



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:59 PM GMT

PDB ID : 4K4V  
Title : Poliovirus polymerase elongation complex (r5+1\_form)  
Authors : Gong, P.; Peersen, O.B.  
Deposited on : 2013-04-12  
Resolution : 2.63 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

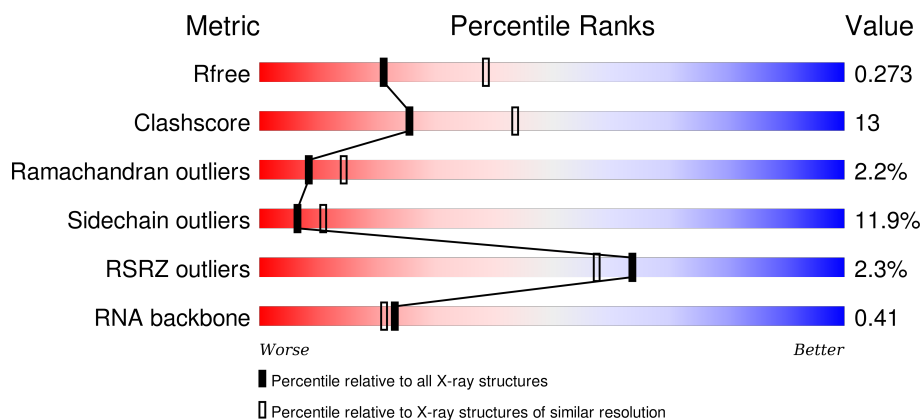
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.63 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.




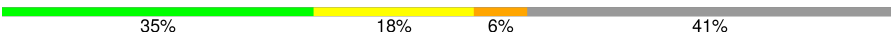
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3377 (2.68-2.60)
Clashscore	102246	3781 (2.68-2.60)
Ramachandran outliers	100387	3722 (2.68-2.60)
Sidechain outliers	100360	3722 (2.68-2.60)
RSRZ outliers	91569	3388 (2.68-2.60)
RNA backbone	2183	1002 (3.06-2.22)

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	471	<div> <div>2%</div> <div>64%</div> <div>30%</div> <div>• •</div> </div>
1	E	471	<div> <div>2%</div> <div>63%</div> <div>30%</div> <div>• • •</div> </div>
2	B	26	<div> <div>•</div> <div>35%</div> <div>12%</div> <div>50%</div> </div>
2	F	26	<div> <div>4%</div> <div>15%</div> <div>31%</div> <div>•</div> <div>50%</div> </div>

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Mol	Chain	Length	Quality of chain
3	C	17	
3	G	17	

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
4	SO4	E	501	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8440 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 RNA-directed RNA polymerase 3D-POL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	462	Total	C	N	O	S	0	0	0
			3703	2374	611	696	22			
1	E	462	Total	C	N	O	S	0	0	0
			3703	2374	611	696	22			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	290	MET	CYS	ENGINEERED MUTATION	UNP P03300
A	446	ASP	LEU	ENGINEERED MUTATION	UNP P03300
A	462	GLY	-	EXPRESSION TAG	UNP P03300
A	463	SER	-	EXPRESSION TAG	UNP P03300
A	464	SER	-	EXPRESSION TAG	UNP P03300
A	465	SER	-	EXPRESSION TAG	UNP P03300
A	466	HIS	-	EXPRESSION TAG	UNP P03300
A	467	HIS	-	EXPRESSION TAG	UNP P03300
A	468	HIS	-	EXPRESSION TAG	UNP P03300
A	469	HIS	-	EXPRESSION TAG	UNP P03300
A	470	HIS	-	EXPRESSION TAG	UNP P03300
A	471	HIS	-	EXPRESSION TAG	UNP P03300
E	290	MET	CYS	ENGINEERED MUTATION	UNP P03300
E	446	ASP	LEU	ENGINEERED MUTATION	UNP P03300
E	462	GLY	-	EXPRESSION TAG	UNP P03300
E	463	SER	-	EXPRESSION TAG	UNP P03300
E	464	SER	-	EXPRESSION TAG	UNP P03300
E	465	SER	-	EXPRESSION TAG	UNP P03300
E	466	HIS	-	EXPRESSION TAG	UNP P03300
E	467	HIS	-	EXPRESSION TAG	UNP P03300
E	468	HIS	-	EXPRESSION TAG	UNP P03300
E	469	HIS	-	EXPRESSION TAG	UNP P03300
E	470	HIS	-	EXPRESSION TAG	UNP P03300
E	471	HIS	-	EXPRESSION TAG	UNP P03300

