



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 02:30 AM EDT

PDB ID : 1M6N  
Title : Crystal structure of the SecA translocation ATPase from *Bacillus subtilis*  
Authors : Hunt, J.F.; Weinkauff, S.; Henry, L.; Fak, J.J.; McNicholas, P.; Oliver, D.B.;  
Deisenhofer, J.  
Deposited on : 2002-07-16  
Resolution : 2.70 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

<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>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

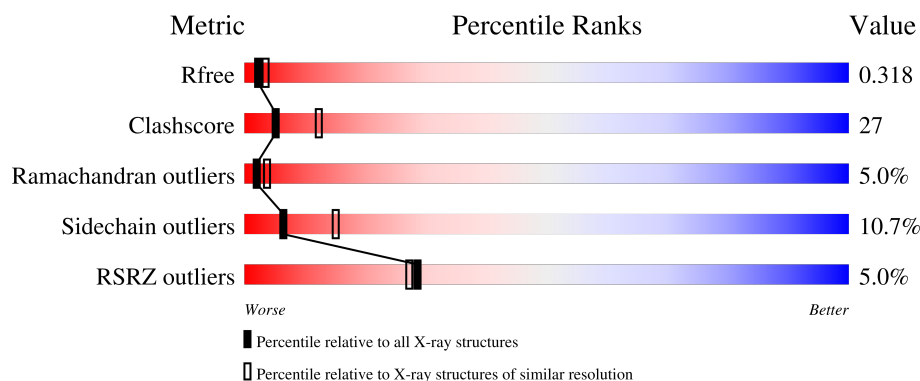
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
$R_{free}$	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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  $\geq 3$ , 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	802	

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	A	1003	-	-	X	-

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6482 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 Preprotein translocase secA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	802	6402	4000	1117	1250	35	0	0	0

- 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	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		

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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		

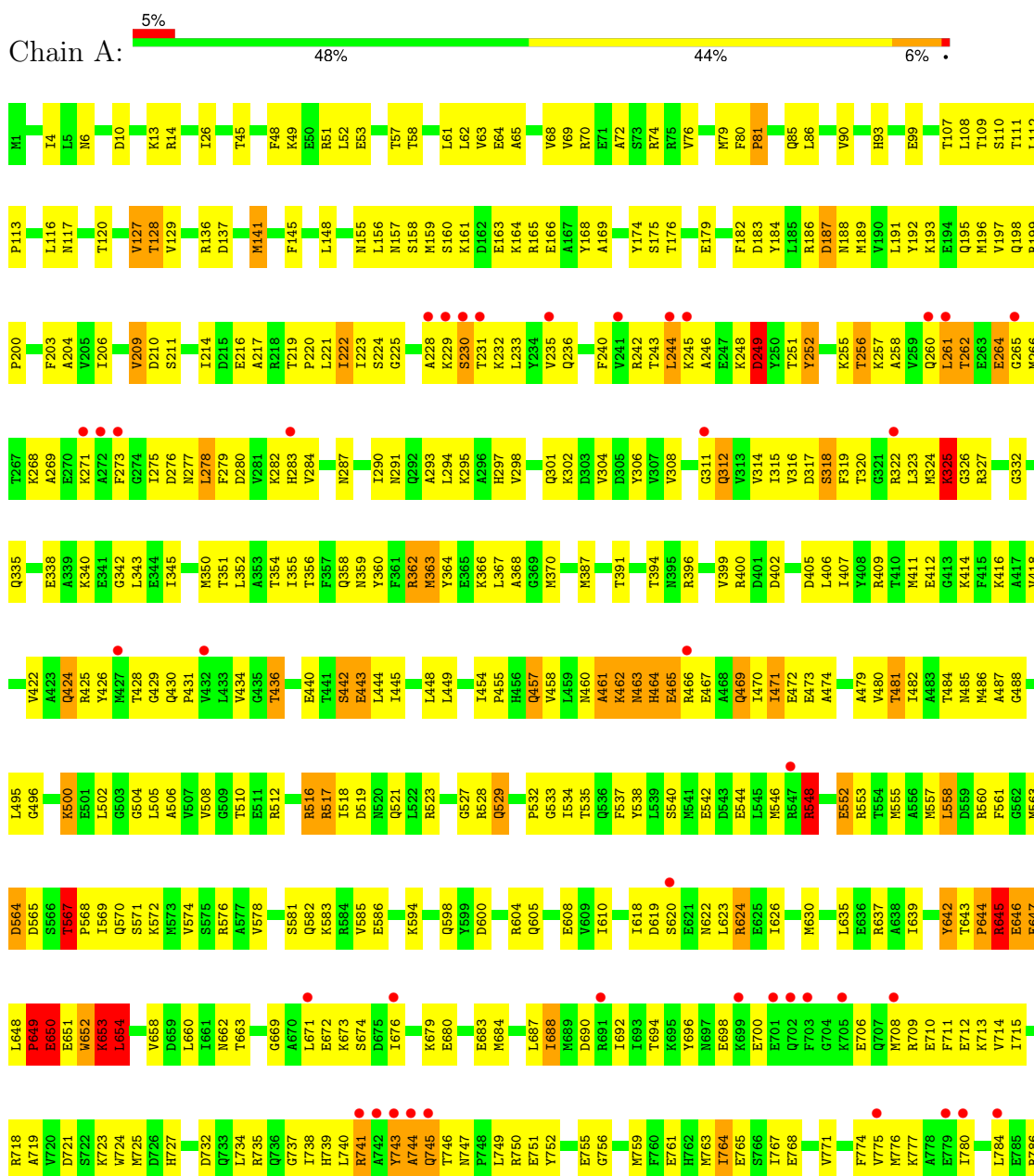
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	45	Total	O	0	0
			45	45		

