



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 01:35 AM GMT

PDB ID : 3DM5  
Title : Structures of SRP54 and SRP19, the two proteins assembling the ribonucleic core of the Signal Recognition Particle from the archaeon *Pyrococcus furiosus*.  
Authors : Egea, P.F.; Napetschnig, J.; Walter, P.; Stroud, R.M.  
Deposited on : 2008-06-30  
Resolution : 2.51 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

---

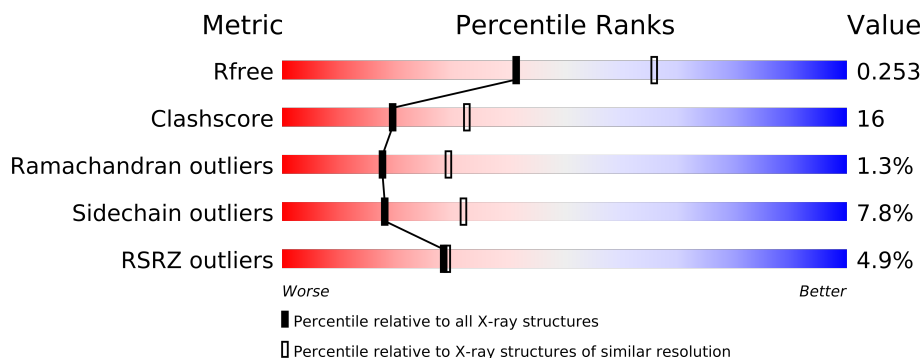
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.51 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))
$R_{free}$	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	443	
1	B	443	

## 2 Entry composition i

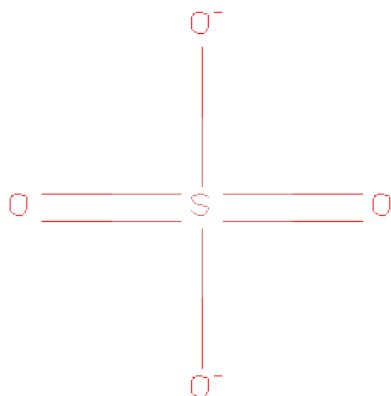
There are 5 unique types of molecules in this entry. The entry contains 6649 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Signal recognition 54 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	416	Total	C	N	O	S	0	0	0
			3192	2028	552	601	11			
1	B	413	Total	C	N	O	S	11	1	0
			3196	2034	556	595	11			

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



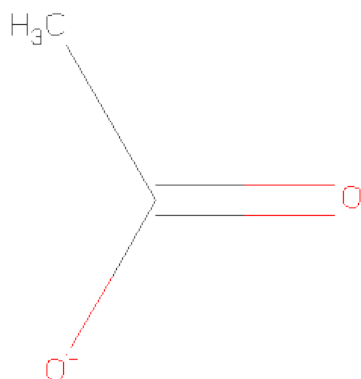
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

*Continued on next page...*

Continued from previous page...

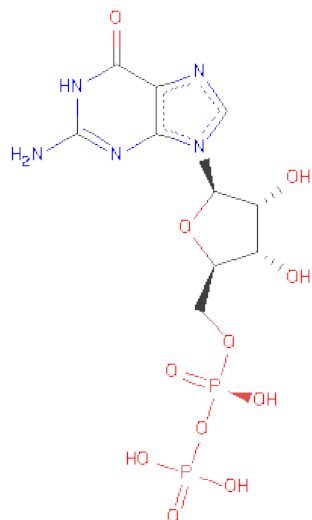
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
4	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 5 is water.

