



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:55 AM UTC

PDB ID : 2020 / pdb_00002o20
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

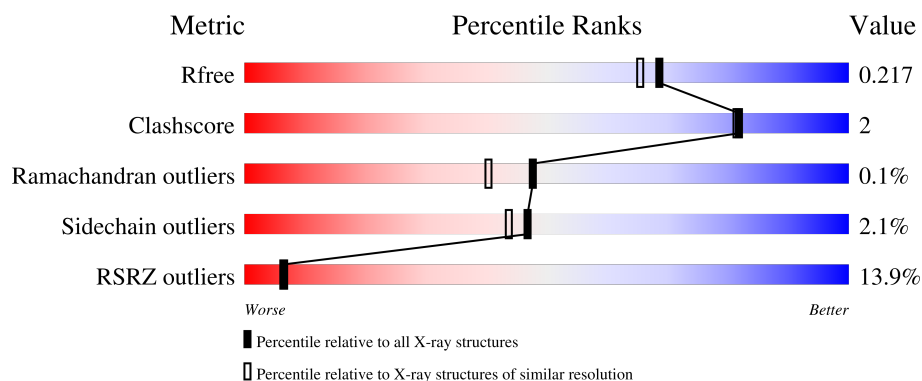
1 Overall quality at a glance

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}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	5% 77% 18%
1	B	332	4% 77% 17%
1	C	332	28% 76% 19%
1	D	332	22% 77% 19%
1	E	332	2% 74% 18%

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Mol	Chain	Length	Quality of chain
1	F	332	5% 77% 5% 18%
1	G	332	5% 77% 5% 18%
1	H	332	21% 77% 5% 18%

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 mutation	UNP Q9CF33
C	89	ALA	ASP	engineered mutation	UNP Q9CF33
D	89	ALA	ASP	engineered mutation	UNP Q9CF33
B	89	ALA	ASP	engineered mutation	UNP Q9CF33
E	89	ALA	ASP	engineered mutation	UNP Q9CF33
F	89	ALA	ASP	engineered mutation	UNP Q9CF33
G	89	ALA	ASP	engineered mutation	UNP Q9CF33
H	89	ALA	ASP	engineered mutation	UNP Q9CF33

- Molecule 2 is SULFATE ION (CCD ID: 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 (CCD ID: CL) (formula: Cl).

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

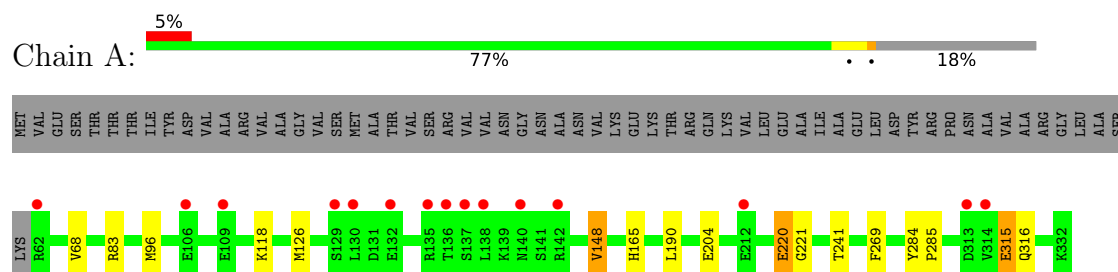
- Molecule 4 is water.

