



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 03:07 AM BST

PDB ID : 6GOX  
Title : SecA  
Authors : White, S.A.; Huber, D.  
Deposited on : 2018-06-04  
Resolution : 3.50 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.

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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  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
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) : 2.13.1

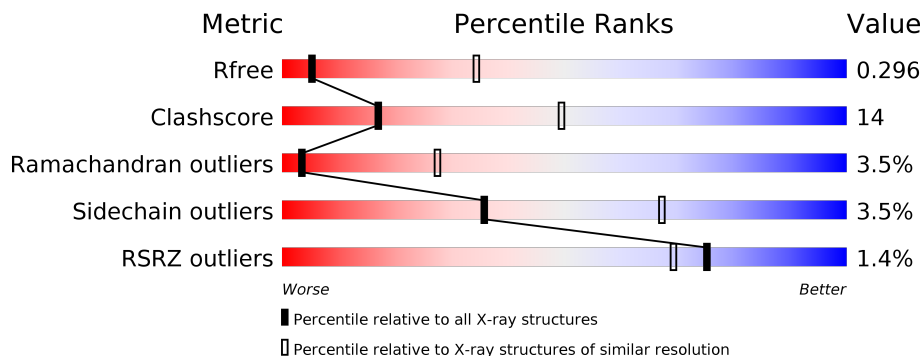
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 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	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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 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	822	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6182 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.

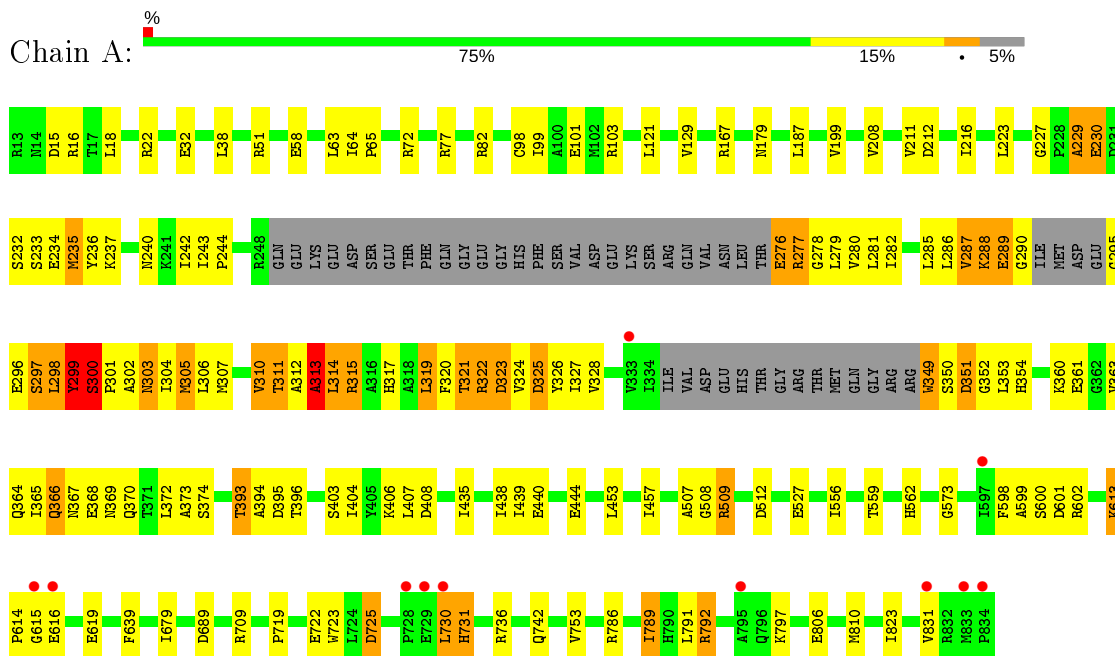
- Molecule 1 is a protein called Protein translocase subunit SecA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	777	6182	3882	1092	1179	29	0	0	0

### 3 Residue-property plots [i](#)

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: Protein translocase subunit SecA



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	163.14Å 106.83Å 75.98Å 90.00° 102.81° 90.00°	Depositor
Resolution (Å)	88.69 – 3.50 47.50 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.7 (88.69-3.50) 99.7 (47.50-3.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.55 (at 3.48Å)	Xtrriage
Refinement program	REFMAC 5.8.0107	Depositor
R, $R_{free}$	0.232 , 0.293 0.233 , 0.296	Depositor DCC
$R_{free}$ test set	785 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	132.1	Xtrriage
Anisotropy	0.037	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 85.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6182	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	158.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% 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](#)