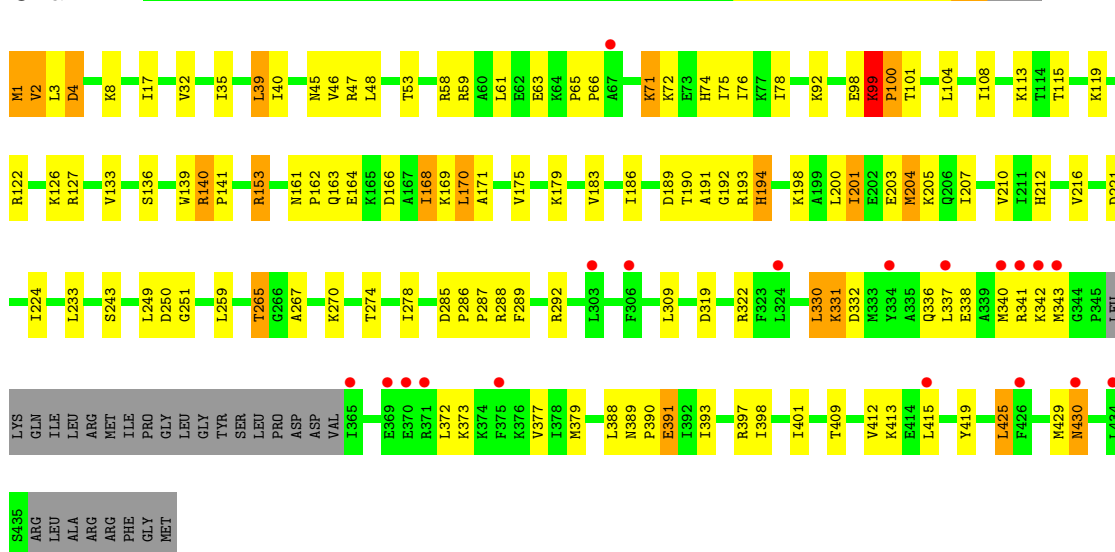
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	72	Total	O	0	0
			72	72		
5	B	70	Total	O	0	0
			70	70		

### 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.

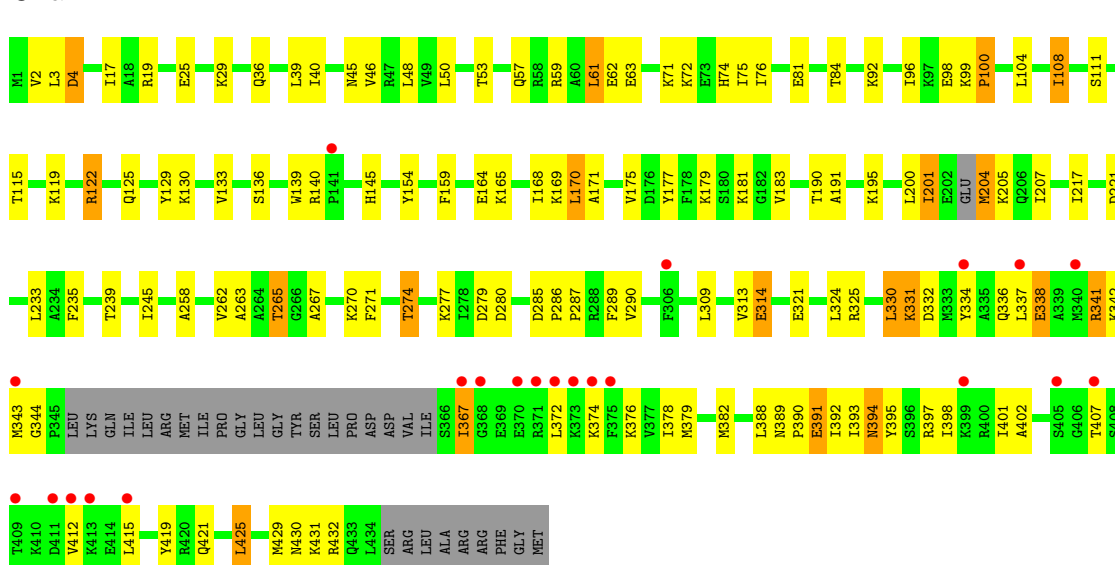
- Molecule 1: Signal recognition 54 kDa protein

Chain A:



- Molecule 1: Signal recognition 54 kDa protein

Chain B:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	127.01Å 127.01Å 186.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	64.74 – 2.51 64.74 – 2.51	Depositor EDS
% Data completeness (in resolution range)	99.5 (64.74-2.51) 99.5 (64.74-2.51)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.76 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.222 , 0.259 0.214 , 0.253	Depositor DCC
$R_{free}$ test set	2000 reflections (3.80%)	DCC
Wilson B-factor (Å <sup>2</sup> )	55.2	Xtriage
Anisotropy	0.163	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 54.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 52652 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6649	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

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

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	0.40	0/3234	0.57	0/4357
1	B	0.40	0/3235	0.57	0/4348
All	All	0.40	0/6469	0.57	0/8705

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3192	0	3248	111	0
1	B	3196	0	3289	100	0
2	A	30	0	0	1	0
2	B	25	0	0	2	0
3	A	4	0	3	0	0
3	B	4	0	3	0	0
4	A	28	0	12	0	0
4	B	28	0	12	0	0
5	A	72	0	0	1	0
5	B	70	0	0	2	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6649	0	6567	211	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 16.