### 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: Preprotein translocase secA



E787	
T794	
T795	
A796	
H797	
Q798	
P799	
G802	

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 1 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	130.83Å 130.83Å 150.35Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.24 – 2.70 45.24 – 2.50	Depositor EDS
% Data completeness (in resolution range)	80.4 (45.24-2.70) 87.3 (45.24-2.50)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.20 (at 2.51Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.220 , 0.301 0.232 , 0.318	Depositor DCC
$R_{free}$ test set	2582 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	74.8	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 95.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.034 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6482	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% 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, 0.333 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

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	0.61	0/6492	0.83	2/8731 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	249	ASP	N-CA-C	-6.87	92.46	111.00
1	A	222	ILE	CB-CA-C	-5.03	101.54	111.60

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	6402	0	6382	344	0
2	A	35	0	0	2	0
3	A	45	0	0	4	0
All	All	6482	0	6382	344	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 27.

All (344) 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:A:431:PRO:HB3	1:A:479:ALA:HB3	1.39	1.04
1:A:724:TRP:HA	1:A:763:MET:HE1	1.41	0.99
1:A:756:GLY:HA2	1:A:759:MET:HE3	1.45	0.95
1:A:635:LEU:HD21	1:A:688:ILE:HG23	1.58	0.83
1:A:425:ARG:O	1:A:428:THR:HG22	1.79	0.82
1:A:261:LEU:HD22	1:A:777:LYS:NZ	1.95	0.81
1:A:571:SER:HB3	1:A:574:VAL:HG12	1.63	0.81
1:A:240:PHE:CZ	1:A:244:LEU:HD11	2.16	0.81
1:A:500:LYS:H	1:A:500:LYS:HD3	1.45	0.80
1:A:643:THR:HA	1:A:652:TRP:CD1	2.17	0.79
1:A:721:ASP:O	1:A:725:MET:HG2	1.82	0.79
1:A:279:PHE:O	1:A:283:HIS:HB3	1.82	0.78
1:A:516:ARG:NH1	1:A:583:LYS:HG2	1.98	0.78
1:A:409:ARG:HG2	1:A:564:ASP:HB3	1.65	0.77
1:A:457:GLN:HG3	1:A:481:THR:HG23	1.66	0.77
1:A:465:GLU:O	1:A:469:GLN:HG2	1.84	0.76
1:A:552:GLU:HA	1:A:555:MET:HE3	1.68	0.76
1:A:301:GLN:HB2	1:A:304:VAL:CG1	2.17	0.75
1:A:738:ILE:HD11	1:A:751:GLU:HB2	1.69	0.75
1:A:265:GLY:O	1:A:269:ALA:HB2	1.85	0.74
1:A:261:LEU:HD22	1:A:777:LYS:HZ1	1.53	0.74
1:A:368:ALA:HA	1:A:387:MET:HE3	1.69	0.73
1:A:261:LEU:HD23	1:A:663:THR:CG2	2.19	0.73
1:A:93:HIS:HD2	1:A:117:ASN:HD21	1.36	0.72
1:A:567:THR:HG23	1:A:568:PRO:HD3	1.72	0.72
1:A:332:GLY:HA2	1:A:335:GLN:NE2	2.05	0.72
1:A:643:THR:N	1:A:644:PRO:HD3	2.05	0.71
1:A:283:HIS:HA	1:A:287:ASN:HB2	1.72	0.71
