



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:45 AM GMT

PDB ID : 2O20  
Title : Crystal structure of transcription regulator CcpA of *Lactococcus lactis*  
Authors : Loll, B.; Kowalczyk, M.; Alings, C.; Chieduch, A.; Bardowski, J.; Saenger, W.; Biesiadka, J.  
Deposited on : 2006-11-29  
Resolution : 1.90 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.

---

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

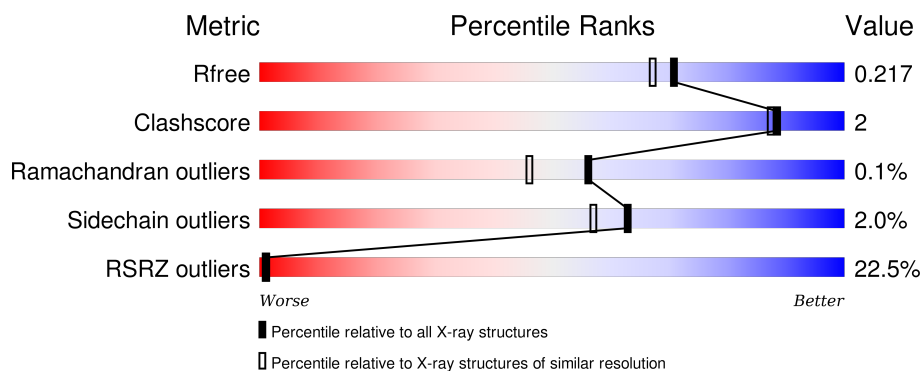
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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	332	<div> <div>12%</div> <div> <div></div> <div>77%</div> <div>• •</div> <div>18%</div> </div> </div>
1	B	332	<div> <div>14%</div> <div> <div></div> <div>77%</div> <div>5% •</div> <div>17%</div> </div> </div>
1	C	332	<div> <div>34%</div> <div> <div></div> <div>77%</div> <div>5%</div> <div>19%</div> </div> </div>
1	D	332	<div> <div>22%</div> <div> <div></div> <div>76%</div> <div>5% •</div> <div>19%</div> </div> </div>
1	E	332	<div> <div>11%</div> <div> <div></div> <div>75%</div> <div>6% •</div> <div>18%</div> </div> </div>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	F	332	
1	G	332	
1	H	332	

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	B	2003	-	-	-	X
2	SO4	F	2002	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 18486 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 Catabolite control protein A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	271	Total	C	N	O	S	0	6	0
			2135	1348	348	430	9			
1	C	270	Total	C	N	O	S	0	2	0
			2106	1327	342	428	9			
1	D	270	Total	C	N	O	S	0	4	0
			2120	1335	347	429	9			
1	B	275	Total	C	N	O	S	0	11	0
			2176	1370	353	444	9			
1	E	271	Total	C	N	O	S	0	11	0
			2151	1358	349	435	9			
1	F	272	Total	C	N	O	S	0	7	0
			2154	1357	356	432	9			
1	G	271	Total	C	N	O	S	0	2	0
			2116	1334	346	427	9			
1	H	272	Total	C	N	O	S	0	6	0
			2152	1355	358	430	9			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	89	ALA	ASP	ENGINEERED	UNP Q9CF33
C	89	ALA	ASP	ENGINEERED	UNP Q9CF33
D	89	ALA	ASP	ENGINEERED	UNP Q9CF33
B	89	ALA	ASP	ENGINEERED	UNP Q9CF33
E	89	ALA	ASP	ENGINEERED	UNP Q9CF33
F	89	ALA	ASP	ENGINEERED	UNP Q9CF33
G	89	ALA	ASP	ENGINEERED	UNP Q9CF33
H	89	ALA	ASP	ENGINEERED	UNP Q9CF33

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	1	Total	Cl	0	0
			1	1		

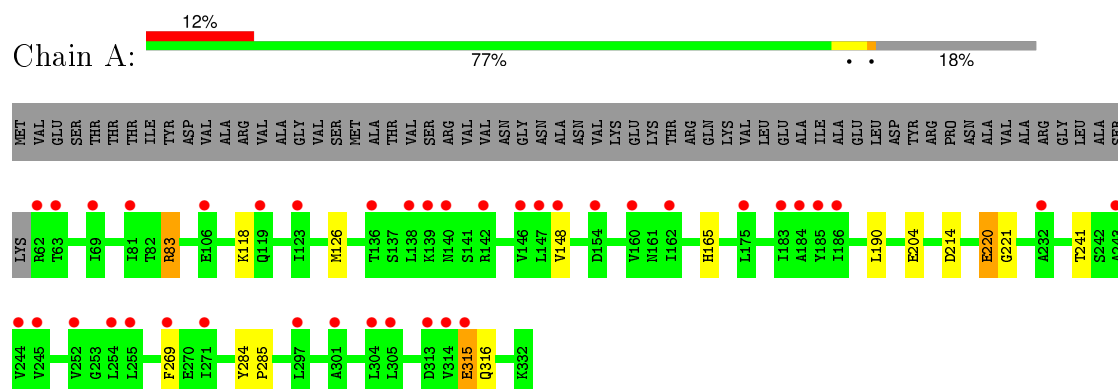
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	244	Total 244	O 244	0	0
4	C	17	Total 17	O 17	0	0
4	D	92	Total 92	O 92	0	0
4	B	217	Total 217	O 217	0	0
4	E	297	Total 297	O 297	0	0
4	F	255	Total 255	O 255	0	0
4	G	137	Total 137	O 137	0	0
4	H	76	Total 76	O 76	0	0

