



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:30 AM GMT

PDB ID : 3IQY
Title : Active site mutants of B. subtilis SecA
Authors : Kim, D.; Hunt, J.F.
Deposited on : 2009-08-21
Resolution : 3.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

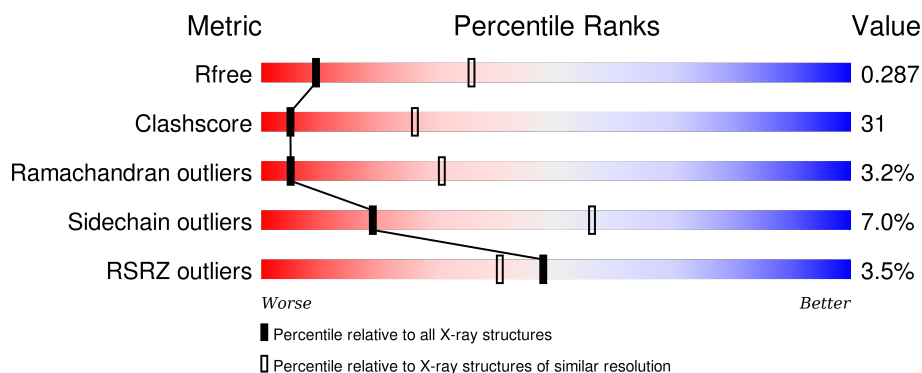
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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}	91344	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	841	

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	901	-	-	X	-

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 6419 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	802	6399	4000	1116	1248	35	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	208	GLN	GLU	ENGINEERED	UNP P28366
A	489	LYS	ARG	ENGINEERED	UNP P28366

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

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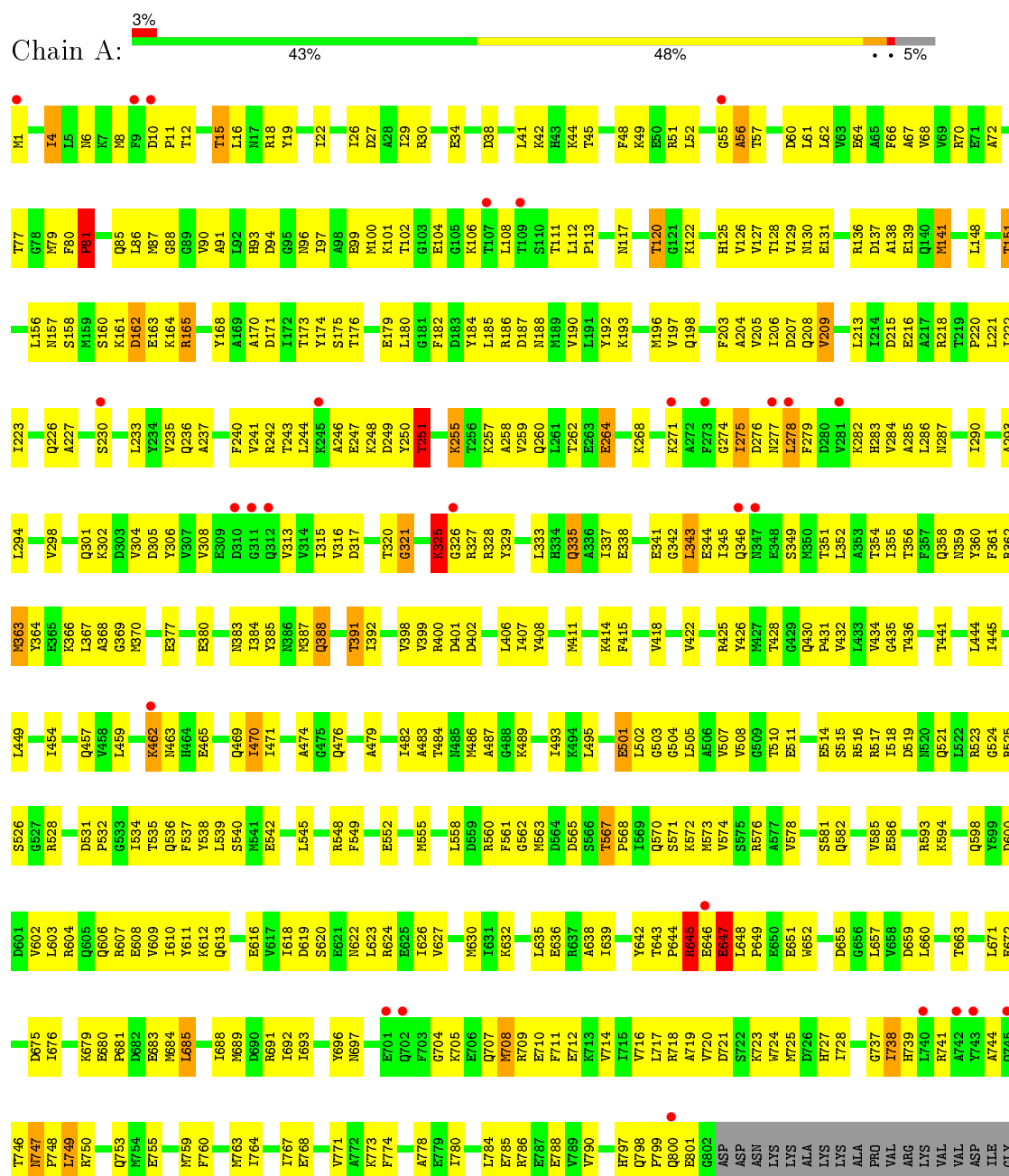
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

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: Protein translocase subunit secA