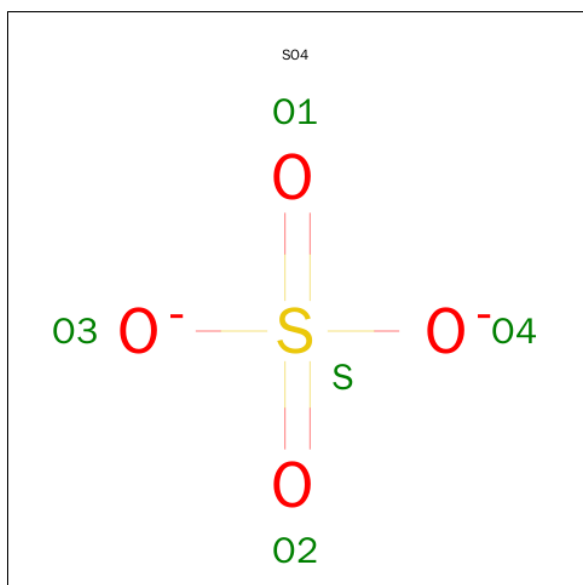
- Molecule 2 is a RNA chain called RNA (5'-R(\*AP\*AP\*GP\*UP\*CP\*UP\*CP\*CP\*AP\*GP\*GP\*UP\*CP\*UP\*CP\*UP\*CP\*UP\*CP\*GP\*UP\*CP\*GP\*AP\*AP\*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	13	Total	C	N	O	P	0	0	0
			271	121	42	95	13			
2	F	13	Total	C	N	O	P	0	0	0
			271	121	42	95	13			

- Molecule 3 is DNA/RNA hybrid called DNA/RNA (5'-R(\*UP\*GP\*UP\*UP\*CP\*GP\*AP\*CP\*GP\*AP\*GP\*AP\*GP\*AP\*GP\*A)-D(P\*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	10	Total	C	N	O	P	0	0	0
			219	98	46	65	10			
3	G	10	Total	C	N	O	P	0	0	0
			219	98	46	65	10			

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	E	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		

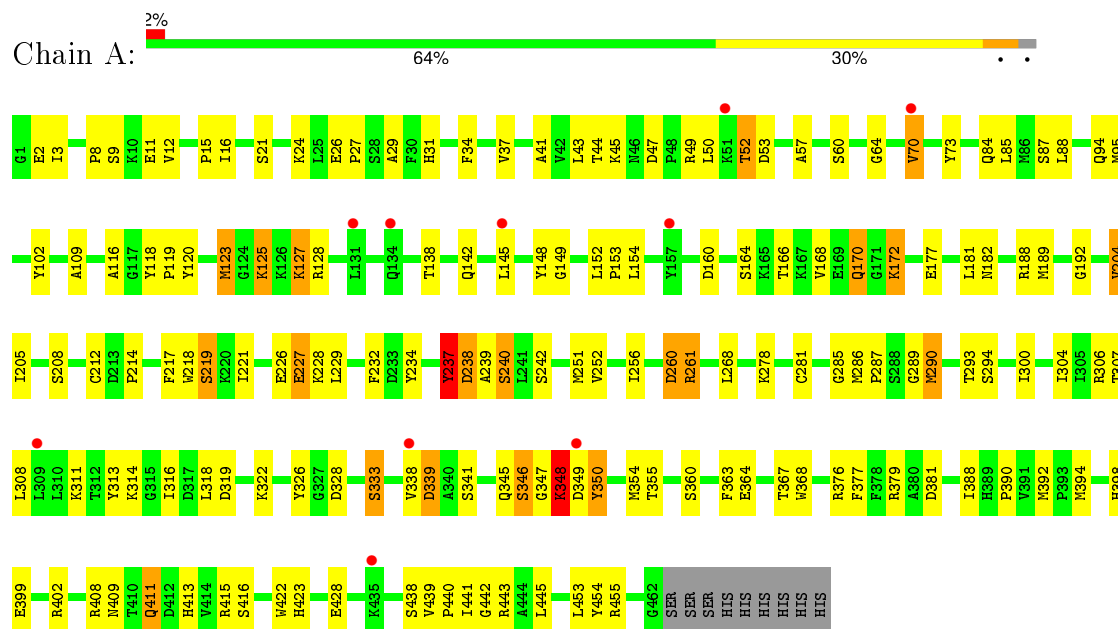
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	30	Total 30	O 30	0	0
5	B	3	Total 3	O 3	0	0
5	C	4	Total 4	O 4	0	0
5	E	6	Total 6	O 6	0	0
5	G	1	Total 1	O 1	0	0

