



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:03 PM GMT

PDB ID : 1NAL  
Title : THE THREE-DIMENSIONAL STRUCTURE OF N-ACETYLNEURAMINATE LYASE FROM ESCHERICHIA COLI  
Authors : Izard, T.; Lawrence, M.C.; Malby, R.L.; Lilley, G.G.; Colman, P.M.  
Deposited on : 1994-02-28  
Resolution : 2.20 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

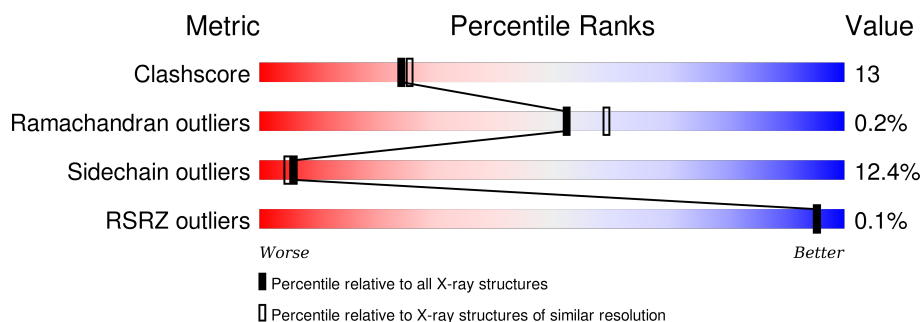
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	1	297	
1	2	297	
1	3	297	
1	4	297	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	1	302	-	-	X	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9072 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 N-ACETYLNEURAMINATE LYASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	291	Total	C	N	O	S	73	0	0
			2248	1433	380	425	10			
1	2	291	Total	C	N	O	S	74	0	0
			2248	1433	380	425	10			
1	3	291	Total	C	N	O	S	70	0	0
			2248	1433	380	425	10			
1	4	291	Total	C	N	O	S	54	0	0
			2248	1433	380	425	10			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	70	GLY	ALA	CONFLICT	UNP P0A6L4
1	84	THR	SER	CONFLICT	UNP P0A6L4
1	282	GLN	LEU	CONFLICT	UNP P0A6L4
2	70	GLY	ALA	CONFLICT	UNP P0A6L4
2	84	THR	SER	CONFLICT	UNP P0A6L4
2	282	GLN	LEU	CONFLICT	UNP P0A6L4
3	70	GLY	ALA	CONFLICT	UNP P0A6L4
3	84	THR	SER	CONFLICT	UNP P0A6L4
3	282	GLN	LEU	CONFLICT	UNP P0A6L4
4	70	GLY	ALA	CONFLICT	UNP P0A6L4
4	84	THR	SER	CONFLICT	UNP P0A6L4
4	282	GLN	LEU	CONFLICT	UNP P0A6L4

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	1	1	Total	O	S	0	0
			5	4	1		
2	2	1	Total	O	S	0	0
			5	4	1		
2	3	1	Total	O	S	0	0
			5	4	1		
2	4	1	Total	O	S	0	0
			5	4	1		

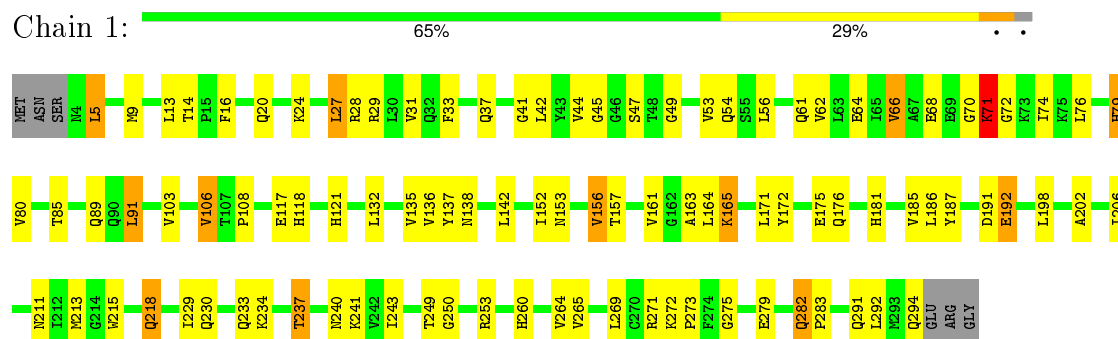
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	1	11	Total	O	0	0
			11	11		
3	2	17	Total	O	0	0
			17	17		
3	3	15	Total	O	0	0
			15	15		
3	4	17	Total	O	0	0
			17	17		