ARG
ASN
ALA
PRO
CYS
HIS
CYS
GLY
SER
GLY
LYS
LYS
TYR
LYS
ASN
CYS
CYS
GLY
ARG
THR
GLU

4 Data and refinement statistics

Property	Value	Source
Space group	P 31 1 2	Depositor
Cell constants a, b, c, α , β , γ	131.01Å 131.01Å 151.97Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.77 – 3.30 29.07 – 3.31	Depositor EDS
% Data completeness (in resolution range)	84.8 (19.77-3.30) 92.9 (29.07-3.31)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.18 (at 3.31Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.207 , 0.269 0.225 , 0.287	Depositor DCC
R_{free} test set	1090 reflections (5.49%)	DCC
Wilson B-factor (Å ²)	86.2	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 67.5	EDS
Estimated twinning fraction	0.042 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 22507 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6419	wwPDB-VP
Average B, all atoms (Å ²)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.51	0/6489	0.66	0/8728

There are no bond length outliers.

There are no bond angle outliers.

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	6399	0	6384	399	0
2	A	20	0	0	2	0
All	All	6419	0	6384	399	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 31.

All (399) 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:648:LEU:HB3	1:A:651:GLU:HB2	1.41	1.00
1:A:162:ASP:HA	1:A:165:ARG:HH12	1.21	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:618:ILE:HD11	1:A:717:LEU:HD11	1.46	0.96
1:A:368:ALA:HA	1:A:387:MET:HE3	1.47	0.94
1:A:356:THR:HG23	1:A:359:ASN:H	1.36	0.85
1:A:274:GLY:HA3	1:A:282:LYS:HZ1	1.40	0.85
1:A:644:PRO:HB2	1:A:647:GLU:HG2	1.57	0.85
1:A:313:VAL:HG11	1:A:337:ILE:HG21	1.62	0.82
1:A:622:ASN:HA	1:A:709:ARG:HE	1.43	0.82
1:A:704:GLY:HA3	1:A:707:GLN:HG2	1.62	0.82
1:A:4:ILE:HD12	1:A:4:ILE:H	1.45	0.82
1:A:165:ARG:NH1	1:A:165:ARG:HB2	1.95	0.81
1:A:165:ARG:HH11	1:A:165:ARG:HB2	1.43	0.81
1:A:240:PHE:HD2	1:A:290:ILE:HD11	1.46	0.81
1:A:136:ARG:HG2	1:A:136:ARG:HH11	1.46	0.81
1:A:616:GLU:O	1:A:620:SER:HB2	1.82	0.80
1:A:489:LYS:HG3	1:A:525:ARG:NH2	1.95	0.80
1:A:425:ARG:O	1:A:428:THR:HG22	1.82	0.80
1:A:401:ASP:HB3	1:A:534:ILE:HG22	1.65	0.79
1:A:168:TYR:CE2	1:A:198:GLN:HG2	2.19	0.78
1:A:763:MET:O	1:A:767:ILE:HG13	1.83	0.78
1:A:274:GLY:HA3	1:A:282:LYS:NZ	2.01	0.76
1:A:175:SER:HB3	1:A:180:LEU:HD21	1.66	0.76
1:A:206:ILE:HD11	1:A:367:LEU:HD11	1.69	0.74
1:A:780:ILE:H	1:A:780:ILE:HD12	1.53	0.74
1:A:571:SER:HB3	1:A:574:VAL:HG12	1.70	0.73
1:A:724:TRP:HA	1:A:763:MET:HE1	1.71	0.73
1:A:594:LYS:O	1:A:598:GLN:HG3	1.89	0.73
1:A:434:VAL:HG12	1:A:508:VAL:HB	1.71	0.72
1:A:301:GLN:HB2	1:A:304:VAL:HG12	1.72	0.71
1:A:128:THR:HG22	1:A:129:VAL:H	1.54	0.70
1:A:137:ASP:HB3	1:A:174:TYR:HE2	1.56	0.70
1:A:301:GLN:HB2	1:A:304:VAL:CG1	2.21	0.70
1:A:552:GLU:HG2	1:A:555:MET:HE3	1.72	0.70
1:A:606:GLN:NE2	1:A:760:PHE:HB2	2.07	0.69
1:A:400:ARG:HD3	1:A:526:SER:O	1.92	0.69
1:A:325:LYS:CE	1:A:325:LYS:H	2.06	0.69
1:A:422:VAL:HG13	1:A:432:VAL:HG21	1.75	0.69
1:A:317:ASP:O	1:A:321:GLY:HA2	1.92	0.68
1:A:518:ILE:HD12	1:A:518:ILE:N	2.09	0.68
1:A:100:MET:HG2	1:A:392:ILE:HB	1.75	0.68
1:A:204:ALA:HB3	1:A:367:LEU:HD12	1.77	0.67
1:A:408:TYR:CD2	1:A:414:LYS:HA	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:THR:HG23	1:A:18:ARG:HH12	1.56	0.67
1:A:248:LYS:O	1:A:262:THR:HG21	1.93	0.67
1:A:260:GLN:OE1	1:A:262:THR:HG22	1.94	0.67
1:A:749:LEU:O	1:A:753:GLN:HG3	1.95	0.67
1:A:315:ILE:H	1:A:315:ILE:HD12	1.60	0.67
1:A:128:THR:HG22	1:A:129:VAL:N	2.10	0.66
1:A:747:ASN:HD21	1:A:750:ARG:HB2	1.61	0.65
1:A:622:ASN:HA	1:A:709:ARG:NE	2.12	0.65
1:A:240:PHE:CD2	1:A:290:ILE:HD11	2.31	0.65
1:A:162:ASP:HA	1:A:165:ARG:NH1	2.04	0.65
1:A:112:LEU:HB2	1:A:113:PRO:HD3	1.77	0.65
1:A:108:LEU:HA	1:A:141:MET:CE	2.27	0.65