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	0.56	1/6283 (0.0%)	0.78	7/8476 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	314	LEU	N-CA	-9.25	1.27	1.46

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	310	VAL	C-N-CA	-7.57	102.79	121.70
1	A	314	LEU	N-CA-CB	-7.50	95.39	110.40
1	A	313	ALA	CA-C-N	-7.02	101.75	117.20
1	A	310	VAL	O-C-N	-5.72	113.54	122.70
1	A	792	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	A	315	ARG	C-N-CA	-5.55	107.82	121.70
1	A	313	ALA	CB-CA-C	-5.09	102.47	110.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	313	ALA	Mainchain

## 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	6182	0	6181	173	0
All	All	6182	0	6181	173	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 14.

All (173) 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:298:LEU:HD11	1:A:307:MET:SD	1.47	1.52
1:A:243:ILE:CD1	1:A:313:ALA:HB1	1.50	1.42
1:A:298:LEU:CD1	1:A:307:MET:SD	2.12	1.37
1:A:279:LEU:HD11	1:A:299:TYR:CE2	1.60	1.34
1:A:304:ILE:HD11	1:A:792:ARG:CZ	1.71	1.17
1:A:279:LEU:CD1	1:A:299:TYR:HE2	1.59	1.15
1:A:321:THR:O	1:A:322:ARG:O	1.63	1.12
1:A:301:PRO:O	1:A:792:ARG:NH2	1.85	1.10
1:A:243:ILE:CG1	1:A:313:ALA:HB1	1.85	1.07
1:A:243:ILE:CD1	1:A:313:ALA:CB	2.35	1.04
1:A:243:ILE:HD13	1:A:313:ALA:HB1	1.36	1.03
1:A:310:VAL:O	1:A:311:THR:C	1.93	0.93
1:A:279:LEU:HD11	1:A:299:TYR:HE2	0.75	0.91
1:A:304:ILE:O	1:A:305:MET:C	2.06	0.90
1:A:304:ILE:O	1:A:306:LEU:N	2.03	0.90
1:A:322:ARG:O	1:A:324:VAL:N	2.05	0.88
1:A:243:ILE:HD11	1:A:313:ALA:HB1	1.54	0.87
1:A:301:PRO:CB	1:A:806:GLU:OE2	2.14	0.86
1:A:311:THR:O	1:A:315:ARG:HB2	1.75	0.86
1:A:301:PRO:O	1:A:792:ARG:CZ	2.24	0.85
1:A:298:LEU:HD12	1:A:307:MET:SD	2.16	0.85
1:A:302:ALA:O	1:A:304:ILE:N	2.09	0.85
1:A:321:THR:O	1:A:325:ASP:OD1	1.93	0.85
1:A:243:ILE:HG12	1:A:313:ALA:HB1	1.58	0.84
1:A:281:LEU:O	1:A:285:LEU:HG	1.76	0.84
1:A:304:ILE:O	1:A:307:MET:N	2.12	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:ILE:HD11	1:A:313:ALA:CB	2.06	0.81
1:A:298:LEU:O	1:A:299:TYR:HB2	1.80	0.81
1:A:321:THR:N	1:A:325:ASP:OD1	2.14	0.81
1:A:229:ALA:O	1:A:230:GLU:HG3	1.83	0.79
1:A:304:ILE:HD11	1:A:792:ARG:NH2	1.98	0.79
1:A:304:ILE:HD11	1:A:792:ARG:NH1	1.98	0.79
1:A:299:TYR:O	1:A:300:SER:HB2	1.82	0.78
1:A:349:TRP:N	1:A:354:HIS:HD1	1.81	0.77
1:A:311:THR:HA	1:A:314:LEU:HD23	1.65	0.77
1:A:300:SER:OG	1:A:301:PRO:HA	1.84	0.77
1:A:233:SER:HA	1:A:365:ILE:HD12	1.68	0.76
1:A:310:VAL:O	1:A:312:ALA:N	2.19	0.74
1:A:689:ASP:OD1	1:A:736:ARG:NH2	2.20	0.74
1:A:310:VAL:C	1:A:312:ALA:N	2.41	0.74
1:A:301:PRO:O	1:A:792:ARG:NH1	2.21	0.73
1:A:279:LEU:CD1	1:A:299:TYR:CE2	2.48	0.73
1:A:15:ASP:HA	1:A:18:LEU:HB2	1.71	0.73
1:A:298:LEU:O	1:A:299:TYR:CB	2.39	0.70
1:A:243:ILE:HG12	1:A:313:ALA:CB	2.21	0.70
1:A:301:PRO:HB2	1:A:806:GLU:OE2	1.90	0.70