1:A:710:GLU:O	1:A:714:VAL:HG23	1.90	0.71
1:A:161:LYS:HE2	1:A:165:ARG:HH22	1.56	0.71
1:A:411:MET:HG3	1:A:542:GLU:HG3	1.71	0.70
1:A:718:ARG:HH21	1:A:787:GLU:HB2	1.56	0.70
1:A:683:GLU:O	1:A:687:LEU:HG	1.92	0.69
1:A:242:ARG:NH1	1:A:245:LYS:HB2	2.07	0.69
1:A:252:TYR:HB3	1:A:256:THR:H	1.57	0.69
1:A:301:GLN:HB2	1:A:304:VAL:HG12	1.74	0.69
1:A:724:TRP:HA	1:A:763:MET:CE	2.20	0.69
1:A:506:ALA:HA	1:A:534:ILE:O	1.93	0.68
1:A:242:ARG:HH11	1:A:245:LYS:HB2	1.57	0.68
1:A:578:VAL:O	1:A:581:SER:HB3	1.93	0.68
1:A:402:ASP:HA	1:A:535:THR:OG1	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:TYR:CD2	1:A:255:LYS:HB2	2.30	0.67
1:A:231:THR:O	1:A:235:VAL:HG23	1.95	0.67
1:A:111:THR:HA	1:A:145:PHE:HZ	1.60	0.67
1:A:412:GLU:O	1:A:416:LYS:HG3	1.95	0.66
1:A:111:THR:HA	1:A:145:PHE:CZ	2.31	0.66
1:A:623:LEU:HD12	1:A:626:ILE:HD12	1.76	0.66
1:A:732:ASP:HA	1:A:735:ARG:HD2	1.78	0.66
1:A:761:GLU:O	1:A:765:GLU:HG3	1.97	0.65
1:A:264:GLU:HG3	1:A:265:GLY:N	2.10	0.65
1:A:517:ARG:HH21	1:A:518:ILE:HD11	1.61	0.65
1:A:445:ILE:O	1:A:449:LEU:HG	1.96	0.64
1:A:248:LYS:O	1:A:264:GLU:HG2	1.98	0.63
1:A:356:THR:HG22	1:A:600:ASP:OD2	1.97	0.63
1:A:424:GLN:HG2	1:A:425:ARG:HG2	1.78	0.63
1:A:679:LYS:HD3	1:A:687:LEU:HD11	1.79	0.63
1:A:630:MET:CE	1:A:771:VAL:HG11	2.29	0.63
1:A:431:PRO:CB	1:A:479:ALA:HB3	2.21	0.63
1:A:449:LEU:CD1	1:A:482:ILE:HD11	2.28	0.63
1:A:159:MET:HB3	1:A:163:GLU:HB2	1.81	0.62
1:A:240:PHE:HZ	1:A:244:LEU:HD11	1.61	0.62
1:A:261:LEU:HD23	1:A:663:THR:HG22	1.80	0.62
1:A:724:TRP:CA	1:A:763:MET:HE1	2.25	0.62
1:A:428:THR:O	1:A:502:LEU:HD22	1.99	0.62
1:A:764:ILE:O	1:A:768:GLU:HG3	2.00	0.62
1:A:519:ASP:HB2	1:A:537:PHE:CZ	2.35	0.62
1:A:571:SER:CB	1:A:574:VAL:HG12	2.30	0.62
1:A:275:ILE:HG22	1:A:275:ILE:O	1.99	0.61
1:A:676:ILE:HG23	1:A:684:MET:SD	2.40	0.61
1:A:252:TYR:HB2	1:A:257:LYS:H	1.66	0.61
1:A:252:TYR:CE2	1:A:642:TYR:HE1	2.19	0.61
1:A:644:PRO:HB3	1:A:645:ARG:HH21	1.64	0.61
1:A:356:THR:HG23	1:A:359:ASN:H	1.65	0.61
1:A:469:GLN:O	1:A:472:GLU:HG2	2.00	0.61
1:A:70:ARG:HG2	1:A:80:PHE:CE1	2.35	0.61
1:A:540:SER:O	1:A:546:MET:HG3	2.01	0.60
1:A:755:GLU:O	1:A:759:MET:HG3	2.01	0.60
1:A:49:LYS:O	1:A:53:GLU:HG2	2.01	0.60
1:A:414:LYS:HD2	1:A:540:SER:HB3	1.84	0.59
1:A:444:LEU:O	1:A:448:LEU:HG	2.02	0.59
1:A:688:ILE:HD13	1:A:688:ILE:O	2.01	0.59
1:A:161:LYS:HE2	1:A:165:ARG:NH2	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:ARG:HG3	1:A:197:VAL:HA	1.85	0.59
1:A:436:THR:HA	1:A:510:THR:OG1	2.02	0.59
1:A:260:GLN:O	1:A:262:THR:N	2.36	0.58
1:A:318:SER:HB2	1:A:319:PHE:HD1	1.68	0.58
1:A:558:LEU:HA	1:A:563:MET:HB2	1.84	0.58
1:A:112:LEU:HB2	1:A:113:PRO:HD3	1.84	0.58
1:A:739:HIS:O	1:A:740:LEU:HD23	2.03	0.58
1:A:128:THR:O	1:A:176:THR:HA	2.03	0.58
1:A:112:LEU:HB2	1:A:113:PRO:CD	2.34	0.58
1:A:157:ASN:HB3	1:A:179:GLU:OE2	2.04	0.58