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

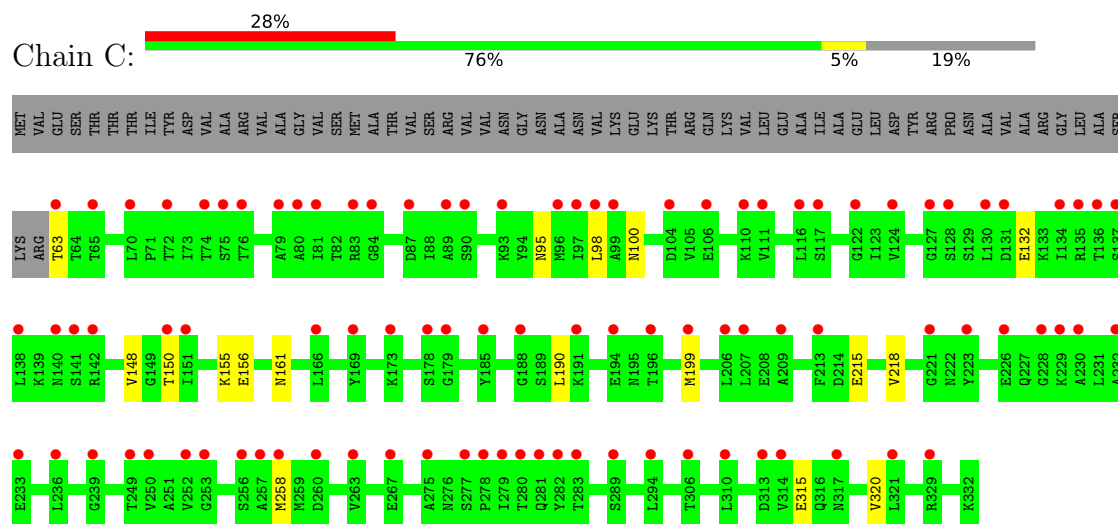
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

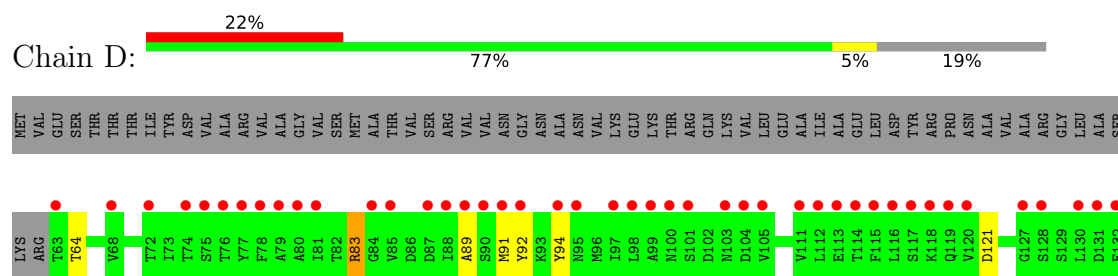
• Molecule 1: Catabolite control protein A

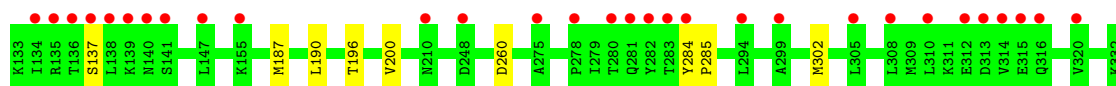


• Molecule 1: Catabolite control protein A

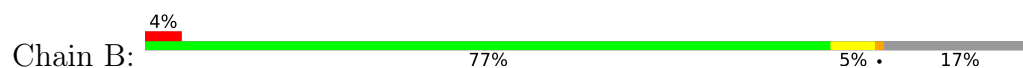


• Molecule 1: Catabolite control protein A

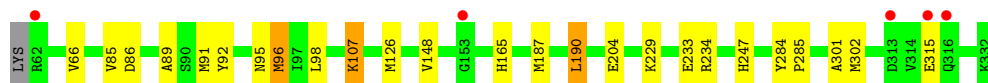
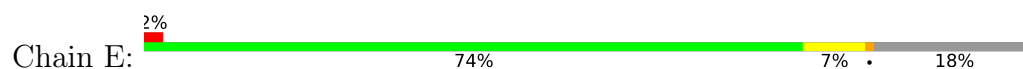




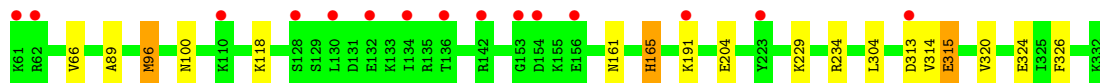
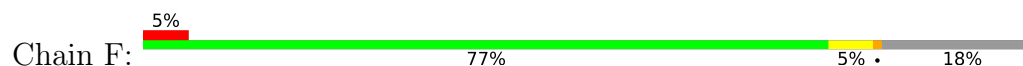
- Molecule 1: Catabolite control protein A



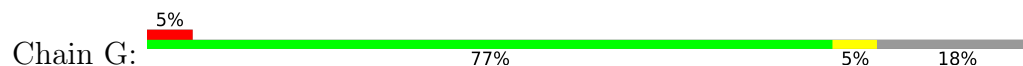
- Molecule 1: Catabolite control protein A



