



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 11:15 pm GMT

PDB ID : 5IXS  
Title : Lactate Dehydrogenase in complex with hydroxylactam inhibitor compound 9: (6R)-3-[(2-chlorophenyl)sulfanyl]-4-hydroxy-6-(3-hydroxyphenyl)-6-(thiophen-3-yl)-5,6-dihydropyridin-2(1H)-one  
Authors : Ultsch, M.; Eigenbrot, C.  
Deposited on : 2016-03-23  
Resolution : 2.05 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

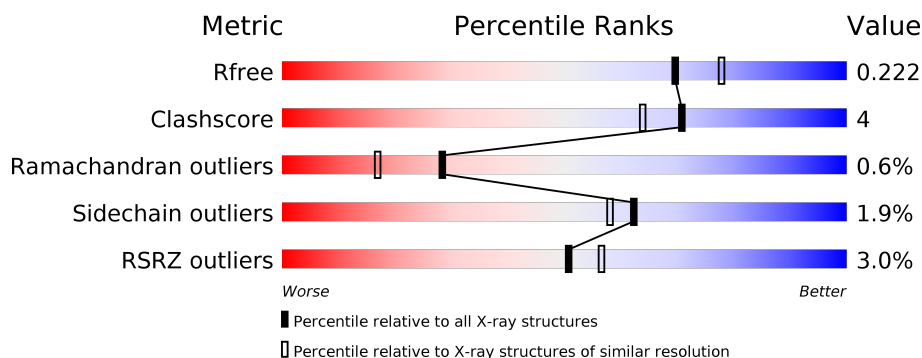
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.05 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))
$R_{free}$	100719	1316 (2.04-2.04)
Clashscore	112137	1394 (2.04-2.04)
Ramachandran outliers	110173	1383 (2.04-2.04)
Sidechain outliers	110143	1383 (2.04-2.04)
RSRZ outliers	101464	1319 (2.04-2.04)

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	331	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 98%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 2px;"> <span>%</span> <span>89%</span> <span>9% ..</span> </div> </div>
1	B	331	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 2%, yellow 1%, green 95%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 2px;"> <span>2%</span> <span>86%</span> <span>11% •</span> </div> </div>
1	C	331	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 6%, orange 6%, yellow 1%, green 87%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 2px;"> <span>6%</span> <span>90%</span> <span>7% ..</span> </div> </div>
1	D	331	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, orange 3%, yellow 1%, green 93%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 2px;"> <span>3%</span> <span>93%</span> <span>5% •</span> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EPE	A	401	-	-	-	X
2	EPE	B	401	-	-	-	X
2	EPE	C	401	-	-	-	X
4	6EY	B	403	-	-	-	X
5	SO4	A	404	-	-	-	X
5	SO4	D	803	-	-	-	X

## 2 Entry composition [i](#)

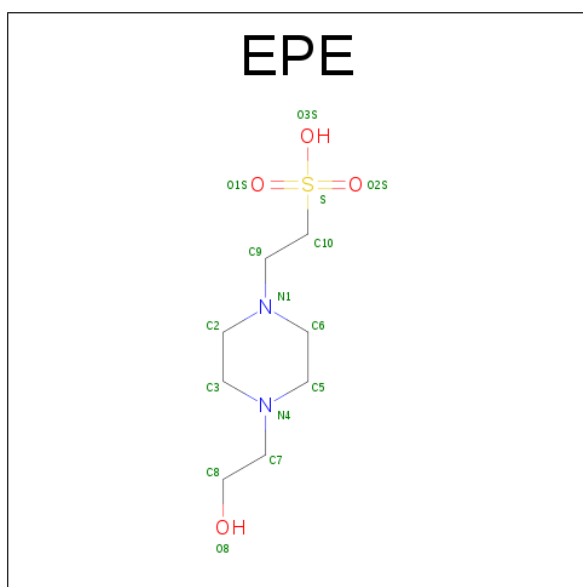
There are 7 unique types of molecules in this entry. The entry contains 11112 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 L-lactate dehydrogenase A chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	327	Total	C	N	O	S	0	4	0
			2556	1635	434	473	14			
1	B	324	Total	C	N	O	S	0	3	0
			2532	1626	430	463	13			
1	C	324	Total	C	N	O	S	0	2	0
			2522	1616	428	465	13			
1	D	330	Total	C	N	O	S	0	4	0
			2580	1650	441	475	14			

- Molecule 2 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).



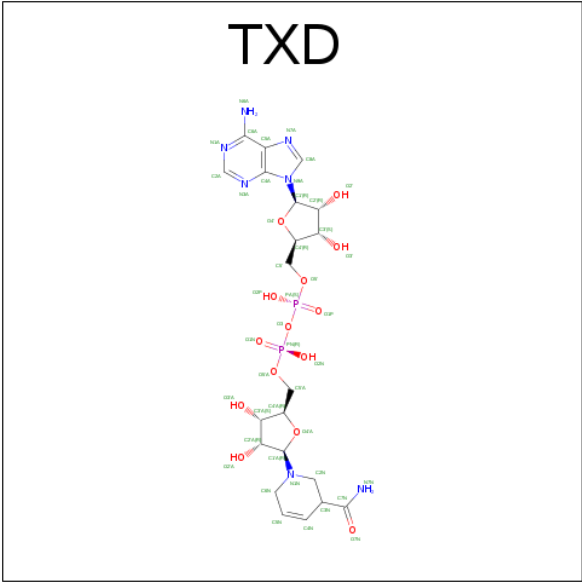
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
2	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