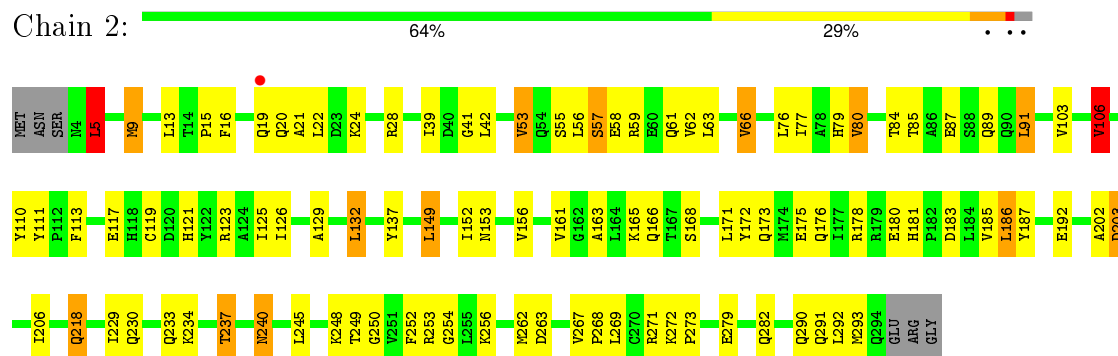
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

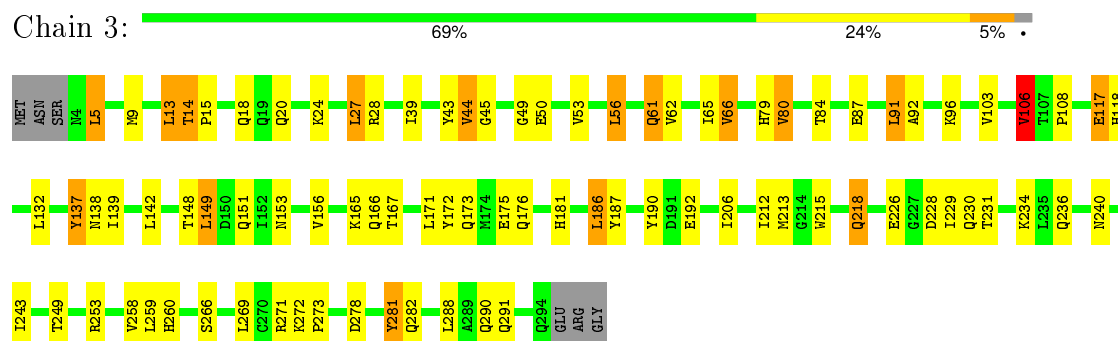
#### • Molecule 1: N-ACETYLNEURAMINATE LYASE



#### • Molecule 1: N-ACETYLNEURAMINATE LYASE



#### • Molecule 1: N-ACETYLNEURAMINATE LYASE

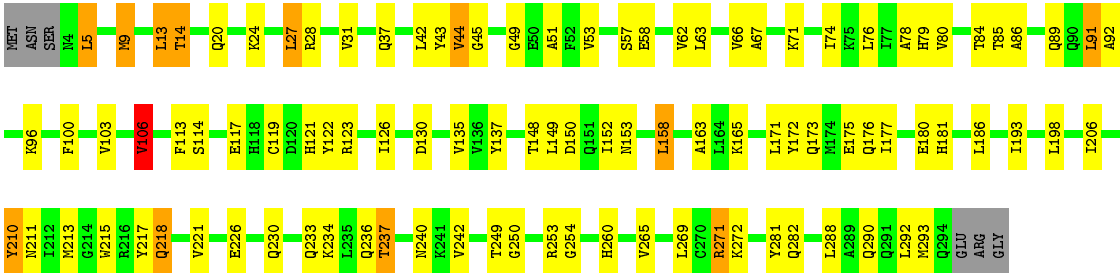


#### • Molecule 1: N-ACETYLNEURAMINATE LYASE

Chain 4: 

64%

29%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	122.80Å 122.80Å 198.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	6.00 – 2.20 20.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (6.00-2.20) 76.8 (20.00-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.208 , (Not available) 0.206 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	29.0	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 80.2	EDS
Estimated twinning fraction	0.057 for -h,-k,l	Xtriage
L-test for twinning <sup>1</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.23$	Xtriage
Outliers	0 of 67898 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9072	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</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