1:A:744:ALA:C	1:A:746:THR:H	2.07	0.57
1:A:637:ARG:HH22	1:A:768:GLU:HB2	1.68	0.57
1:A:658:VAL:HG11	1:A:672:GLU:HA	1.86	0.57
1:A:136:ARG:HG2	1:A:136:ARG:HH11	1.69	0.57
1:A:352:LEU:HD22	1:A:725:MET:HE3	1.85	0.57
1:A:52:LEU:HG	1:A:61:LEU:HD11	1.86	0.57
1:A:461:ALA:HA	1:A:467:GLU:OE1	2.05	0.57
1:A:283:HIS:HA	1:A:287:ASN:CB	2.35	0.57
1:A:414:LYS:HE2	1:A:510:THR:O	2.04	0.57
1:A:700:GLU:HG2	1:A:708:MET:HG2	1.87	0.57
1:A:794:THR:HG22	1:A:795:THR:N	2.18	0.57
1:A:512:ARG:HH21	1:A:523:ARG:NH2	2.03	0.56
1:A:120:THR:HG21	2:A:1003:SO4:S	2.46	0.56
1:A:258:ALA:HB1	1:A:294:LEU:HG	1.88	0.56
1:A:182:PHE:CZ	1:A:221:LEU:HD22	2.41	0.56
1:A:155:ASN:HB3	1:A:175:SER:HB3	1.88	0.55
1:A:654:LEU:N	1:A:654:LEU:HD12	2.20	0.55
1:A:436:THR:HG21	1:A:442:SER:HA	1.87	0.55
1:A:252:TYR:HE2	1:A:642:TYR:HE1	1.54	0.55
1:A:463:ASN:HD22	1:A:466:ARG:NE	2.05	0.55
1:A:225:GLY:HA3	1:A:352:LEU:HD11	1.89	0.55
1:A:646:GLU:O	1:A:648:LEU:N	2.39	0.55
1:A:262:THR:O	1:A:266:MET:HB2	2.07	0.55
1:A:734:LEU:HD23	1:A:759:MET:HE1	1.89	0.55
1:A:727:HIS:HB2	1:A:763:MET:HE2	1.89	0.55
1:A:224:SER:HA	1:A:350:MET:O	2.07	0.55
1:A:516:ARG:HH12	1:A:583:LYS:HG2	1.72	0.55
1:A:440:GLU:HA	1:A:443:GLU:OE2	2.06	0.55
1:A:645:ARG:H	1:A:645:ARG:HE	1.52	0.54
1:A:268:LYS:HA	1:A:271:LYS:HD2	1.90	0.54
1:A:318:SER:HB2	1:A:319:PHE:CD1	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:505:LEU:O	1:A:506:ALA:HB3	2.07	0.54
1:A:557:MET:O	1:A:561:PHE:HB2	2.08	0.54
1:A:434:VAL:CG2	1:A:482:ILE:HG12	2.38	0.54
1:A:630:MET:HE1	1:A:771:VAL:HG21	1.88	0.54
1:A:166:GLU:O	1:A:169:ALA:HB3	2.07	0.54
1:A:45:THR:HG22	1:A:49:LYS:HE3	1.90	0.54
1:A:183:ASP:O	1:A:187:ASP:HB2	2.07	0.54
1:A:563:MET:C	1:A:565:ASP:H	2.11	0.54
1:A:251:THR:HA	1:A:257:LYS:O	2.08	0.53
1:A:654:LEU:HD12	1:A:654:LEU:H	1.73	0.53
1:A:222:ILE:HG22	1:A:223:ILE:N	2.23	0.53
1:A:65:ALA:O	1:A:69:VAL:HG23	2.08	0.53
1:A:268:LYS:HG2	1:A:271:LYS:NZ	2.23	0.53
1:A:582:GLN:O	1:A:586:GLU:HG3	2.09	0.53
1:A:637:ARG:NH1	1:A:765:GLU:HA	2.24	0.53
1:A:658:VAL:O	1:A:662:ASN:HB2	2.09	0.53
1:A:630:MET:HE1	1:A:771:VAL:HG11	1.89	0.53
1:A:222:ILE:HG23	1:A:351:THR:HG23	1.90	0.53
1:A:649:PRO:C	1:A:651:GLU:H	2.12	0.53
1:A:64:GLU:O	1:A:68:VAL:HG23	2.09	0.52
1:A:654:LEU:H	1:A:654:LEU:CD1	2.22	0.52
1:A:723:LYS:HG3	1:A:767:ILE:HG13	1.91	0.52
1:A:52:LEU:HG	1:A:61:LEU:CD1	2.40	0.52
1:A:128:THR:HG22	1:A:129:VAL:H	1.74	0.52
1:A:230:SER:HB2	1:A:233:LEU:HD12	1.91	0.52
1:A:278:LEU:HB2	1:A:282:LYS:HG2	1.91	0.52
1:A:368:ALA:CA	1:A:387:MET:HE3	2.37	0.52
1:A:594:LYS:O	1:A:598:GLN:HG3	2.09	0.52
1:A:643:THR:N	1:A:644:PRO:CD	2.72	0.52
1:A:647:GLU:O	1:A:647:GLU:HG3	2.08	0.52
1:A:161:LYS:HE3	1:A:195:GLN:HG2	1.92	0.52
1:A:165:ARG:HD3	3:A:1117:HOH:O	2.09	0.52
1:A:252:TYR:HE2	1:A:642:TYR:CE1	2.27	0.52