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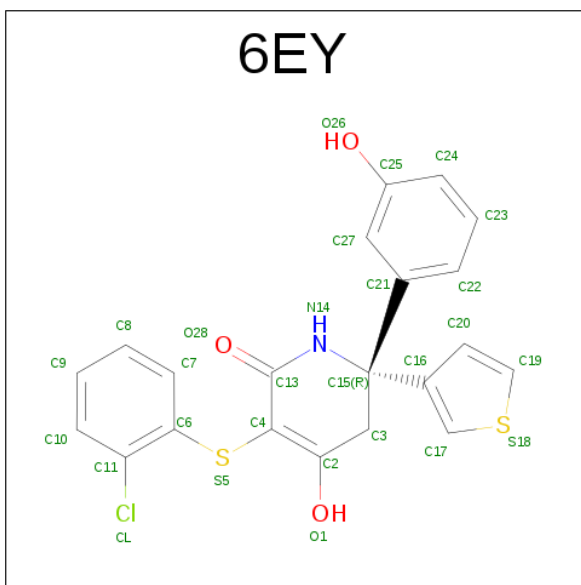
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 3 is 1,4,5,6-TETRAHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: TXD) (formula: C<sub>21</sub>H<sub>31</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



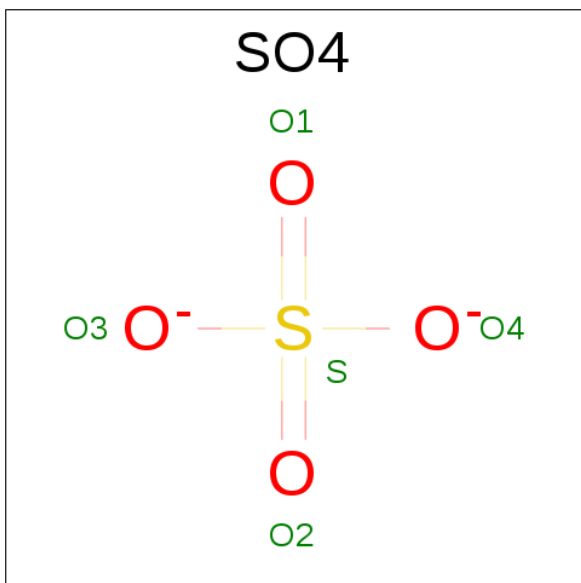
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 4 is (6R)-3-[(2-chlorophenyl)sulfanyl]-4-hydroxy-6-(3-hydroxyphenyl)-6-(thiophen-3-yl)-5,6-dihydropyridin-2(1H)-one (three-letter code: 6EY) (formula: C<sub>21</sub>H<sub>16</sub>ClNO<sub>3</sub>S<sub>2</sub>).



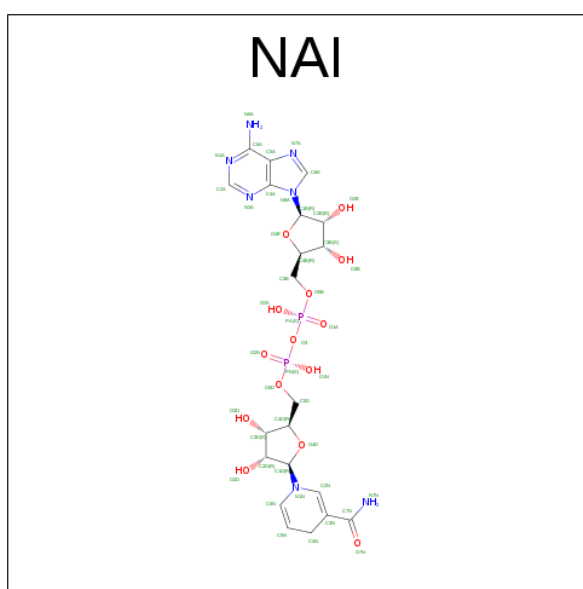
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total 28	C 21	Cl 1	N 1	O 3	S 2	0	0
4	B	1	Total 28	C 21	Cl 1	N 1	O 3	S 2	0	0
4	C	1	Total 28	C 21	Cl 1	N 1	O 3	S 2	0	0
4	D	1	Total 28	C 21	Cl 1	N 1	O 3	S 2	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 6 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: C<sub>21</sub>H<sub>29</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total C N O P 44 21 7 14 2	0	0

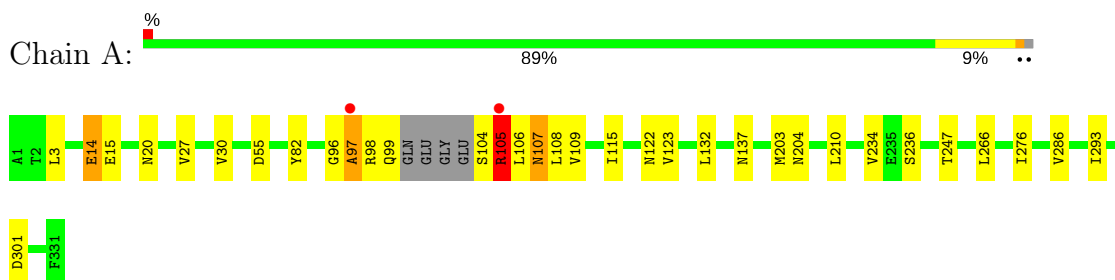
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	158	Total O 158 158	0	0
7	B	159	Total O 159 159	0	0
7	C	98	Total O 98 98	0	0
7	D	154	Total O 154 154	0	0