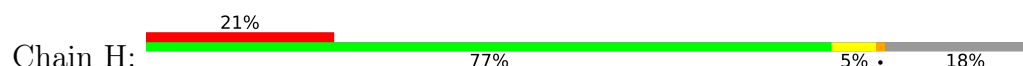
- Molecule 1: Catabolite control protein A

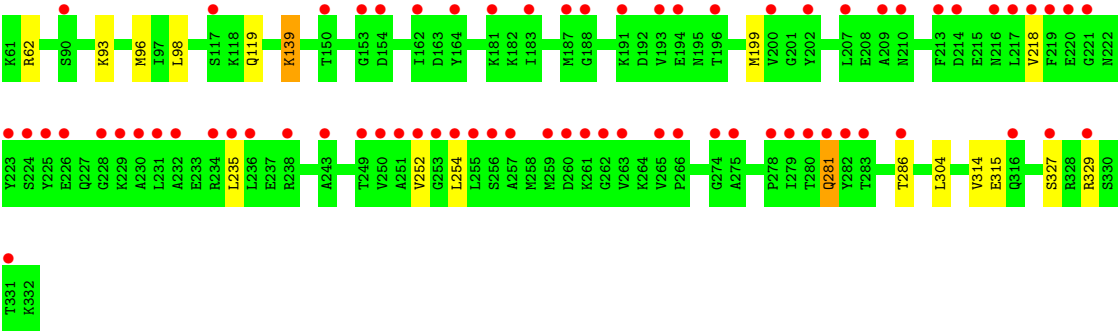


- Molecule 1: Catabolite control protein A



- 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 19.90 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.4 (19.90-1.90) 99.3 (19.90-1.90)	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 (4.67%)	wwPDB-VP
Wilson B-factor (Å ²)	23.2	Xtriage
Anisotropy	0.295	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 53.4	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	0.92	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 [i](#)

5.1 Standard geometry [i](#)

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	0.85	0/2188	0.91	1/2960 (0.0%)
1	B	0.83	1/2248 (0.0%)	0.90	0/3040
1	C	0.53	0/2142	0.76	0/2898
1	D	0.62	0/2164	0.79	0/2927
1	E	0.95	0/2223	0.94	0/3005
1	F	0.88	0/2210	0.91	0/2985
1	G	0.74	0/2152	0.79	0/2911
1	H	0.64	0/2204	0.78	0/2976
All	All	0.77	1/17531 (0.0%)	0.85	1/23702 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	265	VAL	CA-CB	7.05	1.59	1.54

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	148	VAL	CB-CA-C	5.18	117.41	110.42