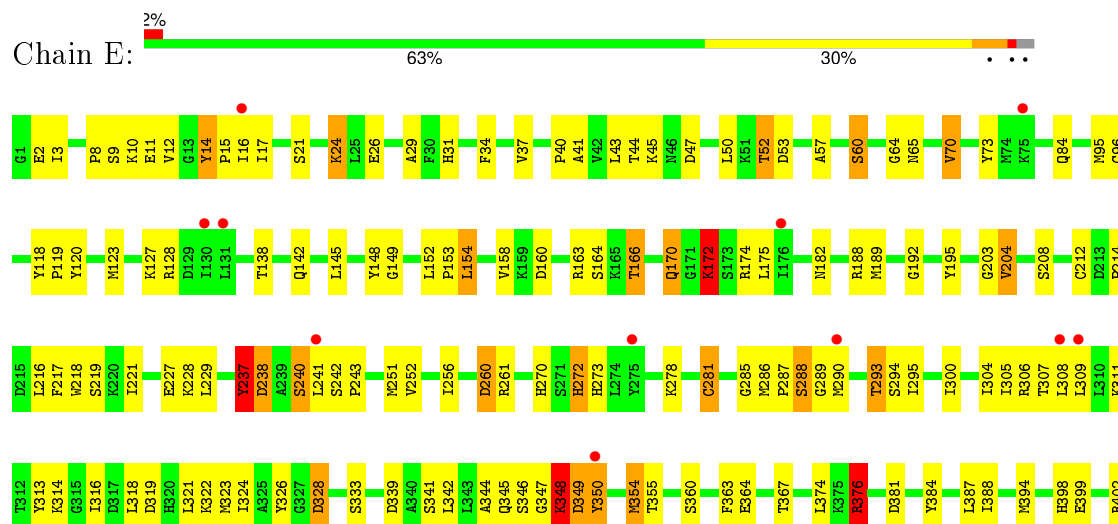
### 3 Residue-property plots

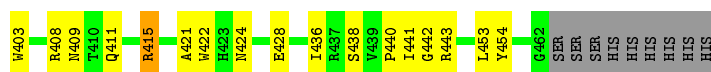
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: RNA-directed RNA polymerase 3D-POL



#### • Molecule 1: RNA-directed RNA polymerase 3D-POL





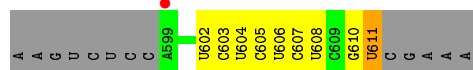
- Molecule 2: RNA (5'-R(\*AP\*AP\*GP\*UP\*CP\*UP\*CP\*CP\*AP\*GP\*GP\*UP\*CP\*UP\*CP\*UP\*CP\*UP\*CP\*GP\*UP\*CP\*GP\*AP\*AP\*A)-3')

Chain B: . 35% 12% 50%



- Molecule 2: RNA (5'-R(\*AP\*AP\*GP\*UP\*CP\*UP\*CP\*CP\*AP\*GP\*GP\*UP\*CP\*UP\*CP\*UP\*CP\*UP\*CP\*GP\*UP\*CP\*GP\*AP\*AP\*A)-3')

Chain F: 4% 15% 31% 50%



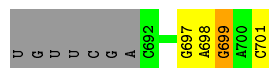
- Molecule 3: DNA/RNA (5'-R(\*UP\*GP\*UP\*UP\*CP\*GP\*AP\*CP\*GP\*AP\*GP\*AP\*GP\*AP\*GP\*AP\*GP\*P\*A)-D(P\*C)-3')

Chain C: 24% 35% 41%



- Molecule 3: DNA/RNA (5'-R(\*UP\*GP\*UP\*UP\*CP\*GP\*AP\*CP\*GP\*AP\*GP\*AP\*GP\*AP\*GP\*AP\*GP\*P\*A)-D(P\*C)-3')

Chain G: 35% 18% 6% 41%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.52Å 63.48Å 101.95Å 73.48° 73.44° 73.64°	Depositor
Resolution (Å)	47.51 – 2.63 47.51 – 2.63	Depositor EDS
% Data completeness (in resolution range)	97.9 (47.51-2.63) 90.7 (47.51-2.63)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.79 (at 2.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.233 , 0.273 0.231 , 0.273	Depositor DCC
$R_{free}$ test set	2116 reflections (5.10%)	DCC
Wilson B-factor (Å <sup>2</sup> )	81.1	Xtriage
Anisotropy	0.348	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 64.8	EDS
Estimated twinning fraction	0.436 for -k,-h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.53$ , $\langle L^2 \rangle = 0.37$	Xtriage
Outliers	0 of 41542 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8440	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.70% 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: SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.50	0/3793	0.65	0/5129
1	E	0.51	0/3793	0.65	1/5129 (0.0%)
2	B	0.70	0/300	1.26	3/464 (0.6%)
2	F	0.68	0/300	1.06	0/464
3	C	0.84	0/246	1.23	1/382 (0.3%)
3	G	0.73	0/246	1.18	1/382 (0.3%)
All	All	0.54	0/8678	0.75	6/11950 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	697	G	N3-C4-C5	-6.46	125.37	128.60
2	B	602	U	N3-C2-O2	5.98	126.39	122.20
1	E	376	ARG	NE-CZ-NH1	-5.79	117.41	120.30
2	B	602	U	N1-C2-O2	-5.75	118.78	122.80
3	C	697	G	OP2-P-O3'	5.05	116.31	105.20
2	B	604	U	C5-C6-N1	-5.03	120.18	122.70