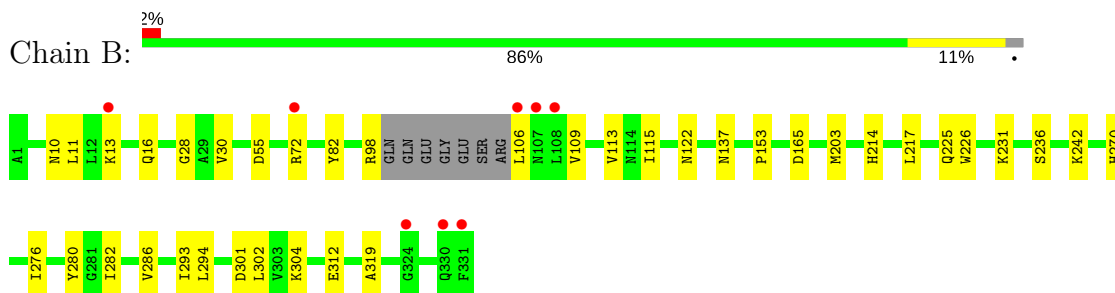
### 3 Residue-property plots [i](#)

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

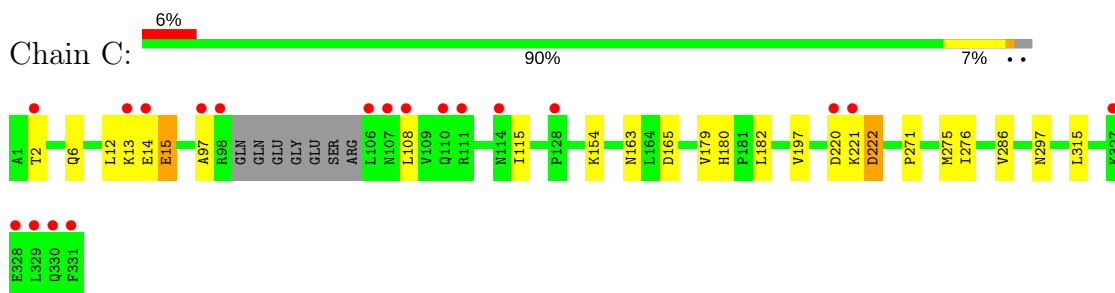
- Molecule 1: L-lactate dehydrogenase A chain



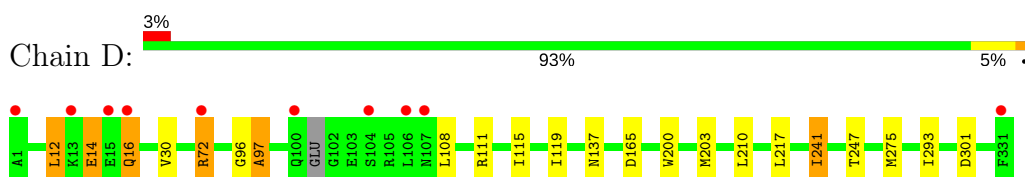
- Molecule 1: L-lactate dehydrogenase A chain



- Molecule 1: L-lactate dehydrogenase A chain



- Molecule 1: L-lactate dehydrogenase A chain





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.62Å 81.23Å 104.80Å 90.00° 97.56° 90.00°	Depositor
Resolution (Å)	37.80 – 2.05 37.83 – 2.05	Depositor EDS
% Data completeness (in resolution range)	98.0 (37.80-2.05) 98.1 (37.83-2.05)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.71 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.174 , 0.221 0.178 , 0.222	Depositor DCC
$R_{free}$ test set	1571 reflections (2.10%)	DCC
Wilson B-factor (Å <sup>2</sup> )	32.7	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 36.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	11112	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% 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, 0.333 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: NAI, TXD, EPE, SO4, 6EY

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	0/2611	0.62	1/3529 (0.0%)
1	B	0.39	0/2585	0.58	1/3495 (0.0%)
1	C	0.37	0/2571	0.56	0/3476
1	D	0.38	0/2635	0.56	0/3560
All	All	0.39	0/10402	0.58	2/14060 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	105	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	B	302	LEU	CA-CB-CG	5.75	128.53	115.30

