	-	3,3,3	0.57	0	2,2,2	0.19	0
3	EDO	A	6	-	3,3,3	0.55	0	2,2,2	0.21	0
3	EDO	A	7	-	3,3,3	0.61	0	2,2,2	0.26	0
3	EDO	A	8	-	3,3,3	0.56	0	2,2,2	0.32	0
3	EDO	A	9	-	3,3,3	0.46	0	2,2,2	0.85	0
5	DMS	B	14	-	3,3,3	2.63	1 (33%)	3,3,3	0.56	0
3	EDO	B	4	-	3,3,3	0.59	0	2,2,2	0.16	0
4	JN8	B	440	-	31,34,34	2.18	9 (29%)	25,47,47	1.44	5 (20%)
3	EDO	B	5	-	3,3,3	0.56	0	2,2,2	0.19	0
3	EDO	B	6	-	3,3,3	0.57	0	2,2,2	0.19	0
6	EPE	C	2	-	14,15,15	0.48	0	18,20,20	2.11	6 (33%)
3	EDO	C	3	-	3,3,3	0.62	0	2,2,2	0.29	0
3	EDO	C	4	-	3,3,3	0.42	0	2,2,2	0.61	0
3	EDO	C	440	-	3,3,3	0.48	0	2,2,2	0.40	0
4	JN8	C	441	-	31,34,34	2.11	7 (22%)	25,47,47	1.36	3 (12%)
3	EDO	C	5	-	3,3,3	0.56	0	2,2,2	0.35	0
3	EDO	C	7	-	3,3,3	0.58	0	2,2,2	0.35	0
3	EDO	C	8	-	3,3,3	0.58	0	2,2,2	0.13	0
3	EDO	C	9	-	3,3,3	0.57	0	2,2,2	0.32	0
3	EDO	D	10	-	3,3,3	0.64	0	2,2,2	0.22	0
3	EDO	D	11	-	3,3,3	0.60	0	2,2,2	0.11	0
4	JN8	D	15	-	31,34,34	2.11	9 (29%)	25,47,47	1.56	5 (20%)
3	EDO	D	2	-	3,3,3	0.49	0	2,2,2	0.53	0
3	EDO	D	3	-	3,3,3	0.39	0	2,2,2	0.90	0
3	EDO	D	4	-	3,3,3	0.60	0	2,2,2	0.27	0
3	EDO	D	440	-	3,3,3	0.47	0	2,2,2	0.20	0
3	EDO	D	5	-	3,3,3	0.56	0	2,2,2	0.28	0
3	EDO	D	6	-	3,3,3	0.53	0	2,2,2	0.50	0
3	EDO	D	7	-	3,3,3	0.59	0	2,2,2	0.31	0
3	EDO	D	8	-	3,3,3	0.68	0	2,2,2	0.05	0
3	EDO	D	9	-	3,3,3	0.53	0	2,2,2	0.11	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
3	EDO	A	2	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	A	4	-	-	0/1/1/1	0/0/0/0
4	JN8	A	440	-	-	0/19/39/39	0/4/4/4
3	EDO	A	441	-	-	0/1/1/1	0/0/0/0
3	EDO	A	442	-	-	0/1/1/1	0/0/0/0
3	EDO	A	5	-	-	0/1/1/1	0/0/0/0
3	EDO	A	6	-	-	0/1/1/1	0/0/0/0
3	EDO	A	7	-	-	0/1/1/1	0/0/0/0
3	EDO	A	8	-	-	0/1/1/1	0/0/0/0
3	EDO	A	9	-	-	0/1/1/1	0/0/0/0
5	DMS	B	14	-	-	0/0/0/0	0/0/0/0
3	EDO	B	4	-	-	0/1/1/1	0/0/0/0
4	JN8	B	440	-	-	0/19/39/39	0/4/4/4
3	EDO	B	5	-	-	0/1/1/1	0/0/0/0
3	EDO	B	6	-	-	0/1/1/1	0/0/0/0
6	EPE	C	2	-	-	0/9/19/19	0/1/1/1
3	EDO	C	3	-	-	0/1/1/1	0/0/0/0
3	EDO	C	4	-	-	0/1/1/1	0/0/0/0
3	EDO	C	440	-	-	0/1/1/1	0/0/0/0
4	JN8	C	441	-	-	0/19/39/39	0/4/4/4
3	EDO	C	5	-	-	0/1/1/1	0/0/0/0
3	EDO	C	7	-	-	0/1/1/1	0/0/0/0
3	EDO	C	8	-	-	0/1/1/1	0/0/0/0