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	3703	0	3666	97	2
1	E	3703	0	3666	95	2
2	B	271	0	139	8	0
2	F	271	0	139	5	0
3	C	219	0	111	5	0
3	G	219	0	111	2	0
4	E	10	0	0	2	0
5	A	30	0	0	10	0
5	B	3	0	0	0	0
5	C	4	0	0	0	0
5	E	6	0	0	1	0
5	G	1	0	0	0	0
All	All	8440	0	7832	203	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (203) 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:84:GLN:OE1	1:A:306:ARG:NH2	2.04	0.91
1:A:15:PRO:O	5:A:516:HOH:O	1.95	0.84
1:A:455:ARG:NH2	5:A:519:HOH:O	2.10	0.80
1:A:394:MET:HB3	1:A:398:HIS:HE1	1.48	0.76
1:E:142:GLN:HA	1:E:145:LEU:HD12	1.67	0.76
1:A:260:ASP:OD1	1:A:260:ASP:N	2.21	0.74
1:E:149:GLY:O	1:E:182:ASN:ND2	2.21	0.71
1:A:142:GLN:HA	1:A:145:LEU:HD12	1.72	0.71
1:E:84:GLN:OE1	1:E:306:ARG:NH2	2.23	0.71
1:E:394:MET:HB3	1:E:398:HIS:CE1	2.26	0.71
1:A:402:ARG:HB2	5:A:520:HOH:O	1.91	0.71
1:A:2:GLU:HB2	1:A:64:GLY:HA2	1.74	0.70
1:A:120:TYR:OH	1:A:182:ASN:OD1	2.10	0.70
1:A:394:MET:HB3	1:A:398:HIS:CE1	2.27	0.69
1:E:120:TYR:OH	1:E:182:ASN:OD1	2.10	0.69
1:A:149:GLY:O	1:A:182:ASN:ND2	2.24	0.68
1:A:52:THR:OG1	1:A:53:ASP:N	2.25	0.68
1:E:394:MET:HB3	1:E:398:HIS:HE1	1.57	0.68
1:E:237:TYR:HD2	1:E:328:ASP:HB3	1.60	0.67
1:E:52:THR:OG1	1:E:53:ASP:N	2.28	0.66
1:E:260:ASP:OD1	1:E:260:ASP:N	2.20	0.66
1:A:347:GLY:O	1:A:350:TYR:N	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:306:ARG:HG2	1:E:318:LEU:HD13	1.78	0.66
1:E:170:GLN:O	1:E:172:LYS:NZ	2.29	0.65
1:E:170:GLN:HG2	1:E:172:LYS:HE2	1.78	0.65
1:E:229:LEU:HD23	1:E:333:SER:HB3	1.77	0.64
1:A:306:ARG:HG2	1:A:318:LEU:HD13	1.80	0.64
1:E:342:LEU:O	1:E:345:GLN:HG2	1.97	0.63
1:E:349:ASP:N	1:E:349:ASP:OD1	2.30	0.63
1:E:339:ASP:OD2	1:E:341:SER:OG	2.12	0.62
1:A:226:GLU:HB2	1:A:333:SER:HB2	1.82	0.62
1:E:2:GLU:HB2	1:E:64:GLY:HA2	1.82	0.61
1:E:381:ASP:OD2	1:E:454:TYR:OH	2.17	0.61
1:E:237:TYR:CD2	1:E:328:ASP:HB3	2.36	0.61
1:A:229:LEU:HD23	1:A:333:SER:HB3	1.82	0.61
1:A:95:MET:N	1:A:189:MET:O	2.21	0.61
1:E:347:GLY:O	1:E:350:TYR:N	2.34	0.60
1:E:204:VAL:HG11	1:E:322:LYS:HB3	1.83	0.59
1:A:204:VAL:HG11	1:A:322:LYS:HB3	1.84	0.58
1:E:24:LYS:HG3	1:E:160:ASP:OD2	2.03	0.58
1:E:203:GLY:HA3	5:E:604:HOH:O	2.03	0.58
1:E:415:ARG:NH2	4:E:501:SO4:S	2.75	0.58
1:A:8:PRO:O	1:A:11:GLU:N	2.32	0.58
1:A:287:PRO:HG2	1:A:290:MET:HB2	1.86	0.58