### 5.1 Standard geometry

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	1	0.77	2/2288 (0.1%)	0.96	6/3097 (0.2%)
1	2	0.69	0/2288	0.92	4/3097 (0.1%)
1	3	0.68	0/2288	0.94	5/3097 (0.2%)
1	4	0.78	1/2288 (0.0%)	0.97	6/3097 (0.2%)
All	All	0.73	3/9152 (0.0%)	0.95	21/12388 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1	0	2
1	2	0	1
1	3	0	1
All	All	0	4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	4	293	MET	CG-SD	5.71	1.96	1.81
1	1	71	LYS	CB-CG	5.39	1.67	1.52
1	1	192	GLU	CB-CG	-5.07	1.42	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4	13	LEU	CA-CB-CG	9.58	137.33	115.30
1	1	13	LEU	CA-CB-CG	7.42	132.37	115.30
1	3	13	LEU	CA-CB-CG	7.07	131.56	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	106	VAL	CB-CA-C	-6.59	98.87	111.40
1	1	71	LYS	CA-C-N	-6.51	103.17	116.20
1	4	106	VAL	CB-CA-C	-6.39	99.26	111.40
1	2	250	GLY	N-CA-C	-6.31	97.32	113.10
1	4	250	GLY	N-CA-C	-6.21	97.57	113.10
1	3	149	LEU	CA-CB-CG	6.04	129.20	115.30
1	2	5	LEU	CA-CB-CG	6.00	129.11	115.30
1	3	106	VAL	CB-CA-C	-5.90	100.18	111.40
1	1	5	LEU	CA-CB-CG	5.83	128.70	115.30
1	1	71	LYS	N-CA-CB	5.60	120.68	110.60
1	4	158	LEU	CA-CB-CG	5.55	128.07	115.30
1	1	250	GLY	N-CA-C	-5.53	99.29	113.10
1	3	56	LEU	CA-CB-CG	5.41	127.74	115.30
1	2	42	LEU	CA-CB-CG	5.28	127.43	115.30
1	4	91	LEU	CA-CB-CG	5.25	127.37	115.30
1	1	79	HIS	N-CA-C	-5.20	96.95	111.00
1	4	43	TYR	N-CA-C	-5.02	97.44	111.00
1	3	186	LEU	CA-CB-CG	5.01	126.83	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	187	TYR	Sidechain
1	1	71	LYS	Mainchain
1	2	272	LYS	Peptide
1	3	281	TYR	Sidechain

## 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	1	2248	0	2266	64	0
1	2	2248	0	2266	60	0
1	3	2248	0	2266	49	0
1	4	2248	0	2266	64	0
2	1	5	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	2	5	0	0	0	0
2	3	5	0	0	1	0
2	4	5	0	0	0	0
3	1	11	0	0	0	0
3	2	17	0	0	0	0
3	3	15	0	0	0	0
3	4	17	0	0	1	0
All	All	9072	0	9064	225	0