1:A:299:TYR:O	1:A:300:SER:CB	2.38	0.70
1:A:232:SER:HB2	1:A:367:ASN:HB3	1.74	0.70
1:A:298:LEU:HA	1:A:303:ASN:HB2	1.76	0.67
1:A:300:SER:CB	1:A:301:PRO:HA	2.24	0.67
1:A:326:TYR:OH	1:A:361:GLU:OE2	2.08	0.67
1:A:234:GLU:O	1:A:236:TYR:N	2.26	0.67
1:A:234:GLU:O	1:A:237:LYS:N	2.28	0.66
1:A:315:ARG:HG2	1:A:319:LEU:HG	1.76	0.66
1:A:232:SER:HB2	1:A:367:ASN:CB	2.26	0.65
1:A:243:ILE:HD13	1:A:313:ALA:CB	2.15	0.65
1:A:351:ASP:O	1:A:353:LEU:N	2.31	0.64
1:A:730:LEU:O	1:A:731:HIS:ND1	2.31	0.64
1:A:457:ILE:HG22	1:A:562:HIS:CE1	2.33	0.63
1:A:322:ARG:CG	1:A:360:LYS:HZ1	2.12	0.62
1:A:457:ILE:HG22	1:A:562:HIS:NE2	2.15	0.62
1:A:278:GLY:O	1:A:282:ILE:HG13	2.00	0.62
1:A:277:ARG:HD3	1:A:278:GLY:H	1.63	0.61
1:A:368:GLU:HG2	1:A:369:ASN:N	2.14	0.61
1:A:32:GLU:CD	1:A:72:ARG:NH1	2.54	0.61
1:A:350:SER:O	1:A:353:LEU:HB3	2.02	0.60
1:A:508:GLY:O	1:A:509:ARG:HG2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:GLU:O	1:A:235:MET:C	2.40	0.59
1:A:598:PHE:O	1:A:600:SER:N	2.36	0.59
1:A:321:THR:CA	1:A:325:ASP:OD1	2.50	0.58
1:A:321:THR:HB	1:A:324:VAL:HB	1.85	0.58
1:A:103:ARG:NH1	1:A:573:GLY:O	2.37	0.58
1:A:354:HIS:CD2	1:A:366:GLN:OE1	2.56	0.58
1:A:302:ALA:CB	1:A:810:MET:HE2	2.34	0.57
1:A:232:SER:CB	1:A:367:ASN:HB3	2.36	0.56
1:A:287:VAL:O	1:A:287:VAL:HG12	2.04	0.56
1:A:322:ARG:HG2	1:A:360:LYS:HZ1	1.71	0.56
1:A:232:SER:O	1:A:233:SER:OG	2.20	0.56
1:A:287:VAL:HG13	1:A:709:ARG:NH1	2.21	0.56
1:A:304:ILE:CD1	1:A:792:ARG:CZ	2.66	0.55
1:A:438:ILE:HD13	1:A:559:THR:HG22	1.88	0.55
1:A:300:SER:OG	1:A:792:ARG:NH2	2.40	0.55
1:A:227:GLY:O	1:A:369:ASN:HA	2.07	0.55
1:A:232:SER:CB	1:A:367:ASN:CB	2.85	0.55
1:A:613:LYS:O	1:A:615:GLY:N	2.40	0.55
1:A:304:ILE:CD1	1:A:792:ARG:NH2	2.69	0.55
1:A:404:ILE:HD11	1:A:639:PHE:HE1	1.72	0.55
1:A:679:ILE:HG13	1:A:823:ILE:HD11	1.89	0.54
1:A:304:ILE:CD1	1:A:792:ARG:NH1	2.69	0.54
1:A:310:VAL:C	1:A:312:ALA:H	2.11	0.54
1:A:315:ARG:CG	1:A:319:LEU:HG	2.38	0.54
1:A:302:ALA:HB2	1:A:810:MET:HE2	1.90	0.53
1:A:349:TRP:N	1:A:354:HIS:ND1	2.54	0.53
1:A:789:ILE:HG23	1:A:789:ILE:O	2.09	0.53
1:A:242:ILE:HD11	1:A:288:LYS:HD2	1.89	0.53
1:A:298:LEU:CD1	1:A:307:MET:CG	2.87	0.53
1:A:229:ALA:HB2	1:A:370:GLN:HG2	1.90	0.52
1:A:38:LEU:O	1:A:77:ARG:NH2	2.37	0.52
1:A:227:GLY:HA3	1:A:372:LEU:HD11	1.92	0.52
1:A:276:GLU:CG	1:A:280:VAL:HG23	2.39	0.51
1:A:302:ALA:O	1:A:304:ILE:HG13	2.10	0.51
1:A:322:ARG:HG3	1:A:360:LYS:HZ1	1.75	0.51
1:A:298:LEU:HA	1:A:303:ASN:CB	2.39	0.51
1:A:240:ASN:HA	1:A:243:ILE:HD12	1.93	0.50
1:A:167:ARG:HG2	1:A:199:VAL:HA	1.93	0.50
1:A:310:VAL:O	1:A:314:LEU:HB3	2.11	0.50
1:A:243:ILE:HD11	1:A:313:ALA:HB2	1.91	0.50
1:A:212:ASP:O	1:A:216:ILE:HB	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:GLU:HG3	1:A:290:GLY:N	2.28	0.49
1:A:243:ILE:N	1:A:244:PRO:HD2	2.28	0.49
1:A:321:THR:C	1:A:325:ASP:OD1	2.49	0.49