1:E:219:SER:HG	1:E:388:ILE:H	1.51	0.57
1:A:170:GLN:O	1:A:172:LYS:NZ	2.35	0.57
1:A:339:ASP:HB3	5:A:514:HOH:O	2.03	0.57
1:A:308:LEU:HD22	1:A:346:SER:HB2	1.87	0.57
1:A:445:LEU:O	5:A:526:HOH:O	2.17	0.57
1:A:376:ARG:HD3	1:A:390:PRO:HB2	1.87	0.57
1:E:339:ASP:HB3	1:E:342:LEU:HD12	1.86	0.56
1:E:8:PRO:O	1:E:11:GLU:N	2.31	0.56
1:E:252:VAL:O	1:E:256:ILE:HG12	2.06	0.56
1:A:24:LYS:HG3	1:A:160:ASP:OD2	2.05	0.56
1:E:73:TYR:OH	1:E:314:LYS:HE3	2.05	0.56
2:F:606:U:H2'	2:F:607:C:C6	2.41	0.55
1:E:237:TYR:HE1	1:E:241:LEU:HD11	1.71	0.54
1:E:308:LEU:HD22	1:E:346:SER:HB2	1.88	0.54
1:A:286:MET:HG3	1:A:287:PRO:HD2	1.88	0.54
1:A:84:GLN:O	1:A:87:SER:OG	2.18	0.54
1:A:394:MET:C	1:A:398:HIS:HD1	2.10	0.54
1:E:237:TYR:CE2	1:E:328:ASP:HA	2.43	0.54
1:A:422:TRP:CD1	1:A:453:LEU:HD13	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:SER:HG	1:A:388:ILE:H	1.53	0.53
1:A:422:TRP:CZ2	1:A:423:HIS:CE1	2.97	0.53
1:E:421:ALA:O	1:E:424:ASN:ND2	2.31	0.52
1:A:268:LEU:O	5:A:511:HOH:O	2.19	0.52
1:E:95:MET:SD	1:E:192:GLY:HA3	2.50	0.52
1:A:85:LEU:HA	1:A:88:LEU:HD12	1.91	0.51
1:A:232:PHE:CD2	1:A:354:MET:HE3	2.45	0.51
1:E:95:MET:N	1:E:189:MET:O	2.27	0.51
1:A:347:GLY:O	1:A:349:ASP:N	2.43	0.51
1:A:73:TYR:OH	1:A:314:LYS:HE3	2.10	0.51
2:B:602:U:H2'	2:B:603:C:C6	2.46	0.50
1:E:57:ALA:O	1:E:60:SER:HB3	2.11	0.50
1:A:217:PHE:O	1:A:221:ILE:HG13	2.12	0.50
1:E:163:ARG:HH12	1:E:174:ARG:NH1	2.09	0.50
1:A:252:VAL:O	1:A:256:ILE:HG12	2.11	0.50
1:E:2:GLU:HG2	1:E:3:ILE:O	2.12	0.50
1:A:170:GLN:HG2	1:A:172:LYS:HE2	1.93	0.49
1:A:345:GLN:O	1:A:348:LYS:HG3	2.12	0.49
2:B:606:U:H2'	2:B:607:C:C6	2.48	0.49
1:E:237:TYR:HD2	1:E:328:ASP:CB	2.26	0.49
1:A:47:ASP:O	1:A:50:LEU:HB2	2.13	0.49
1:E:34:PHE:HD2	1:E:398:HIS:CD2	2.31	0.49
1:A:238:ASP:C	1:A:240:SER:H	2.17	0.49
1:A:381:ASP:OD2	1:A:454:TYR:OH	2.26	0.49
1:E:47:ASP:O	1:E:50:LEU:HB2	2.12	0.49
1:E:37:VAL:N	1:E:399:GLU:OE2	2.46	0.49
1:A:229:LEU:HD11	1:A:368:TRP:CE2	2.48	0.48
1:A:152:LEU:HB3	1:A:153:PRO:HD2	1.95	0.48
1:A:116:ALA:O	1:A:181:LEU:N	2.42	0.48
1:E:349:ASP:HB2	1:E:350:TYR:HD1	1.78	0.48
1:E:10:LYS:HG3	1:E:11:GLU:N	2.28	0.48
1:E:345:GLN:O	1:E:348:LYS:HG3	2.13	0.48
1:A:345:GLN:HG3	1:A:346:SER:H	1.78	0.48
1:E:288:SER:OG	1:E:289:GLY:N	2.47	0.48
1:E:347:GLY:O	1:E:349:ASP:N	2.46	0.48
1:A:289:GLY:O	2:B:600:G:O2'	2.29	0.48