1:A:571:SER:HB3	1:A:574:VAL:CG1	2.27	0.65
1:A:635:LEU:HD11	1:A:688:ILE:HD11	1.79	0.64
1:A:259:VAL:HG11	1:A:663:THR:HG22	1.80	0.64
1:A:671:LEU:HD21	1:A:676:ILE:HD11	1.80	0.64
1:A:325:LYS:H	1:A:325:LYS:HE2	1.61	0.64
1:A:93:HIS:HD2	1:A:117:ASN:HD21	1.46	0.64
1:A:780:ILE:N	1:A:780:ILE:HD12	2.12	0.63
1:A:574:VAL:O	1:A:578:VAL:HG23	1.97	0.63
1:A:6:ASN:ND2	1:A:6:ASN:O	2.31	0.63
1:A:571:SER:O	1:A:574:VAL:HG12	1.99	0.63
1:A:515:SER:HB2	1:A:518:ILE:HD13	1.80	0.63
1:A:207:ASP:O	1:A:208:GLN:HB2	1.98	0.63
1:A:493:ILE:O	1:A:528:ARG:HD3	1.99	0.63
1:A:716:VAL:O	1:A:720:VAL:HG23	1.98	0.63
1:A:15:THR:HG23	1:A:18:ARG:NH1	2.14	0.63
1:A:275:ILE:CG2	1:A:278:LEU:HD12	2.29	0.62
1:A:176:THR:O	1:A:180:LEU:HG	1.98	0.62
1:A:449:LEU:CD1	1:A:482:ILE:HD11	2.29	0.62
1:A:313:VAL:HG11	1:A:337:ILE:CG2	2.28	0.62
1:A:66:PHE:CE2	1:A:112:LEU:HB3	2.35	0.62
1:A:99:GLU:OE1	1:A:391:THR:HG23	2.00	0.61
1:A:462:LYS:HD3	1:A:463:ASN:H	1.63	0.61
1:A:463:ASN:ND2	1:A:465:GLU:HB3	2.15	0.61
1:A:727:HIS:HB2	1:A:763:MET:CE	2.29	0.61
1:A:747:ASN:N	1:A:747:ASN:HD22	1.97	0.61
1:A:79:MET:CE	1:A:108:LEU:HD22	2.31	0.61
1:A:8:MET:O	1:A:11:PRO:HD2	2.00	0.61
1:A:738:ILE:O	1:A:738:ILE:HD13	2.01	0.60
1:A:435:GLY:HA2	1:A:483:ALA:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:GLN:O	1:A:362:ARG:HG3	2.01	0.60
1:A:226:GLN:HA	1:A:349:SER:HA	1.83	0.60
1:A:4:ILE:CD1	1:A:4:ILE:H	2.15	0.60
1:A:203:PHE:CE2	1:A:205:VAL:HG23	2.37	0.60
1:A:630:MET:HE3	1:A:771:VAL:HG11	1.84	0.59
1:A:274:GLY:C	1:A:276:ASP:H	2.06	0.59
1:A:704:GLY:CA	1:A:707:GLN:HG2	2.32	0.59
1:A:356:THR:CG2	1:A:359:ASN:H	2.10	0.59
1:A:635:LEU:HD11	1:A:688:ILE:CD1	2.33	0.59
1:A:182:PHE:CZ	1:A:221:LEU:HD22	2.37	0.59
1:A:571:SER:CB	1:A:574:VAL:HG12	2.32	0.59
1:A:514:GLU:HB3	1:A:585:VAL:HG11	1.84	0.59
1:A:486:MET:CE	1:A:525:ARG:HE	2.15	0.59
1:A:244:LEU:HD11	1:A:264:GLU:HB2	1.85	0.58
1:A:624:ARG:HG2	1:A:696:TYR:OH	2.03	0.58
1:A:136:ARG:HG2	1:A:136:ARG:NH1	2.14	0.58
1:A:127:VAL:HB	1:A:180:LEU:HD11	1.84	0.58
1:A:385:TYR:O	1:A:387:MET:HG3	2.04	0.58
1:A:411:MET:HB2	1:A:542:GLU:HB2	1.83	0.58
1:A:70:ARG:HD2	1:A:86:LEU:HD21	1.85	0.58
1:A:504:GLY:HA3	1:A:532:PRO:O	2.03	0.58
1:A:220:PRO:HG2	1:A:222:ILE:HD11	1.85	0.58
1:A:108:LEU:HA	1:A:141:MET:HE2	1.86	0.57
1:A:175:SER:CB	1:A:180:LEU:HD21	2.33	0.57
1:A:360:TYR:O	1:A:363:MET:HG3	2.05	0.57
1:A:380:GLU:HG3	1:A:384:ILE:HD12	1.86	0.57
1:A:4:ILE:HD12	1:A:4:ILE:N	2.17	0.57
1:A:275:ILE:HD12	1:A:275:ILE:H	1.69	0.57
1:A:230:SER:OG	1:A:233:LEU:HD13	2.05	0.57
1:A:704:GLY:HA3	1:A:707:GLN:HE21	1.69	0.56
1:A:315:ILE:HG22	1:A:316:VAL:H	1.69	0.56
1:A:64:GLU:O	1:A:68:VAL:HG23	2.04	0.56
1:A:724:TRP:HA	1:A:763:MET:CE	2.36	0.56
1:A:268:LYS:HA	1:A:271:LYS:HE3	1.87	0.56
1:A:747:ASN:ND2	1:A:750:ARG:HB2	2.21	0.56
1:A:251:THR:HA	1:A:257:LYS:O	2.06	0.56
1:A:368:ALA:CA	1:A:387:MET:HE3	2.30	0.56
1:A:623:LEU:HD23	1:A:712:GLU:HB3	1.86	0.56
1:A:516:ARG:NH1	1:A:586:GLU:OE1	2.38	0.56
1:A:727:HIS:CB	1:A:763:MET:HE1	2.35	0.56
1:A:567:THR:HG23	1:A:568:PRO:HD3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:755:GLU:O	1:A:759:MET:HG3	2.05	0.56
1:A:636:GLU:HB2	1:A:685:LEU:HD21	1.86	0.56
1:A:704:GLY:CA	1:A:707:GLN:HE21	2.19	0.56
1:A:563:MET:HA	1:A:563:MET:CE	2.36	0.56
1:A:519:ASP:HB2	1:A:537:PHE:CZ	2.41	0.56
1:A:30:ARG:O	1:A:34:GLU:HB2	2.06	0.55
1:A:275:ILE:HG21	1:A:278:LEU:HD12	1.86	0.55
1:A:635:LEU:O	1:A:639:ILE:HG12	2.06	0.55
1:A:203:PHE:CE2	1:A:205:VAL:CG2	2.89	0.55
1:A:411:MET:O	1:A:414:LYS:HB3	2.06	0.55
1:A:72:ALA:HB2	1:A:148:LEU:HD21	1.88	0.55
1:A:343:LEU:HD23	1:A:344:GLU:H	1.71	0.55
1:A:129:VAL:HG23	1:A:130:ASN:N	2.22	0.55
1:A:262:THR:HG23	1:A:264:GLU:HG3	1.87	0.55
1:A:489:LYS:HG3	1:A:525:ARG:HH22	1.71	0.55
1:A:434:VAL:CG2	1:A:482:ILE:HG12	2.37	0.55
1:A:431:PRO:HB3	1:A:476:GLN:O	2.06	0.55