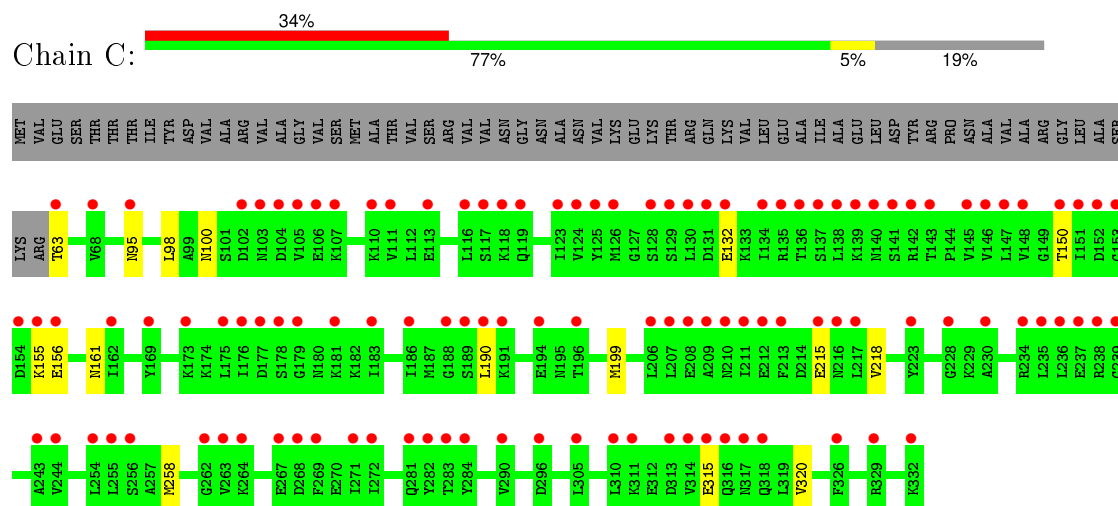
### 3 Residue-property plots

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.

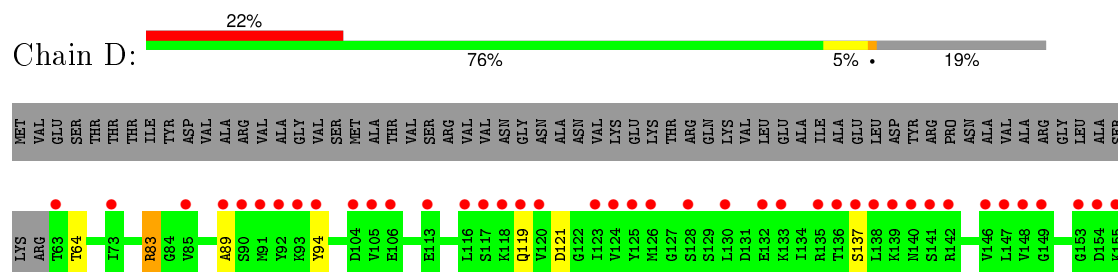
#### • Molecule 1: Catabolite control protein A



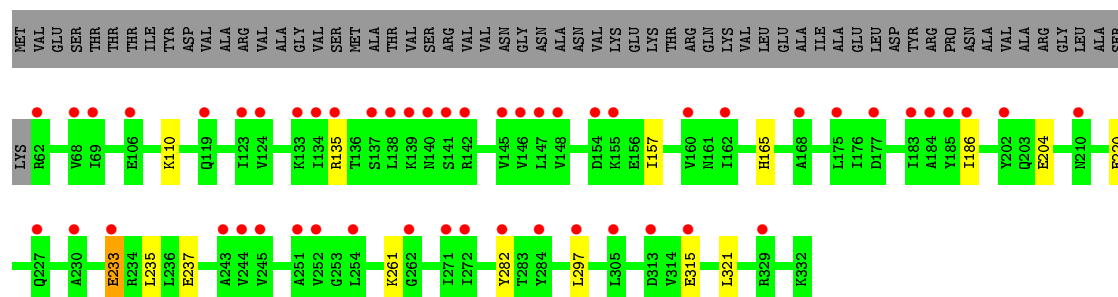
#### • Molecule 1: Catabolite control protein A



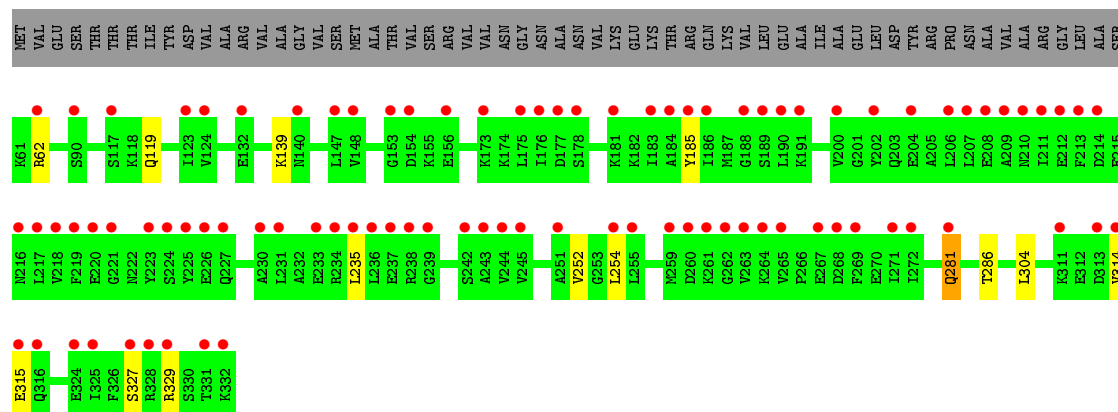
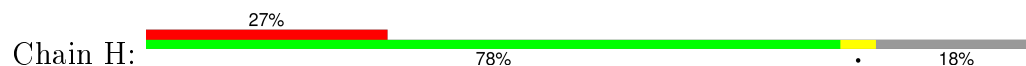
#### • Molecule 1: Catabolite control protein A