1:E:44:THR:HG22	1:E:45:LYS:H	1.79	0.48
1:A:44:THR:HG22	1:A:45:LYS:H	1.78	0.47
1:E:422:TRP:CD1	1:E:453:LEU:HD13	2.50	0.47
1:A:413:HIS:O	1:A:416:SER:HB3	2.14	0.47
1:A:24:LYS:HG2	2:B:599:A:H61	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:ALA:HB1	1:A:441:ILE:HG21	1.96	0.47
1:A:177:GLU:HB2	1:A:287:PRO:O	2.14	0.47
1:E:440:PRO:HA	1:E:443:ARG:NH1	2.30	0.47
1:A:29:ALA:CB	1:A:441:ILE:HG21	2.45	0.46
1:A:37:VAL:N	1:A:399:GLU:OE2	2.47	0.46
1:E:286:MET:HG2	1:E:293:THR:HG22	1.97	0.46
1:E:29:ALA:HB1	1:E:441:ILE:HG21	1.98	0.46
1:E:40:PRO:HD3	1:E:403:TRP:CH2	2.50	0.46
1:A:341:SER:HA	1:A:363:PHE:CD2	2.50	0.46
1:A:84:GLN:NE2	1:A:205:ILE:O	2.47	0.46
1:A:127:LYS:HG3	1:A:181:LEU:HD22	1.97	0.46
1:A:338:VAL:O	1:A:338:VAL:HG23	2.15	0.46
1:A:411:GLN:HB3	5:A:525:HOH:O	2.16	0.46
1:A:416:SER:OG	3:C:698:A:H1'	2.15	0.46
1:A:261:ARG:H	1:A:261:ARG:HG2	1.49	0.46
1:A:394:MET:O	1:A:398:HIS:ND1	2.38	0.45
1:A:212:CYS:HB2	1:A:217:PHE:CG	2.51	0.45
1:E:415:ARG:NH2	4:E:501:SO4:O1	2.49	0.45
2:F:602:U:H2'	2:F:603:C:C6	2.51	0.45
1:E:326:TYR:CD1	3:G:701:DC:H1'	2.51	0.45
1:E:384:TYR:HB2	1:E:387:LEU:HD12	1.98	0.45
1:E:436:ILE:O	1:E:442:GLY:HA3	2.17	0.45
1:E:270:HIS:NE2	1:E:281:CYS:SG	2.89	0.45
1:E:95:MET:HB3	1:E:189:MET:HA	1.99	0.45
1:E:158:VAL:HA	1:E:175:LEU:HD23	1.99	0.45
1:A:413:HIS:CD2	3:C:698:A:H4'	2.52	0.45
1:A:313:TYR:HB3	1:A:316:ILE:HB	1.99	0.45
1:E:309:LEU:HD12	1:E:321:LEU:HD22	1.99	0.44
1:E:374:LEU:O	1:E:376:ARG:HD2	2.17	0.44
1:E:237:TYR:CD2	1:E:328:ASP:HA	2.52	0.44
2:F:611:U:O5'	2:F:611:U:H6	2.01	0.44
1:A:439:VAL:HG23	1:A:442:GLY:H	1.82	0.44
1:A:49:ARG:NH1	1:A:168:VAL:HG11	2.32	0.44
1:E:188:ARG:NH1	2:F:602:U:OP1	2.46	0.44
1:E:238:ASP:C	1:E:240:SER:H	2.20	0.44
1:A:57:ALA:O	1:A:60:SER:HB3	2.18	0.44
1:A:237:TYR:CD1	1:A:237:TYR:C	2.91	0.44
2:B:604:U:H2'	2:B:605:C:C6	2.51	0.44
1:E:212:CYS:O	1:E:214:PRO:HD3	2.18	0.44
1:E:8:PRO:O	1:E:10:LYS:N	2.51	0.43
1:A:70:VAL:HG21	1:A:251:MET:CE	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:166:THR:O	1:E:170:GLN:N	2.30	0.43
1:A:95:MET:HB3	1:A:189:MET:HA	1.99	0.43
1:E:195:TYR:HA	1:E:295:ILE:CD1	2.48	0.43
1:E:41:ALA:O	1:E:43:LEU:HD13	2.18	0.43
2:F:604:U:H2'	2:F:605:C:C6	2.53	0.43
1:A:379:ARG:NH2	5:A:522:HOH:O	2.51	0.43
1:A:227:GLU:HB3	1:A:228:LYS:NZ	2.34	0.43