1:A:6:ASN:HD21	1:A:13:LYS:NZ	2.08	0.51
1:A:164:LYS:NZ	1:A:179:GLU:OE1	2.43	0.51
1:A:193:LYS:O	1:A:196:MET:HG3	2.10	0.51
1:A:644:PRO:O	1:A:646:GLU:N	2.44	0.51
1:A:203:PHE:HA	1:A:366:LYS:O	2.10	0.51
1:A:264:GLU:CG	1:A:265:GLY:N	2.73	0.51
1:A:637:ARG:HH12	1:A:765:GLU:HA	1.74	0.51
1:A:137:ASP:O	1:A:141:MET:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:620:SER:OG	1:A:713:LYS:HG3	2.11	0.51
1:A:639:ILE:HD11	1:A:688:ILE:HG21	1.93	0.51
1:A:574:VAL:O	1:A:578:VAL:HG23	2.11	0.50
1:A:620:SER:HB2	1:A:623:LEU:HB2	1.94	0.50
1:A:358:GLN:O	1:A:362:ARG:HB2	2.10	0.50
1:A:471:ILE:HD12	1:A:488:GLY:HA3	1.92	0.50
1:A:26:ILE:CG1	1:A:63:VAL:HG13	2.41	0.50
1:A:252:TYR:HB3	1:A:256:THR:N	2.25	0.50
1:A:268:LYS:HG2	1:A:271:LYS:HZ1	1.76	0.50
1:A:294:LEU:O	1:A:298:VAL:HG23	2.11	0.50
1:A:558:LEU:CA	1:A:563:MET:HB2	2.41	0.50
1:A:26:ILE:HG12	1:A:63:VAL:HG13	1.93	0.50
1:A:434:VAL:HG22	1:A:482:ILE:HG12	1.93	0.50
1:A:604:ARG:HG3	1:A:605:GLN:N	2.27	0.50
1:A:210:ASP:O	1:A:214:ILE:HB	2.12	0.50
1:A:569:ILE:HG22	1:A:570:GLN:N	2.26	0.50
1:A:72:ALA:O	1:A:76:VAL:HG23	2.12	0.49
1:A:623:LEU:HD23	1:A:712:GLU:HB3	1.93	0.49
1:A:360:TYR:O	1:A:363:MET:HB2	2.12	0.49
1:A:290:ILE:O	1:A:294:LEU:HB2	2.13	0.49
1:A:794:THR:HG22	1:A:795:THR:H	1.78	0.49
1:A:127:VAL:HG13	1:A:206:ILE:HA	1.95	0.49
1:A:406:LEU:HD12	1:A:538:TYR:CE1	2.48	0.49
1:A:332:GLY:HA2	1:A:335:GLN:HE22	1.74	0.49
1:A:246:ALA:HB3	1:A:264:GLU:OE2	2.13	0.48
1:A:271:LYS:C	1:A:273:PHE:H	2.15	0.48
1:A:400:ARG:HG3	1:A:533:GLY:HA3	1.94	0.48
1:A:517:ARG:O	1:A:521:GLN:HG3	2.13	0.48
1:A:436:THR:HA	1:A:510:THR:HG1	1.76	0.48
1:A:449:LEU:HD11	1:A:482:ILE:HD11	1.94	0.48
1:A:713:LYS:HD2	1:A:786:ARG:NH2	2.28	0.48
1:A:111:THR:CG2	1:A:141:MET:HG3	2.43	0.48
1:A:184:TYR:O	1:A:188:ASN:ND2	2.45	0.48
1:A:434:VAL:HG12	1:A:508:VAL:HB	1.95	0.48
1:A:565:ASP:O	1:A:567:THR:HG22	2.13	0.48
1:A:168:TYR:CE2	1:A:198:GLN:HG2	2.49	0.48
1:A:204:ALA:HB3	1:A:367:LEU:HD12	1.94	0.48
1:A:284:VAL:HG11	1:A:718:ARG:HD2	1.95	0.48
1:A:622:ASN:HA	1:A:709:ARG:HH21	1.79	0.48
1:A:431:PRO:HB2	1:A:505:LEU:HD12	1.95	0.48
1:A:204:ALA:HB2	1:A:364:TYR:CE2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:680:GLU:O	1:A:684:MET:HG3	2.14	0.47
1:A:743:TYR:O	1:A:745:GLN:N	2.47	0.47
1:A:108:LEU:HA	1:A:141:MET:HE3	1.95	0.47
1:A:727:HIS:CB	1:A:763:MET:CE	2.92	0.47
1:A:734:LEU:HD23	1:A:759:MET:CE	2.43	0.47
1:A:161:LYS:HB2	1:A:165:ARG:NH2	2.29	0.47
1:A:261:LEU:HD22	1:A:777:LYS:HZ2	1.75	0.47
1:A:527:GLY:O	1:A:529:GLN:N	2.47	0.47
1:A:248:LYS:C	1:A:262:THR:HG21	2.35	0.47
1:A:471:ILE:O	1:A:474:ALA:HB3	2.14	0.47
1:A:744:ALA:O	1:A:745:GLN:HG2	2.14	0.47
1:A:750:ARG:NH1	3:A:1104:HOH:O	2.47	0.47
1:A:738:ILE:C	1:A:740:LEU:H	2.17	0.47
1:A:764:ILE:N	1:A:764:ILE:HD13	2.30	0.47