• Molecule 1: Catabolite control protein A



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	117.76Å 74.27Å 160.30Å 90.00° 102.36° 90.00°	Depositor
Resolution (Å)	19.90 – 1.90 19.87 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.4 (19.90-1.90) 99.5 (19.87-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.89 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.176 , 0.211 0.185 , 0.217	Depositor DCC
$R_{free}$ test set	10565 reflections (5.25%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.2	Xtriage
Anisotropy	0.295	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 55.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 211692 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	18486	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, CL

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	0.68	0/2188	0.77	3/2960 (0.1%)
1	B	0.62	0/2248	0.73	2/3040 (0.1%)
1	C	0.39	0/2142	0.54	0/2898
1	D	0.46	0/2164	0.61	0/2927
1	E	0.77	2/2223 (0.1%)	0.83	4/3005 (0.1%)
1	F	0.67	0/2210	0.75	3/2985 (0.1%)
1	G	0.58	0/2152	0.63	0/2911
1	H	0.48	0/2204	0.59	0/2976
All	All	0.60	2/17531 (0.0%)	0.69	12/23702 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	226	GLU	CD-OE1	5.18	1.31	1.25
1	E	226	GLU	CG-CD	5.17	1.59	1.51

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	83	ARG	NE-CZ-NH1	10.68	125.64	120.30
1	E	234	ARG	NE-CZ-NH2	-9.72	115.44	120.30
1	F	234	ARG	NE-CZ-NH2	-9.24	115.68	120.30
1	A	83	ARG	NE-CZ-NH2	-8.35	116.12	120.30
1	B	238	ARG	NE-CZ-NH1	7.85	124.23	120.30
1	E	234	ARG	NE-CZ-NH1	7.71	124.16	120.30
1	F	234	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	E	248	ASP	CB-CG-OD1	5.87	123.58	118.30
1	F	163	ASP	CB-CG-OD1	5.77	123.49	118.30
1	B	234	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	E	214	ASP	CB-CG-OD1	5.48	123.23	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	214	ASP	CB-CG-OD1	5.05	122.84	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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	2135	0	2148	10	0
1	B	2176	0	2178	16	0
1	C	2106	0	2116	4	0
1	D	2120	0	2130	12	0
1	E	2151	0	2164	23	0
1	F	2154	0	2172	9	0
1	G	2116	0	2134	7	0
1	H	2152	0	2178	9	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
2	E	5	0	0	0	0
2	F	10	0	0	0	0
2	G	5	0	0	0	0
3	E	1	0	0	0	0
4	A	244	0	0	2	0
4	B	217	0	0	3	0
4	C	17	0	0	0	0
4	D	92	0	0	4	0
4	E	297	0	0	9	0
4	F	255	0	0	1	0
4	G	137	0	0	1	0
4	H	76	0	0	0	0
All	All	18486	0	17220	85	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 2.

All (85) 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:B:226[A]:GLU:OE1	4:B:2079:HOH:O	1.65	1.14
1:D:119[A]:GLN:CD	4:D:415:HOH:O	1.90	1.08
1:E:303[A]:ARG:NE	4:E:2302:HOH:O	1.88	1.06
1:E:86[A]:ASP:OD1	4:E:2295:HOH:O	1.73	1.05
1:E:303[A]:ARG:CZ	4:E:2302:HOH:O	2.05	1.04
1:D:119[A]:GLN:OE1	4:D:415:HOH:O	1.76	1.03
1:E:303[A]:ARG:NH2	4:E:2302:HOH:O	1.94	1.01
1:B:317[B]:ASN:OD1	4:B:2115:HOH:O	1.79	1.00
1:E:86[A]:ASP:CG	4:E:2295:HOH:O	2.08	0.91
1:B:238:ARG:HG3	1:B:238:ARG:HH11	1.45	0.81
1:B:116:LEU:HD21	1:B:141:SER:HB3	1.68	0.76
1:E:204[B]:GLU:HG3	4:E:2131:HOH:O	1.85	0.74
1:E:86[A]:ASP:OD2	1:F:100:ASN:ND2	2.32	0.63
1:F:229:LYS:HE2	4:F:2203:HOH:O	2.02	0.60
1:E:89:ALA:HB2	1:E:302:MET:CE	2.31	0.60
1:H:304:LEU:HD11	1:H:314:VAL:HG11	1.84	0.59
1:B:131:ASP:HB3	1:B:134:ILE:HG12	1.88	0.56
1:E:315:GLU:OE1	1:E:315:GLU:N	2.28	0.56
1:B:112:LEU:O	1:B:116:LEU:HD13	2.07	0.55
1:E:89:ALA:HB2	1:E:302:MET:HE2	1.88	0.55
1:F:165:HIS:HE1	1:F:204:GLU:OE1	1.90	0.55
1:H:315:GLU:H	1:H:315:GLU:CD	2.10	0.55
1:E:233:GLU:OE1	4:E:2168:HOH:O	2.19	0.53
1:D:119[A]:GLN:CG	4:D:415:HOH:O	2.46	0.53
1:F:66:VAL:HB	1:F:96:MET:HE2	1.91	0.53
1:E:86[B]:ASP:OD1	1:E:96:MET:CE	2.58	0.52
1:B:329:ARG:NH1	4:B:2145:HOH:O	2.42	0.52
1:E:95:ASN:HD21	1:F:118[A]:LYS:NZ	2.09	0.51
1:E:126:MET:HG2	1:E:148[B]:VAL:HG23	1.91	0.51
1:B:238:ARG:HG3	1:B:238:ARG:NH1	2.20	0.50
1:H:286:THR:OG1	1:H:329:ARG:HG2	2.12	0.50
1:E:126:MET:CG	1:E:148[B]:VAL:HG23	2.42	0.49
1:D:89:ALA:HB2	1:D:302:MET:CE	2.42	0.48
1:B:112:LEU:HD11	1:B:134:ILE:HG23	1.94	0.48
1:E:187:MET:SD	1:E:190:LEU:HD13	2.54	0.48
1:G:282:TYR:CG	1:H:252:VAL:HG11	2.49	0.48
1:A:165:HIS:HD2	4:A:2111:HOH:O	1.97	0.47
1:E:89:ALA:HB2	1:E:302:MET:HE3	1.97	0.47
1:F:304:LEU:HD11	1:F:314:VAL:HG11	1.97	0.46
1:B:304:LEU:CD1	1:B:314:VAL:HG11	2.46	0.46
1:H:62:ARG:NH1	1:H:119:GLN:NE2	2.64	0.46
1:B:314:VAL:HB	1:B:317[B]:ASN:HD21	1.81	0.46