1:A:441:THR:HG21	1:A:511:GLU:OE2	2.07	0.55
1:A:645:ARG:O	1:A:647:GLU:N	2.40	0.54
1:A:671:LEU:HA	1:A:691:ARG:NH1	2.21	0.54
1:A:279:PHE:C	1:A:283:HIS:HB2	2.26	0.54
1:A:727:HIS:HB2	1:A:763:MET:HE1	1.89	0.54
1:A:518:ILE:N	1:A:518:ILE:CD1	2.70	0.54
1:A:624:ARG:HH21	1:A:709:ARG:HH22	1.56	0.54
1:A:632:LYS:HE3	1:A:685:LEU:HD12	1.90	0.54
1:A:38:ASP:O	1:A:42:LYS:HG3	2.08	0.54
1:A:138:ALA:HB2	1:A:174:TYR:CG	2.42	0.54
1:A:79:MET:HE3	1:A:108:LEU:HD22	1.90	0.54
1:A:328:ARG:HH22	1:A:346:GLN:HB3	1.73	0.54
1:A:161:LYS:HG3	1:A:165:ARG:HH22	1.73	0.54
1:A:444:LEU:C	1:A:444:LEU:HD12	2.28	0.54
1:A:411:MET:HG2	1:A:415:PHE:HE1	1.72	0.54
1:A:414:LYS:HD3	1:A:540:SER:HB3	1.89	0.54
1:A:639:ILE:HD11	1:A:688:ILE:HD11	1.89	0.54
1:A:246:ALA:O	1:A:249:ASP:HB3	2.08	0.54
1:A:679:LYS:HG2	1:A:683:GLU:HG2	1.90	0.54
1:A:137:ASP:HB3	1:A:174:TYR:CE2	2.39	0.53
1:A:463:ASN:HD21	1:A:465:GLU:HB3	1.73	0.53
1:A:549:PHE:CE1	1:A:581:SER:HB3	2.44	0.53
1:A:259:VAL:HG11	1:A:663:THR:CG2	2.38	0.53
1:A:693:ILE:HG22	1:A:697:ASN:HD21	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:558:LEU:O	1:A:563:MET:HB2	2.08	0.53
1:A:244:LEU:HD12	1:A:268:LYS:HD2	1.91	0.53
1:A:27:ASP:O	1:A:30:ARG:HG2	2.09	0.53
1:A:97:ILE:HD12	1:A:387:MET:HB3	1.91	0.53
1:A:192:TYR:CD2	1:A:786:ARG:NH1	2.76	0.53
1:A:356:THR:HG22	1:A:600:ASP:OD2	2.09	0.52
1:A:602:VAL:O	1:A:606:GLN:HG3	2.09	0.52
1:A:308:VAL:HG13	1:A:343:LEU:HD12	1.91	0.52
1:A:101:LYS:O	1:A:104:GLU:HG2	2.09	0.52
1:A:62:LEU:O	1:A:66:PHE:HD1	1.92	0.52
1:A:632:LYS:HG3	1:A:685:LEU:HD11	1.90	0.52
1:A:81:PRO:HA	1:A:85:GLN:OE1	2.07	0.52
1:A:502:LEU:N	1:A:502:LEU:HD12	2.24	0.52
1:A:131:GLU:OE2	1:A:156:LEU:HD22	2.10	0.52
1:A:301:GLN:CB	1:A:304:VAL:HG12	2.39	0.52
1:A:680:GLU:HB3	1:A:681:PRO:HD2	1.91	0.52
1:A:643:THR:HA	1:A:652:TRP:CD1	2.45	0.52
1:A:635:LEU:HD21	1:A:688:ILE:CG1	2.40	0.52
1:A:719:ALA:O	1:A:723:LYS:HG2	2.09	0.52
1:A:325:LYS:HD2	1:A:738:ILE:HG12	1.91	0.52
1:A:226:GLN:HG2	1:A:227:ALA:N	2.25	0.51
1:A:315:ILE:HG22	1:A:316:VAL:N	2.24	0.51
1:A:356:THR:HG22	1:A:359:ASN:HB2	1.92	0.51
1:A:449:LEU:HD12	1:A:482:ILE:HD11	1.92	0.51
1:A:359:ASN:OD1	1:A:604:ARG:HD3	2.10	0.51
1:A:260:GLN:HG3	1:A:260:GLN:O	2.11	0.51
1:A:704:GLY:N	1:A:707:GLN:HE21	2.08	0.51
1:A:425:ARG:HD3	1:A:430:GLN:OE1	2.10	0.51
1:A:305:ASP:O	1:A:316:VAL:HG12	2.11	0.51
1:A:747:ASN:HB2	1:A:748:PRO:HD2	1.93	0.51
1:A:86:LEU:O	1:A:90:VAL:HG23	2.10	0.50
1:A:764:ILE:O	1:A:768:GLU:HG3	2.11	0.50
1:A:88:GLY:O	1:A:91:ALA:HB3	2.11	0.50
1:A:258:ALA:HB1	1:A:294:LEU:HG	1.93	0.50
1:A:724:TRP:CZ2	1:A:728:ILE:HD11	2.46	0.50
1:A:112:LEU:HB2	1:A:113:PRO:CD	2.42	0.50
1:A:623:LEU:HD23	1:A:712:GLU:CB	2.41	0.50
1:A:747:ASN:HD22	1:A:747:ASN:H	1.60	0.50
1:A:431:PRO:O	1:A:505:LEU:HD12	2.11	0.50
1:A:111:THR:CG2	1:A:141:MET:HG3	2.40	0.50
1:A:164:LYS:O	1:A:165:ARG:C	2.49	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:517:ARG:O	1:A:521:GLN:HG3	2.12	0.50
1:A:108:LEU:HA	1:A:141:MET:HE1	1.94	0.50
1:A:218:ARG:HE	1:A:801:GLU:HG3	1.75	0.50
1:A:495:LEU:HD13	1:A:531:ASP:OD2	2.12	0.50
1:A:459:LEU:HD21	1:A:470:ILE:HG21	1.94	0.50
1:A:255:LYS:HD2	1:A:257:LYS:CE	2.41	0.49
1:A:79:MET:HE1	1:A:108:LEU:HD22	1.94	0.49
1:A:315:ILE:HD12	1:A:315:ILE:N	2.25	0.49
1:A:157:ASN:HB3	1:A:179:GLU:OE2	2.13	0.49
1:A:168:TYR:CZ	1:A:198:GLN:HG2	2.47	0.49
1:A:127:VAL:HB	1:A:180:LEU:CD1	2.42	0.49
1:A:760:PHE:CZ	1:A:764:ILE:HD11	2.48	0.49
1:A:710:GLU:O	1:A:714:VAL:HG23	2.12	0.49
1:A:635:LEU:HD21	1:A:688:ILE:HG13	1.95	0.49
1:A:51:ARG:O	1:A:56:ALA:HB3	2.13	0.49
1:A:672:GLU:O	1:A:675:ASP:HB2	2.13	0.49
1:A:255:LYS:HD2	1:A:257:LYS:HE2	1.95	0.49
1:A:545:LEU:HG	1:A:549:PHE:CE2	2.48	0.48
1:A:184:TYR:O	1:A:188:ASN:ND2	2.46	0.48
1:A:302:LYS:HA	1:A:306:TYR:CZ	2.48	0.48