3	EDO	C	9	-	-	0/1/1/1	0/0/0/0
3	EDO	D	10	-	-	0/1/1/1	0/0/0/0
3	EDO	D	11	-	-	0/1/1/1	0/0/0/0
4	JN8	D	15	-	-	0/19/39/39	0/4/4/4
3	EDO	D	2	-	-	0/1/1/1	0/0/0/0
3	EDO	D	3	-	-	0/1/1/1	0/0/0/0
3	EDO	D	4	-	-	0/1/1/1	0/0/0/0
3	EDO	D	440	-	-	0/1/1/1	0/0/0/0
3	EDO	D	5	-	-	0/1/1/1	0/0/0/0
3	EDO	D	6	-	-	0/1/1/1	0/0/0/0
3	EDO	D	7	-	-	0/1/1/1	0/0/0/0
3	EDO	D	8	-	-	0/1/1/1	0/0/0/0
3	EDO	D	9	-	-	0/1/1/1	0/0/0/0

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	440	JN8	O20-C19	-3.55	1.27	1.34
4	D	15	JN8	C12-C13	-3.25	1.48	1.51
4	C	441	JN8	O20-C19	-3.08	1.28	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	440	JN8	C6-C5	-3.05	1.48	1.51
4	D	15	JN8	O20-C19	-3.00	1.28	1.34
4	A	440	JN8	O20-C19	-2.97	1.28	1.34
4	B	440	JN8	O20-C27	-2.75	1.39	1.46
4	D	15	JN8	C6-C5	-2.64	1.48	1.51
4	D	15	JN8	C6-N7	-2.31	1.42	1.46
4	C	441	JN8	O20-C27	-2.19	1.41	1.46
4	D	15	JN8	O20-C27	-2.14	1.41	1.46
4	A	440	JN8	C6-C5	-2.12	1.49	1.51
4	A	440	JN8	O20-C27	-2.04	1.41	1.46
4	B	440	JN8	C6-N7	-2.04	1.43	1.46
4	B	440	JN8	C2-C3	2.03	1.46	1.41
4	D	15	JN8	C24-N28	2.18	1.45	1.33
4	A	440	JN8	C24-N28	2.21	1.46	1.33
4	B	440	JN8	C24-N28	2.21	1.46	1.33
4	A	440	JN8	C2-C3	2.24	1.46	1.41
4	C	441	JN8	C24-N28	2.27	1.46	1.33
4	C	441	JN8	C2-C3	2.55	1.47	1.41
4	B	440	JN8	C11-N10	3.42	1.43	1.35
4	D	15	JN8	C11-N10	3.63	1.44	1.35
4	C	441	JN8	C11-N10	3.69	1.44	1.35
4	A	440	JN8	C11-N10	3.80	1.44	1.35
5	B	14	DMS	O-S	4.40	1.80	1.50
4	D	15	JN8	C24-N7	5.00	1.46	1.36
4	A	440	JN8	C24-N7	5.43	1.47	1.36
4	C	441	JN8	C24-N7	5.75	1.47	1.36
4	B	440	JN8	C24-N7	5.85	1.47	1.36
4	A	440	JN8	C2-C1	6.72	1.53	1.39
4	C	441	JN8	C2-C1	6.80	1.53	1.39
4	D	15	JN8	C2-C1	6.86	1.53	1.39
4	B	440	JN8	C2-C1	6.94	1.54	1.39

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	440	JN8	C2-C1-C5	-3.78	109.67	113.61
4	C	441	JN8	C2-C1-C5	-3.65	109.81	113.61
4	D	15	JN8	C2-C1-C5	-3.27	110.21	113.61
4	B	440	JN8	C15-C16-S17	-3.19	109.70	113.23
4	A	440	JN8	C2-C1-C5	-2.94	110.55	113.61
4	A	440	JN8	O29-C24-N7	-2.87	117.39	121.77
4	D	15	JN8	C15-C16-S17	-2.56	110.40	113.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	441	JN8	C15-C16-S17	-2.35	110.63	113.23