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2135	0	2148	11	0
1	B	2176	0	2178	14	0
1	C	2106	0	2116	4	0
1	D	2120	0	2130	9	0
1	E	2151	0	2164	23	0
1	F	2154	0	2172	11	0
1	G	2116	0	2134	8	0
1	H	2152	0	2178	11	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	1	0
4	C	17	0	0	0	0
4	D	92	0	0	0	0
4	E	297	0	0	4	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	86	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 (86) 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:E:89:ALA:HB2	1:E:302:MET:HE3	1.39	1.02
1:B:238:ARG:HH11	1:B:238:ARG:HG3	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:85:VAL:CG1	1:E:302:MET:HE2	2.23	0.68
1:E:85:VAL:HG12	1:E:302:MET:HE2	1.79	0.63
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:H:315:GLU:H	1:H:315:GLU:CD	2.10	0.59
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:66:VAL:HG11	1:E:302:MET:HE1	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:91:MET:HE3	1:E:92:TYR:CE1	2.42	0.55
1:F:165:HIS:HE1	1:F:204:GLU:OE1	1.90	0.55
1:E:233:GLU:OE1	4:E:2168:HOH:O	2.19	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:E:315:GLU:H	1:E:315:GLU:CD	2.18	0.50
1:H:286:THR:OG1	1:H:329:ARG:HG2	2.12	0.50
1:A:315:GLU:H	1:A:315:GLU:CD	2.19	0.50
1:C:199:MET:HE1	1:C:218:VAL:HG21	1.93	0.50
1:F:66:VAL:HB	1:F:96:MET:HE2	1.93	0.49
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:H:96:MET:HE3	1:H:98:LEU:HD11	1.94	0.48
1:D:284:TYR:HA	1:D:285:PRO:C	2.39	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: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
1:B:314:VAL:HB	1:B:317[B]:ASN:HD21	1.81	0.46
1:A:284:TYR:HA	1:A:285:PRO:C	2.40	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:E:98:LEU:C	1:E:98:LEU:HD23	2.42	0.45
1:H:286:THR:HG1	1:H:329:ARG:HG2	1.80	0.45
1:E:85:VAL:HG13	1:E:302:MET:HE2	1.97	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:G:233:GLU:HG3	1:G:261:LYS:HZ2	1.80	0.44
1:D:91:MET:HE3	1:D:92:TYR:CZ	2.51	0.44
1:H:281:GLN:HE21	1:H:281:GLN:HA	1.82	0.44
1:D:89:ALA:HB2	1:D:302:MET:HE3	1.99	0.44
1:E:165:HIS:CD2	1:E:165:HIS:C	2.95	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:107[B]:LYS:HD3	4:E:2298:HOH:O	2.16	0.44
1:F:89:ALA:CB	1:F:96:MET:HE1	2.48	0.44
1:A:68:VAL:HG21	1:A:96:MET:HE1	1.99	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:E:284:TYR:HA	1:E:285:PRO:C	2.43	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:135:ARG:HG3	1:G:157:ILE:HD11	2.02	0.42
1:H:199:MET:HE1	1:H:218:VAL:HG11	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:D:64:THR:HB	1:D:94:TYR:CD1	2.54	0.41
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:F:324:GLU:HG3	1:F:326:PHE:CE1	2.56	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:F:315:GLU:H	1:F:315:GLU:CD	2.29	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%)	30	22
1	B	284/332 (86%)	277 (98%)	6 (2%)	1 (0%)	30	22
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%)	30	22
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%)	48	40

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 [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	A	243/286 (85%)	240 (99%)	3 (1%)	63	63
1	B	250/286 (87%)	245 (98%)	5 (2%)	48	46
1	C	238/286 (83%)	228 (96%)	10 (4%)	26	19
1	D	240/286 (84%)	237 (99%)	3 (1%)	61	61
1	E	247/286 (86%)	241 (98%)	6 (2%)	43	38
1	F	244/286 (85%)	239 (98%)	5 (2%)	48	46
1	G	239/286 (84%)	234 (98%)	5 (2%)	47	44
1	H	244/286 (85%)	240 (98%)	4 (2%)	55	54
All	All	1945/2288 (85%)	1904 (98%)	41 (2%)	47	44

All (41) 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	148	VAL
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	260	ASP
1	B	156	GLU
1	B	238	ARG
1	B	287[A]	LEU
1	B	287[B]	LEU
1	B	315	GLU
1	E	96	MET
1	E	107[A]	LYS
1	E	107[B]	LYS
1	E	190	LEU
1	E	229	LYS
1	E	234	ARG
1	F	96	MET
1	F	165	HIS
1	F	191	LYS
1	F	234	ARG
1	F	313	ASP
1	G	106	GLU
1	G	148	VAL
1	G	233	GLU
1	G	237	GLU
1	G	315	GLU
1	H	93	LYS
1	H	139	LYS
1	H	281	GLN
1	H	327	SER