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	2556	0	2656	32	0
1	B	2532	0	2639	29	0
1	C	2522	0	2623	18	0
1	D	2580	0	2687	16	0
2	A	15	0	17	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	15	0	17	1	0
2	C	15	0	18	0	0
3	A	44	0	27	6	0
3	B	44	0	27	6	0
3	D	44	0	27	2	0
4	A	28	0	0	2	0
4	B	28	0	0	2	0
4	C	28	0	0	0	0
4	D	28	0	0	0	0
5	A	5	0	0	0	0
5	B	5	0	0	0	0
5	C	5	0	0	0	0
5	D	5	0	0	0	0
6	C	44	0	26	1	0
7	A	158	0	0	2	0
7	B	159	0	0	5	0
7	C	98	0	0	1	0
7	D	154	0	0	0	0
All	All	11112	0	10764	87	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (87) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:ARG:HG2	1:A:105:ARG:HH11	1.23	0.97
1:A:20:ASN:OD1	7:A:501:HOH:O	2.01	0.78
1:B:98:ARG:HG3	4:B:403:6EY:C24	2.16	0.76
1:B:276:ILE:HD11	1:B:286:VAL:HG23	1.66	0.76
1:A:14:GLU:HB3	1:A:15:GLU:HB2	1.69	0.74
1:B:203:MET:HB2	7:B:654:HOH:O	1.91	0.70
1:B:30:VAL:HG21	3:B:402:TXD:H6N1	1.71	0.70
1:A:105:ARG:HG2	1:A:105:ARG:NH1	1.93	0.69
1:B:203:MET:SD	7:B:654:HOH:O	2.52	0.67
1:A:247:THR:HG23	3:A:402:TXD:H5N	1.78	0.66
1:A:293:ILE:CD1	1:C:179:VAL:HG22	2.25	0.65
1:B:10:ASN:OD1	1:B:13:LYS:HG2	1.97	0.64
1:A:99:GLN:HG2	1:A:108:LEU:HD22	1.82	0.62
1:B:72[A]:ARG:NH1	7:B:502:HOH:O	2.32	0.61
1:A:247:THR:CG2	3:A:402:TXD:H5N	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:96:GLY:O	1:D:111:ARG:NH1	2.36	0.59
1:A:3:LEU:HD13	1:B:214:HIS:HB2	1.84	0.59
1:D:203[A]:MET:HE2	1:D:217:LEU:HD21	1.86	0.58
1:D:203[A]:MET:HG2	1:D:210:LEU:HD22	1.85	0.58
1:B:137:ASN:ND2	3:B:402:TXD:H2N1	2.18	0.58
1:A:105:ARG:HG3	1:A:106:LEU:N	2.19	0.57
1:C:13:LYS:O	1:C:15:GLU:N	2.37	0.57
4:A:403:6EY:O26	7:A:502:HOH:O	2.17	0.56
1:B:98:ARG:CG	4:B:403:6EY:C24	2.84	0.56
1:B:276:ILE:HD13	1:B:282:ILE:HD13	1.87	0.56
1:B:225:GLN:NE2	7:B:503:HOH:O	2.38	0.56
1:C:276:ILE:HD11	1:C:286:VAL:HG23	1.88	0.56
1:A:293:ILE:HD12	1:C:179:VAL:HG22	1.87	0.55
1:A:105:ARG:CG	1:A:105:ARG:HH11	2.08	0.55
1:A:14:GLU:HB3	1:A:15:GLU:CB	2.35	0.55
1:A:204:ASN:HA	1:A:210:LEU:HD13	1.90	0.54
1:A:30:VAL:HG21	3:A:402:TXD:H6N1	1.89	0.54
1:D:30:VAL:HG21	3:D:801:TXD:H6N1	1.89	0.53
1:C:154[B]:LYS:HE2	1:C:275:MET:SD	2.49	0.52
1:C:182:LEU:HD11	1:D:72[B]:ARG:NH2	2.24	0.52
1:D:203[A]:MET:CE	1:D:217:LEU:HD21	2.40	0.52
1:D:115:ILE:HG22	1:D:119:ILE:HD12	1.93	0.51
1:D:200:TRP:CE3	1:D:203[B]:MET:SD	3.04	0.51
1:A:104:SER:O	1:A:105:ARG:HB3	2.11	0.50
1:A:293:ILE:HG13	1:A:301:ASP:HB2	1.93	0.50
