



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 04:08 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

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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

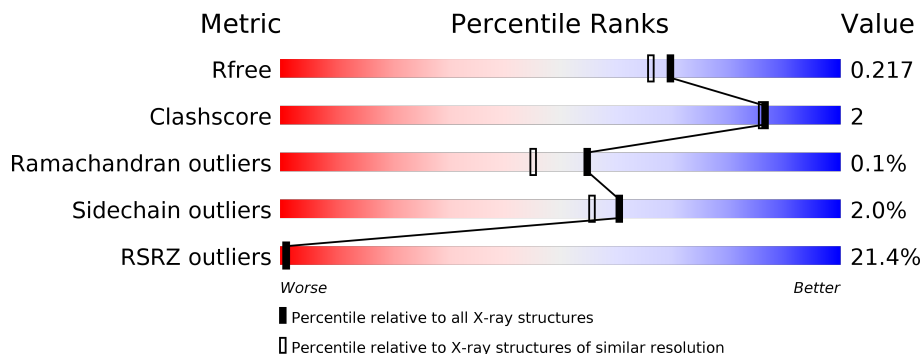
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	100719	5047 (1.90-1.90)
Clashscore	112137	5731 (1.90-1.90)
Ramachandran outliers	110173	5669 (1.90-1.90)
Sidechain outliers	110143	5670 (1.90-1.90)
RSRZ outliers	101464	5100 (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 ≥ 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>33%</div> <div> <div></div> <div>77%</div> <div>5%</div> <div>19%</div> </div> </div>
1	D	332	<div> <div>21%</div> <div> <div></div> <div>76%</div> <div>5% •</div> <div>19%</div> </div> </div>
1	E	332	<div> <div>10%</div> <div> <div></div> <div>75%</div> <div>6% •</div> <div>18%</div> </div> </div>
1	F	332	<div> <div>10%</div> <div> <div></div> <div>77%</div> <div>5% •</div> <div>18%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
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: O₄S).



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		

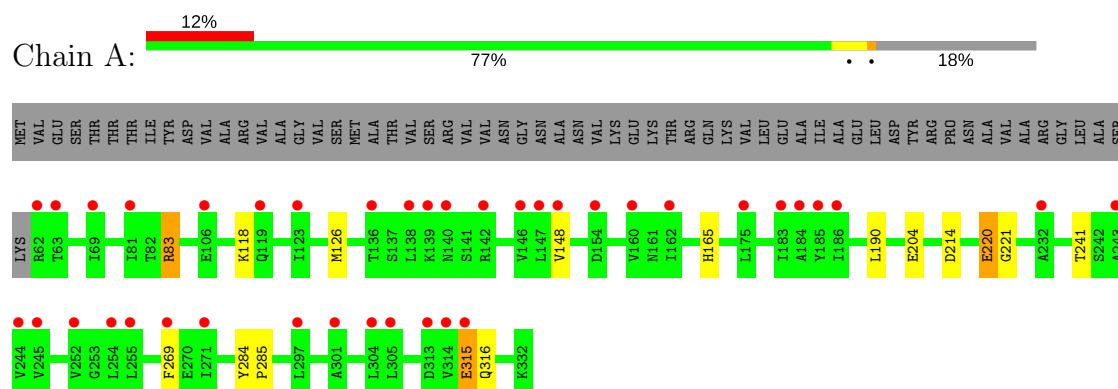
- Molecule 4 is water.