All (211) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:341:ARG:HH11	1:A:341:ARG:HG3	1.27	0.99
1:B:341:ARG:HH11	1:B:341:ARG:HG3	1.36	0.91
1:A:99:LYS:O	1:A:100:PRO:C	2.09	0.90
1:B:330:LEU:HD12	1:B:390:PRO:HG3	1.54	0.86
1:A:265:THR:HG22	1:A:267:ALA:H	1.40	0.85
1:B:324:LEU:HD22	1:B:429:MET:HB2	1.60	0.83
1:A:127:ARG:HH11	1:A:127:ARG:HG3	1.43	0.82
1:A:99:LYS:HG3	1:A:100:PRO:HD3	1.62	0.81
1:B:99:LYS:HG3	1:B:100:PRO:HD3	1.61	0.81
1:B:168:ILE:HD13	1:B:207:ILE:HG12	1.63	0.80
1:A:168:ILE:HD13	1:A:207:ILE:HG12	1.66	0.77
1:B:341:ARG:HG3	1:B:341:ARG:NH1	1.97	0.77
1:A:113:LYS:HE2	1:A:189:ASP:OD1	1.85	0.76
1:A:341:ARG:NH1	1:A:341:ARG:HG3	1.97	0.74
1:A:330:LEU:HD12	1:A:390:PRO:HG3	1.70	0.72
1:A:45:ASN:HD22	1:A:48:LEU:H	1.38	0.72
1:A:193:ARG:HG3	1:A:200:LEU:HD12	1.71	0.71
1:B:398:ILE:HG23	1:B:412:VAL:HG11	1.74	0.70
1:A:92:LYS:O	1:A:270:LYS:HD3	1.93	0.68
1:B:99:LYS:O	1:B:100:PRO:C	2.33	0.67
1:A:265:THR:CG2	1:A:267:ALA:H	2.07	0.67
1:A:153:ARG:HG2	5:A:505:HOH:O	1.95	0.66
1:A:2:VAL:H	1:A:250:ASP:HA	1.61	0.66
1:A:390:PRO:HG2	1:A:419:TYR:CZ	2.29	0.66
1:B:71:LYS:O	1:B:75:ILE:HG12	1.96	0.66
1:B:104:LEU:HD11	1:B:190:THR:CG2	2.26	0.66
1:B:111:SER:HA	1:B:221:ASP:HB2	1.77	0.66
1:B:334:TYR:OH	1:B:376:LYS:HE2	1.96	0.65
1:B:382:MET:HG2	1:B:401:ILE:HD13	1.79	0.65
1:A:136:SER:HA	1:A:170:LEU:HD13	1.79	0.65
1:B:330:LEU:HD21	1:B:415:LEU:HD21	1.80	0.64
1:A:164:GLU:OE1	1:A:164:GLU:HA	1.97	0.63
1:A:341:ARG:HD3	1:A:372:LEU:HD22	1.80	0.63
1:A:1:MET:O	1:A:2:VAL:HG12	1.99	0.62
1:B:136:SER:HA	1:B:170:LEU:HD13	1.81	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:59:ARG:O	1:A:63:GLU:HB2	1.98	0.62
1:A:32:VAL:HG13	1:A:53:THR:HB	1.81	0.62
1:A:99:LYS:O	1:A:101:THR:N	2.32	0.62
1:B:245:ILE:HG12	1:B:271:PHE:HB2	1.81	0.62
1:A:203:GLU:O	1:A:207:ILE:HG13	1.99	0.62
1:B:100:PRO:HG2	1:B:179:LYS:HG3	1.81	0.61
1:B:324:LEU:CD2	1:B:429:MET:HB2	2.30	0.61
1:A:40:ILE:HD12	1:A:46:VAL:HG22	1.83	0.60
1:A:166:ASP:HB3	1:A:169:LYS:HB2	1.83	0.60
1:B:277:LYS:HE2	5:B:535:HOH:O	2.01	0.60
1:B:341:ARG:HH11	1:B:341:ARG:CG	2.14	0.60
1:B:398:ILE:HG23	1:B:412:VAL:CG1	2.32	0.60
1:A:127:ARG:HH11	1:A:127:ARG:CG	2.15	0.60
1:B:63:GLU:OE1	1:B:74:HIS:HE1	1.85	0.60
1:B:45:ASN:HD22	1:B:48:LEU:H	1.51	0.59
1:B:330:LEU:HD12	1:B:390:PRO:CG	2.31	0.59
1:A:285:ASP:OD1	1:A:287:PRO:HD2	2.03	0.59
1:B:337:LEU:HB3	1:B:372:LEU:HD12	1.85	0.58
1:A:71:LYS:H	1:A:71:LYS:HD2	1.68	0.58
1:A:286:PRO:HB2	1:A:287:PRO:HD3	1.85	0.58
1:A:139:TRP:HB2	1:A:191:ALA:HB1	1.85	0.57
1:A:58:ARG:HH12	1:A:59:ARG:HG2	1.69	0.57
1:A:99:LYS:CG	1:A:100:PRO:HD3	2.35	0.56
1:B:274:THR:HG22	1:B:280:ASP:HB3	1.87	0.56
1:B:25:GLU:O	1:B:29:LYS:HG2	2.04	0.56
1:A:127:ARG:NH1	1:A:127:ARG:HG3	2.19	0.56
1:B:29:LYS:HD2	1:B:57:GLN:HE21	1.71	0.55
1:B:59:ARG:O	1:B:63:GLU:HB2	2.05	0.55
1:A:340:MET:HA	1:A:343:MET:HE3	1.90	0.54
1:A:98:GLU:C	1:A:99:LYS:O	2.43	0.54
1:A:3:LEU:HD22	1:A:289:PHE:HZ	1.72	0.54
1:B:139:TRP:HB2	1:B:191:ALA:HB1	1.89	0.53
1:A:2:VAL:H	1:A:251:GLY:H	1.57	0.53
1:A:249:LEU:HD11	1:A:259:LEU:HD21	1.91	0.53
1:B:100:PRO:CG	1:B:179:LYS:HG3	2.38	0.53
1:A:100:PRO:HG2	1:A:179:LYS:HG3	1.90	0.52