1:A:704:GLY:H	1:A:707:GLN:NE2	2.11	0.48
1:A:727:HIS:HB2	1:A:763:MET:HE3	1.94	0.48
1:A:287:ASN:O	1:A:290:ILE:HG22	2.13	0.48
1:A:262:THR:CG2	1:A:264:GLU:HG3	2.43	0.48
1:A:197:VAL:HG23	1:A:198:GLN:N	2.28	0.48
1:A:624:ARG:HG2	1:A:696:TYR:CE2	2.47	0.48
1:A:284:VAL:HG11	1:A:718:ARG:HD2	1.94	0.48
1:A:516:ARG:O	1:A:517:ARG:C	2.51	0.48
1:A:644:PRO:HB3	1:A:645:ARG:HH21	1.78	0.48
1:A:244:LEU:HD21	1:A:264:GLU:OE1	2.14	0.48
1:A:57:THR:OG1	1:A:60:ASP:OD1	2.29	0.48
1:A:91:ALA:O	1:A:94:ASP:HB2	2.14	0.47
1:A:106:LYS:HG3	2:A:901:SO4:O3	2.14	0.47
1:A:418:VAL:O	1:A:422:VAL:HG23	2.14	0.47
1:A:441:THR:O	1:A:445:ILE:HG22	2.14	0.47
1:A:430:GLN:HG3	1:A:504:GLY:O	2.13	0.47
1:A:723:LYS:C	1:A:763:MET:HE2	2.35	0.47
1:A:400:ARG:HE	1:A:535:THR:HG21	1.79	0.47
1:A:341:GLU:C	1:A:343:LEU:H	2.18	0.47
1:A:106:LYS:O	1:A:370:MET:HE1	2.14	0.47
1:A:676:ILE:HG23	1:A:684:MET:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:780:ILE:H	1:A:780:ILE:CD1	2.23	0.46
1:A:10:ASP:N	1:A:11:PRO:HD2	2.30	0.46
1:A:241:VAL:HG21	1:A:293:ALA:HB3	1.95	0.46
1:A:399:VAL:HG12	1:A:399:VAL:O	2.16	0.46
1:A:524:GLY:C	1:A:526:SER:H	2.19	0.46
1:A:66:PHE:CD2	1:A:112:LEU:HB3	2.51	0.46
1:A:52:LEU:HG	1:A:61:LEU:HD11	1.97	0.46
1:A:168:TYR:CD2	1:A:198:GLN:HA	2.51	0.46
1:A:425:ARG:NH1	1:A:534:ILE:HD11	2.31	0.46
1:A:406:LEU:HD12	1:A:538:TYR:CE1	2.50	0.46
1:A:788:GLU:HG2	1:A:790:VAL:H	1.81	0.46
1:A:426:TYR:CD2	1:A:454:ILE:HG23	2.51	0.46
1:A:19:TYR:O	1:A:87:MET:HG2	2.15	0.46
1:A:436:THR:HB	1:A:441:THR:HB	1.97	0.46
1:A:354:THR:CG2	1:A:355:ILE:N	2.79	0.46
1:A:608:GLU:O	1:A:612:LYS:HB3	2.16	0.45
1:A:545:LEU:HG	1:A:549:PHE:CZ	2.51	0.45
1:A:165:ARG:HG3	1:A:197:VAL:HA	1.97	0.45
1:A:402:ASP:HA	1:A:535:THR:OG1	2.16	0.45
1:A:518:ILE:H	1:A:518:ILE:CD1	2.29	0.45
1:A:327:ARG:HD2	1:A:755:GLU:OE1	2.15	0.45
1:A:400:ARG:NH1	1:A:400:ARG:HB3	2.31	0.45
1:A:48:PHE:CE1	1:A:68:VAL:HG21	2.52	0.45
1:A:642:TYR:C	1:A:644:PRO:HD3	2.37	0.45
1:A:610:ILE:HG13	1:A:724:TRP:CE3	2.51	0.45
1:A:335:GLN:HA	1:A:338:GLU:OE1	2.17	0.45
1:A:120:THR:HB	1:A:122:LYS:HG3	1.98	0.45
1:A:618:ILE:HD12	1:A:717:LEU:HD21	1.98	0.45
1:A:190:VAL:HG11	1:A:196:MET:HG3	1.99	0.45
1:A:721:ASP:O	1:A:725:MET:HG2	2.16	0.45
1:A:724:TRP:N	1:A:763:MET:HE2	2.32	0.45
1:A:431:PRO:HB3	1:A:479:ALA:HB3	1.99	0.45
1:A:510:THR:O	1:A:511:GLU:HB3	2.17	0.45
1:A:406:LEU:HG	1:A:536:GLN:NE2	2.32	0.45
1:A:352:LEU:HD22	1:A:725:MET:HE3	1.98	0.45
1:A:618:ILE:CD1	1:A:717:LEU:HD11	2.34	0.44
1:A:561:PHE:O	1:A:562:GLY:C	2.55	0.44
1:A:693:ILE:N	1:A:693:ILE:HD12	2.32	0.44
1:A:22:ILE:O	1:A:26:ILE:HG13	2.16	0.44
1:A:507:VAL:CG1	1:A:535:THR:HG22	2.47	0.44
1:A:738:ILE:C	1:A:738:ILE:HD13	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:671:LEU:HA	1:A:691:ARG:HH12	1.82	0.44
1:A:247:GLU:C	1:A:249:ASP:H	2.20	0.44
1:A:459:LEU:HD21	1:A:470:ILE:CG2	2.48	0.44
1:A:711:PHE:HD1	1:A:784:LEU:HD11	1.82	0.44
1:A:325:LYS:H	1:A:325:LYS:HE3	1.80	0.44
1:A:77:THR:C	1:A:79:MET:H	2.21	0.44
1:A:255:LYS:NZ	1:A:638:ALA:HA	2.32	0.44
1:A:380:GLU:HG3	1:A:384:ILE:CD1	2.48	0.44
1:A:407:ILE:HA	1:A:539:LEU:O	2.17	0.44
1:A:222:ILE:HD13	1:A:799:PRO:CD	2.48	0.44
1:A:275:ILE:N	1:A:282:LYS:HZ2	2.16	0.44
1:A:676:ILE:CG2	1:A:684:MET:SD	3.06	0.44
1:A:718:ARG:HH11	1:A:718:ARG:HG2	1.83	0.44
1:A:326:GLY:HA3	1:A:737:GLY:HA3	1.99	0.44
1:A:275:ILE:HG22	1:A:275:ILE:O	2.18	0.43
1:A:434:VAL:O	1:A:434:VAL:HG23	2.18	0.43
1:A:251:THR:HG21	1:A:298:VAL:HG11	1.99	0.43
1:A:774:PHE:O	1:A:778:ALA:HB3	2.18	0.43
1:A:489:LYS:HE2	1:A:521:GLN:NE2	2.33	0.43
1:A:561:PHE:O	1:A:563:MET:HG2	2.18	0.43
1:A:501:GLU:C	1:A:503:GLY:H	2.20	0.43
1:A:160:SER:OG	1:A:163:GLU:HG3	2.18	0.43
1:A:380:GLU:OE1	1:A:593:ARG:NH1	2.50	0.43
1:A:192:TYR:CE2	1:A:786:ARG:HD2	2.53	0.43
1:A:603:LEU:O	1:A:607:ARG:HG3	2.18	0.43