1:A:296:GLU:HB3	1:A:297:SER:HB2	1.96	0.48
1:A:320:PHE:HE1	1:A:353:LEU:HD21	1.79	0.48
1:A:350:SER:O	1:A:353:LEU:CB	2.60	0.48
1:A:300:SER:CB	1:A:301:PRO:CA	2.90	0.48
1:A:276:GLU:HG2	1:A:280:VAL:HG23	1.95	0.47
1:A:440:GLU:O	1:A:444:GLU:HG3	2.14	0.47
1:A:276:GLU:HG2	1:A:280:VAL:CG2	2.44	0.47
1:A:99:ILE:HD11	1:A:407:LEU:HD13	1.96	0.47
1:A:233:SER:O	1:A:237:LYS:CD	2.62	0.47
1:A:304:ILE:CG1	1:A:792:ARG:NH2	2.78	0.47
1:A:232:SER:OG	1:A:367:ASN:HB2	2.15	0.46
1:A:322:ARG:HG2	1:A:360:LYS:NZ	2.30	0.46
1:A:286:LEU:C	1:A:288:LYS:H	2.18	0.46
1:A:351:ASP:C	1:A:353:LEU:H	2.18	0.46
1:A:349:TRP:HB2	1:A:354:HIS:HD1	1.80	0.46
1:A:298:LEU:O	1:A:299:TYR:CD2	2.69	0.46
1:A:129:VAL:HB	1:A:208:VAL:HA	1.98	0.45
1:A:295:GLY:C	1:A:296:GLU:CG	2.84	0.45
1:A:301:PRO:HD2	1:A:806:GLU:HG2	1.98	0.45
1:A:310:VAL:HG12	1:A:311:THR:N	2.30	0.45
1:A:354:HIS:HD2	1:A:366:GLN:OE1	1.97	0.45
1:A:232:SER:CB	1:A:367:ASN:HB2	2.47	0.45
1:A:313:ALA:HB3	1:A:314:LEU:H	1.32	0.45
1:A:223:LEU:O	1:A:374:SER:HA	2.17	0.45
1:A:286:LEU:HD23	1:A:290:GLY:N	2.31	0.45
1:A:435:ILE:O	1:A:439:ILE:HG12	2.17	0.45
1:A:786:ARG:O	1:A:789:ILE:HG22	2.15	0.45
1:A:58:GLU:HG2	1:A:63:LEU:HD21	1.98	0.44
1:A:304:ILE:CG1	1:A:792:ARG:HH22	2.31	0.44
1:A:243:ILE:N	1:A:244:PRO:CD	2.80	0.44
1:A:51:ARG:HG2	1:A:121:LEU:O	2.16	0.44
1:A:363:VAL:HG12	1:A:364:GLN:N	2.33	0.44
1:A:298:LEU:HD12	1:A:307:MET:CG	2.48	0.44
1:A:403:SER:O	1:A:406:LYS:NZ	2.41	0.44
1:A:101:GLU:OE2	1:A:393:THR:HA	2.18	0.43
1:A:453:LEU:HB3	1:A:556:ILE:HD13	1.99	0.43
1:A:301:PRO:HD2	1:A:806:GLU:CG	2.47	0.43
1:A:722:GLU:HA	1:A:725:ASP:OD2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:613:LYS:HD3	1:A:616:GLU:OE1	2.19	0.43
1:A:277:ARG:HD3	1:A:278:GLY:N	2.33	0.43
1:A:281:LEU:HG	1:A:285:LEU:HD11	2.00	0.43
1:A:286:LEU:C	1:A:288:LYS:N	2.72	0.43
1:A:276:GLU:HG3	1:A:280:VAL:HG23	2.01	0.42
1:A:351:ASP:C	1:A:353:LEU:N	2.72	0.42
1:A:302:ALA:HB1	1:A:810:MET:HE2	2.01	0.42
1:A:99:ILE:HD12	1:A:211:VAL:HG21	2.01	0.42
1:A:232:SER:HB2	1:A:367:ASN:HB2	1.99	0.42
1:A:278:GLY:O	1:A:282:ILE:CG1	2.68	0.42
1:A:32:GLU:HB2	1:A:72:ARG:NH1	2.35	0.42
1:A:797:LYS:HB2	1:A:797:LYS:HE2	1.95	0.41
1:A:753:VAL:HG11	1:A:831:VAL:CG1	2.50	0.41
1:A:98:CYS:HA	1:A:408:ASP:O	2.19	0.41
1:A:719:PRO:HG2	1:A:723:TRP:NE1	2.35	0.41
1:A:187:LEU:HD22	1:A:373:ALA:HB1	2.03	0.41
1:A:32:GLU:OE1	1:A:82:ARG:NH1	2.54	0.41
1:A:179:ASN:N	1:A:179:ASN:OD1	2.53	0.41
1:A:64:ILE:HB	1:A:65:PRO:HD3	2.03	0.41
1:A:327:ILE:HG22	1:A:328:VAL:N	2.35	0.41
1:A:298:LEU:HD12	1:A:307:MET:HG2	2.03	0.40
1:A:243:ILE:HD13	1:A:313:ALA:CA	2.51	0.40
1:A:276:GLU:O	1:A:279:LEU:HB3	2.22	0.40
1:A:304:ILE:C	1:A:306:LEU:N	2.70	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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	769/822 (94%)	703 (91%)	39 (5%)	27 (4%)	<b>3</b> <b>27</b>