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

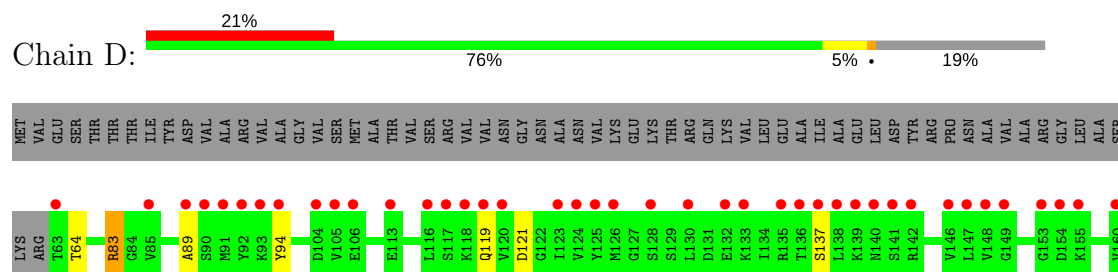
• Molecule 1: Catabolite control protein A

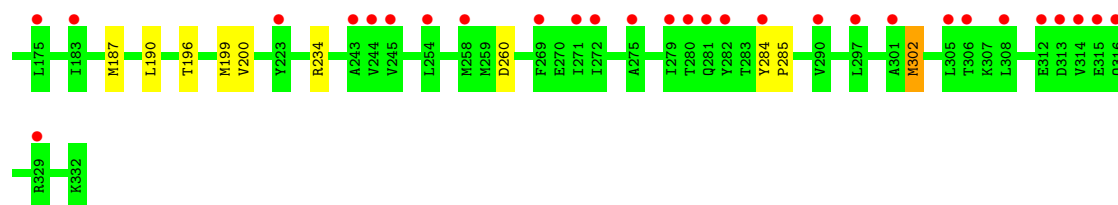


• Molecule 1: Catabolite control protein A

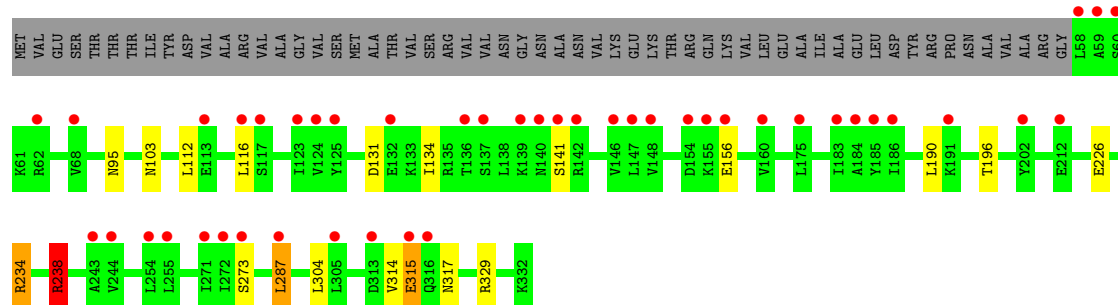
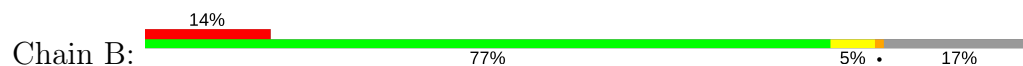


• Molecule 1: Catabolite control protein A

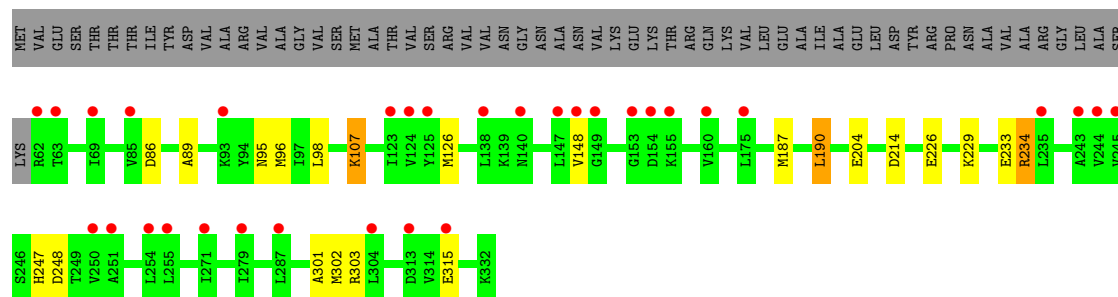
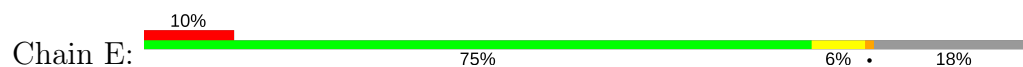