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

All (225) 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)
1:2:80:VAL:HG22	1:2:91:LEU:HB3	1.53	0.90
1:1:80:VAL:HG22	1:1:91:LEU:HB3	1.53	0.88
1:4:153:ASN:OD1	1:4:181:HIS:HE1	1.62	0.81
1:4:79:HIS:CE1	1:4:106:VAL:HG22	2.15	0.81
1:1:153:ASN:OD1	1:1:181:HIS:HE1	1.63	0.81
1:2:110:TYR:O	1:3:142:LEU:HD12	1.80	0.81
1:4:79:HIS:HE1	1:4:106:VAL:HG22	1.45	0.80
1:3:80:VAL:HG22	1:3:91:LEU:HB3	1.64	0.80
1:3:62:VAL:O	1:3:66:VAL:HG13	1.83	0.78
1:1:108:PRO:HD2	1:1:118:HIS:HD2	1.50	0.77
1:1:14:THR:HG21	1:1:54:GLN:NE2	2.00	0.76
1:2:149:LEU:HD13	1:2:153:ASN:HD21	1.50	0.75
1:3:108:PRO:HD2	1:3:118:HIS:HD2	1.52	0.74
1:3:27:LEU:HD11	1:3:62:VAL:HG13	1.69	0.74
1:2:153:ASN:OD1	1:2:181:HIS:HE1	1.70	0.74
1:1:47:SER:HB2	2:1:302:SO4:O1	1.88	0.74
1:3:108:PRO:HD2	1:3:118:HIS:CD2	2.24	0.73
1:1:294:GLN:O	1:1:294:GLN:HG3	1.89	0.72
1:1:14:THR:HG21	1:1:54:GLN:HE22	1.55	0.72
1:2:171:LEU:HD12	1:4:171:LEU:HD12	1.73	0.70
1:2:56:LEU:HD21	1:2:87:GLU:HB3	1.74	0.70
1:2:273:PRO:O	1:3:117:GLU:HG2	1.91	0.70
1:2:24:LYS:O	1:2:28:ARG:HG3	1.90	0.70
1:3:173:GLN:HA	1:3:176:GLN:HE21	1.56	0.70
1:3:153:ASN:OD1	1:3:181:HIS:HE1	1.75	0.69
1:2:119:CYS:O	1:2:123:ARG:HG3	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:85:THR:O	1:4:89:GLN:HG3	1.93	0.68
1:1:62:VAL:O	1:1:66:VAL:HG13	1.94	0.68
1:4:249:THR:O	1:4:253:ARG:HD2	1.94	0.68
1:4:218:GLN:HA	1:4:218:GLN:HE21	1.60	0.66
1:1:273:PRO:HG2	1:4:113:PHE:CZ	2.31	0.66
1:1:218:GLN:HA	1:1:218:GLN:HE21	1.60	0.66
1:1:108:PRO:HD2	1:1:118:HIS:CD2	2.32	0.65
1:2:173:GLN:HA	1:2:176:GLN:HE21	1.62	0.65
1:3:14:THR:HG23	1:3:49:GLY:O	1.95	0.65
1:2:163:ALA:HB2	1:2:185:VAL:HB	1.78	0.65
1:4:121:HIS:HE1	3:4:447:HOH:O	1.80	0.63
1:2:233:GLN:O	1:2:237:THR:HG23	1.99	0.63
1:3:165:LYS:HE3	2:3:306:SO4:O4	2.00	0.61
1:4:119:CYS:O	1:4:123:ARG:HG3	2.00	0.61
1:4:5:LEU:HD23	1:4:5:LEU:H	1.65	0.61
1:3:84:THR:HB	1:3:87:GLU:HB2	1.82	0.61
1:2:55:SER:OG	1:2:58:GLU:HG3	2.01	0.61
1:2:149:LEU:HD13	1:2:153:ASN:ND2	2.15	0.60
1:1:171:LEU:HD12	1:3:171:LEU:HD12	1.82	0.60
1:1:192:GLU:HA	1:1:240:ASN:HD21	1.67	0.59
1:2:85:THR:OG1	1:2:121:HIS:HD2	1.86	0.59
1:2:9:MET:CE	1:2:77:ILE:HD11	2.33	0.58
1:3:236:GLN:HE21	1:3:240:ASN:ND2	2.02	0.58
1:2:9:MET:O	1:2:206:ILE:HA	2.03	0.58
1:4:165:LYS:HG2	1:4:206:ILE:HD12	1.84	0.58
1:3:45:GLY:O	1:3:79:HIS:HD2	1.87	0.58
1:3:142:LEU:HD22	1:3:142:LEU:N	2.18	0.57
1:4:122:TYR:O	1:4:126:ILE:HG13	2.03	0.57
1:1:279:GLU:HA	1:1:282:GLN:HE22	1.69	0.57
1:3:24:LYS:O	1:3:28:ARG:HG3	2.03	0.57
1:3:139:ILE:HD11	1:3:142:LEU:HD23	1.85	0.57
1:1:249:THR:O	1:1:253:ARG:HD2	2.04	0.57
1:1:279:GLU:HA	1:1:282:GLN:NE2	2.18	0.57
1:3:44:VAL:HG11	1:3:66:VAL:HG21	1.87	0.57
1:3:236:GLN:HE21	1:3:240:ASN:HD21	1.51	0.56
1:2:218:GLN:HE21	1:2:218:GLN:HA	1.71	0.56
1:2:62:VAL:O	1:2:66:VAL:HG12	2.06	0.56
1:4:114:SER:OG	1:4:117:GLU:HG3	2.06	0.56
1:1:9:MET:O	1:1:206:ILE:HA	2.05	0.56
1:3:9:MET:O	1:3:206:ILE:HA	2.05	0.55
1:3:80:VAL:HG21	1:3:92:ALA:HA	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:14:THR:CG2	1:4:49:GLY:O	2.54	0.55
1:2:121:HIS:CE1	1:2:125:ILE:HD11	2.42	0.55
1:4:217:TYR:O	1:4:221:VAL:HG23	2.06	0.55
1:4:173:GLN:O	1:4:177:ILE:HG13	2.07	0.54
1:4:67:ALA:O	1:4:71:LYS:HB2	2.06	0.54
1:4:44:VAL:HG22	1:4:63:LEU:HD23	1.89	0.53
1:4:27:LEU:O	1:4:31:VAL:HG23	2.09	0.53
1:4:135:VAL:HG22	1:4:163:ALA:HB3	1.90	0.53