1:B:96:ILE:HG21	1:B:129:TYR:CE1	2.45	0.52
1:A:99:LYS:HB3	1:A:100:PRO:CD	2.39	0.52
1:A:265:THR:HG22	1:A:267:ALA:N	2.18	0.52
1:B:334:TYR:HD1	1:B:379:MET:CE	2.23	0.52
1:B:130:LYS:HG2	1:B:183:VAL:HG12	1.90	0.52
1:A:104:LEU:HD11	1:A:190:THR:HG21	1.91	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:35:ILE:HG22	1:A:39:LEU:HD22	1.92	0.52
1:A:192:GLY:O	1:A:193:ARG:HG2	2.10	0.51
1:A:40:ILE:CD1	1:A:46:VAL:HG22	2.40	0.51
1:B:394:ASN:O	1:B:398:ILE:HG13	2.10	0.51
1:B:262:VAL:O	1:B:265:THR:HG22	2.11	0.51
1:B:92:LYS:O	1:B:270:LYS:HD3	2.10	0.51
1:A:341:ARG:NH1	1:A:341:ARG:CG	2.72	0.51
1:B:164:GLU:HG2	1:B:170:LEU:HG	1.93	0.51
1:A:288:ARG:O	1:A:292:ARG:HG2	2.10	0.51
1:A:2:VAL:O	1:A:4:ASP:N	2.42	0.50
1:B:338:GLU:O	1:B:341:ARG:HG2	2.11	0.50
1:B:334:TYR:HE1	1:B:376:LYS:HG3	1.77	0.50
1:B:84:THR:HA	1:B:290:VAL:HG21	1.94	0.50
1:A:198:LYS:HE2	2:A:448:SO4:O4	2.11	0.50
1:B:36:GLN:OE1	1:B:53:THR:HG21	2.11	0.49
1:A:74:HIS:O	1:A:78:ILE:HG13	2.12	0.49
1:B:99:LYS:HG3	1:B:100:PRO:CD	2.37	0.49
1:B:235:PHE:O	1:B:239:THR:HG22	2.11	0.49
1:B:397:ARG:O	1:B:401:ILE:HG13	2.12	0.49
1:A:122:ARG:CZ	1:A:126:LYS:HG3	2.41	0.49
1:B:285:ASP:OD1	1:B:287:PRO:HD2	2.13	0.49
1:B:258:ALA:O	1:B:262:VAL:HG23	2.13	0.48
1:A:17:ILE:CD1	1:A:75:ILE:HG21	2.43	0.48
1:A:104:LEU:HD23	1:A:216:VAL:HG22	1.95	0.48
1:A:115:THR:HG22	1:A:119:LYS:HE3	1.95	0.48
1:B:36:GLN:CG	1:B:53:THR:HG21	2.44	0.48
1:B:342:LYS:C	1:B:344:GLY:H	2.16	0.48
1:A:164:GLU:CG	1:A:170:LEU:HG	2.43	0.48
1:A:127:ARG:CG	1:A:127:ARG:NH1	2.73	0.48
1:B:263:ALA:C	1:B:265:THR:H	2.17	0.48
1:B:430:ASN:C	1:B:432:ARG:H	2.16	0.48
1:B:390:PRO:HG2	1:B:419:TYR:CZ	2.50	0.47
1:B:331:LYS:HE3	1:B:388:LEU:HD21	1.96	0.47
1:A:99:LYS:HA	1:A:99:LYS:HD2	1.49	0.47
1:B:332:ASP:O	1:B:336:GLN:HG2	2.15	0.47
1:A:104:LEU:HD11	1:A:190:THR:CG2	2.44	0.47
1:A:397:ARG:O	1:A:401:ILE:HG13	2.15	0.47
1:A:71:LYS:H	1:A:71:LYS:CD	2.23	0.47
1:A:331:LYS:HE3	1:A:388:LEU:HD21	1.96	0.47
1:B:390:PRO:O	1:B:393:ILE:HG13	2.15	0.47
1:B:334:TYR:HD1	1:B:379:MET:HE3	1.80	0.47
1:B:99:LYS:HD2	1:B:99:LYS:HA	1.59	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:243:SER:HB3	1:A:270:LYS:HE3	1.97	0.47
1:A:161:ASN:O	1:A:163:GLN:N	2.48	0.47
1:A:204:MET:HG3	1:A:205:LYS:N	2.30	0.47
1:B:25:GLU:HG3	1:B:61:LEU:HD11	1.97	0.46
1:B:29:LYS:HD2	1:B:57:GLN:NE2	2.30	0.46
1:B:104:LEU:HD11	1:B:190:THR:HG21	1.97	0.46
1:A:390:PRO:O	1:A:393:ILE:HG13	2.15	0.46
1:A:1:MET:HG3	1:A:250:ASP:HB2	1.97	0.46
1:B:108:ILE:HG22	1:B:200:LEU:CD1	2.45	0.46
1:A:175:VAL:O	1:A:179:LYS:HB2	2.14	0.46
1:B:201:ILE:HA	1:B:204:MET:HG2	1.98	0.46
1:B:367:ILE:HD11	1:B:372:LEU:HB2	1.97	0.46
1:A:161:ASN:C	1:A:163:GLN:H	2.19	0.46
1:B:122:ARG:O	1:B:122:ARG:HD2	2.15	0.46
1:B:430:ASN:O	1:B:432:ARG:N	2.48	0.45
1:A:319:ASP:O	1:A:322:ARG:HB2	2.15	0.45
1:A:373:LYS:O	1:A:377:VAL:HG23	2.17	0.45
1:B:425:LEU:O	1:B:429:MET:HG2	2.16	0.45
1:B:3:LEU:HD22	1:B:289:PHE:HZ	1.81	0.45
1:A:99:LYS:CB	1:A:100:PRO:CD	2.94	0.45
1:A:164:GLU:OE2	1:A:169:LYS:HE2	2.16	0.45
1:A:3:LEU:HD22	1:A:289:PHE:CZ	2.52	0.45
1:B:59:ARG:HH12	1:B:81:GLU:CD	2.20	0.45
1:B:374:LYS:O	1:B:378:ILE:HG13	2.17	0.45