1:A:104:SER:HB2	1:A:107:ASN:HB2	1.92	0.50
1:A:97:ALA:HA	3:A:402:TXD:O2P	2.12	0.50
1:C:115:ILE:HG23	6:C:402:NAI:N6A	2.27	0.49
1:A:96:GLY:O	1:A:97:ALA:CB	2.61	0.49
1:A:96:GLY:O	1:A:97:ALA:HB3	2.13	0.49
1:B:153:PRO:HA	2:B:401:EPE:H92	1.96	0.48
1:A:115:ILE:HG23	3:A:402:TXD:N6A	2.29	0.48
1:D:97:ALA:HB3	1:D:111:ARG:HH12	1.80	0.47
1:D:293[A]:ILE:HD12	1:D:301:ASP:HB2	1.96	0.47
1:A:82:TYR:CG	1:A:122:ASN:HB3	2.49	0.47
1:A:203:MET:HG2	1:A:210:LEU:HD22	1.96	0.47
1:D:137:ASN:ND2	3:D:801:TXD:H2N1	2.29	0.47
1:C:182:LEU:HD11	1:D:72[B]:ARG:CZ	2.46	0.46
1:C:197:VAL:HG21	1:C:315:LEU:HD23	1.96	0.46
1:B:109:VAL:O	1:B:113:VAL:HG23	2.15	0.46
1:D:12:LEU:HD22	1:D:14:GLU:HG2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:154[B]:LYS:HE3	7:C:515:HOH:O	2.15	0.46
1:B:293:ILE:HD12	1:B:301:ASP:HB2	1.98	0.46
1:B:270:HIS:CD2	1:B:294:LEU:HD12	2.52	0.45
1:B:98:ARG:NH2	3:B:402:TXD:O1P	2.49	0.45
1:D:108:LEU:HD12	1:D:111:ARG:HH21	1.82	0.45
1:D:241:ILE:CD1	1:D:247:THR:HG23	2.47	0.45
1:A:98:ARG:O	1:A:99:GLN:C	2.54	0.45
1:B:16:GLN:HE21	1:C:297:ASN:HD22	1.65	0.44
1:B:115:ILE:HG23	3:B:402:TXD:N6A	2.33	0.44
1:A:98:ARG:HG2	4:A:403:6EY:O26	2.17	0.44
1:A:137:ASN:ND2	3:A:402:TXD:H2N1	2.33	0.43
1:B:82:TYR:CG	1:B:122:ASN:HB3	2.53	0.43
1:A:14:GLU:HB3	1:A:15:GLU:CA	2.48	0.43
1:B:231:LYS:HA	1:B:231:LYS:HD3	1.89	0.43
1:D:203[A]:MET:HE1	1:D:217:LEU:HD11	2.01	0.43
1:B:137:ASN:HD21	3:B:402:TXD:H2N1	1.81	0.43
1:A:123:VAL:HG11	1:A:132:LEU:HD21	2.01	0.42
1:A:276:ILE:HG22	1:A:286:VAL:HG23	2.01	0.42
1:B:242:LYS:NZ	7:B:509:HOH:O	2.52	0.42
1:B:28:GLY:HA3	3:B:402:TXD:O5'	2.19	0.42
1:B:280:TYR:HB3	1:B:312:GLU:HG3	2.00	0.42
1:C:221:LYS:O	1:C:222:ASP:C	2.58	0.42
1:C:163:ASN:HA	1:C:271:PRO:HG2	2.01	0.42
1:A:266:LEU:O	1:C:180:HIS:HB2	2.20	0.41
1:A:105:ARG:O	1:A:109:VAL:N	2.48	0.41
1:B:304:LYS:HE3	1:C:6:GLN:O	2.21	0.41
1:B:217:LEU:HD12	1:B:226:TRP:HB2	2.03	0.41
1:B:286:VAL:HG21	1:B:319:ALA:HB1	2.03	0.41
1:C:2:THR:O	1:C:6:GLN:HG3	2.21	0.41
1:C:12:LEU:HD12	1:C:12:LEU:O	2.20	0.40
1:B:11:LEU:HD23	1:C:154[A]:LYS:HG3	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	327/331 (99%)	315 (96%)	9 (3%)	3 (1%)	20	10
1	B	323/331 (98%)	317 (98%)	6 (2%)	0	100	100
1	C	322/331 (97%)	312 (97%)	7 (2%)	3 (1%)	20	10
1	D	330/331 (100%)	322 (98%)	6 (2%)	2 (1%)	28	17
All	All	1302/1324 (98%)	1266 (97%)	28 (2%)	8 (1%)	28	17