1:2:249:THR:O	1:2:253:ARG:HD2	2.09	0.53
1:4:80:VAL:HG21	1:4:92:ALA:HA	1.91	0.53
1:1:165:LYS:HE2	1:1:206:ILE:HG21	1.91	0.52
1:2:117:GLU:OE2	1:3:253:ARG:NH2	2.42	0.52
1:3:79:HIS:HE1	1:3:106:VAL:H	1.57	0.52
1:2:172:TYR:O	1:2:176:GLN:HG3	2.09	0.52
1:1:45:GLY:O	1:1:79:HIS:CD2	2.62	0.52
1:1:45:GLY:O	1:1:79:HIS:HD2	1.93	0.52
1:4:45:GLY:O	1:4:51:ALA:HB2	2.10	0.52
1:1:54:GLN:HA	1:1:271:ARG:HH21	1.74	0.52
1:4:13:LEU:HD22	1:4:211:ASN:ND2	2.25	0.52
1:3:56:LEU:HD21	1:3:87:GLU:HB3	1.92	0.51
1:4:20:GLN:HE22	1:4:272:LYS:HG2	1.75	0.51
1:4:106:VAL:HG13	1:4:137:TYR:CD2	2.46	0.51
1:3:20:GLN:HE22	1:3:272:LYS:HG2	1.74	0.51
1:2:9:MET:HG3	1:2:41:GLY:C	2.31	0.51
1:1:29:ARG:HD2	1:1:264:VAL:O	2.11	0.51
1:4:42:LEU:HG	1:4:74:ILE:HD12	1.93	0.51
1:1:85:THR:O	1:1:89:GLN:HG3	2.09	0.51
1:4:5:LEU:CD2	1:4:5:LEU:H	2.23	0.51
1:2:252:PHE:O	1:2:256:LYS:HG3	2.11	0.50
1:3:153:ASN:OD1	1:3:181:HIS:CE1	2.61	0.50
1:4:172:TYR:O	1:4:176:GLN:HG3	2.11	0.50
1:2:9:MET:HE3	1:2:77:ILE:HD11	1.92	0.50
1:4:236:GLN:HE21	1:4:240:ASN:HD21	1.60	0.50
1:4:79:HIS:HE1	1:4:106:VAL:H	1.58	0.50
1:3:45:GLY:O	1:3:79:HIS:CD2	2.64	0.50
1:3:43:TYR:CD1	1:3:206:ILE:HD13	2.46	0.50
1:3:228:ASP:OD1	1:3:231:THR:HG23	2.11	0.50
1:4:24:LYS:O	1:4:28:ARG:HG3	2.12	0.49
1:3:137:TYR:CD1	1:3:165:LYS:HD3	2.48	0.49
1:1:198:LEU:HD23	1:1:202:ALA:HB3	1.95	0.49
1:1:292:LEU:C	1:1:294:GLN:H	2.16	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:117:GLU:OE2	1:4:253:ARG:NH2	2.46	0.49
1:3:218:GLN:HE21	1:3:218:GLN:HA	1.77	0.49
1:2:245:LEU:O	1:2:248:LYS:HB2	2.13	0.48
1:2:111:TYR:OH	1:3:50:GLU:HA	2.13	0.48
1:4:260:HIS:HD2	1:4:265:VAL:O	1.96	0.48
1:4:85:THR:OG1	1:4:121:HIS:HD2	1.97	0.48
1:4:62:VAL:O	1:4:66:VAL:HG13	2.13	0.48
1:3:249:THR:O	1:3:253:ARG:HD2	2.12	0.48
1:2:267:VAL:CG1	1:2:269:LEU:HD23	2.43	0.48
1:4:78:ALA:HB2	1:4:100:PHE:CD2	2.48	0.48
1:4:84:THR:HG22	1:4:86:ALA:H	1.79	0.48
1:1:27:LEU:HD11	1:1:62:VAL:HG13	1.96	0.47
1:1:273:PRO:HG2	1:4:113:PHE:CE1	2.48	0.47
1:1:85:THR:OG1	1:1:121:HIS:HD2	1.97	0.47
1:2:267:VAL:HG12	1:2:269:LEU:HD23	1.97	0.47
1:1:24:LYS:O	1:1:28:ARG:HG3	2.14	0.47
1:4:236:GLN:HE21	1:4:240:ASN:ND2	2.12	0.47
1:3:192:GLU:HG3	1:3:243:ILE:HD13	1.95	0.47
1:1:20:GLN:HE22	1:1:272:LYS:HG2	1.78	0.47
1:1:27:LEU:O	1:1:31:VAL:HG23	2.15	0.47
1:4:233:GLN:O	1:4:237:THR:HG23	2.15	0.47
1:2:19:GLN:O	1:2:20:GLN:HB2	2.16	0.46
1:2:178:ARG:NH2	1:2:203:ASP:OD1	2.48	0.46
1:3:212:ILE:HG22	1:3:259:LEU:HG	1.97	0.46
1:1:9:MET:HG2	1:1:41:GLY:N	2.31	0.46
1:2:163:ALA:CB	1:2:185:VAL:HB	2.43	0.46
1:4:148:THR:O	1:4:152:ILE:HG13	2.15	0.46
1:4:14:THR:HG22	1:4:49:GLY:O	2.16	0.45
1:4:242:VAL:HG13	1:4:288:LEU:HD21	1.99	0.45
1:2:152:ILE:O	1:2:156:VAL:HB	2.16	0.45
1:3:258:VAL:HG21	1:3:288:LEU:HD23	1.99	0.45
1:1:260:HIS:HD2	1:1:265:VAL:O	2.00	0.45
1:4:213:MET:HA	1:4:215:TRP:CZ3	2.51	0.45
1:1:163:ALA:HB2	1:1:185:VAL:HB	1.97	0.45
1:1:152:ILE:O	1:1:156:VAL:HB	2.17	0.45
1:4:292:LEU:HD23	1:4:292:LEU:HA	1.81	0.45
1:1:172:TYR:O	1:1:176:GLN:HG3	2.17	0.45
1:4:96:LYS:HD2	1:4:130:ASP:HB3	1.98	0.45
1:4:253:ARG:HG3	1:4:254:GLY:N	2.31	0.45
1:2:9:MET:HE2	1:2:77:ILE:HD11	1.98	0.45
1:2:262:MET:O	1:2:263:ASP:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:294:GLN:CG	1:1:294:GLN:O	2.59	0.44
1:1:253:ARG:NH2	1:4:117:GLU:OE2	2.50	0.44
1:1:42:LEU:HG	1:1:74:ILE:HD12	2.00	0.44
1:2:153:ASN:OD1	1:2:181:HIS:CE1	2.61	0.44