1:A:161:LYS:HB2	1:A:165:ARG:HH22	1.80	0.47
1:A:219:THR:HB	1:A:220:PRO:HD2	1.96	0.47
1:A:458:VAL:HG22	1:A:482:ILE:HB	1.95	0.47
1:A:581:SER:O	1:A:585:VAL:HG23	2.13	0.47
1:A:610:ILE:HG13	1:A:724:TRP:CE3	2.49	0.47
1:A:86:LEU:O	1:A:90:VAL:HG23	2.13	0.47
1:A:311:GLY:C	1:A:312:GLN:HG2	2.33	0.47
1:A:163:GLU:O	1:A:166:GLU:HB3	2.14	0.47
1:A:434:VAL:HA	1:A:508:VAL:O	2.14	0.47
1:A:652:TRP:H	1:A:654:LEU:HD11	1.80	0.47
1:A:108:LEU:HA	1:A:141:MET:CE	2.45	0.46
1:A:424:GLN:HG2	1:A:425:ARG:N	2.30	0.46
1:A:287:ASN:OD1	1:A:291:ASN:ND2	2.49	0.46
1:A:317:ASP:HB3	1:A:320:THR:OG1	2.15	0.46
1:A:466:ARG:O	1:A:470:ILE:HG13	2.15	0.46
1:A:572:LYS:O	1:A:576:ARG:HG3	2.16	0.46
1:A:649:PRO:O	1:A:651:GLU:N	2.49	0.46
1:A:684:MET:O	1:A:688:ILE:HG22	2.15	0.46
1:A:741:ARG:HD3	1:A:741:ARG:C	2.36	0.46
1:A:62:LEU:HA	1:A:116:LEU:HD22	1.98	0.46
1:A:242:ARG:HA	1:A:242:ARG:HD3	1.76	0.46
1:A:306:TYR:OH	1:A:340:LYS:HE2	2.15	0.46
1:A:136:ARG:HG2	1:A:136:ARG:NH1	2.30	0.46
1:A:445:ILE:HA	1:A:448:LEU:HG	1.98	0.46
1:A:148:LEU:HD23	1:A:148:LEU:HA	1.84	0.46
1:A:429:GLY:C	1:A:502:LEU:HD13	2.37	0.46
1:A:268:LYS:HA	1:A:271:LYS:CD	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:VAL:HG13	1:A:343:LEU:HD11	1.99	0.45
1:A:431:PRO:O	1:A:505:LEU:O	2.34	0.45
1:A:155:ASN:HB3	1:A:175:SER:CB	2.46	0.45
1:A:199:ARG:CG	1:A:200:PRO:HD2	2.47	0.45
1:A:72:ALA:HB2	1:A:148:LEU:HD11	1.98	0.45
1:A:338:GLU:OE1	1:A:345:ILE:HA	2.17	0.45
1:A:774:PHE:N	1:A:774:PHE:CD1	2.85	0.45
1:A:108:LEU:O	1:A:111:THR:OG1	2.28	0.45
1:A:454:ILE:HA	1:A:455:PRO:HD3	1.81	0.45
1:A:653:LYS:HD2	1:A:653:LYS:C	2.37	0.45
1:A:780:ILE:HD13	1:A:784:LEU:HD11	1.98	0.45
1:A:48:PHE:CE1	1:A:68:VAL:HG21	2.52	0.44
1:A:261:LEU:HD23	1:A:663:THR:HG23	1.96	0.44
1:A:251:THR:OG1	1:A:252:TYR:N	2.50	0.44
1:A:322:ARG:HG3	1:A:323:LEU:N	2.32	0.44
1:A:252:TYR:CB	1:A:257:LYS:H	2.28	0.44
1:A:710:GLU:HG3	1:A:714:VAL:HG23	1.99	0.44
1:A:741:ARG:HD3	1:A:741:ARG:O	2.18	0.44
1:A:692:ILE:HG23	1:A:776:MET:HE1	1.99	0.44
1:A:308:VAL:HG13	1:A:343:LEU:CD1	2.47	0.44
1:A:643:THR:HA	1:A:652:TRP:CG	2.52	0.44
1:A:110:SER:O	1:A:113:PRO:HD2	2.18	0.44
1:A:192:TYR:CE2	1:A:786:ARG:HD2	2.52	0.44
1:A:252:TYR:HD2	1:A:255:LYS:N	2.16	0.44
1:A:436:THR:HG21	1:A:442:SER:CA	2.46	0.44
1:A:775:VAL:HG12	1:A:775:VAL:O	2.17	0.44
1:A:604:ARG:O	1:A:608:GLU:HG3	2.17	0.44
1:A:85:GLN:HG2	1:A:109:THR:OG1	2.18	0.43
1:A:658:VAL:CG1	1:A:672:GLU:HA	2.47	0.43
1:A:279:PHE:O	1:A:283:HIS:CB	2.61	0.43
1:A:563:MET:C	1:A:565:ASP:N	2.71	0.43
1:A:327:ARG:HD2	1:A:755:GLU:OE1	2.18	0.43
1:A:257:LYS:HD2	1:A:660:LEU:HD11	2.01	0.43
1:A:409:ARG:CG	1:A:564:ASP:HB3	2.43	0.43
1:A:711:PHE:HD1	1:A:784:LEU:HD22	1.83	0.43
1:A:744:ALA:C	1:A:746:THR:N	2.72	0.43
1:A:10:ASP:O	1:A:14:ARG:HG3	2.19	0.43