1:B:115:THR:HG22	1:B:119:LYS:HE3	1.99	0.45
1:B:145:HIS:HE1	2:B:445:SO4:O4	1.99	0.44
1:B:389:ASN:HB3	1:B:391:GLU:OE2	2.17	0.44
1:A:425:LEU:HD22	1:A:429:MET:CE	2.48	0.44
1:B:171:ALA:O	1:B:175:VAL:HG23	2.18	0.44
1:A:99:LYS:HG3	1:A:100:PRO:CD	2.42	0.44
1:A:65:PRO:HG3	1:A:71:LYS:HA	1.99	0.44
1:A:1:MET:HA	1:A:251:GLY:H	1.83	0.44
1:B:72:LYS:O	1:B:76:ILE:HG12	2.19	0.43
1:B:62:GLU:O	1:B:62:GLU:HG3	2.19	0.43
1:A:1:MET:HA	1:A:251:GLY:N	2.33	0.43
1:A:161:ASN:C	1:A:163:GLN:N	2.72	0.43
1:A:65:PRO:HA	1:A:66:PRO:HD2	1.86	0.43
1:A:72:LYS:O	1:A:76:ILE:HG12	2.18	0.43
1:B:313:VAL:HG13	1:B:314:GLU:H	1.82	0.43
1:B:342:LYS:C	1:B:344:GLY:N	2.72	0.43
1:A:2:VAL:N	1:A:250:ASP:HA	2.29	0.43
1:B:17:ILE:HD13	1:B:75:ILE:HG21	2.00	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:243:SER:CB	1:A:270:LYS:HE3	2.49	0.43
1:B:279:ASP:HB2	5:B:545:HOH:O	2.18	0.43
1:A:164:GLU:HG3	1:A:170:LEU:HG	2.00	0.43
1:B:367:ILE:HD11	1:B:372:LEU:CA	2.49	0.43
1:B:125:GLN:NE2	1:B:154:TYR:O	2.51	0.43
1:A:274:THR:CG2	1:A:274:THR:O	2.67	0.43
1:A:343:MET:O	1:A:343:MET:HG2	2.19	0.42
1:A:221:ASP:O	1:A:224:ILE:HG12	2.18	0.42
1:A:415:LEU:HD23	1:A:415:LEU:O	2.19	0.42
1:A:164:GLU:OE1	1:A:164:GLU:CA	2.64	0.42
1:B:195:LYS:HB3	1:B:195:LYS:HE2	1.76	0.42
1:B:177:TYR:OH	1:B:181:LYS:HE2	2.19	0.42
1:B:389:ASN:O	1:B:392:ILE:HG12	2.20	0.42
1:B:337:LEU:HB3	1:B:372:LEU:CD1	2.49	0.42
1:A:278:ILE:O	1:A:278:ILE:HG13	2.19	0.42
1:A:183:VAL:HG21	1:A:186:ILE:HG12	2.02	0.42
1:B:265:THR:CG2	1:B:267:ALA:H	2.33	0.42
1:B:313:VAL:HG13	1:B:314:GLU:N	2.35	0.42
1:B:50:LEU:HA	1:B:50:LEU:HD23	1.84	0.42
1:A:389:ASN:HB3	1:A:391:GLU:OE2	2.20	0.42
1:B:177:TYR:CD2	1:B:177:TYR:C	2.92	0.42
1:A:337:LEU:HB3	1:A:372:LEU:HD11	2.02	0.41
1:A:171:ALA:O	1:A:175:VAL:HG23	2.20	0.41
1:A:168:ILE:HG21	1:A:210:VAL:HG21	2.02	0.41
1:A:198:LYS:HA	1:A:201:ILE:HD11	2.01	0.41
1:A:338:GLU:O	1:A:342:LYS:HD3	2.20	0.41
1:B:159:PHE:CD2	1:B:159:PHE:C	2.93	0.41
1:B:36:GLN:O	1:B:40:ILE:HG12	2.20	0.41
1:B:402:ALA:HB1	1:B:407:THR:O	2.20	0.41
1:B:71:LYS:HG3	2:B:448:SO4:O1	2.20	0.41
1:A:398:ILE:HG23	1:A:412:VAL:HG11	2.02	0.41
1:A:139:TRP:HH2	1:A:194:HIS:ND1	2.18	0.41
1:A:409:THR:O	1:A:413:LYS:HG3	2.20	0.41
1:A:99:LYS:HB3	1:A:100:PRO:HD3	2.02	0.41
1:B:98:GLU:C	1:B:99:LYS:O	2.58	0.41
1:B:204:MET:HG3	1:B:205:LYS:N	2.35	0.41
1:A:337:LEU:HB3	1:A:372:LEU:CD1	2.50	0.41
1:B:63:GLU:OE1	1:B:74:HIS:CE1	2.69	0.41
1:B:286:PRO:HB2	1:B:287:PRO:HD3	2.03	0.41
1:A:332:ASP:O	1:A:336:GLN:HG2	2.21	0.41
1:B:274:THR:HG22	1:B:280:ASP:CB	2.51	0.41
1:A:99:LYS:CB	1:A:100:PRO:HD3	2.51	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:8:LYS:HB3	1:A:8:LYS:HE3	1.85	0.40
1:A:98:GLU:O	1:A:99:LYS:O	2.39	0.40
1:A:2:VAL:HG13	1:A:2:VAL:O	2.20	0.40
1:A:140:ARG:HA	1:A:141:PRO:HD2	1.87	0.40
1:A:309:LEU:HD12	1:A:309:LEU:HA	1.85	0.40
1:B:40:ILE:HD11	1:B:46:VAL:HG23	2.02	0.40
1:A:379:MET:HG3	1:A:415:LEU:HD11	2.03	0.40
1:B:321:GLU:O	1:B:325:ARG:HG3	2.22	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	412/443 (93%)	383 (93%)	23 (6%)	6 (2%)	15	25
1	B	408/443 (92%)	380 (93%)	23 (6%)	5 (1%)	19	32
All	All	820/886 (93%)	763 (93%)	46 (6%)	11 (1%)	18	29