1:E:118:TYR:CD1	1:E:119:PRO:HA	2.54	0.43
1:E:305:ILE:HD13	1:E:323:MET:HE1	2.01	0.43
2:B:611:U:H6	2:B:611:U:O5'	2.02	0.43
1:A:73:TYR:CE2	1:A:311:LYS:HD3	2.54	0.42
1:E:217:PHE:O	1:E:221:ILE:HG13	2.19	0.42
1:A:326:TYR:CD1	3:C:701:DC:H1'	2.54	0.42
1:E:31:HIS:CE1	1:E:402:ARG:NH2	2.87	0.42
1:E:345:GLN:CG	1:E:346:SER:N	2.82	0.42
2:B:609:C:H42	3:C:693:G:H1	1.68	0.42
1:E:73:TYR:CE2	1:E:311:LYS:HD3	2.55	0.42
3:G:698:A:H2'	3:G:699:G:C8	2.55	0.42
1:E:65:ASN:HB3	1:E:243:PRO:HD2	2.02	0.42
1:E:272:HIS:N	1:E:272:HIS:ND1	2.68	0.42
1:A:27:PRO:HB3	1:A:31:HIS:CG	2.53	0.42
1:A:2:GLU:HG2	1:A:3:ILE:O	2.20	0.42
1:A:49:ARG:HH11	1:A:168:VAL:HG11	1.85	0.42
1:A:188:ARG:NH1	2:B:602:U:OP1	2.49	0.42
1:E:14:TYR:HA	1:E:15:PRO:HD3	1.77	0.42
1:E:313:TYR:HB3	1:E:316:ILE:HB	2.02	0.42
1:E:394:MET:C	1:E:398:HIS:HD1	2.20	0.42
1:E:341:SER:HA	1:E:363:PHE:CD2	2.55	0.42
1:A:212:CYS:O	1:A:214:PRO:HD3	2.20	0.42
1:E:152:LEU:HB3	1:E:153:PRO:HD2	2.02	0.41
1:E:154:LEU:O	1:E:273:HIS:HA	2.20	0.41
1:A:377:PHE:HB3	5:A:521:HOH:O	2.19	0.41
1:E:118:TYR:CG	1:E:119:PRO:HA	2.55	0.41
1:E:70:VAL:HG21	1:E:251:MET:CE	2.50	0.41
1:A:300:ILE:O	1:A:304:ILE:HG13	2.20	0.41
1:A:399:GLU:HA	5:A:520:HOH:O	2.20	0.41
1:E:212:CYS:HB2	1:E:217:PHE:CG	2.54	0.41
1:E:344:ALA:HA	1:E:354:MET:SD	2.61	0.41
1:E:300:ILE:O	1:E:304:ILE:HG13	2.21	0.41
1:E:345:GLN:HG3	1:E:346:SER:N	2.36	0.41
1:A:123:MET:CE	1:A:125:LYS:HD2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:TYR:CD2	1:A:328:ASP:HB3	2.56	0.41
1:E:350:TYR:N	1:E:350:TYR:CD1	2.88	0.41
1:A:118:TYR:CD1	1:A:119:PRO:HA	2.56	0.41
1:A:41:ALA:O	1:A:43:LEU:HD13	2.20	0.41
1:E:241:LEU:HD23	1:E:241:LEU:HA	1.81	0.41
3:C:692:C:H2'	3:C:693:G:H8	1.86	0.41
1:A:392:MET:HB2	1:A:392:MET:HE2	1.88	0.41
1:E:216:LEU:HA	1:E:216:LEU:HD23	1.80	0.41
1:A:234:TYR:CD2	1:A:237:TYR:HD2	2.39	0.40
1:A:440:PRO:HA	1:A:443:ARG:NH1	2.36	0.40
1:A:148:TYR:O	1:A:152:LEU:HD21	2.21	0.40
1:E:237:TYR:C	1:E:237:TYR:CD1	2.95	0.40
1:A:95:MET:SD	1:A:192:GLY:HA3	2.62	0.40
1:A:148:TYR:HB2	1:A:182:ASN:HD21	1.85	0.40
1:E:349:ASP:HB2	1:E:350:TYR:CD1	2.56	0.40
1:A:34:PHE:HD2	1:A:398:HIS:CD2	2.39	0.40
1:A:102:TYR:O	1:A:109:ALA:HB2	2.21	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:VAL:O	1:E:148:TYR:OH[1_446]	1.91	0.29
1:A:148:TYR:OH	1:E:12:VAL:O[1_446]	1.95	0.25