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:HIS:HE1	1:A:204:GLU:OE1	1.99	0.46
1:D:119[A]:GLN:HG3	4:D:415:HOH:O	2.12	0.46
1:C:100:ASN:HB3	1:D:83:ARG:NH2	2.30	0.46
1:B:273:SER:HB2	1:B:287[B]:LEU:HD21	1.98	0.46
1:D:89:ALA:HB2	1:D:302:MET:HE2	1.99	0.45
1:E:126:MET:HG3	1:E:148[B]:VAL:CG2	2.47	0.45
1:H:139:LYS:N	1:H:139:LYS:HD3	2.31	0.45
1:A:315:GLU:H	1:A:315:GLU:CD	2.19	0.45
1:C:199:MET:HE1	1:C:218:VAL:HG21	1.98	0.45
1:H:281:GLN:HA	1:H:281:GLN:HE21	1.82	0.44
1:E:107[B]:LYS:HD3	4:E:2298:HOH:O	2.16	0.44
1:D:187:MET:SD	1:D:190:LEU:HD13	2.58	0.44
1:A:220:GLU:HG3	1:A:221:GLY:N	2.33	0.44
1:C:63:THR:CG2	1:C:95:ASN:ND2	2.81	0.43
1:D:284:TYR:HA	1:D:285:PRO:C	2.39	0.43
1:H:286:THR:HG1	1:H:329:ARG:HG2	1.82	0.43
1:H:235:LEU:HD12	1:H:254:LEU:HD11	1.99	0.43
1:E:247:HIS:HE1	4:E:2192:HOH:O	2.01	0.43
1:A:118:LYS:NZ	1:B:95:ASN:HD21	2.17	0.43
1:F:161:ASN:O	1:F:320:VAL:HA	2.19	0.42
1:G:186:ILE:HD11	1:G:235:LEU:HD21	2.01	0.42
1:C:161:ASN:O	1:C:320:VAL:HA	2.18	0.42
1:G:233:GLU:HG3	1:G:261:LYS:HZ2	1.83	0.42
1:E:86[B]:ASP:OD1	1:E:96:MET:HE2	2.19	0.42
1:G:135:ARG:HG3	1:G:157:ILE:HD11	2.02	0.42
1:G:165:HIS:HE1	1:G:204:GLU:OE1	2.02	0.42
1:E:148[B]:VAL:HG11	1:E:301:ALA:CB	2.50	0.42
1:A:316[B]:GLN:NE2	4:A:2095:HOH:O	2.53	0.42
1:A:126:MET:CG	1:A:148:VAL:HG13	2.50	0.42
1:B:116:LEU:HD21	1:B:141:SER:CB	2.45	0.41
1:D:64:THR:HB	1:D:94:TYR:CD1	2.54	0.41
1:F:324:GLU:HG3	1:F:326:PHE:CE1	2.56	0.41
1:B:190:LEU:O	1:B:196:THR:HG23	2.20	0.41
1:A:284:TYR:HA	1:A:285:PRO:C	2.40	0.41
1:E:98:LEU:HD23	1:E:98:LEU:C	2.42	0.41
1:G:297:LEU:HD23	1:G:321:LEU:HD12	2.02	0.41
1:D:196:THR:O	1:D:200:VAL:HG23	2.20	0.40
1:D:64:THR:HA	1:D:121:ASP:OD2	2.21	0.40
1:A:241:THR:O	1:A:269:PHE:HA	2.21	0.40
1:G:110:LYS:NZ	4:G:2075:HOH:O	2.54	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	275/332 (83%)	271 (98%)	3 (1%)	1 (0%)	39	27
1	B	284/332 (86%)	277 (98%)	6 (2%)	1 (0%)	39	27
1	C	270/332 (81%)	263 (97%)	7 (3%)	0	100	100
1	D	272/332 (82%)	265 (97%)	7 (3%)	0	100	100
1	E	280/332 (84%)	276 (99%)	4 (1%)	0	100	100
1	F	277/332 (83%)	272 (98%)	4 (1%)	1 (0%)	39	27
1	G	271/332 (82%)	267 (98%)	4 (2%)	0	100	100
1	H	276/332 (83%)	271 (98%)	5 (2%)	0	100	100
All	All	2205/2656 (83%)	2162 (98%)	40 (2%)	3 (0%)	56	46

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	315	GLU
1	A	315	GLU
1	B	315	GLU