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	99	LYS
1	B	4	ASP
1	B	100	PRO
1	B	394	ASN
1	A	430	ASN
1	B	431	LYS
1	A	4	ASP
1	B	421	GLN
1	A	100	PRO
1	A	2	VAL
1	A	162	PRO

### 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	332/378 (88%)	309 (93%)	23 (7%)	22	39
1	B	333/378 (88%)	304 (91%)	29 (9%)	15	27
All	All	665/756 (88%)	613 (92%)	52 (8%)	18	32

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	39	LEU
1	A	47	ARG
1	A	61	LEU
1	A	71	LYS
1	A	99	LYS
1	A	108	ILE
1	A	133	VAL
1	A	140	ARG
1	A	153	ARG
1	A	168	ILE
1	A	170	LEU
1	A	194	HIS
1	A	201	ILE
1	A	204	MET
1	A	212	HIS
1	A	233	LEU
1	A	265	THR
1	A	330	LEU
1	A	331	LYS
1	A	391	GLU
1	A	425	LEU
1	A	430	ASN
1	B	2	VAL
1	B	4	ASP
1	B	19	ARG
1	B	39	LEU
1	B	61	LEU
1	B	108	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	122	ARG
1	B	133	VAL
1	B	140	ARG
1	B	165	LYS
1	B	169	LYS
1	B	170	LEU
1	B	201	ILE
1	B	204	MET
1	B	217	ILE
1	B	233	LEU
1	B	265	THR
1	B	274	THR
1	B	309	LEU
1	B	314	GLU
1	B	330	LEU
1	B	331	LYS
1	B	338	GLU
1	B	341	ARG
1	B	343	MET
1	B	367	ILE
1	B	391	GLU
1	B	395	TYR
1	B	425	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	GLN
1	A	45	ASN
1	A	74	HIS
1	A	209	ASN
1	A	226	GLN
1	A	418	GLN
1	B	45	ASN
1	B	57	GLN
1	B	74	HIS
1	B	145	HIS
1	B	163	GLN
1	B	226	GLN
1	B	336	GLN



### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

15 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	SO4	A	444	-	4,4,4	0.11	0	6,6,6	0.10	0
2	SO4	A	445	-	4,4,4	0.06	0	6,6,6	0.14	0
2	SO4	A	446	-	4,4,4	0.08	0	6,6,6	0.22	0
2	SO4	A	447	-	4,4,4	0.23	0	6,6,6	0.37	0
2	SO4	A	448	-	4,4,4	0.18	0	6,6,6	0.19	0
2	SO4	A	449	-	4,4,4	0.13	0	6,6,6	0.13	0
3	ACT	A	450	-	1,3,3	1.66	0	0,3,3	0.00	-
4	GDP	A	501	-	30,30,30	1.57	3 (10%)	44,47,47	4.19	7 (15%)
2	SO4	B	444	-	4,4,4	0.14	0	6,6,6	0.14	0
2	SO4	B	445	-	4,4,4	0.12	0	6,6,6	0.31	0
2	SO4	B	446	-	4,4,4	0.15	0	6,6,6	0.08	0
2	SO4	B	447	-	4,4,4	0.13	0	6,6,6	0.20	0
2	SO4	B	448	-	4,4,4	0.15	0	6,6,6	0.22	0
3	ACT	B	449	-	1,3,3	1.15	0	0,3,3	0.00	-
4	GDP	B	501	-	30,30,30	1.29	3 (10%)	44,47,47	2.76	7 (15%)

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	444	-	-	0/0/0/0	0/0/0/0
2	SO4	A	445	-	-	0/0/0/0	0/0/0/0
2	SO4	A	446	-	-	0/0/0/0	0/0/0/0
2	SO4	A	447	-	-	0/0/0/0	0/0/0/0
2	SO4	A	448	-	-	0/0/0/0	0/0/0/0
2	SO4	A	449	-	-	0/0/0/0	0/0/0/0
3	ACT	A	450	-	-	0/0/0/0	0/0/0/0
4	GDP	A	501	-	-	0/16/32/32	0/1/3/3
2	SO4	B	444	-	-	0/0/0/0	0/0/0/0
2	SO4	B	445	-	-	0/0/0/0	0/0/0/0
2	SO4	B	446	-	-	0/0/0/0	0/0/0/0
2	SO4	B	447	-	-	0/0/0/0	0/0/0/0
2	SO4	B	448	-	-	0/0/0/0	0/0/0/0
3	ACT	B	449	-	-	0/0/0/0	0/0/0/0
4	GDP	B	501	-	-	0/16/32/32	0/1/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	501	GDP	C6-C5	4.85	1.49	1.41
4	A	501	GDP	C4-N9	-3.84	1.32	1.37
4	B	501	GDP	C6-C5	3.59	1.47	1.41
4	B	501	GDP	C5-C4	3.00	1.47	1.40
4	A	501	GDP	C5-C4	2.93	1.47	1.40
4	B	501	GDP	C4-N9	-2.85	1.33	1.37