4	D	15	JN8	O29-C24-N7	-2.33	118.20	121.77
4	B	440	JN8	O18-C11-N10	-2.27	119.66	123.72
6	C	2	EPE	C9-N1-C2	-2.03	106.06	111.27
4	B	440	JN8	O20-C19-O31	-2.01	120.17	123.53
4	B	440	JN8	C27-O20-C19	2.08	121.46	117.67
4	C	441	JN8	C27-O20-C19	2.42	122.08	117.67
6	C	2	EPE	C7-N4-C3	2.44	117.51	111.27
4	D	15	JN8	O20-C19-C2	2.65	119.47	113.03
6	C	2	EPE	C5-N4-C3	2.83	115.03	108.90
6	C	2	EPE	C7-N4-C5	3.03	119.02	111.27
4	D	15	JN8	C27-O20-C19	3.50	124.06	117.67
6	C	2	EPE	O2S-S-C10	3.82	110.17	106.91
4	A	440	JN8	C27-O20-C19	4.50	125.88	117.67
6	C	2	EPE	O1S-S-C10	5.50	111.60	106.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

23 monomers are involved in 51 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2	EDO	1	0
4	A	440	JN8	3	0
3	A	442	EDO	3	0
3	A	5	EDO	1	0
4	B	440	JN8	2	0
3	B	5	EDO	4	0
6	C	2	EPE	3	0
3	C	3	EDO	2	0
3	C	4	EDO	1	0
3	C	440	EDO	1	0
4	C	441	JN8	2	0
3	C	7	EDO	2	0
3	C	8	EDO	2	0
3	D	10	EDO	2	0
3	D	11	EDO	4	0
4	D	15	JN8	4	0
3	D	3	EDO	5	0
3	D	4	EDO	2	0
3	D	440	EDO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	5	EDO	2	0
3	D	7	EDO	1	0
3	D	8	EDO	1	0
3	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%)	0.23	10 (3%) 52 51	23, 37, 73, 111	0
1	B	325/361 (90%)	0.28	10 (3%) 52 51	26, 48, 69, 103	0
1	C	325/361 (90%)	0.24	10 (3%) 52 51	28, 46, 79, 104	0
1	D	324/361 (89%)	0.15	4 (1%) 81 82	23, 35, 65, 90	0
All	All	1301/1444 (90%)	0.22	34 (2%) 59 59	23, 42, 71, 111	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	296	GLY	8.2
1	C	295	SER	7.1
1	A	295	SER	6.7
1	A	297	VAL	5.9
1	C	296	GLY	5.6
1	C	297	VAL	5.1
1	A	357	MET	4.7
1	C	353	GLU	4.6
1	A	294	SER	4.2
1	A	353	GLU	4.1
1	C	294	SER	3.9
1	A	356	PRO	3.5
1	A	293	THR	3.5
1	D	362	ASN	3.2
1	C	293	THR	3.0
1	A	409	THR	2.9
1	B	88	GLN	2.8
1	B	96	LEU	2.5
1	C	356	PRO	2.5
1	B	139	VAL	2.4
1	A	358	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	94	LYS	2.4
1	C	357	MET	2.4
1	D	354	ILE	2.4
1	C	362	ASN	2.3
1	B	296	GLY	2.3
1	B	295	SER	2.3
1	B	147	MET	2.2
1	D	353	GLU	2.2
1	B	112	LEU	2.2
1	C	363	ALA	2.1
1	B	143	ILE	2.1
1	B	328	LEU	2.0