### 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	243/286 (85%)	240 (99%)	3 (1%)	78	76
1	B	250/286 (87%)	244 (98%)	6 (2%)	57	49

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	238/286 (83%)	229 (96%)	9 (4%)	40	28
1	D	240/286 (84%)	234 (98%)	6 (2%)	55	47
1	E	247/286 (86%)	242 (98%)	5 (2%)	63	57
1	F	244/286 (85%)	240 (98%)	4 (2%)	70	66
1	G	239/286 (84%)	235 (98%)	4 (2%)	68	64
1	H	244/286 (85%)	241 (99%)	3 (1%)	78	76
All	All	1945/2288 (85%)	1905 (98%)	40 (2%)	63	55

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	ARG
1	A	190	LEU
1	A	220	GLU
1	C	98	LEU
1	C	132	GLU
1	C	150	THR
1	C	155	LYS
1	C	156	GLU
1	C	190	LEU
1	C	215	GLU
1	C	258	MET
1	C	315	GLU
1	D	83	ARG
1	D	137	SER
1	D	199	MET
1	D	234	ARG
1	D	260	ASP
1	D	302	MET
1	B	156	GLU
1	B	234	ARG
1	B	238	ARG
1	B	287[A]	LEU
1	B	287[B]	LEU
1	B	315	GLU
1	E	107[A]	LYS
1	E	107[B]	LYS
1	E	190	LEU
1	E	229	LYS
1	E	234	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	F	165	HIS
1	F	234	ARG
1	F	238	ARG
1	F	313	ASP
1	G	220	GLU
1	G	233	GLU
1	G	237	GLU
1	G	315	GLU
1	H	185	TYR
1	H	281	GLN
1	H	327	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	ASN
1	A	216	ASN
1	A	247	HIS
1	C	95	ASN
1	C	216	ASN
1	C	247	HIS
1	C	316	GLN
1	D	95	ASN
1	D	103	ASN
1	D	247	HIS
1	B	95	ASN
1	B	103	ASN
1	B	216	ASN
1	E	95	ASN
1	E	210	ASN
1	E	247	HIS
1	F	95	ASN
1	F	103	ASN
1	F	165	HIS
1	F	216	ASN
1	F	247	HIS
1	G	247	HIS
1	H	95	ASN
1	H	119	GLN
1	H	247	HIS
1	H	281	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 ⓘ

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	SO4	A	2006	-	4,4,4	0.16	0	6,6,6	0.14	0
2	SO4	A	2007	-	4,4,4	0.23	0	6,6,6	0.20	0
2	SO4	B	2001	-	4,4,4	0.36	0	6,6,6	0.64	0
2	SO4	B	2003	-	4,4,4	0.11	0	6,6,6	0.17	0
2	SO4	E	2004	-	4,4,4	0.22	0	6,6,6	0.26	0
2	SO4	F	2002	-	4,4,4	0.25	0	6,6,6	0.43	0
2	SO4	F	2005	-	4,4,4	0.14	0	6,6,6	0.16	0
2	SO4	G	2008	-	4,4,4	0.13	0	6,6,6	0.19	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	SO4	A	2006	-	-	0/0/0/0	0/0/0/0
2	SO4	A	2007	-	-	0/0/0/0	0/0/0/0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	B	2001	-	-	0/0/0/0	0/0/0/0
2	SO4	B	2003	-	-	0/0/0/0	0/0/0/0
2	SO4	E	2004	-	-	0/0/0/0	0/0/0/0
2	SO4	F	2002	-	-	0/0/0/0	0/0/0/0
2	SO4	F	2005	-	-	0/0/0/0	0/0/0/0
2	SO4	G	2008	-	-	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.

No monomer is involved in short contacts.

## 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	271/332 (81%)	0.92	39 (14%) 3 4	15, 22, 40, 45	0
1	B	275/332 (82%)	1.02	46 (16%) 2 2	15, 23, 44, 52	0
1	C	270/332 (81%)	1.96	114 (42%) 0 0	47, 54, 65, 70	1 (0%)
1	D	270/332 (81%)	1.38	74 (27%) 1 1	28, 40, 56, 60	1 (0%)
1	E	271/332 (81%)	0.84	36 (13%) 4 5	13, 18, 31, 42	0
1	F	272/332 (81%)	0.96	38 (13%) 4 4	14, 21, 38, 44	0
1	G	271/332 (81%)	1.02	52 (19%) 2 2	20, 31, 44, 49	0
1	H	272/332 (81%)	1.62	90 (33%) 0 0	24, 43, 65, 67	1 (0%)
All	All	2172/2656 (81%)	1.21	489 (22%) 1 1	13, 29, 58, 70	3 (0%)