Sometimes 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	247	HIS
1	C	95	ASN
1	C	216	ASN
1	C	316	GLN
1	D	95	ASN
1	D	103	ASN
1	D	180	ASN
1	D	247	HIS
1	B	95	ASN
1	B	103	ASN
1	B	216	ASN
1	E	95	ASN
1	E	247	HIS
1	E	318	GLN
1	F	103	ASN
1	F	165	HIS
1	F	216	ASN
1	F	247	HIS
1	F	318	GLN
1	G	281	GLN
1	G	318	GLN
1	H	95	ASN
1	H	119	GLN
1	H	210	ASN
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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	G	2008	-	4,4,4	0.30	0	6,6,6	0.24	0
2	SO4	B	2001	-	4,4,4	0.33	0	6,6,6	0.73	0
2	SO4	A	2007	-	4,4,4	0.29	0	6,6,6	0.28	0
2	SO4	B	2003	-	4,4,4	0.29	0	6,6,6	0.15	0
2	SO4	F	2002	-	4,4,4	0.20	0	6,6,6	0.50	0
2	SO4	A	2006	-	4,4,4	0.28	0	6,6,6	0.13	0
2	SO4	E	2004	-	4,4,4	0.34	0	6,6,6	0.27	0
2	SO4	F	2005	-	4,4,4	0.23	0	6,6,6	0.17	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%)	0.32	15 (5%) 30 32	11, 22, 39, 45	6 (2%)
1	B	275/332 (82%)	0.41	13 (4%) 36 39	13, 23, 42, 52	11 (4%)
1	C	270/332 (81%)	1.80	94 (34%) 1 0	25, 54, 65, 70	2 (0%)
1	D	270/332 (81%)	1.30	74 (27%) 1 1	16, 40, 56, 60	4 (1%)
1	E	271/332 (81%)	0.02	5 (1%) 67 71	9, 18, 31, 42	11 (4%)
1	F	272/332 (81%)	0.42	15 (5%) 30 32	12, 21, 38, 44	7 (2%)
1	G	271/332 (81%)	0.62	15 (5%) 30 32	19, 31, 44, 49	2 (0%)
1	H	272/332 (81%)	1.30	71 (26%) 1 1	14, 43, 65, 67	6 (2%)
All	All	2172/2656 (81%)	0.77	302 (13%) 6 6	9, 29, 58, 70	49 (2%)

All (302) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	256[A]	SER	7.4
1	F	313	ASP	7.1
1	A	136	THR	6.5
1	H	90[A]	SER	5.5
1	C	228	GLY	5.0
1	D	141	SER	5.0
1	D	63	THR	4.9
1	B	140	ASN	4.7
1	D	136	THR	4.5
1	B	59	ALA	4.5
1	B	141	SER	4.3
1	H	230	ALA	4.3
1	F	61	LYS	4.3
1	C	280	THR	4.2
1	H	225	TYR	4.2
1	A	313	ASP	4.2