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	501	GDP	C6-C5-N7	25.64	137.59	134.14
4	B	501	GDP	C6-C5-N7	14.94	136.15	134.14
4	B	501	GDP	N3-C4-N9	5.38	134.81	126.91
4	B	501	GDP	C5-C4-N3	-4.40	119.56	125.94
4	A	501	GDP	N3-C4-N9	4.17	133.02	126.91
4	A	501	GDP	C5-C4-N3	-3.93	120.25	125.94
4	A	501	GDP	C4-C5-N7	-3.82	106.25	109.52
4	B	501	GDP	C2-N3-C4	3.67	120.25	115.09
4	A	501	GDP	C2-N3-C4	3.60	120.15	115.09
4	A	501	GDP	C8-N9-C4	2.88	109.10	106.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	501	GDP	C1'-N9-C4	-2.83	121.74	126.64
4	B	501	GDP	C4-C5-N7	-2.58	107.31	109.52
4	B	501	GDP	C8-N9-C4	2.54	108.83	106.90
4	B	501	GDP	O4'-C1'-C2'	-2.01	103.69	106.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	416/443 (93%)	0.33	19 (4%) 31 32	35, 59, 112, 141	0
1	B	413/443 (93%)	0.40	22 (5%) 25 26	33, 64, 111, 132	0
All	All	829/886 (93%)	0.37	41 (4%) 28 29	33, 61, 112, 141	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	367	ILE	7.1
1	A	365	ILE	6.6
1	B	372	LEU	4.5
1	A	426	PHE	4.3
1	B	371	ARG	4.2
1	B	415	LEU	4.0
1	B	373	LYS	3.7
1	B	334	TYR	3.6
1	A	342	LYS	3.4
1	A	341	ARG	3.4
1	B	337	LEU	3.3
1	A	343	MET	3.2
1	B	407	THR	3.2
1	A	67	ALA	3.1
1	A	306	PHE	3.0
1	A	371	ARG	2.9
1	A	324	LEU	2.9
1	A	340	MET	2.8
1	A	434	LEU	2.7
1	B	343	MET	2.6
1	B	306	PHE	2.6
1	B	412	VAL	2.6
1	B	405	SER	2.5
1	B	409	THR	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	374	LYS	2.4
1	A	375	PHE	2.4
1	B	141	PRO	2.4
1	A	369	GLU	2.4
1	A	415	LEU	2.3
1	A	370	GLU	2.3
1	B	413	LYS	2.3
1	A	334	TYR	2.3
1	B	340	MET	2.3
1	B	370	GLU	2.3
1	B	375	PHE	2.3
1	A	337	LEU	2.2
1	B	399	LYS	2.2
1	B	368	GLY	2.1
1	A	430	ASN	2.0
1	A	303	LEU	2.0
1	B	411	ASP	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 ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	ACT	A	450	4/4	0.16	1.11	59,78,84,87	0
4	GDP	A	501	28/28	0.17	0.41	37,45,49,51	0
4	GDP	B	501	28/28	0.16	0.38	35,41,51,64	0
2	SO4	B	444	5/5	0.15	-0.35	87,89,112,122	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	B	446	5/5	0.16	-0.55	107,109,125,135	0
2	SO4	B	445	5/5	0.12	-0.59	73,73,103,111	0
2	SO4	A	444	5/5	0.14	-0.70	97,101,106,122	0
2	SO4	A	448	5/5	0.11	-0.88	87,89,105,112	0
3	ACT	B	449	4/4	0.13	-1.04	58,78,79,80	0
2	SO4	B	447	5/5	0.13	-1.27	79,85,89,101	0
2	SO4	A	446	5/5	0.11	-1.37	90,92,109,123	0
2	SO4	A	447	5/5	0.12	-2.09	65,76,87,90	0
2	SO4	A	449	5/5	0.10	-2.32	88,99,117,124	0
2	SO4	B	448	5/5	0.12	-2.86	105,106,116,132	0
2	SO4	A	445	5/5	0.11	-4.26	89,91,110,118	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.