All (489) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	58	LEU	8.6
1	F	313	ASP	8.0
1	C	313	ASP	7.6
1	C	140	ASN	7.5
1	H	230	ALA	7.3
1	C	154	ASP	7.0
1	H	223	TYR	6.9
1	H	209	ALA	6.9
1	B	313	ASP	6.8
1	H	183	ILE	6.7
1	F	61	LYS	6.6
1	B	60	SER	6.5
1	C	63	THR	6.5
1	B	140	ASN	6.3
1	D	140	ASN	6.3
1	D	314	VAL	6.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	313	ASP	6.0
1	C	256[A]	SER	6.0
1	H	216	ASN	6.0
1	H	190	LEU	5.9
1	C	131	ASP	5.9
1	C	141	SER	5.8
1	C	191	LYS	5.8
1	H	153	GLY	5.8
1	G	244	VAL	5.6
1	C	106	GLU	5.5
1	H	243	ALA	5.4
1	H	181	LYS	5.4
1	H	191	LYS	5.3
1	B	59	ALA	5.2
1	H	244	VAL	5.2
1	C	190	LEU	5.2
1	A	313	ASP	5.2
1	H	154	ASP	5.1
1	H	313	ASP	5.0
1	A	62	ARG	5.0
1	C	119	GLN	5.0
1	C	315	GLU	4.9
1	C	138	LEU	4.9
1	B	62	ARG	4.9
1	D	141	SER	4.9
1	D	63	THR	4.8
1	H	260	ASP	4.8
1	D	136	THR	4.8
1	D	315	GLU	4.8
1	C	116	LEU	4.7
1	H	186	ILE	4.7
1	H	207	LEU	4.7
1	C	132	GLU	4.7
1	C	176	ILE	4.6
1	D	271	ILE	4.6
1	C	124	VAL	4.6
1	H	237	GLU	4.6
1	C	314	VAL	4.5
1	C	223	TYR	4.5
1	C	271	ILE	4.5
1	H	189	SER	4.5
1	H	184	ALA	4.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	G	271	ILE	4.4
1	H	178	SER	4.4
1	H	314	VAL	4.4
1	H	233	GLU	4.4
1	D	139	LYS	4.4
1	D	147	LEU	4.3
1	C	207	LEU	4.3
1	D	146	VAL	4.3
1	H	235	LEU	4.3
1	H	254	LEU	4.3
1	A	136	THR	4.3
1	A	244	VAL	4.2
1	F	62	ARG	4.2
1	G	62	ARG	4.2
1	G	313	ASP	4.2
1	C	254	LEU	4.2
1	H	271	ILE	4.2
1	H	255	LEU	4.1
1	B	116	LEU	4.1
1	H	236	LEU	4.1
1	C	188	GLY	4.1
1	C	105	VAL	4.1
1	B	244	VAL	4.1
1	D	91	MET	4.0
1	C	128	SER	4.0
1	A	140[A]	ASN	4.0
1	G	284	TYR	4.0
1	C	316	GLN	4.0
1	C	142	ARG	4.0
1	C	189	SER	4.0
1	B	136	THR	4.0
1	C	139	LYS	3.9
1	C	228	GLY	3.9
1	C	282	TYR	3.9
1	G	138	LEU	3.9
1	B	271	ILE	3.9
1	C	237	GLU	3.9
1	H	234[A]	ARG	3.8
1	H	212	GLU	3.8
1	H	211	ILE	3.8
1	D	305	LEU	3.8
1	F	154	ASP	3.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	209	ALA	3.8
1	D	119[A]	GLN	3.8
1	F	271	ILE	3.8
1	C	156	GLU	3.8
1	D	132	GLU	3.7
1	C	151	ILE	3.7
1	C	210	ASN	3.7
1	G	140	ASN	3.7
1	B	117	SER	3.7
1	B	141	SER	3.7
1	G	142	ARG	3.7
1	D	138	LEU	3.6
1	A	154	ASP	3.6
1	G	154	ASP	3.6
1	D	254	LEU	3.6
1	H	206	LEU	3.6
1	A	271	ILE	3.6
1	H	214	ASP	3.6
1	C	243	ALA	3.6
1	H	231	LEU	3.6
1	D	243	ALA	3.6
1	C	147	LEU	3.6
1	G	139	LYS	3.6
1	H	261	LYS	3.6
1	C	238	ARG	3.6
1	H	272	ILE	3.5
1	E	315	GLU	3.5
1	D	123	ILE	3.5
1	D	142	ARG	3.5
1	C	123	ILE	3.5
1	H	221	GLY	3.5
1	C	117	SER	3.5
1	D	118	LYS	3.5
1	F	191	LYS	3.5
1	C	134	ILE	3.5
1	H	328	ARG	3.5
1	G	243	ALA	3.5
1	C	264	LYS	3.4
1	D	272	ILE	3.4
1	G	148	VAL	3.4
1	C	255	LEU	3.4
1	D	137	SER	3.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	255[A]	LEU	3.4
1	D	116	LEU	3.4
1	G	315	GLU	3.4
1	D	133	LYS	3.4
1	H	202	TYR	3.4
1	A	305	LEU	3.4
1	C	206	LEU	3.4
1	C	104	ASP	3.4
1	H	262	GLY	3.3
1	D	148	VAL	3.3
1	B	272	ILE	3.3
1	B	148	VAL	3.3
1	D	155	LYS	3.3
1	D	316	GLN	3.3
1	C	215	GLU	3.3
1	D	124	VAL	3.3
1	D	312	GLU	3.3
1	C	272	ILE	3.3
1	G	254	LEU	3.2
1	A	243	ALA	3.2
1	C	213	PHE	3.2
1	H	219	PHE	3.2
1	C	175	LEU	3.2
1	H	210	ASN	3.2
1	C	148	VAL	3.2
1	D	85	VAL	3.2
1	H	177	ASP	3.2
1	H	315	GLU	3.2
1	C	111	VAL	3.2