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	105	ARG
1	C	14	GLU
1	A	97	ALA
1	D	97	ALA
1	C	222	ASP
1	C	97	ALA
1	D	16	GLN
1	A	27	VAL

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	288/287 (100%)	281 (98%)	7 (2%)	54	48
1	B	284/287 (99%)	280 (99%)	4 (1%)	71	70
1	C	283/287 (99%)	279 (99%)	4 (1%)	71	70
1	D	290/287 (101%)	282 (97%)	8 (3%)	49	42
All	All	1145/1148 (100%)	1122 (98%)	23 (2%)	62	56

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

Mol	Chain	Res	Type
1	A	14	GLU
1	A	55[A]	ASP
1	A	55[B]	ASP
1	A	105	ARG
1	A	107	ASN
1	A	234	VAL
1	A	236	SER
1	B	55	ASP
1	B	106	LEU
1	B	165	ASP
1	B	236	SER
1	C	15	GLU
1	C	108	LEU
1	C	165	ASP
1	C	220	ASP
1	D	12	LEU
1	D	14	GLU
1	D	16	GLN
1	D	72[A]	ARG
1	D	72[B]	ARG
1	D	165	ASP
1	D	241	ILE
1	D	275	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	16	GLN
1	D	330	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

15 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	EPE	A	401	-	15,15,15	1.72	1 (6%)	18,20,20	6.28	9 (50%)
3	TXD	A	402	-	43,48,48	2.16	10 (23%)	44,73,73	2.78	12 (27%)
4	6EY	A	403	-	27,31,31	1.26	2 (7%)	29,45,45	1.79	4 (13%)
5	SO4	A	404	-	4,4,4	0.23	0	6,6,6	0.10	0
2	EPE	B	401	-	15,15,15	1.58	1 (6%)	18,20,20	6.36	12 (66%)
3	TXD	B	402	-	43,48,48	2.36	13 (30%)	44,73,73	2.68	9 (20%)
4	6EY	B	403	-	27,31,31	1.41	2 (7%)	29,45,45	2.28	4 (13%)
5	SO4	B	404	-	4,4,4	0.30	0	6,6,6	0.12	0
2	EPE	C	401	-	15,15,15	1.65	1 (6%)	18,20,20	6.86	9 (50%)
6	NAI	C	402	-	40,48,48	2.35	12 (30%)	41,73,73	2.55	7 (17%)
4	6EY	C	403	-	27,31,31	1.37	2 (7%)	29,45,45	1.77	2 (6%)
5	SO4	C	404	-	4,4,4	0.40	0	6,6,6	0.30	0
3	TXD	D	801	-	43,48,48	2.30	12 (27%)	44,73,73	2.72	11 (25%)
4	6EY	D	802	-	27,31,31	1.34	2 (7%)	29,45,45	1.83	4 (13%)
5	SO4	D	803	-	4,4,4	0.37	0	6,6,6	0.20	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	EPE	A	401	-	-	0/9/19/19	0/1/1/1
3	TXD	A	402	-	-	0/26/72/72	0/5/5/5
4	6EY	A	403	-	-	0/10/34/34	0/4/4/4
5	SO4	A	404	-	-	0/0/0/0	0/0/0/0
2	EPE	B	401	-	-	0/9/19/19	0/1/1/1
3	TXD	B	402	-	-	0/26/72/72	0/5/5/5
4	6EY	B	403	-	-	0/10/34/34	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SO4	B	404	-	-	0/0/0/0	0/0/0/0
2	EPE	C	401	-	-	0/9/19/19	0/1/1/1
6	NAI	C	402	-	-	0/25/72/72	0/5/5/5
4	6EY	C	403	-	-	0/10/34/34	0/4/4/4
5	SO4	C	404	-	-	0/0/0/0	0/0/0/0
3	TXD	D	801	-	-	0/26/72/72	0/5/5/5
4	6EY	D	802	-	-	0/10/34/34	0/4/4/4
5	SO4	D	803	-	-	0/0/0/0	0/0/0/0

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	EPE	C10-S	-6.05	1.68	1.77
3	B	402	TXD	C2N-C3N	-5.99	1.47	1.53
2	C	401	EPE	C10-S	-5.65	1.69	1.77
2	B	401	EPE	C10-S	-5.43	1.69	1.77
3	A	402	TXD	C2N-C3N	-4.83	1.48	1.53
4	D	802	6EY	C17-C16	-4.78	1.34	1.37
3	D	801	TXD	C2'-C3'	-4.77	1.40	1.53
3	B	402	TXD	C2'-C3'	-4.62	1.41	1.53
3	A	402	TXD	C2'-C3'	-4.60	1.41	1.53
3	D	801	TXD	C2N-C3N	-4.44	1.48	1.53
6	C	402	NAI	C2B-C3B	-4.32	1.42	1.53
3	D	801	TXD	C2N-N1N	-4.25	1.40	1.47
3	B	402	TXD	C2N-N1N	-4.25	1.40	1.47
4	B	403	6EY	C17-C16	-4.22	1.34	1.37
4	C	403	6EY	C17-C16	-3.98	1.34	1.37
3	D	801	TXD	O2'A-C2'A	-3.92	1.33	1.43
4	A	403	6EY	C17-C16	-3.59	1.34	1.37
6	C	402	NAI	O2D-C2D	-3.48	1.34	1.43
3	A	402	TXD	C2N-N1N	-3.46	1.41	1.47
3	B	402	TXD	O2'A-C2'A	-3.44	1.35	1.43
6	C	402	NAI	C5D-C4D	-2.80	1.42	1.51
3	A	402	TXD	O2'A-C2'A	-2.79	1.36	1.43
3	A	402	TXD	C5'A-C4'A	-2.78	1.42	1.51
3	D	801	TXD	C3N-C7N	-2.74	1.49	1.53
3	D	801	TXD	C5'A-C4'A	-2.68	1.43	1.51
3	D	801	TXD	C3'A-C2'A	-2.51	1.46	1.53
3	B	402	TXD	C3N-C7N	-2.50	1.50	1.53
3	B	402	TXD	C5'A-C4'A	-2.35	1.44	1.51
6	C	402	NAI	O3D-C3D	-2.32	1.37	1.43
6	C	402	NAI	C2D-C3D	-2.24	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	TXD	C2'-C1'	-2.21	1.50	1.53
3	A	402	TXD	C3'A-C2'A	-2.14	1.47	1.53
3	D	801	TXD	C2'-C1'	-2.14	1.50	1.53
6	C	402	NAI	C2B-C1B	-2.12	1.50	1.53
3	D	801	TXD	O2'-C2'	-2.08	1.38	1.43
3	B	402	TXD	C3'A-C2'A	-2.07	1.48	1.53
3	A	402	TXD	C3N-C7N	-2.06	1.50	1.53
6	C	402	NAI	O4B-C4B	-2.04	1.40	1.45
3	B	402	TXD	C5'-C4'	-2.04	1.45	1.51
3	B	402	TXD	C1'A-N1N	2.06	1.48	1.41
6	C	402	NAI	C6N-N1N	2.52	1.44	1.37
3	A	402	TXD	C6A-N6A	2.62	1.44	1.34
3	D	801	TXD	C6A-N6A	2.65	1.44	1.34
6	C	402	NAI	C6A-N6A	2.82	1.45	1.34
3	B	402	TXD	C6A-N6A	2.82	1.45	1.34
6	C	402	NAI	C7N-N7N	3.62	1.43	1.33
4	D	802	6EY	C17-S18	3.62	1.75	1.70
4	A	403	6EY	C17-S18	4.53	1.76	1.70
6	C	402	NAI	C2N-C3N	4.84	1.48	1.34
4	C	403	6EY	C17-S18	4.88	1.77	1.70
3	A	402	TXD	C7N-N7N	5.06	1.42	1.32
4	B	403	6EY	C17-S18	5.18	1.77	1.70
3	B	402	TXD	C7N-N7N	5.56	1.43	1.32
3	D	801	TXD	C7N-N7N	5.59	1.43	1.32
3	D	801	TXD	C4N-C5N	6.79	1.50	1.32
3	A	402	TXD	C4N-C5N	6.79	1.50	1.32
3	B	402	TXD	C4N-C5N	6.93	1.50	1.32
6	C	402	NAI	C6N-C5N	9.15	1.50	1.33