1:A:774:PHE:N	1:A:774:PHE:HD1	2.16	0.43
1:A:323:LEU:HD23	1:A:323:LEU:HA	1.78	0.43
1:A:425:ARG:HB3	1:A:430:GLN:HB3	2.01	0.43
1:A:256:THR:HG22	1:A:295:LYS:HE3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:GLU:O	1:A:548:ARG:HB2	2.17	0.43
1:A:623:LEU:CD1	1:A:626:ILE:HD12	2.47	0.43
1:A:301:GLN:HB2	1:A:304:VAL:HG11	2.00	0.42
1:A:648:LEU:CB	1:A:651:GLU:HB2	2.49	0.42
1:A:325:LYS:HB2	1:A:325:LYS:HE2	1.38	0.42
1:A:571:SER:HB3	1:A:574:VAL:CG1	2.40	0.42
1:A:743:TYR:C	1:A:745:GLN:H	2.22	0.42
1:A:650:GLU:HA	1:A:654:LEU:HD21	2.00	0.42
1:A:109:THR:O	1:A:113:PRO:HD2	2.20	0.42
1:A:155:ASN:O	1:A:156:LEU:HD23	2.19	0.42
1:A:203:PHE:CE1	1:A:366:LYS:HE3	2.54	0.42
1:A:186:ARG:HA	1:A:189:MET:CE	2.50	0.42
1:A:462:LYS:HD3	1:A:462:LYS:N	2.35	0.42
1:A:652:TRP:O	1:A:653:LYS:CB	2.68	0.42
1:A:74:ARG:HD3	1:A:80:PHE:HB2	2.01	0.42
1:A:293:ALA:O	1:A:297:HIS:ND1	2.53	0.42
1:A:738:ILE:HD13	1:A:752:TYR:HB2	2.01	0.42
1:A:57:THR:HB	3:A:1106:HOH:O	2.19	0.42
1:A:182:PHE:CD2	1:A:796:ALA:HB1	2.55	0.42
1:A:630:MET:HB2	1:A:630:MET:HE2	1.84	0.42
1:A:426:TYR:C	1:A:428:THR:H	2.23	0.42
1:A:504:GLY:HA3	1:A:532:PRO:O	2.19	0.42
1:A:418:VAL:O	1:A:422:VAL:HG23	2.20	0.42
1:A:431:PRO:HA	1:A:479:ALA:O	2.20	0.42
1:A:727:HIS:CB	1:A:763:MET:HE3	2.49	0.42
1:A:306:TYR:HB2	1:A:314:VAL:O	2.19	0.41
1:A:394:THR:HG22	1:A:396:ARG:O	2.20	0.41
1:A:315:ILE:HG22	1:A:316:VAL:N	2.35	0.41
1:A:460:ASN:OD1	1:A:460:ASN:N	2.53	0.41
1:A:694:THR:O	1:A:698:GLU:HG3	2.21	0.41
1:A:206:ILE:HB	1:A:209:VAL:HG13	2.02	0.41
1:A:354:THR:CG2	1:A:355:ILE:N	2.83	0.41
1:A:630:MET:HE2	1:A:771:VAL:HG11	2.02	0.41
1:A:654:LEU:N	1:A:654:LEU:CD1	2.82	0.41
1:A:284:VAL:HG11	1:A:718:ARG:HH11	1.85	0.41
1:A:414:LYS:CD	1:A:540:SER:HB3	2.49	0.41
1:A:569:ILE:CG2	1:A:570:GLN:N	2.84	0.41
1:A:620:SER:CB	1:A:623:LEU:HB2	2.51	0.41
1:A:715:ILE:HD13	1:A:715:ILE:HA	1.91	0.41
1:A:798:GLN:HA	1:A:799:PRO:HD3	1.89	0.41
1:A:326:GLY:HA3	1:A:737:GLY:HA3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:MET:HE1	3:A:1115:HOH:O	2.20	0.41
1:A:563:MET:O	1:A:565:ASP:N	2.53	0.41
1:A:248:LYS:O	1:A:262:THR:HG21	2.22	0.40
1:A:711:PHE:HD1	1:A:784:LEU:CD2	2.34	0.40
1:A:217:ALA:HB1	1:A:358:GLN:HE22	1.86	0.40
1:A:484:THR:O	1:A:485:ASN:HB2	2.22	0.40
1:A:79:MET:O	1:A:81:PRO:HD3	2.22	0.40
1:A:93:HIS:CD2	1:A:117:ASN:HD21	2.26	0.40
1:A:120:THR:HG21	2:A:1003:SO4:O4	2.20	0.40
1:A:174:TYR:O	1:A:175:SER:HB3	2.21	0.40
1:A:232:LYS:O	1:A:236:GLN:HB2	2.21	0.40
1:A:516:ARG:O	1:A:517:ARG:C	2.59	0.40
1:A:671:LEU:O	1:A:672:GLU:HG3	2.21	0.40
1:A:642:TYR:C	1:A:644:PRO:HD3	2.40	0.40
1:A:744:ALA:O	1:A:746:THR:N	2.54	0.40
1:A:645:ARG:O	1:A:647:GLU:N	2.55	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	800/802 (100%)	654 (82%)	106 (13%)	40 (5%)	<b>2</b> <b>4</b>