1	B	94	LYS	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
3	EDO	D	9	4/4	0.92	0.26	9.96	31,35,38,40	0
3	EDO	D	3	4/4	0.92	0.40	8.72	29,30,38,39	0
3	EDO	C	8	4/4	0.77	0.34	8.28	49,53,54,60	0
3	EDO	B	4	4/4	0.85	0.46	8.15	51,53,59,61	0
3	EDO	D	4	4/4	0.81	0.29	7.72	40,48,51,56	0
3	EDO	D	11	4/4	0.79	0.44	5.66	44,49,54,57	0
3	EDO	D	10	4/4	0.75	0.23	5.03	46,48,49,49	0
3	EDO	D	8	4/4	0.82	0.27	4.61	42,46,48,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	EDO	C	440	4/4	0.95	0.23	4.13	54,55,56,59	0
3	EDO	A	9	4/4	0.97	0.23	4.08	32,34,38,48	0
3	EDO	A	8	4/4	0.74	0.23	4.03	52,52,53,58	0
3	EDO	B	5	4/4	0.75	0.29	3.95	50,55,56,57	0
6	EPE	C	2	15/15	0.93	0.26	3.35	47,68,82,83	0
3	EDO	D	440	4/4	0.93	0.21	2.98	34,35,38,39	0
3	EDO	A	442	4/4	0.95	0.25	2.17	37,39,40,43	0
3	EDO	A	6	4/4	0.93	0.19	1.74	33,40,41,42	0
3	EDO	C	5	4/4	0.92	0.19	1.39	42,44,47,48	0
3	EDO	C	4	4/4	0.95	0.18	1.31	49,50,53,54	0
3	EDO	A	5	4/4	0.84	0.17	1.25	47,48,50,51	0
3	EDO	C	7	4/4	0.62	0.27	1.25	46,53,55,56	0
4	JN8	A	440	31/31	0.93	0.26	1.18	36,49,72,78	0
3	EDO	A	4	4/4	0.94	0.17	1.15	39,43,45,47	0
3	EDO	C	3	4/4	0.85	0.20	1.13	41,44,48,53	0
2	ZN	B	7	1/1	0.99	0.16	1.07	43,43,43,43	0
4	JN8	B	440	31/31	0.93	0.19	0.99	29,39,55,60	0
3	EDO	A	7	4/4	0.81	0.20	0.72	47,48,51,54	0
4	JN8	C	441	31/31	0.90	0.19	0.66	34,48,63,67	0
2	ZN	C	11	1/1	0.99	0.16	0.34	40,40,40,40	0
3	EDO	D	6	4/4	0.92	0.16	0.34	38,39,40,46	0
3	EDO	C	9	4/4	0.91	0.17	0.26	50,52,52,55	0
4	JN8	D	15	31/31	0.92	0.17	0.15	27,48,64,75	0
2	ZN	D	13	1/1	1.00	0.15	-0.14	37,37,37,37	0
3	EDO	A	441	4/4	0.96	0.15	-0.29	27,31,32,34	0
2	ZN	A	10	1/1	0.99	0.15	-0.83	35,35,35,35	0
2	ZN	C	10	1/1	0.97	0.13	-0.92	65,65,65,65	0
2	ZN	D	12	1/1	0.99	0.12	-2.31	59,59,59,59	0
3	EDO	D	7	4/4	0.95	0.13	-2.85	35,39,39,41	0
2	ZN	B	8	1/1	0.97	0.12	-2.95	64,64,64,64	0
2	ZN	A	11	1/1	0.99	0.09	-3.83	54,54,54,54	0
3	EDO	D	5	4/4	0.82	0.19	-	47,48,50,55	0
3	EDO	B	6	4/4	0.81	0.22	-	53,56,56,59	0
3	EDO	A	2	4/4	0.90	0.15	-	49,53,55,57	0
3	EDO	D	2	4/4	0.94	0.17	-	34,40,40,42	0
5	DMS	B	14	4/4	0.85	0.19	-	69,69,75,80	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.