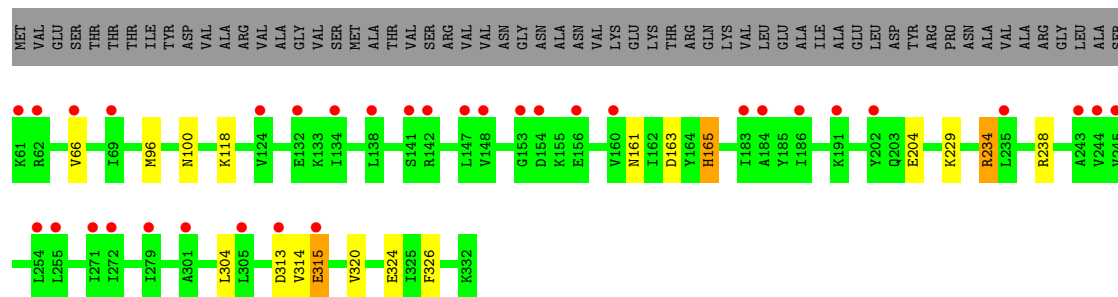
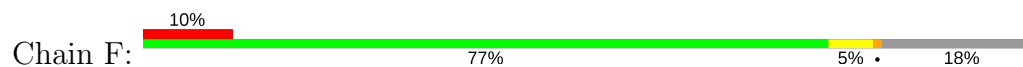
• Molecule 1: Catabolite control protein A



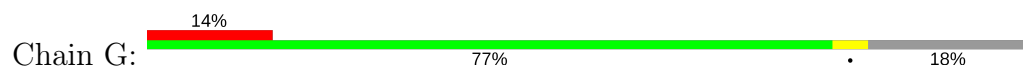
• Molecule 1: Catabolite control protein A

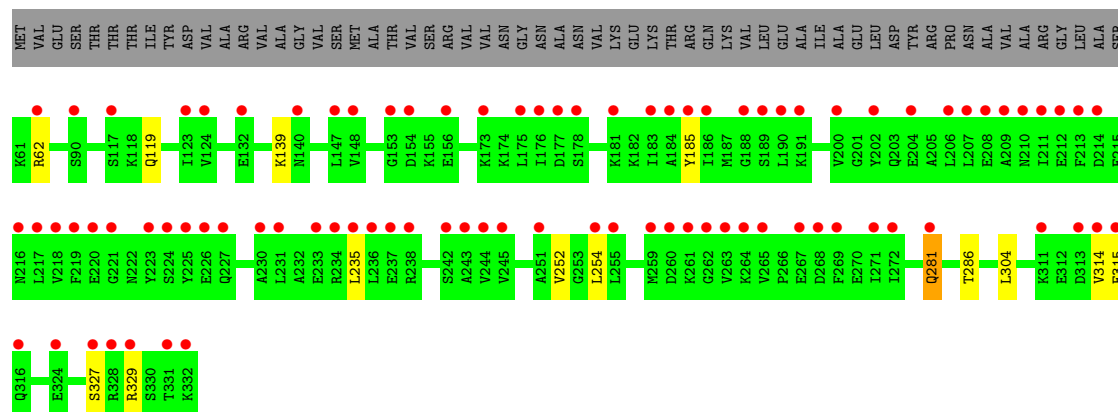


• Molecule 1: Catabolite control protein A



• 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	23.2	Xtriage
Anisotropy	0.295	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 55.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	18486	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