1	C	155	LYS	3.2
1	D	89	ALA	3.2
1	G	124	VAL	3.2
1	H	148	VAL	3.2
1	C	317	ASN	3.2
1	H	281	GLN	3.2
1	F	183	ILE	3.2
1	H	175	LEU	3.2
1	B	132	GLU	3.1
1	E	271	ILE	3.1
1	A	254	LEU	3.1
1	B	137[A]	SER	3.1
1	H	185	TYR	3.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	E	148[A]	VAL	3.1
1	H	263	VAL	3.1
1	C	268	ASP	3.1
1	H	213	PHE	3.1
1	D	117	SER	3.1
1	C	311	LYS	3.1
1	C	244	VAL	3.1
1	C	235	LEU	3.1
1	C	196	THR	3.1
1	F	243	ALA	3.1
1	G	123	ILE	3.0
1	D	281	GLN	3.0
1	H	227	GLN	3.0
1	F	153	GLY	3.0
1	C	267	GLU	3.0
1	C	183	ILE	3.0
1	C	211	ILE	3.0
1	C	107	LYS	3.0
1	B	139	LYS	3.0
1	F	124	VAL	3.0
1	H	327	SER	3.0
1	D	93	LYS	3.0
1	G	272	ILE	3.0
1	C	113	GLU	3.0
1	D	183	ILE	3.0
1	E	287	LEU	3.0
1	A	142	ARG	2.9
1	C	135	ARG	2.9
1	G	147	LEU	2.9
1	E	123	ILE	2.9
1	H	176	ILE	2.9
1	D	104	ASP	2.9
1	H	220	GLU	2.9
1	C	153	GLY	2.9
1	C	212	GLU	2.9
1	A	138	LEU	2.9
1	H	245	VAL	2.9
1	B	202	TYR	2.9
1	H	188	GLY	2.9
1	F	254	LEU	2.9
1	D	90	SER	2.9
1	A	245	VAL	2.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	F	184	ALA	2.9
1	H	226	GLU	2.8
1	H	268	ASP	2.8
1	C	318	GLN	2.8
1	G	168	ALA	2.8
1	E	244	VAL	2.8
1	C	125	TYR	2.8
1	H	90[A]	SER	2.8
1	D	175	LEU	2.8
1	H	140	ASN	2.8
1	B	315	GLU	2.8
1	D	284	TYR	2.8
1	A	175	LEU	2.8
1	E	251	ALA	2.8
1	H	123	ILE	2.8
1	C	130	LEU	2.8
1	A	63	THR	2.8
1	D	105	VAL	2.8
1	H	329	ARG	2.8
1	F	235	LEU	2.7
1	H	217	LEU	2.7
1	C	177	ASP	2.7
1	A	186	ILE	2.7
1	C	110	LYS	2.7
1	G	185	TYR	2.7
1	C	136	THR	2.7
1	D	154	ASP	2.7
1	B	243	ALA	2.7
1	D	126	MET	2.7
1	D	153	GLY	2.7
1	E	255[A]	LEU	2.7
1	D	297	LEU	2.7
1	B	316	GLN	2.7
1	D	125	TYR	2.7
1	H	225	TYR	2.7
1	B	255	LEU	2.7
1	F	272	ILE	2.7
1	H	208	GLU	2.7
1	D	106	GLU	2.6
1	C	234	ARG	2.6
1	A	139	LYS	2.6
1	B	254	LEU	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	305	LEU	2.6
1	B	113	GLU	2.6
1	E	279	ILE	2.6
1	F	244	VAL	2.6
1	H	124	VAL	2.6
1	H	265	VAL	2.6
1	B	184	ALA	2.6
1	E	243	ALA	2.6
1	C	262	GLY	2.6
1	E	313	ASP	2.6
1	C	118	LYS	2.6
1	C	129	SER	2.6
1	G	137	SER	2.6
1	D	135[A]	ARG	2.6
1	G	230	ALA	2.6
1	H	332	LYS	2.6
1	A	123	ILE	2.6
1	E	245	VAL	2.6
1	C	194[A]	GLU	2.6
1	G	282	TYR	2.6
1	C	102	ASP	2.6
1	A	160	VAL	2.6
1	B	175	LEU	2.6
1	A	314	VAL	2.6
1	C	68	VAL	2.6
1	B	123	ILE	2.6
1	D	128	SER	2.6
1	E	154	ASP	2.6
1	A	183	ILE	2.5
1	D	130	LEU	2.5
1	G	305	LEU	2.5
1	G	210	ASN	2.5
1	C	186	ILE	2.5
1	F	134	ILE	2.5
1	H	264	LYS	2.5
1	C	236	LEU	2.5
1	D	269	PHE	2.5
1	C	145	VAL	2.5
1	B	124	VAL	2.5
1	G	183	ILE	2.5
1	G	329	ARG	2.5
1	G	175	LEU	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	H	324	GLU	2.5
1	D	120	VAL	2.5
1	D	245	VAL	2.5
1	B	160	VAL	2.5
1	C	173	LYS	2.5
1	G	135	ARG	2.4
1	D	244	VAL	2.4
1	H	117	SER	2.4
1	D	94	TYR	2.4
1	H	238[A]	ARG	2.4
1	A	304	LEU	2.4
1	C	269	PHE	2.4
1	H	242	SER	2.4
1	A	148	VAL	2.4
1	G	252	VAL	2.4
1	C	152	ASP	2.4
1	C	179	GLY	2.4
1	C	239	GLY	2.4
1	G	162	ILE	2.4
1	E	62	ARG	2.4
1	B	146	VAL	2.4
1	D	301	ALA	2.4
1	G	227	GLN	2.4
1	D	280	THR	2.4
1	H	331	THR	2.4
1	B	154	ASP	2.4
1	G	141	SER	2.4
1	C	146	VAL	2.4
1	H	311	LYS	2.4
1	C	103	ASN	2.4
1	D	282	TYR	2.4
1	B	185	TYR	2.4
1	H	269	PHE	2.4
1	A	162	ILE	2.3
1	B	186	ILE	2.3