1:1:47:SER:CB	2:1:302:SO4:O1	2.62	0.44
1:4:44:VAL:HG11	1:4:66:VAL:HG21	1.99	0.44
1:1:47:SER:N	2:1:302:SO4:O1	2.51	0.44
1:1:33:PHE:HE2	1:1:211:ASN:O	2.00	0.44
1:3:5:LEU:HB3	1:3:187:TYR:OH	2.18	0.44
1:1:70:GLY:O	1:1:71:LYS:C	2.55	0.44
1:1:135:VAL:HA	1:1:163:ALA:O	2.18	0.44
1:3:148:THR:HG23	1:3:151:GLN:OE1	2.18	0.44
1:1:153:ASN:OD1	1:1:181:HIS:CE1	2.55	0.43
1:1:37:GLN:HG3	1:1:215:TRP:HE3	1.82	0.43
1:2:186:LEU:HB3	1:2:202:ALA:HA	1.99	0.43
1:2:85:THR:O	1:2:89:GLN:HG3	2.18	0.43
1:4:9:MET:O	1:4:206:ILE:HA	2.18	0.43
1:2:165:LYS:HA	1:2:187:TYR:HB2	2.00	0.43
1:2:57:SER:O	1:2:61:GLN:HB2	2.18	0.43
1:2:79:HIS:NE2	1:2:106:VAL:HG22	2.33	0.43
1:2:59:ARG:O	1:2:63:LEU:HG	2.18	0.43
1:3:137:TYR:CE1	1:3:165:LYS:HD3	2.54	0.43
1:3:39:ILE:HD12	1:3:39:ILE:HA	1.92	0.43
1:2:292:LEU:HD23	1:2:292:LEU:HA	1.88	0.43
1:2:58:GLU:CD	1:2:271:ARG:HH22	2.22	0.43
1:4:84:THR:HG22	1:4:86:ALA:N	2.33	0.43
1:1:156:VAL:HA	1:1:161:VAL:HG11	1.99	0.43
1:2:53:VAL:O	1:2:53:VAL:HG13	2.19	0.43
1:4:58:GLU:CD	1:4:271:ARG:HH22	2.22	0.43
1:3:167:THR:HG22	1:3:190:TYR:CE1	2.54	0.43
1:4:14:THR:HG21	1:4:49:GLY:O	2.17	0.42
1:2:126:ILE:HD11	1:2:161:VAL:HG23	2.01	0.42
1:1:64:GLU:O	1:1:68:GLU:HG3	2.20	0.42
1:2:15:PRO:O	1:2:22:LEU:HD12	2.19	0.42
1:2:192:GLU:CD	1:2:192:GLU:H	2.22	0.42
1:4:253:ARG:HG3	1:4:254:GLY:H	1.84	0.42
1:1:237:THR:O	1:1:241:LYS:HG3	2.19	0.42
1:2:129:ALA:O	1:2:132:LEU:HB2	2.19	0.42
1:1:165:LYS:HG3	1:1:206:ILE:HD12	2.02	0.42
1:4:45:GLY:O	1:4:79:HIS:HD2	2.02	0.42
1:1:153:ASN:O	1:1:157:THR:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:213:MET:HA	1:3:215:TRP:CZ3	2.55	0.42
1:3:278:ASP:HB3	1:3:281:TYR:CD2	2.54	0.42
1:4:180:GLU:HB3	1:4:181:HIS:CE1	2.55	0.41
1:2:113:PHE:CZ	1:3:273:PRO:HG2	2.55	0.41
1:4:249:THR:HG22	1:4:281:TYR:CG	2.55	0.41
1:4:42:LEU:HG	1:4:74:ILE:CD1	2.51	0.41
1:2:39:ILE:HA	1:2:39:ILE:HD12	1.78	0.41
1:4:106:VAL:HG13	1:4:137:TYR:CE2	2.54	0.41
1:2:267:VAL:HG12	1:2:269:LEU:CD2	2.51	0.41
1:1:233:GLN:O	1:1:237:THR:CG2	2.68	0.41
1:3:260:HIS:CD2	1:3:266:SER:O	2.73	0.41
1:1:14:THR:CG2	1:1:49:GLY:O	2.69	0.41
1:3:61:GLN:O	1:3:65:ILE:HG13	2.19	0.41
1:1:292:LEU:HD23	1:1:292:LEU:HA	1.88	0.41
1:1:80:VAL:HB	1:1:103:VAL:HG22	2.02	0.41
1:4:198:LEU:HD11	1:4:221:VAL:HG22	2.02	0.41
1:2:253:ARG:HG3	1:2:254:GLY:N	2.36	0.41
1:4:171:LEU:HD21	1:4:193:ILE:HD12	2.02	0.41
1:1:192:GLU:HG3	1:1:243:ILE:HG21	2.02	0.41
1:1:42:LEU:HG	1:1:74:ILE:CD1	2.51	0.41
1:3:14:THR:HA	1:3:15:PRO:HD3	1.89	0.40
1:4:210:TYR:N	1:4:210:TYR:CD1	2.89	0.40
1:1:16:PHE:CE2	1:1:271:ARG:HG3	2.56	0.40
1:3:240:ASN:HD22	1:3:240:ASN:N	2.19	0.40
1:1:213:MET:HA	1:1:215:TRP:CH2	2.57	0.40
1:2:192:GLU:HA	1:2:240:ASN:HD21	1.85	0.40
1:2:279:GLU:HA	1:2:282:GLN:NE2	2.36	0.40
1:2:16:PHE:HA	1:2:21:ALA:O	2.20	0.40
1:1:275:GLY:N	1:4:117:GLU:OE2	2.51	0.40
1:2:132:LEU:HD12	1:2:132:LEU:HA	1.78	0.40
1:2:5:LEU:HD23	1:2:185:VAL:HG21	2.03	0.40
1:1:136:VAL:O	1:1:164:LEU:HD12	2.22	0.40
1:1:106:VAL:HG13	1:1:137:TYR:CE2	2.56	0.40
1:2:5:LEU:H	1:2:5:LEU:CD2	2.35	0.40
1:1:136:VAL:HG23	1:1:161:VAL:HG13	2.02	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	1	289/297 (97%)	275 (95%)	13 (4%)	1 (0%)	46	50
1	2	289/297 (97%)	276 (96%)	12 (4%)	1 (0%)	46	50
1	3	289/297 (97%)	273 (94%)	16 (6%)	0	100	100
1	4	289/297 (97%)	279 (96%)	10 (4%)	0	100	100
All	All	1156/1188 (97%)	1103 (95%)	51 (4%)	2 (0%)	52	59