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

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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:126:MET:HG2	1:E:148[B]:VAL:HG23	1.91	0.51
1:E:95:ASN:HD21	1:F:118[A]:LYS:NZ	2.09	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:A:165:HIS:HE1	1:A:204:GLU:OE1	1.99	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:314:VAL:HB	1:B:317[B]:ASN:HD21	1.81	0.46
1:B:273:SER:HB2	1:B:287[B]:LEU:HD21	1.98	0.46
1:C:100:ASN:HB3	1:D:83:ARG:NH2	2.30	0.46
1:D:119[A]:GLN:HG3	4:D:415:HOH:O	2.12	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:A:220:GLU:HG3	1:A:221:GLY:N	2.33	0.44
1:D:187:MET:SD	1:D:190:LEU:HD13	2.58	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:235:LEU:HD12	1:H:254:LEU:HD11	1.99	0.43
1:H:286:THR:HG1	1:H:329:ARG:HG2	1.82	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:126:MET:CG	1:A:148:VAL:HG13	2.50	0.42
1:A:316[B]:GLN:NE2	4:A:2095:HOH:O	2.53	0.42
1:B:116:LEU:HD21	1:B:141:SER:CB	2.45	0.41
1:B:190:LEU:O	1:B:196:THR:HG23	2.20	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: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:A:241:THR:O	1:A:269:PHE:HA	2.21	0.40
1:D:64:THR:HA	1:D:121:ASP:OD2	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%)	38	26
1	B	284/332 (86%)	277 (98%)	6 (2%)	1 (0%)	38	26
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%)	38	26
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%)	55	45

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%)	75	75
1	B	250/286 (87%)	244 (98%)	6 (2%)	54	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	238/286 (83%)	229 (96%)	9 (4%)	38	27
1	D	240/286 (84%)	234 (98%)	6 (2%)	53	45
1	E	247/286 (86%)	242 (98%)	5 (2%)	60	55
1	F	244/286 (85%)	240 (98%)	4 (2%)	68	65
1	G	239/286 (84%)	235 (98%)	4 (2%)	66	62
1	H	244/286 (85%)	241 (99%)	3 (1%)	75	75
All	All	1945/2288 (85%)	1905 (98%)	40 (2%)	60	53

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

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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	0.21	0	6,6,6	0.10	0
2	SO4	A	2007	-	4,4,4	0.21	0	6,6,6	0.28	0
2	SO4	B	2001	-	4,4,4	0.25	0	6,6,6	0.68	0
2	SO4	B	2003	-	4,4,4	0.21	0	6,6,6	0.15	0
2	SO4	E	2004	-	4,4,4	0.27	0	6,6,6	0.23	0
2	SO4	F	2002	-	4,4,4	0.14	0	6,6,6	0.47	0
2	SO4	F	2005	-	4,4,4	0.16	0	6,6,6	0.19	0
2	SO4	G	2008	-	4,4,4	0.24	0	6,6,6	0.22	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

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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, 95th 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 ²)	Q<0.9
1	A	271/332 (81%)	0.87	39 (14%) 3 3	15, 22, 40, 45	0
1	B	275/332 (82%)	0.98	45 (16%) 2 2	15, 23, 44, 52	0
1	C	270/332 (81%)	1.90	109 (40%) 0 0	47, 54, 65, 70	1 (0%)
1	D	270/332 (81%)	1.33	70 (25%) 1 1	28, 40, 56, 60	1 (0%)
1	E	271/332 (81%)	0.80	32 (11%) 5 5	13, 18, 31, 42	0
1	F	272/332 (81%)	0.91	34 (12%) 4 5	14, 21, 38, 44	0
1	G	271/332 (81%)	0.98	48 (17%) 2 2	20, 31, 44, 49	0
1	H	272/332 (81%)	1.57	88 (32%) 0 0	24, 43, 65, 67	1 (0%)
All	All	2172/2656 (81%)	1.17	465 (21%) 1 1	13, 29, 58, 70	3 (0%)

All (465) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	58	LEU	8.4
1	F	313	ASP	7.9
1	C	313	ASP	7.5
1	C	140	ASN	7.4
1	H	230	ALA	7.1
1	C	154	ASP	6.9
1	H	223	TYR	6.9
1	H	209	ALA	6.7
1	B	313	ASP	6.6
1	H	183	ILE	6.5
1	F	61	LYS	6.5
1	C	63	THR	6.4
1	B	60	SER	6.4
1	B	140	ASN	6.2
1	D	140	ASN	6.2
1	D	313	ASP	5.9