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	228	ALA
1	A	261	LEU
1	A	302	LYS
1	A	325	LYS

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Mol	Chain	Res	Type
1	A	528	ARG
1	A	567	THR
1	A	645	ARG
1	A	646	GLU
1	A	647	GLU
1	A	649	PRO
1	A	653	LYS
1	A	312	GLN
1	A	342	GLY
1	A	461	ALA
1	A	487	ALA
1	A	644	PRO
1	A	650	GLU
1	A	669	GLY
1	A	744	ALA
1	A	230	SER
1	A	244	LEU
1	A	249	ASP
1	A	256	THR
1	A	276	ASP
1	A	496	GLY
1	A	654	LEU
1	A	673	LYS
1	A	229	LYS
1	A	278	LEU
1	A	463	ASN
1	A	464	HIS
1	A	548	ARG
1	A	243	THR
1	A	564	ASP
1	A	624	ARG
1	A	719	ALA
1	A	216	GLU
1	A	324	MET
1	A	480	VAL

### 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	689/689 (100%)	615 (89%)	74 (11%)	6 15

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	ARG
1	A	58	THR
1	A	81	PRO
1	A	99	GLU
1	A	107	THR
1	A	127	VAL
1	A	128	THR
1	A	141	MET
1	A	158	SER
1	A	160	SER
1	A	187	ASP
1	A	191	LEU
1	A	209	VAL
1	A	211	SER
1	A	249	ASP
1	A	252	TYR
1	A	262	THR
1	A	264	GLU
1	A	277	ASN
1	A	280	ASP
1	A	318	SER
1	A	325	LYS
1	A	362	ARG
1	A	363	MET
1	A	370	MET
1	A	391	THR
1	A	399	VAL
1	A	405	ASP
1	A	407	ILE
1	A	424	GLN
1	A	436	THR
1	A	442	SER
1	A	443	GLU
1	A	457	GLN
1	A	462	LYS
1	A	464	HIS

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Mol	Chain	Res	Type
1	A	465	GLU
1	A	469	GLN
1	A	471	ILE
1	A	473	GLU
1	A	481	THR
1	A	486	MET
1	A	495	LEU
1	A	500	LYS
1	A	516	ARG
1	A	517	ARG
1	A	529	GLN
1	A	548	ARG
1	A	552	GLU
1	A	553	ARG
1	A	558	LEU
1	A	560	ARG
1	A	567	THR
1	A	618	ILE
1	A	619	ASP
1	A	624	ARG
1	A	642	TYR
1	A	645	ARG
1	A	649	PRO
1	A	650	GLU
1	A	652	TRP
1	A	653	LYS
1	A	654	LEU
1	A	674	SER
1	A	688	ILE
1	A	690	ASP
1	A	696	TYR
1	A	706	GLU
1	A	741	ARG
1	A	743	TYR
1	A	745	GLN
1	A	747	ASN
1	A	749	LEU
1	A	764	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	93	HIS
1	A	287	ASN
1	A	291	ASN
1	A	335	GLN
1	A	386	ASN
1	A	424	GLN
1	A	463	ASN
1	A	469	GLN
1	A	513	HIS
1	A	570	GLN
1	A	589	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

7 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	1006	-	4,4,4	0.33	0	6,6,6	0.37	0
2	SO4	A	1005	-	4,4,4	0.30	0	6,6,6	0.19	0
2	SO4	A	1001	-	4,4,4	0.32	0	6,6,6	0.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	SO4	A	1004	-	4,4,4	0.25	0	6,6,6	0.48	0
2	SO4	A	1007	-	4,4,4	0.31	0	6,6,6	0.20	0
2	SO4	A	1003	-	4,4,4	0.26	0	6,6,6	0.27	0
2	SO4	A	1002	-	4,4,4	0.29	0	6,6,6	0.18	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.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1003	SO4	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 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	802/802 (100%)	0.06	40 (4%)	28 27	35, 92, 168, 207	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	703	PHE	8.2
1	A	273	PHE	6.1
1	A	261	LEU	5.8
1	A	241	VAL	5.7
1	A	701	GLU	5.6
1	A	742	ALA	5.2
1	A	676	ILE	4.8
1	A	702	GLN	4.7
1	A	743	TYR	4.6
1	A	260	GLN	4.6
1	A	228	ALA	4.3
1	A	620	SER	4.1
1	A	244	LEU	4.0
1	A	427	MET	3.7
1	A	744	ALA	3.7
1	A	229	LYS	3.6
1	A	691	ARG	3.1
1	A	245	LYS	3.0
1	A	235	VAL	2.9
1	A	784	LEU	2.9
1	A	311	GLY	2.9
1	A	271	LYS	2.8
1	A	671	LEU	2.8
1	A	779	GLU	2.8
1	A	741	ARG	2.8
1	A	432	VAL	2.6
1	A	283	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	230	SER	2.6
1	A	272	ALA	2.5
1	A	547	ARG	2.5
1	A	699	LYS	2.5
1	A	745	GLN	2.4
1	A	265	GLY	2.4
1	A	705	LYS	2.2
1	A	708	MET	2.2
1	A	322	ARG	2.2
1	A	466	ARG	2.1
1	A	780	ILE	2.1
1	A	231	THR	2.1
1	A	775	VAL	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 monosaccharides 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, 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	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	A	1007	5/5	0.90	0.39	107,112,116,130	0
2	SO4	A	1003	5/5	0.93	0.10	95,96,110,111	0
2	SO4	A	1005	5/5	0.95	0.14	111,114,117,118	0
2	SO4	A	1006	5/5	0.96	0.15	78,93,98,100	0
2	SO4	A	1004	5/5	0.98	0.08	75,76,83,105	0
2	SO4	A	1002	5/5	0.98	0.07	93,99,108,110	0
2	SO4	A	1001	5/5	0.99	0.18	46,63,71,78	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.