1:A:604:ARG:NH1	1:A:608:GLU:OE2	2.51	0.43
1:A:626:ILE:HG22	1:A:630:MET:HE2	2.00	0.43
1:A:279:PHE:CA	1:A:283:HIS:HB2	2.49	0.43
1:A:102:THR:HG21	1:A:525:ARG:NH1	2.33	0.43
1:A:62:LEU:HD23	1:A:66:PHE:CD1	2.53	0.43
1:A:380:GLU:O	1:A:383:ASN:HB3	2.18	0.43
1:A:774:PHE:H	1:A:774:PHE:HD1	1.65	0.43
1:A:125:HIS:HA	1:A:173:THR:O	2.18	0.43
1:A:377:GLU:CG	1:A:517:ARG:HD3	2.49	0.43
1:A:723:LYS:HD3	1:A:723:LYS:N	2.34	0.43
1:A:567:THR:HG23	1:A:568:PRO:CD	2.47	0.43
1:A:328:ARG:HH22	1:A:346:GLN:CB	2.30	0.43
1:A:377:GLU:CD	1:A:517:ARG:HH11	2.22	0.43
1:A:112:LEU:N	1:A:113:PRO:HD2	2.34	0.43
1:A:335:GLN:HE21	1:A:345:ILE:HG23	1.82	0.43
1:A:708:MET:HE2	1:A:711:PHE:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:572:LYS:HE2	1:A:576:ARG:NH2	2.34	0.43
1:A:704:GLY:H	1:A:707:GLN:HE21	1.66	0.43
1:A:48:PHE:CZ	1:A:68:VAL:HG21	2.54	0.43
1:A:237:ALA:O	1:A:241:VAL:HG23	2.19	0.43
1:A:235:VAL:HG23	1:A:236:GLN:N	2.33	0.43
1:A:607:ARG:O	1:A:611:TYR:HB2	2.19	0.43
1:A:255:LYS:HZ1	1:A:638:ALA:HA	1.82	0.43
1:A:689:MET:HE3	1:A:692:ILE:HB	2.01	0.43
1:A:209:VAL:CG1	1:A:369:GLY:HA3	2.49	0.43
1:A:62:LEU:O	1:A:66:PHE:CD1	2.72	0.42
1:A:185:LEU:HB3	1:A:223:ILE:HD12	2.02	0.42
1:A:283:HIS:O	1:A:287:ASN:HB3	2.18	0.42
1:A:471:ILE:O	1:A:474:ALA:HB3	2.19	0.42
1:A:102:THR:HG21	1:A:525:ARG:HH11	1.85	0.42
1:A:630:MET:CE	1:A:771:VAL:HG11	2.48	0.42
1:A:360:TYR:O	1:A:362:ARG:N	2.52	0.42
1:A:514:GLU:O	1:A:582:GLN:HB3	2.20	0.42
1:A:165:ARG:HH11	1:A:165:ARG:CB	2.22	0.42
1:A:767:ILE:O	1:A:771:VAL:HG23	2.20	0.42
1:A:41:LEU:O	1:A:44:LYS:HB2	2.20	0.42
1:A:727:HIS:HB3	1:A:763:MET:HE1	2.01	0.42
1:A:127:VAL:HG13	1:A:206:ILE:HA	2.01	0.42
1:A:70:ARG:HG2	1:A:80:PHE:CE1	2.54	0.42
1:A:222:ILE:HG23	1:A:351:THR:HG23	2.01	0.42
1:A:523:ARG:HG3	1:A:523:ARG:HH11	1.85	0.42
1:A:97:ILE:HD12	1:A:387:MET:CB	2.49	0.42
1:A:274:GLY:CA	1:A:282:LYS:NZ	2.78	0.42
1:A:127:VAL:CG1	1:A:206:ILE:HG12	2.49	0.42
1:A:96:ASN:HB3	1:A:388:GLN:O	2.20	0.42
1:A:276:ASP:HB3	1:A:277:ASN:H	1.57	0.42
1:A:128:THR:O	1:A:176:THR:HA	2.19	0.42
1:A:469:GLN:H	1:A:469:GLN:HG2	1.69	0.42
1:A:329:TYR:HB3	1:A:333:LEU:HB3	2.01	0.42
1:A:204:ALA:HB3	1:A:367:LEU:CD1	2.48	0.41
1:A:462:LYS:H	1:A:462:LYS:HD3	1.84	0.41
1:A:220:PRO:O	1:A:798:GLN:HG3	2.20	0.41
1:A:623:LEU:O	1:A:627:VAL:HG23	2.20	0.41
1:A:449:LEU:HD11	1:A:482:ILE:HD11	2.01	0.41
1:A:203:PHE:CE1	1:A:366:LYS:HG2	2.56	0.41
1:A:45:THR:O	1:A:49:LYS:HG3	2.20	0.41
1:A:430:GLN:HE21	1:A:504:GLY:H	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:GLN:HG2	1:A:227:ALA:H	1.84	0.41
1:A:193:LYS:HD2	1:A:619:ASP:HB2	2.03	0.41
1:A:711:PHE:CD1	1:A:784:LEU:HD11	2.56	0.41
1:A:398:VAL:HG12	1:A:400:ARG:H	1.86	0.41
1:A:469:GLN:HE21	1:A:469:GLN:HB3	1.67	0.41
1:A:355:ILE:HG12	1:A:356:THR:N	2.35	0.41
1:A:627:VAL:O	1:A:630:MET:N	2.46	0.41
1:A:462:LYS:H	1:A:462:LYS:CD	2.34	0.41
1:A:563:MET:C	1:A:565:ASP:H	2.23	0.41
1:A:657:LEU:O	1:A:660:LEU:N	2.54	0.41
1:A:213:LEU:HA	1:A:213:LEU:HD23	1.86	0.41
1:A:222:ILE:HD13	1:A:799:PRO:HD3	2.01	0.41
1:A:64:GLU:O	1:A:67:ALA:HB3	2.22	0.41
1:A:800:GLN:HG2	1:A:801:GLU:N	2.36	0.41
1:A:151:THR:HB	1:A:171:ASP:H	1.86	0.41
1:A:626:ILE:O	1:A:630:MET:HG3	2.21	0.40
1:A:431:PRO:HA	1:A:479:ALA:O	2.21	0.40
1:A:471:ILE:O	1:A:474:ALA:CB	2.70	0.40
1:A:111:THR:HG21	1:A:141:MET:HG3	2.04	0.40
1:A:572:LYS:HE2	1:A:576:ARG:HH21	1.87	0.40
1:A:12:THR:O	1:A:16:LEU:HD12	2.22	0.40
1:A:106:LYS:HE3	2:A:901:SO4:S	2.61	0.40
1:A:355:ILE:HG13	1:A:607:ARG:NH2	2.36	0.40
1:A:462:LYS:HG2	1:A:463:ASN:N	2.37	0.40
1:A:126:VAL:HG12	1:A:126:VAL:O	2.21	0.40
1:A:609:VAL:O	1:A:613:GLN:HB3	2.21	0.40
1:A:204:ALA:HB2	1:A:364:TYR:CE2	2.56	0.40
1:A:406:LEU:HD23	1:A:570:GLN:HG2	2.03	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	800/841 (95%)	680 (85%)	94 (12%)	26 (3%)	5	30