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Mol	Chain	Res	Type	RSRZ
1	H	216	ASN	5.9
1	C	256[A]	SER	5.9
1	D	314	VAL	5.9
1	H	190	LEU	5.8
1	C	131	ASP	5.8
1	C	191	LYS	5.7
1	C	141	SER	5.7
1	H	153	GLY	5.7
1	G	244	VAL	5.4
1	C	106	GLU	5.4
1	H	181	LYS	5.3
1	H	243	ALA	5.3
1	H	191	LYS	5.2
1	B	59	ALA	5.1
1	H	244	VAL	5.1
1	A	313	ASP	5.1
1	C	190	LEU	5.1
1	H	154	ASP	5.0
1	A	62	ARG	4.9
1	H	313	ASP	4.9
1	C	119	GLN	4.9
1	C	315	GLU	4.9
1	B	62	ARG	4.9
1	C	138	LEU	4.8
1	D	141	SER	4.8
1	D	63	THR	4.8
1	D	315	GLU	4.7
1	H	260	ASP	4.7
1	D	136	THR	4.7
1	C	132	GLU	4.7
1	C	116	LEU	4.6
1	H	186	ILE	4.6
1	H	207	LEU	4.6
1	H	237	GLU	4.5
1	C	176	ILE	4.5
1	D	271	ILE	4.5
1	C	124	VAL	4.5
1	C	223	TYR	4.4
1	C	314	VAL	4.4
1	H	189	SER	4.4
1	D	139	LYS	4.4
1	C	271	ILE	4.4