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	72	GLY
1	2	268	PRO

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	240/245 (98%)	213 (89%)	27 (11%)	7	6
1	2	240/245 (98%)	209 (87%)	31 (13%)	5	4
1	3	240/245 (98%)	206 (86%)	34 (14%)	4	3
1	4	240/245 (98%)	213 (89%)	27 (11%)	7	6
All	All	960/980 (98%)	841 (88%)	119 (12%)	6	5

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	5	LEU
1	1	27	LEU
1	1	44	VAL
1	1	53	VAL
1	1	56	LEU
1	1	61	GLN
1	1	66	VAL
1	1	76	LEU
1	1	91	LEU
1	1	106	VAL
1	1	132	LEU
1	1	138	ASN
1	1	142	LEU
1	1	156	VAL
1	1	165	LYS
1	1	175	GLU
1	1	186	LEU
1	1	191	ASP
1	1	218	GLN
1	1	229	ILE
1	1	230	GLN
1	1	234	LYS
1	1	237	THR
1	1	269	LEU
1	1	282	GLN
1	1	283	PRO
1	1	291	GLN
1	2	5	LEU
1	2	9	MET
1	2	13	LEU
1	2	53	VAL
1	2	57	SER
1	2	66	VAL
1	2	76	LEU
1	2	80	VAL
1	2	84	THR
1	2	91	LEU
1	2	103	VAL
1	2	106	VAL
1	2	132	LEU
1	2	137	TYR
1	2	149	LEU
1	2	166	GLN

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Mol	Chain	Res	Type
1	2	168	SER
1	2	175	GLU
1	2	180	GLU
1	2	183	ASP
1	2	186	LEU
1	2	203	ASP
1	2	218	GLN
1	2	229	ILE
1	2	230	GLN
1	2	234	LYS
1	2	237	THR
1	2	240	ASN
1	2	290	GLN
1	2	291	GLN
1	2	293	MET
1	3	5	LEU
1	3	13	LEU
1	3	14	THR
1	3	18	GLN
1	3	27	LEU
1	3	44	VAL
1	3	53	VAL
1	3	61	GLN
1	3	66	VAL
1	3	80	VAL
1	3	91	LEU
1	3	96	LYS
1	3	103	VAL
1	3	106	VAL
1	3	117	GLU
1	3	132	LEU
1	3	137	TYR
1	3	138	ASN
1	3	149	LEU
1	3	156	VAL
1	3	166	GLN
1	3	172	TYR
1	3	175	GLU
1	3	186	LEU
1	3	218	GLN
1	3	226	GLU
1	3	229	ILE