## 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	460/471 (98%)	402 (87%)	49 (11%)	9 (2%)	9	16
1	E	460/471 (98%)	407 (88%)	42 (9%)	11 (2%)	7	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	920/942 (98%)	809 (88%)	91 (10%)	20 (2%)	8	14

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	SER
1	A	237	TYR
1	E	9	SER
1	E	70	VAL
1	E	288	SER
1	A	70	VAL
1	A	227	GLU
1	A	339	ASP
1	A	348	LYS
1	E	228	LYS
1	E	237	TYR
1	A	239	ALA
1	E	227	GLU
1	E	348	LYS
1	E	172	LYS
1	E	307	THR
1	A	307	THR
1	E	287	PRO
1	E	285	GLY
1	A	285	GLY

### 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	403/412 (98%)	358 (89%)	45 (11%)	7	12
1	E	403/412 (98%)	352 (87%)	51 (13%)	5	9
All	All	806/824 (98%)	710 (88%)	96 (12%)	6	11

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ILE
1	A	21	SER
1	A	26	GLU
1	A	52	THR
1	A	94	GLN
1	A	123	MET
1	A	125	LYS
1	A	127	LYS
1	A	128	ARG
1	A	138	THR
1	A	154	LEU
1	A	164	SER
1	A	166	THR
1	A	170	GLN
1	A	172	LYS
1	A	204	VAL
1	A	208	SER
1	A	218	TRP
1	A	219	SER
1	A	237	TYR
1	A	238	ASP
1	A	240	SER
1	A	242	SER
1	A	260	ASP
1	A	261	ARG
1	A	278	LYS
1	A	281	CYS
1	A	290	MET
1	A	293	THR
1	A	294	SER
1	A	319	ASP
1	A	333	SER
1	A	346	SER
1	A	348	LYS
1	A	350	TYR
1	A	355	THR
1	A	360	SER
1	A	364	GLU
1	A	367	THR
1	A	408	ARG
1	A	409	ASN
1	A	411	GLN
1	A	415	ARG

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Mol	Chain	Res	Type
1	A	428	GLU
1	A	438	SER
1	E	14	TYR
1	E	16	ILE
1	E	17	ILE
1	E	21	SER
1	E	24	LYS
1	E	26	GLU
1	E	52	THR
1	E	60	SER
1	E	96	CYS
1	E	123	MET
1	E	127	LYS
1	E	128	ARG
1	E	138	THR
1	E	154	LEU
1	E	164	SER
1	E	166	THR
1	E	170	GLN
1	E	172	LYS
1	E	204	VAL
1	E	208	SER
1	E	218	TRP
1	E	237	TYR
1	E	238	ASP
1	E	240	SER
1	E	242	SER
1	E	260	ASP
1	E	261	ARG
1	E	272	HIS
1	E	278	LYS
1	E	281	CYS
1	E	290	MET
1	E	293	THR
1	E	294	SER
1	E	319	ASP
1	E	324	ILE
1	E	328	ASP
1	E	348	LYS
1	E	349	ASP
1	E	350	TYR
1	E	354	MET

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Mol	Chain	Res	Type
1	E	355	THR
1	E	360	SER
1	E	364	GLU
1	E	367	THR
1	E	376	ARG
1	E	408	ARG
1	E	409	ASN
1	E	411	GLN
1	E	415	ARG
1	E	428	GLU
1	E	438	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	12/26 (46%)	3 (25%)	0
2	F	12/26 (46%)	3 (25%)	0
3	C	8/17 (47%)	1 (12%)	0
3	G	8/17 (47%)	1 (12%)	0
All	All	40/86 (46%)	8 (20%)	0

All (8) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	608	U
2	B	610	G
2	B	611	U
3	C	699	G
2	F	608	U
2	F	610	G
2	F	611	U
3	G	699	G

There are no RNA pucker outliers to report.

## 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 ⓘ

2 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	$\# Z  > 2$
4	SO4	E	501	-	4,4,4	0.15	0	6,6,6	0.22	0
4	SO4	E	502	-	4,4,4	0.14	0	6,6,6	0.17	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
4	SO4	E	501	-	-	0/0/0/0	0/0/0/0
4	SO4	E	502	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	501	SO4	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	462/471 (98%)	0.03	10 (2%) 65 59	58, 91, 122, 138	0
1	E	462/471 (98%)	0.12	11 (2%) 62 56	58, 90, 122, 138	0
2	B	13/26 (50%)	-0.38	0 100 100	71, 79, 120, 127	0
2	F	13/26 (50%)	-0.21	1 (7%) 16 12	73, 80, 121, 129	0
3	C	10/17 (58%)	-0.55	0 100 100	72, 78, 124, 129	0
3	G	10/17 (58%)	-0.65	0 100 100	71, 78, 125, 129	0
All	All	970/1028 (94%)	0.05	22 (2%) 64 57	58, 90, 122, 138	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	130	ILE	6.6
1	E	176	ILE	3.8
1	A	134	GLN	3.5
1	A	338	VAL	3.2
1	A	309	LEU	2.9
1	E	131	LEU	2.8
1	E	241	LEU	2.7
1	A	349	ASP	2.5
1	E	290	MET	2.4
1	E	275	TYR	2.4
1	E	16	ILE	2.3
1	A	51	LYS	2.3
1	E	308	LEU	2.3
1	A	157	TYR	2.2
1	A	435	LYS	2.2
1	E	309	LEU	2.2
1	E	350	TYR	2.2
1	A	145	LEU	2.1
1	E	75	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	131	LEU	2.1
1	A	70	VAL	2.0
2	F	599	A	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
4	SO4	E	501	5/5	0.98	0.06	-3.68	101,110,115,118	0
4	SO4	E	502	5/5	0.95	0.07	-	110,117,135,135	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.