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Mol	Chain	Res	Type	RSRZ
1	H	233	GLU	4.4
1	H	184	ALA	4.3
1	H	178	SER	4.3
1	G	271	ILE	4.3
1	H	314	VAL	4.3
1	D	147	LEU	4.2
1	F	62	ARG	4.2
1	G	62	ARG	4.2
1	A	136	THR	4.2
1	C	207	LEU	4.2
1	H	235	LEU	4.2
1	H	254	LEU	4.2
1	D	146	VAL	4.2
1	G	313	ASP	4.1
1	C	254	LEU	4.1
1	A	244	VAL	4.1
1	H	271	ILE	4.1
1	H	255	LEU	4.0
1	D	91	MET	4.0
1	B	116	LEU	4.0
1	H	236	LEU	4.0
1	C	188	GLY	4.0
1	C	142	ARG	4.0
1	C	105	VAL	4.0
1	G	284	TYR	3.9
1	A	140[A]	ASN	3.9
1	C	128	SER	3.9
1	C	316	GLN	3.9
1	B	244	VAL	3.9
1	C	189	SER	3.9
1	B	136	THR	3.9
1	C	139	LYS	3.9
1	C	282	TYR	3.9
1	C	228	GLY	3.8
1	H	234[A]	ARG	3.8
1	C	237	GLU	3.8
1	H	212	GLU	3.8
1	G	138	LEU	3.8
1	B	271	ILE	3.8
1	D	119[A]	GLN	3.8
1	F	154	ASP	3.7
1	H	211	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	156	GLU	3.7
1	D	305	LEU	3.7
1	C	209	ALA	3.7
1	D	132	GLU	3.7
1	F	271	ILE	3.7
1	C	210	ASN	3.7
1	G	142	ARG	3.6
1	G	140	ASN	3.6
1	C	151	ILE	3.6
1	B	117	SER	3.6
1	B	141	SER	3.6
1	A	154	ASP	3.5
1	G	154	ASP	3.5
1	D	138	LEU	3.5
1	H	214	ASP	3.5
1	C	238	ARG	3.5
1	G	139	LYS	3.5
1	H	261	LYS	3.5
1	D	254	LEU	3.5
1	H	206	LEU	3.5
1	C	243	ALA	3.5
1	A	271	ILE	3.5
1	E	315	GLU	3.5
1	H	231	LEU	3.5
1	D	243	ALA	3.5
1	C	147	LEU	3.5
1	D	142	ARG	3.5
1	D	118	LYS	3.4
1	F	191	LYS	3.4
1	H	328	ARG	3.4
1	H	272	ILE	3.4
1	H	221	GLY	3.4
1	C	264	LYS	3.4
1	C	117	SER	3.4
1	D	123	ILE	3.4
1	C	123	ILE	3.4
1	G	243	ALA	3.4
1	C	134	ILE	3.4
1	D	133	LYS	3.3
1	G	315	GLU	3.3
1	D	272	ILE	3.3
1	D	137	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	H	202	TYR	3.3
1	C	255	LEU	3.3
1	G	148	VAL	3.3
1	C	104	ASP	3.3
1	A	255[A]	LEU	3.3
1	D	116	LEU	3.3
1	H	262	GLY	3.3
1	A	305	LEU	3.3
1	C	206	LEU	3.3
1	D	155	LYS	3.3
1	C	215	GLU	3.2
1	D	316	GLN	3.2
1	D	312	GLU	3.2
1	B	272	ILE	3.2
1	D	148	VAL	3.2
1	B	148	VAL	3.2
1	D	124	VAL	3.2
1	H	315	GLU	3.2
1	H	210	ASN	3.2
1	H	177	ASP	3.2
1	A	243	ALA	3.2
1	C	155	LYS	3.2
1	C	272	ILE	3.2
1	G	254	LEU	3.1
1	C	213	PHE	3.1
1	H	219	PHE	3.1
1	C	175	LEU	3.1
1	C	317	ASN	3.1
1	H	281	GLN	3.1
1	C	148	VAL	3.1
1	D	85	VAL	3.1
1	B	132	GLU	3.1
1	D	89	ALA	3.1
1	C	111	VAL	3.1
1	H	185	TYR	3.1
1	B	137[A]	SER	3.1
1	G	124	VAL	3.1
1	H	148	VAL	3.1
1	H	175	LEU	3.1
1	F	183	ILE	3.1
1	C	311	LYS	3.1
1	C	268	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	254	LEU	3.0
1	E	271	ILE	3.0
1	D	117	SER	3.0
1	E	148[A]	VAL	3.0
1	H	263	VAL	3.0
1	H	213	PHE	3.0
1	C	196	THR	3.0
1	C	267	GLU	3.0
1	D	281	GLN	3.0
1	H	227	GLN	3.0
1	C	107	LYS	3.0