1	F	186	ILE	2.3
1	G	155	LYS	2.3
1	F	255	LEU	2.3
1	H	251	ALA	2.3
1	E	250	VAL	2.3
1	F	132	GLU	2.3
1	H	200	VAL	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	H	316	GLN	2.3
1	G	69	ILE	2.3
1	C	216	ASN	2.3
1	C	230	ALA	2.3
1	A	252	VAL	2.3
1	C	263	VAL	2.3
1	A	81	ILE	2.3
1	C	169	TYR	2.3
1	F	202	TYR	2.3
1	B	142	ARG	2.3
1	A	147	LEU	2.3
1	B	287[A]	LEU	2.3
1	E	149	GLY	2.3
1	A	106	GLU	2.3
1	F	315	GLU	2.3
1	B	68	VAL	2.3
1	F	160	VAL	2.3
1	A	119	GLN	2.3
1	A	269	PHE	2.3
1	D	113	GLU	2.3
1	H	132	GLU	2.3
1	C	310	LEU	2.3
1	D	308	LEU	2.3
1	G	297	LEU	2.3
1	E	85	VAL	2.3
1	G	245	VAL	2.3
1	C	137	SER	2.3
1	C	283	THR	2.3
1	C	296	ASP	2.2
1	G	68	VAL	2.2
1	E	93	LYS	2.2
1	A	232	ALA	2.2
1	B	183	ILE	2.2
1	G	202	TYR	2.2
1	B	273	SER	2.2
1	E	147	LEU	2.2
1	E	235	LEU	2.2
1	H	147	LEU	2.2
1	G	119	GLN	2.2
1	D	290	VAL	2.2
1	H	156	GLU	2.2
1	C	329	ARG	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	E	63	THR	2.2
1	A	301	ALA	2.2
1	C	162	ILE	2.2
1	E	69	ILE	2.2
1	F	279	ILE	2.2
1	B	125	TYR	2.2
1	F	138	LEU	2.2
1	F	305	LEU	2.2
1	C	332	LYS	2.2
1	G	160	VAL	2.2
1	A	184	ALA	2.2
1	F	69	ILE	2.2
1	E	304	LEU	2.2
1	C	143	THR	2.2
1	F	156	GLU	2.2
1	H	204	GLU	2.2
1	E	160	VAL	2.2
1	F	245	VAL	2.2
1	H	259	MET	2.2
1	F	301	ALA	2.2
1	G	262	GLY	2.2
1	A	69	ILE	2.2
1	C	150	THR	2.2
1	E	254	LEU	2.2
1	F	147	LEU	2.2
1	D	329	ARG	2.2
1	E	124	VAL	2.2
1	H	224	SER	2.2
1	B	212[A]	GLU	2.1
1	E	140	ASN	2.1
1	H	267	GLU	2.1
1	C	281	GLN	2.1
1	F	142	ARG	2.1
1	G	186	ILE	2.1
1	G	133	LYS	2.1
1	D	92	TYR	2.1
1	E	125	TYR	2.1
1	A	315	GLU	2.1
1	C	178	SER	2.1
1	E	138	LEU	2.1
1	D	160	VAL	2.1
1	G	146	VAL	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	223	TYR	2.1
1	A	297	LEU	2.1
1	C	305	LEU	2.1
1	D	149	GLY	2.1
1	D	275	ALA	2.1
1	B	191	LYS	2.1
1	A	146	VAL	2.1
1	F	66	VAL	2.1
1	F	148	VAL	2.1
1	H	218	VAL	2.1
1	G	233	GLU	2.1
1	D	306	THR	2.1
1	C	126	MET	2.1
1	D	279	ILE	2.1
1	E	153	GLY	2.1
1	A	185	TYR	2.1
1	B	147	LEU	2.1
1	E	175	LEU	2.1
1	G	184	ALA	2.1
1	E	146	VAL	2.1
1	F	146	VAL	2.1
1	G	177	ASP	2.1
1	F	141	SER	2.1
1	H	173	LYS	2.1
1	D	258	MET	2.1
1	C	217	LEU	2.1
1	C	181	LYS	2.1
1	B	155	LYS	2.1
1	G	145	VAL	2.1
1	C	95	ASN	2.0
1	B	156	GLU	2.0
1	C	326	PHE	2.0
1	D	73	ILE	2.0
1	D	186	ILE	2.0
1	G	251	ALA	2.0
1	H	62	ARG	2.0
1	C	284	TYR	2.0
1	F	217	LEU	2.0
1	C	290	VAL	2.0
1	B	245	VAL	2.0
1	F	314	VAL	2.0
1	H	239	GLY	2.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	E	155	LYS	2.0
1	E	184	ALA	2.0
1	G	134	ILE	2.0
1	D	235	LEU	2.0
1	E	305	LEU	2.0
1	G	106	GLU	2.0
1	F	85	VAL	2.0
1	E	171[A]	SER	2.0
1	C	208	GLU	2.0
1	D	184	ALA	2.0
1	H	325	ILE	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	SO4	F	2002	5/5	0.96	0.23	4.81	36,39,44,44	0
2	SO4	B	2003	5/5	0.96	0.25	4.03	55,56,57,57	0
2	SO4	B	2001	5/5	0.97	0.17	0.87	34,36,39,41	0
3	CL	E	2010	1/1	0.99	0.07	-3.71	20,20,20,20	0
2	SO4	G	2008	5/5	0.81	0.35	-	61,63,65,66	0
2	SO4	E	2004	5/5	0.93	0.26	-	57,59,60,60	0
2	SO4	A	2006	5/5	0.84	0.30	-	81,81,82,82	0
2	SO4	A	2007	5/5	0.90	0.30	-	80,80,80,81	0
2	SO4	F	2005	5/5	0.82	0.34	-	74,74,75,76	0

## 6.5 Other polymers

There are no such residues in this entry.