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	229	ALA
1	A	235	MET
1	A	303	ASN
1	A	305	MET
1	A	322	ARG
1	A	323	ASP
1	A	394	ALA
1	A	396	THR
1	A	507	ALA
1	A	599	ALA
1	A	614	PRO
1	A	730	LEU
1	A	230	GLU
1	A	299	TYR
1	A	311	THR
1	A	351	ASP
1	A	352	GLY
1	A	395	ASP
1	A	791	LEU
1	A	289	GLU
1	A	297	SER
1	A	288	LYS
1	A	300	SER
1	A	619	GLU
1	A	789	ILE
1	A	287	VAL
1	A	613	LYS

### 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	659/700 (94%)	636 (96%)	23 (4%)	36 67

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ARG
1	A	22	ARG
1	A	276	GLU
1	A	277	ARG
1	A	298	LEU
1	A	299	TYR
1	A	300	SER
1	A	317	HIS
1	A	319	LEU
1	A	321	THR
1	A	323	ASP
1	A	325	ASP
1	A	349	TRP
1	A	366	GLN
1	A	393	THR
1	A	509	ARG
1	A	512	ASP
1	A	527	GLU
1	A	601	ASP
1	A	602	ARG
1	A	725	ASP
1	A	731	HIS
1	A	742	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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](#)

There are no ligands in this entry.

## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	777/822 (94%)	-0.29	11 (1%) 75 69	95, 147, 233, 302	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	833	MET	5.0
1	A	831	VAL	4.5
1	A	834	PRO	4.3
1	A	728	PRO	4.0
1	A	730	LEU	3.9
1	A	616	GLU	3.2
1	A	597	ILE	2.3
1	A	795	ALA	2.3
1	A	615	GLY	2.2
1	A	729	GLU	2.1
1	A	333	VAL	2.1

### 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](#)

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.