1	C	244	VAL	3.0
1	F	243	ALA	3.0
1	C	235	LEU	3.0
1	B	139	LYS	3.0
1	F	153	GLY	3.0
1	D	93	LYS	3.0
1	G	123	ILE	2.9
1	C	113	GLU	2.9
1	C	183	ILE	2.9
1	C	211	ILE	2.9
1	H	327	SER	2.9
1	A	142	ARG	2.9
1	C	135	ARG	2.9
1	F	124	VAL	2.9
1	G	272	ILE	2.9
1	H	220	GLU	2.9
1	C	212	GLU	2.9
1	E	287	LEU	2.9
1	D	104	ASP	2.9
1	D	183	ILE	2.9
1	C	153	GLY	2.8
1	G	147	LEU	2.8
1	E	123	ILE	2.8
1	H	176	ILE	2.8
1	B	202	TYR	2.8
1	H	226	GLU	2.8
1	H	188	GLY	2.8
1	D	90	SER	2.8
1	A	138	LEU	2.8
1	C	318	GLN	2.8
1	C	125	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	315	GLU	2.8
1	H	268	ASP	2.8
1	H	245	VAL	2.8
1	F	184	ALA	2.8
1	F	254	LEU	2.8
1	H	140	ASN	2.8
1	H	90[A]	SER	2.8
1	D	284	TYR	2.8
1	A	245	VAL	2.8
1	G	168	ALA	2.7
1	E	244	VAL	2.7
1	D	175	LEU	2.7
1	H	329	ARG	2.7
1	A	63	THR	2.7
1	E	251	ALA	2.7
1	C	110	LYS	2.7
1	A	175	LEU	2.7
1	D	126	MET	2.7
1	H	123	ILE	2.7
1	G	185	TYR	2.7
1	C	130	LEU	2.7
1	C	177	ASP	2.7
1	C	136	THR	2.7
1	D	154	ASP	2.7
1	D	105	VAL	2.7
1	D	153	GLY	2.7
1	F	235	LEU	2.7
1	H	217	LEU	2.7
1	A	186	ILE	2.6
1	B	243	ALA	2.6
1	B	316	GLN	2.6
1	D	125	TYR	2.6
1	H	225	TYR	2.6
1	H	208	GLU	2.6
1	E	255[A]	LEU	2.6
1	D	297	LEU	2.6
1	D	106	GLU	2.6
1	C	234	ARG	2.6
1	A	139	LYS	2.6
1	B	113	GLU	2.6
1	B	255	LEU	2.6
1	F	272	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	118	LYS	2.6
1	D	135[A]	ARG	2.6
1	H	332	LYS	2.6
1	C	194[A]	GLU	2.6
1	E	313	ASP	2.6
1	C	262	GLY	2.6
1	G	282	TYR	2.5
1	B	184	ALA	2.5
1	B	254	LEU	2.5
1	B	305	LEU	2.5
1	E	243	ALA	2.5
1	C	129	SER	2.5
1	G	137	SER	2.5
1	E	279	ILE	2.5
1	F	244	VAL	2.5
1	H	124	VAL	2.5
1	H	265	VAL	2.5
1	G	230	ALA	2.5
1	C	102	ASP	2.5
1	A	123	ILE	2.5
1	E	245	VAL	2.5
1	D	128	SER	2.5
1	E	154	ASP	2.5
1	A	160	VAL	2.5
1	B	175	LEU	2.5
1	H	264	LYS	2.5
1	G	210	ASN	2.5
1	B	123	ILE	2.5
1	A	314	VAL	2.5
1	C	68	VAL	2.5
1	G	329	ARG	2.5
1	A	183	ILE	2.4
1	H	324	GLU	2.4
1	D	130	LEU	2.4
1	G	305	LEU	2.4
1	C	173	LYS	2.4
1	C	186	ILE	2.4
1	F	134	ILE	2.4
1	G	135	ARG	2.4
1	C	236	LEU	2.4
1	D	269	PHE	2.4
1	H	238[A]	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	183	ILE	2.4
1	C	145	VAL	2.4
1	B	124	VAL	2.4
1	G	175	LEU	2.4
1	D	94	TYR	2.4
1	H	117	SER	2.4
1	E	62	ARG	2.4
1	D	120	VAL	2.4
1	D	245	VAL	2.4
1	B	160	VAL	2.4
1	H	242	SER	2.4
1	C	152	ASP	2.4
1	C	179	GLY	2.4
1	C	239	GLY	2.4
1	G	227	GLN	2.4
1	D	244	VAL	2.4
1	A	304	LEU	2.3
1	C	269	PHE	2.3
1	H	311	LYS	2.3
1	D	280	THR	2.3
1	H	331	THR	2.3
1	B	154	ASP	2.3
1	A	148	VAL	2.3
1	G	141	SER	2.3
1	G	162	ILE	2.3
1	G	252	VAL	2.3
1	C	103	ASN	2.3
1	D	301	ALA	2.3