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Mol	Chain	Res	Type
1	3	230	GLN
1	3	234	LYS
1	3	269	LEU
1	3	271	ARG
1	3	282	GLN
1	3	290	GLN
1	3	291	GLN
1	4	5	LEU
1	4	9	MET
1	4	14	THR
1	4	27	LEU
1	4	37	GLN
1	4	44	VAL
1	4	53	VAL
1	4	57	SER
1	4	76	LEU
1	4	91	LEU
1	4	103	VAL
1	4	106	VAL
1	4	149	LEU
1	4	150	ASP
1	4	158	LEU
1	4	175	GLU
1	4	186	LEU
1	4	210	TYR
1	4	218	GLN
1	4	226	GLU
1	4	230	GLN
1	4	234	LYS
1	4	237	THR
1	4	269	LEU
1	4	271	ARG
1	4	282	GLN
1	4	290	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	20	GLN
1	1	54	GLN
1	1	79	HIS
1	1	89	GLN

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Mol	Chain	Res	Type
1	1	90	GLN
1	1	118	HIS
1	1	121	HIS
1	1	138	ASN
1	1	166	GLN
1	1	181	HIS
1	1	218	GLN
1	1	240	ASN
1	1	260	HIS
1	1	282	GLN
1	2	54	GLN
1	2	121	HIS
1	2	138	ASN
1	2	153	ASN
1	2	166	GLN
1	2	176	GLN
1	2	181	HIS
1	2	218	GLN
1	2	240	ASN
1	2	260	HIS
1	2	282	GLN
1	3	18	GLN
1	3	20	GLN
1	3	79	HIS
1	3	118	HIS
1	3	121	HIS
1	3	138	ASN
1	3	166	GLN
1	3	176	GLN
1	3	181	HIS
1	3	188	ASN
1	3	218	GLN
1	3	240	ASN
1	3	260	HIS
1	4	18	GLN
1	4	20	GLN
1	4	54	GLN
1	4	79	HIS
1	4	118	HIS
1	4	121	HIS
1	4	138	ASN
1	4	166	GLN

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Mol	Chain	Res	Type
1	4	176	GLN
1	4	181	HIS
1	4	218	GLN
1	4	240	ASN
1	4	260	HIS

### 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](#)

4 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	SO4	1	302	-	4,4,4	1.26	0	6,6,6	1.07	1 (16%)
2	SO4	2	304	-	4,4,4	1.46	1 (25%)	6,6,6	0.72	0
2	SO4	3	306	-	4,4,4	1.12	0	6,6,6	0.74	0
2	SO4	4	308	-	4,4,4	1.35	0	6,6,6	0.99	1 (16%)

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	SO4	1	302	-	-	0/0/0/0	0/0/0/0
2	SO4	2	304	-	-	0/0/0/0	0/0/0/0
2	SO4	3	306	-	-	0/0/0/0	0/0/0/0
2	SO4	4	308	-	-	0/0/0/0	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	304	SO4	O1-S	-2.55	1.38	1.47

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	302	SO4	O2-S-O1	-2.15	102.69	109.50
2	4	308	SO4	O2-S-O1	2.01	115.86	109.50

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	1	302	SO4	3	0
2	3	306	SO4	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	1	291/297 (97%)	-0.79	0 <a href="#">100</a> <a href="#">100</a>	14, 27, 45, 58	17 (5%)
1	2	291/297 (97%)	-0.68	1 (0%) <a href="#">94</a> <a href="#">94</a>	16, 29, 48, 73	17 (5%)
1	3	291/297 (97%)	-0.65	0 <a href="#">100</a> <a href="#">100</a>	18, 30, 51, 68	17 (5%)
1	4	291/297 (97%)	-0.78	0 <a href="#">100</a> <a href="#">100</a>	11, 25, 46, 65	13 (4%)
All	All	1164/1188 (97%)	-0.72	1 (0%) <a href="#">95</a> <a href="#">95</a>	11, 28, 48, 73	64 (5%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	2	19	GLN	2.3

### 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( $\text{\AA}^2$ )	Q<0.9
2	SO4	2	304	5/5	0.99	0.07	-0.06	44,46,50,51	0
2	SO4	1	302	5/5	0.98	0.07	-0.14	35,38,44,47	0
2	SO4	4	308	5/5	0.99	0.06	-1.63	33,33,38,41	0
2	SO4	3	306	5/5	0.99	0.05	-1.85	38,40,43,46	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.