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	243	THR
1	A	278	LEU
1	A	321	GLY
1	A	325	LYS
1	A	646	GLU
1	A	649	PRO
1	A	56	ALA
1	A	275	ILE
1	A	285	ALA
1	A	320	THR
1	A	487	ALA
1	A	744	ALA
1	A	215	ASP
1	A	216	GLU
1	A	251	THR
1	A	361	PHE
1	A	647	GLU
1	A	55	GLY
1	A	81	PRO
1	A	739	HIS
1	A	170	ALA
1	A	342	GLY
1	A	645	ARG
1	A	773	LYS
1	A	4	ILE
1	A	29	ILE

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	689/721 (96%)	641 (93%)	48 (7%)	19	56

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	15	THR
1	A	81	PRO
1	A	120	THR
1	A	139	GLU
1	A	141	MET
1	A	151	THR
1	A	158	SER
1	A	162	ASP
1	A	165	ARG
1	A	186	ARG
1	A	187	ASP
1	A	209	VAL
1	A	242	ARG
1	A	250	TYR
1	A	251	THR
1	A	255	LYS
1	A	264	GLU
1	A	286	LEU
1	A	325	LYS
1	A	335	GLN
1	A	343	LEU
1	A	363	MET
1	A	388	GLN
1	A	391	THR
1	A	457	GLN
1	A	462	LYS
1	A	470	ILE
1	A	484	THR
1	A	501	GLU
1	A	548	ARG
1	A	560	ARG
1	A	567	THR
1	A	573	MET
1	A	645	ARG
1	A	647	GLU
1	A	655	ASP
1	A	659	ASP
1	A	685	LEU
1	A	705	LYS
1	A	708	MET
1	A	738	ILE