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Mol	Chain	Res	Type	RSRZ
1	C	136	THR	4.1
1	D	140	ASN	4.1
1	D	314	VAL	4.0
1	B	313	ASP	4.0
1	D	139	LYS	4.0
1	D	210[A]	ASN	3.9
1	D	117	SER	3.9
1	B	60	SER	3.9
1	D	284	TYR	3.8
1	B	132	GLU	3.8
1	C	196	THR	3.7
1	C	89	ALA	3.7
1	D	137	SER	3.7
1	F	132	GLU	3.7
1	H	228	GLY	3.7
1	C	278	PRO	3.7
1	G	284	TYR	3.7
1	H	275	ALA	3.7
1	D	75	SER	3.6
1	C	110	LYS	3.6
1	C	130	LEU	3.6
1	C	188	GLY	3.6
1	C	263	VAL	3.6
1	D	275	ALA	3.5
1	H	224	SER	3.5
1	A	135	ARG	3.5
1	G	138	LEU	3.5
1	H	281	GLN	3.5
1	A	137	SER	3.5
1	C	137	SER	3.5
1	D	316	GLN	3.5
1	B	62	ARG	3.5
1	H	236	LEU	3.5
1	C	141	SER	3.4
1	C	277	SER	3.4
1	F	153	GLY	3.4
1	H	229	LYS	3.3
1	B	58	LEU	3.3
1	C	74	THR	3.3
1	A	132	GLU	3.3
1	H	207	LEU	3.3
1	D	89	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	G	313	ASP	3.3
1	C	249	THR	3.2
1	D	313	ASP	3.2
1	H	243	ALA	3.2
1	C	80	ALA	3.2
1	C	63	THR	3.2
1	C	282	TYR	3.2
1	D	114	THR	3.2
1	C	111	VAL	3.1
1	G	137	SER	3.1
1	D	132	GLU	3.1
1	D	72	THR	3.1
1	D	98	LEU	3.1
1	F	130	LEU	3.1
1	B	136	THR	3.1
1	D	104	ASP	3.1
1	D	74	THR	3.1
1	D	111	VAL	3.0
1	G	282	TYR	3.0
1	D	95	ASN	3.0
1	D	312	GLU	3.0
1	D	128	SER	3.0
1	C	93	LYS	3.0
1	D	80	ALA	3.0
1	H	257	ALA	3.0
1	C	279	ILE	3.0
1	B	116	LEU	3.0
1	C	127	GLY	3.0
1	D	84	GLY	3.0
1	G	253	GLY	3.0
1	A	142	ARG	3.0
1	H	216	ASN	3.0
1	H	278	PRO	2.9
1	C	138	LEU	2.9
1	C	310	LEU	2.9
1	D	155	LYS	2.9
1	A	140[A]	ASN	2.9
1	C	140	ASN	2.9
1	H	209	ALA	2.9
1	H	154	ASP	2.9
1	A	138	LEU	2.9
1	H	153	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	62	ARG	2.9
1	H	238[A]	ARG	2.9
1	C	207	LEU	2.9
1	C	84	GLY	2.9
1	C	314	VAL	2.8
1	D	134	ILE	2.8
1	D	138	LEU	2.8
1	D	283	THR	2.8
1	D	87	ASP	2.8
1	C	223	TYR	2.8
1	D	113	GLU	2.8
1	H	214	ASP	2.8
1	D	77	TYR	2.7
1	C	233	GLU	2.7
1	H	262	GLY	2.7
1	C	72	THR	2.7
1	D	97	ILE	2.7
1	F	154	ASP	2.7
1	H	187	MET	2.7
1	H	256	SER	2.7
1	C	253	GLY	2.7
1	C	131	ASP	2.7
1	C	116	LEU	2.7
1	D	119[A]	GLN	2.7
1	D	100	ASN	2.7
1	D	120	VAL	2.7
1	H	218	VAL	2.7
1	D	79	ALA	2.7
1	C	96	MET	2.7
1	A	130	LEU	2.7
1	D	310	LEU	2.7
1	H	231	LEU	2.7
1	H	279	ILE	2.7
1	C	87	ASP	2.6
1	D	94	TYR	2.6
1	H	213	PHE	2.6
1	G	128	SER	2.6
1	D	116	LEU	2.6
1	H	188	GLY	2.6
1	H	251	ALA	2.6
1	D	115	PHE	2.6
1	G	135	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	221	GLY	2.6
1	A	314	VAL	2.6
1	H	193	VAL	2.6
1	C	117	SER	2.6
1	H	283	THR	2.6
1	H	327	SER	2.6
1	C	98	LEU	2.6
1	C	79	ALA	2.6
1	D	85	VAL	2.6
1	C	178	SER	2.6
1	D	90	SER	2.6
1	H	210	ASN	2.6
1	C	83	ARG	2.5
1	C	166	LEU	2.5
1	C	236	LEU	2.5
1	D	131	ASP	2.5
1	D	147	LEU	2.5
1	C	257	ALA	2.5
1	H	250	VAL	2.5
1	H	196	THR	2.5
1	D	112	LEU	2.5
1	D	130	LEU	2.5
1	D	294	LEU	2.5
1	D	320	VAL	2.5
1	D	278	PRO	2.5
1	C	104	ASP	2.5
1	F	223	TYR	2.5
1	H	217	LEU	2.5
1	C	317	ASN	2.5
1	D	81	ILE	2.5
1	H	162	ILE	2.5
1	A	106	GLU	2.5
1	H	280	THR	2.5
1	H	260	ASP	2.5
1	D	282	TYR	2.4