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	EPE	O1S-S-C10	-19.77	89.81	106.79
2	C	401	EPE	O2S-S-C10	-19.51	90.04	106.79
2	A	401	EPE	O1S-S-C10	-17.52	91.75	106.79
2	C	401	EPE	O3S-S-C10	-13.97	88.87	106.06
2	C	401	EPE	O1S-S-C10	-13.57	95.13	106.79
2	A	401	EPE	O2S-S-C10	-13.01	95.62	106.79
2	A	401	EPE	O3S-S-C10	-11.12	92.38	106.06
2	B	401	EPE	O2S-S-C10	-10.86	97.46	106.79
3	A	402	TXD	N3A-C2A-N1A	-8.59	121.38	128.86
6	C	402	NAI	N3A-C2A-N1A	-8.19	121.73	128.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	EPE	O3S-S-C10	-8.12	96.07	106.06
3	B	402	TXD	N3A-C2A-N1A	-7.54	122.29	128.86
3	B	402	TXD	C3N-C4N-C5N	-7.48	112.54	123.15
3	D	801	TXD	N3A-C2A-N1A	-7.34	122.47	128.86
6	C	402	NAI	C1D-N1N-C6N	-7.09	105.38	120.77
3	D	801	TXD	C3N-C4N-C5N	-7.00	113.22	123.15
3	A	402	TXD	C3N-C4N-C5N	-6.94	113.31	123.15
3	D	801	TXD	C4'-O4'-C1'	-5.76	103.64	109.77
4	D	802	6EY	C16-C17-S18	-5.37	108.83	112.29
3	B	402	TXD	C4'-O4'-C1'	-5.24	104.19	109.77
4	B	403	6EY	C16-C17-S18	-4.93	109.11	112.29
3	A	402	TXD	C4'-O4'-C1'	-4.90	104.56	109.77
2	A	401	EPE	C6-C5-N4	-4.81	100.90	110.63
4	A	403	6EY	C16-C17-S18	-3.96	109.74	112.29
6	C	402	NAI	C4B-O4B-C1B	-3.93	105.59	109.77
4	C	403	6EY	C16-C17-S18	-3.53	110.01	112.29
3	D	801	TXD	C4A-C5A-N7A	-2.97	106.54	109.41
6	C	402	NAI	C4D-O4D-C1D	-2.92	102.97	109.47
2	C	401	EPE	C2-C3-N4	-2.88	104.81	110.63
3	A	402	TXD	C4'A-O4'A-C1'A	-2.88	103.05	109.47
3	D	801	TXD	C4'A-O4'A-C1'A	-2.75	103.35	109.47
3	A	402	TXD	O7N-C7N-N7N	-2.72	118.90	123.06
4	B	403	6EY	C24-C25-C27	-2.49	117.44	120.20
6	C	402	NAI	C4A-C5A-N7A	-2.30	107.19	109.41
3	B	402	TXD	C4'A-O4'A-C1'A	-2.20	104.56	109.47
3	A	402	TXD	C4A-C5A-N7A	-2.18	107.30	109.41
3	A	402	TXD	C3'A-C2'A-C1'A	-2.05	97.50	101.43
4	A	403	6EY	C6-S5-C4	2.06	105.48	102.68
3	D	801	TXD	O5'-C5'-C4'	2.21	116.84	109.00
4	B	403	6EY	C3-C15-N14	2.22	110.80	108.11
3	B	402	TXD	O5'A-C5'A-C4'A	2.28	117.08	109.00
4	D	802	6EY	C3-C15-N14	2.42	111.04	108.11
3	D	801	TXD	C3N-C7N-N7N	2.48	119.52	117.03
2	B	401	EPE	O3S-S-O2S	2.56	117.23	111.37
2	C	401	EPE	C7-N4-C3	2.59	117.90	111.26
2	B	401	EPE	O2S-S-O1S	2.62	122.94	113.86
3	A	402	TXD	C3N-C7N-N7N	2.66	119.70	117.03
2	B	401	EPE	O3S-S-O1S	2.92	118.07	111.37
3	A	402	TXD	C5N-C6N-N1N	3.03	117.96	110.91
2	C	401	EPE	C5-C6-N1	3.20	117.11	110.63
2	A	401	EPE	C3-C2-N1	3.26	117.23	110.63
4	A	403	6EY	C3-C15-N14	3.28	112.08	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	802	6EY	C6-S5-C4	3.28	107.13	102.68
2	A	401	EPE	C7-N4-C5	3.40	119.98	111.26
2	C	401	EPE	O3S-S-O1S	3.42	119.22	111.37
2	A	401	EPE	O3S-S-O2S	3.60	119.61	111.37
3	D	801	TXD	C5N-C6N-N1N	3.64	119.38	110.91
3	B	402	TXD	C5N-C6N-N1N	3.68	119.49	110.91
3	D	801	TXD	C4N-C3N-C7N	3.81	120.64	110.08
2	C	401	EPE	O3S-S-O2S	3.93	120.38	111.37
2	B	401	EPE	C3-C2-N1	4.07	118.86	110.63
3	A	402	TXD	C4N-C3N-C7N	4.22	121.77	110.08
2	B	401	EPE	C5-N4-C3	4.32	118.66	108.87
2	B	401	EPE	C2-C3-N4	4.50	119.74	110.63
2	A	401	EPE	O3S-S-O1S	4.65	122.02	111.37
2	B	401	EPE	C5-C6-N1	4.66	120.06	110.63
2	B	401	EPE	C6-N1-C2	4.68	119.47	108.87
2	B	401	EPE	C6-C5-N4	4.71	120.16	110.63
3	B	402	TXD	C2N-C3N-C4N	4.73	115.52	108.68
2	C	401	EPE	C6-N1-C2	4.93	120.04	108.87
2	A	401	EPE	C6-N1-C2	5.03	120.26	108.87
6	C	402	NAI	O4D-C1D-N1N	5.11	118.37	108.07
3	B	402	TXD	C4N-C3N-C7N	5.12	124.25	110.08
4	D	802	6EY	C15-N14-C13	5.72	120.43	117.24
3	A	402	TXD	C2N-C3N-C4N	6.33	117.84	108.68
3	D	801	TXD	C2N-C3N-C4N	6.52	118.11	108.68
4	A	403	6EY	C15-N14-C13	6.77	121.02	117.24
4	C	403	6EY	C15-N14-C13	8.03	121.73	117.24
6	C	402	NAI	C1D-N1N-C2N	8.38	135.30	121.09
3	D	801	TXD	C2N-N1N-C1'A	8.63	136.03	115.26
3	A	402	TXD	C2N-N1N-C1'A	8.74	136.29	115.26
3	B	402	TXD	C2N-N1N-C1'A	9.05	137.03	115.26
4	B	403	6EY	C15-N14-C13	9.82	122.73	117.24