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Mol	Chain	Res	Type
1	A	741	ARG
1	A	746	THR
1	A	747	ASN
1	A	749	LEU
1	A	785	GLU
1	A	797	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	17	ASN
1	A	43	HIS
1	A	93	HIS
1	A	226	GLN
1	A	236	GLN
1	A	287	ASN
1	A	291	ASN
1	A	297	HIS
1	A	335	GLN
1	A	395	ASN
1	A	463	ASN
1	A	469	GLN
1	A	570	GLN
1	A	697	ASN
1	A	707	GLN
1	A	733	GLN
1	A	747	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

4 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	901	-	4,4,4	0.19	0	6,6,6	0.12	0
2	SO4	A	902	-	4,4,4	0.38	0	6,6,6	0.14	0
2	SO4	A	903	-	4,4,4	0.23	0	6,6,6	0.07	0
2	SO4	A	904	-	4,4,4	0.21	0	6,6,6	0.10	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	901	-	-	0/0/0/0	0/0/0/0
2	SO4	A	902	-	-	0/0/0/0	0/0/0/0
2	SO4	A	903	-	-	0/0/0/0	0/0/0/0
2	SO4	A	904	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	SO4	2	0

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, 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	802/841 (95%)	-0.01	28 (3%) 48 40	47, 97, 146, 177	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	312	GLN	4.9
1	A	702	GLN	4.6
1	A	1	MET	3.9
1	A	273	PHE	3.6
1	A	9	PHE	3.6
1	A	55	GLY	3.6
1	A	310	ASP	3.4
1	A	740	LEU	3.3
1	A	281	VAL	2.9
1	A	701	GLU	2.9
1	A	743	TYR	2.7
1	A	230	SER	2.7
1	A	742	ALA	2.5
1	A	10	ASP	2.5
1	A	745	GLN	2.5
1	A	311	GLY	2.5
1	A	107	THR	2.4
1	A	347	ASN	2.3
1	A	245	LYS	2.3
1	A	278	LEU	2.2
1	A	109	THR	2.2
1	A	326	GLY	2.2
1	A	462	LYS	2.2
1	A	646	GLU	2.1
1	A	271	LYS	2.1
1	A	800	GLN	2.1
1	A	277	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	346	GLN	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 carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	SO4	A	901	5/5	0.95	0.32	0.66	66,77,82,84	0
2	SO4	A	902	5/5	0.96	0.16	-1.96	107,116,122,123	0
2	SO4	A	904	5/5	0.72	0.38	-	159,164,168,172	1
2	SO4	A	903	5/5	0.57	0.35	-	171,172,177,179	0

6.5 Other polymers [i](#)

There are no such residues in this entry.