1	H	223	TYR	2.4
1	C	213	PHE	2.4
1	C	321	LEU	2.4
1	F	134	ILE	2.4
1	C	173	LYS	2.4
1	D	280	THR	2.4
1	F	136	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	206	LEU	2.4
1	B	138	LEU	2.4
1	D	76	THR	2.4
1	D	99	ALA	2.4
1	E	62	ARG	2.4
1	C	106	GLU	2.4
1	D	68	VAL	2.4
1	G	140	ASN	2.4
1	F	128	SER	2.4
1	C	229	LYS	2.4
1	D	305	LEU	2.4
1	C	81	ILE	2.4
1	C	329	ARG	2.4
1	H	286	THR	2.4
1	D	315	GLU	2.4
1	F	156	GLU	2.4
1	F	62	ARG	2.3
1	H	235	LEU	2.3
1	C	194[A]	GLU	2.3
1	C	275	ALA	2.3
1	H	253	GLY	2.3
1	F	110	LYS	2.3
1	A	129	SER	2.3
1	C	70	LEU	2.3
1	H	316	GLN	2.3
1	C	97	ILE	2.3
1	H	183	ILE	2.3
1	F	142	ARG	2.3
1	H	234[A]	ARG	2.3
1	C	313	ASP	2.3
1	A	109	GLU	2.3
1	A	212	GLU	2.3
1	D	308	LEU	2.3
1	D	118	LYS	2.3
1	H	219	PHE	2.3
1	H	232	ALA	2.3
1	C	239	GLY	2.3
1	F	191	LYS	2.3
1	H	181	LYS	2.3
1	C	135	ARG	2.2
1	D	127	GLY	2.2
1	E	315	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	221	GLY	2.2
1	H	282	TYR	2.2
1	C	75	SER	2.2
1	C	289	SER	2.2
1	D	88	ILE	2.2
1	H	252	VAL	2.2
1	H	263	VAL	2.2
1	C	76	THR	2.2
1	C	90	SER	2.2
1	C	209	ALA	2.2
1	C	260	ASP	2.2
1	H	117	SER	2.2
1	H	266	PRO	2.2
1	C	267	GLU	2.2
1	B	113	GLU	2.2
1	H	254	LEU	2.2
1	C	179	GLY	2.2
1	D	248	ASP	2.2
1	C	99	ALA	2.2
1	C	230	ALA	2.2
1	D	78	PHE	2.2
1	H	202	TYR	2.2
1	C	226	GLU	2.2
1	G	132	GLU	2.2
1	E	316	GLN	2.2
1	C	150	THR	2.2
1	G	136	THR	2.2
1	D	299	ALA	2.2
1	G	142	ARG	2.2
1	H	150	THR	2.1
1	C	142	ARG	2.1
1	C	199	MET	2.1
1	H	194	GLU	2.1
1	H	259	MET	2.1
1	C	151	ILE	2.1
1	C	128	SER	2.1
1	C	283	THR	2.1
1	D	101	SER	2.1
1	H	331	THR	2.1
1	D	135[A]	ARG	2.1
1	H	329	ARG	2.1
1	D	103	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	230	ALA	2.1
1	C	134	ILE	2.1
1	D	92	TYR	2.1
1	C	65	THR	2.1
1	C	191	LYS	2.1
1	H	220	GLU	2.1
1	H	226	GLU	2.1
1	C	124	VAL	2.1
1	C	252	VAL	2.1
1	D	281	GLN	2.1
1	C	294	LEU	2.1
1	H	255	LEU	2.1
1	B	129	SER	2.0
1	H	261	LYS	2.0
1	H	164	TYR	2.0
1	C	258	MET	2.0
1	D	91	MET	2.0
1	E	153	GLY	2.0
1	H	274	GLY	2.0
1	H	200	VAL	2.0
1	H	265	VAL	2.0
1	C	232	ALA	2.0
1	G	209	ALA	2.0
1	E	313	ASP	2.0
1	G	139	LYS	2.0
1	H	191	LYS	2.0
1	C	122	GLY	2.0
1	C	281	GLN	2.0
1	C	306	THR	2.0
1	H	249	THR	2.0
1	C	169	TYR	2.0
1	C	185	TYR	2.0
1	C	250	VAL	2.0
1	D	105	VAL	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 [i](#)

There are no oligosaccharides 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. 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	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	A	2007	5/5	0.64	0.19	80,80,80,81	0
2	SO4	F	2005	5/5	0.74	0.17	74,74,75,76	0
2	SO4	G	2008	5/5	0.74	0.16	61,63,65,66	0
2	SO4	A	2006	5/5	0.77	0.15	81,81,82,82	0
2	SO4	E	2004	5/5	0.83	0.17	57,59,60,60	0
2	SO4	B	2003	5/5	0.88	0.18	55,56,57,57	0
2	SO4	F	2002	5/5	0.93	0.19	36,39,44,44	0
2	SO4	B	2001	5/5	0.94	0.17	34,36,39,41	0
3	CL	E	2010	1/1	0.99	0.17	20,20,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.