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	TXD	6	0
4	A	403	6EY	2	0
2	B	401	EPE	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	402	TXD	6	0
4	B	403	6EY	2	0
6	C	402	NAI	1	0
3	D	801	TXD	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	327/331 (98%)	-0.28	2 (0%) 89 91	18, 30, 59, 88	0
1	B	324/331 (97%)	-0.27	8 (2%) 58 63	19, 30, 60, 108	0
1	C	324/331 (97%)	0.04	19 (5%) 23 25	21, 38, 83, 135	0
1	D	330/331 (99%)	-0.32	10 (3%) 51 56	20, 30, 68, 119	0
All	All	1305/1324 (98%)	-0.21	39 (2%) 51 56	18, 32, 71, 135	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	97	ALA	7.4
1	B	108	LEU	4.9
1	C	14	GLU	4.7
1	D	15	GLU	4.3
1	D	1	ALA	4.2
1	C	329	LEU	3.7
1	D	100	GLN	3.5
1	D	107	ASN	3.2
1	C	107	ASN	3.1
1	D	104	SER	3.1
1	C	330	GLN	3.1
1	D	331	PHE	3.0
1	A	97	ALA	3.0
1	D	13	LYS	2.9
1	B	13	LYS	2.9
1	C	2	THR	2.9
1	C	110	GLN	2.8
1	A	105	ARG	2.8
1	C	13	LYS	2.8
1	D	106	LEU	2.8
1	B	106	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	327	LYS	2.6
1	C	108	LEU	2.6
1	C	331	PHE	2.5
1	B	330	GLN	2.5
1	B	72[A]	ARG	2.5
1	B	107	ASN	2.5
1	C	328	GLU	2.3
1	C	221	LYS	2.3
1	B	331	PHE	2.3
1	C	106	LEU	2.3
1	C	128	PRO	2.3
1	C	111	ARG	2.3
1	C	98	ARG	2.2
1	B	324	GLY	2.2
1	D	16	GLN	2.1
1	C	114	ASN	2.0
1	D	72[A]	ARG	2.0
1	C	220	ASP	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	EPE	A	401	15/15	0.84	0.19	5.47	34,57,65,67	15
4	6EY	B	403	28/28	0.91	0.17	4.52	34,57,72,83	0
2	EPE	C	401	15/15	0.77	0.21	4.47	49,76,92,95	15

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	EPE	B	401	15/15	0.93	0.14	3.02	43,57,81,94	15
5	SO4	A	404	5/5	0.99	0.18	2.26	23,24,29,35	4
5	SO4	D	803	5/5	0.99	0.16	2.03	21,23,26,32	4
5	SO4	B	404	5/5	0.99	0.17	1.82	20,24,26,32	4
5	SO4	C	404	5/5	0.99	0.15	1.43	24,24,31,36	4
4	6EY	D	802	28/28	0.95	0.12	0.18	31,38,59,71	0
4	6EY	A	403	28/28	0.94	0.11	0.11	26,37,47,57	0
3	TXD	B	402	44/44	0.96	0.10	0.08	24,34,40,45	0
4	6EY	C	403	28/28	0.94	0.13	-0.04	26,51,71,84	0
6	NAI	C	402	44/44	0.92	0.14	-0.04	34,50,60,68	0
3	TXD	D	801	44/44	0.96	0.09	-0.20	22,34,40,53	0
3	TXD	A	402	44/44	0.97	0.08	-0.76	21,30,38,44	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.