1	D	282	TYR	2.3
1	B	185	TYR	2.3
1	G	155	LYS	2.3
1	B	146	VAL	2.3
1	F	132	GLU	2.3
1	H	316	GLN	2.3
1	C	146	VAL	2.3
1	C	216	ASN	2.3
1	H	269	PHE	2.3
1	B	142	ARG	2.3
1	A	162	ILE	2.3
1	B	186	ILE	2.3
1	F	186	ILE	2.3
1	H	251	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	106	GLU	2.3
1	F	255	LEU	2.3
1	F	315	GLU	2.3
1	C	169	TYR	2.2
1	F	202	TYR	2.2
1	A	119	GLN	2.2
1	D	113	GLU	2.2
1	H	132	GLU	2.2
1	C	230	ALA	2.2
1	E	250	VAL	2.2
1	H	200	VAL	2.2
1	G	69	ILE	2.2
1	E	149	GLY	2.2
1	A	252	VAL	2.2
1	C	263	VAL	2.2
1	A	81	ILE	2.2
1	A	147	LEU	2.2
1	B	287[A]	LEU	2.2
1	E	93	LYS	2.2
1	A	269	PHE	2.2
1	C	137	SER	2.2
1	C	283	THR	2.2
1	B	68	VAL	2.2
1	F	160	VAL	2.2
1	C	310	LEU	2.2
1	C	329	ARG	2.2
1	D	308	LEU	2.2
1	G	297	LEU	2.2
1	C	296	ASP	2.2
1	H	156	GLU	2.2
1	G	119	GLN	2.2
1	G	202	TYR	2.2
1	E	85	VAL	2.2
1	G	245	VAL	2.2
1	C	332	LYS	2.2
1	B	273	SER	2.2
1	E	63	THR	2.2
1	A	232	ALA	2.2
1	B	125	TYR	2.2
1	G	68	VAL	2.2
1	B	183	ILE	2.1
1	F	279	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	259	MET	2.1
1	E	147	LEU	2.1
1	E	235	LEU	2.1
1	F	156	GLU	2.1
1	H	147	LEU	2.1
1	H	204	GLU	2.1
1	A	301	ALA	2.1
1	D	290	VAL	2.1
1	D	329	ARG	2.1
1	C	143	THR	2.1
1	C	162	ILE	2.1
1	E	69	ILE	2.1
1	F	138	LEU	2.1
1	F	305	LEU	2.1
1	A	184	ALA	2.1
1	B	212[A]	GLU	2.1
1	H	267	GLU	2.1
1	F	142	ARG	2.1
1	G	133	LYS	2.1
1	E	140	ASN	2.1
1	G	160	VAL	2.1
1	G	262	GLY	2.1
1	C	150	THR	2.1
1	C	281	GLN	2.1
1	A	315	GLU	2.1
1	F	69	ILE	2.1
1	E	304	LEU	2.1
1	F	301	ALA	2.1
1	H	224	SER	2.1
1	D	92	TYR	2.1
1	E	125	TYR	2.1
1	E	160	VAL	2.1
1	F	245	VAL	2.1
1	B	191	LYS	2.1
1	A	69	ILE	2.1
1	C	178	SER	2.1
1	E	254	LEU	2.1
1	F	147	LEU	2.1
1	G	233	GLU	2.1
1	D	223	TYR	2.1
1	C	126	MET	2.1
1	E	124	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	186	ILE	2.1
1	E	138	LEU	2.1
1	D	149	GLY	2.1
1	H	173	LYS	2.1
1	D	258	MET	2.0
1	D	306	THR	2.0
1	A	185	TYR	2.0
1	D	160	VAL	2.0
1	G	146	VAL	2.0
1	C	181	LYS	2.0
1	D	275	ALA	2.0
1	B	155	LYS	2.0
1	E	153	GLY	2.0
1	A	297	LEU	2.0
1	C	305	LEU	2.0
1	G	177	ASP	2.0
1	F	141	SER	2.0
1	A	146	VAL	2.0
1	F	66	VAL	2.0
1	F	148	VAL	2.0
1	H	62	ARG	2.0
1	H	218	VAL	2.0
1	B	156	GLU	2.0
1	G	184	ALA	2.0
1	C	95	ASN	2.0
1	D	279	ILE	2.0
1	B	147	LEU	2.0
1	E	175	LEU	2.0
1	E	155	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

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, 95th 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 ²)	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 [i](#)

There are no such residues in this entry.