



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 02:09 AM UTC

PDB ID : 3IQY / pdb_00003iqy
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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

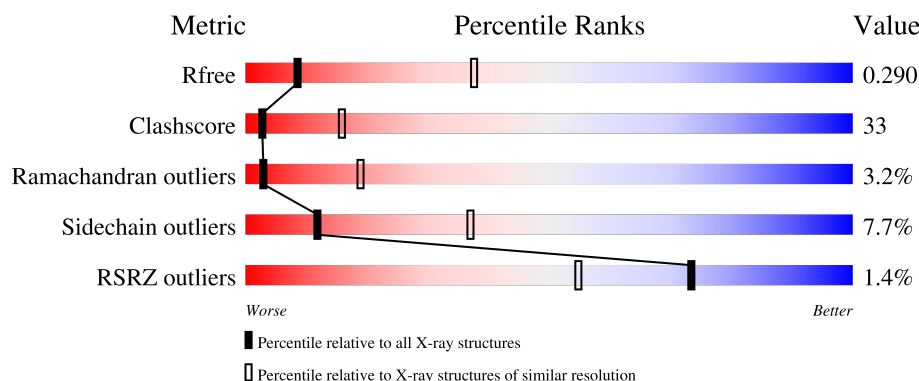
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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

Mol	Chain	Length	Quality of chain
1	A	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 mutation	UNP P28366
A	489	LYS	ARG	engineered mutation	UNP P28366

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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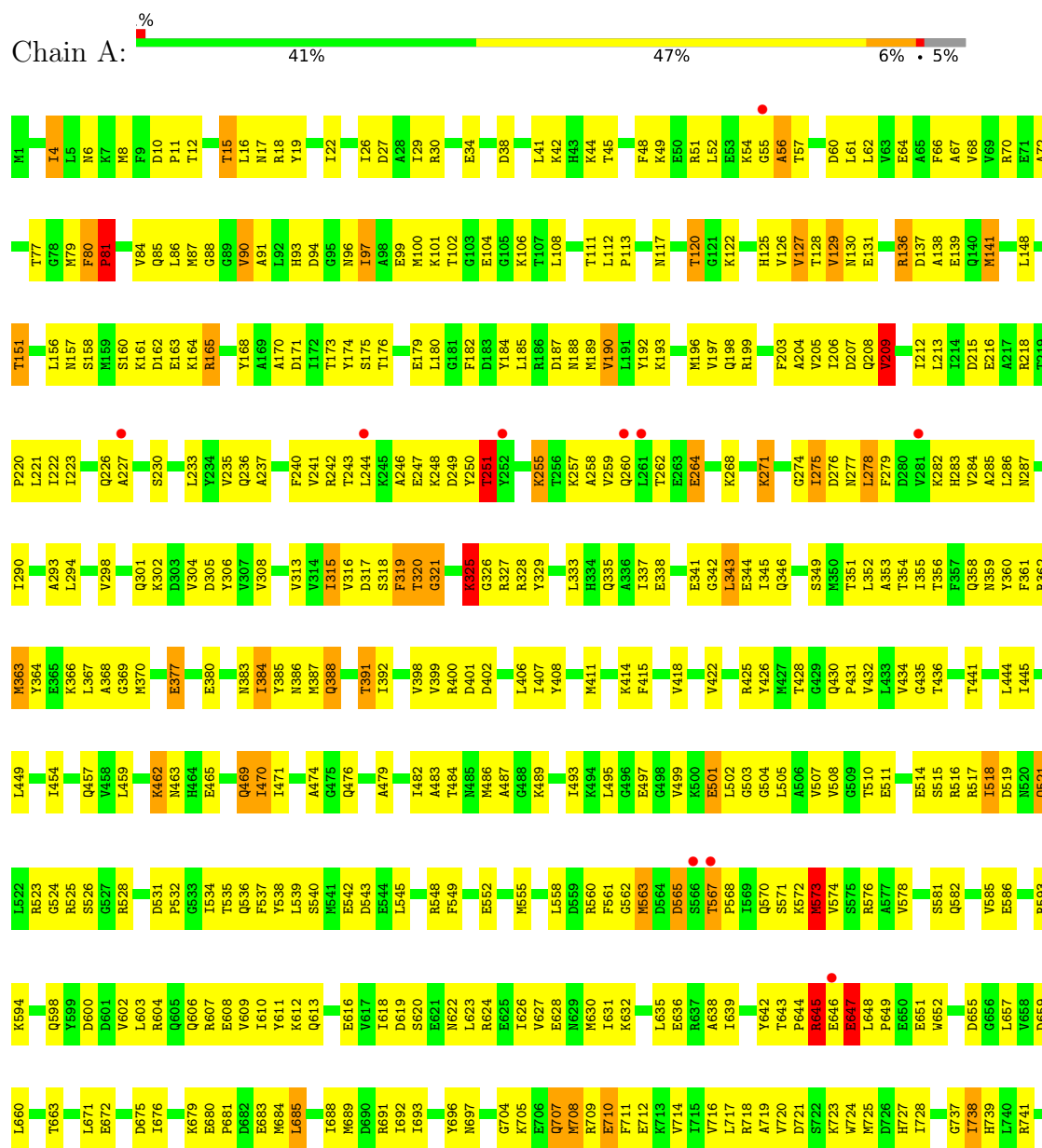
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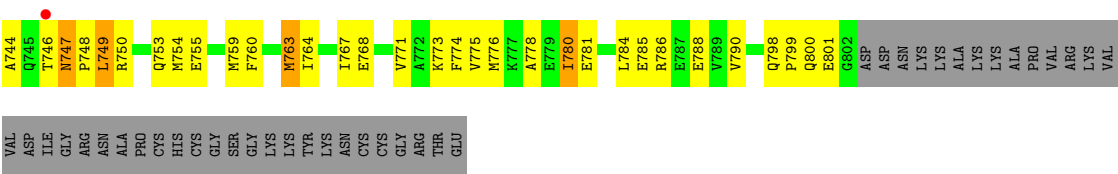
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

3 Residue-property plots

These plots are drawn for all protein, RNA, 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	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 19.77 – 3.31	Depositor EDS
% Data completeness (in resolution range)	84.8 (19.77-3.30) 92.4 (19.77-3.31)	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 0.223 , 0.290	Depositor DCC
R_{free} test set	1090 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	86.2	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 61.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.042 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0.65	1/6489 (0.0%)	1.00	17/8728 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	573	MET	SD-CE	5.16	1.92	1.79

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	129	VAL	N-CA-C	10.09	120.02	110.53
1	A	80	PHE	CA-C-N	7.54	129.26	119.84
1	A	80	PHE	C-N-CA	7.54	129.26	119.84
1	A	54	LYS	N-CA-C	-6.64	100.37	110.14
1	A	518	ILE	N-CA-C	6.48	116.64	110.42
1	A	781	GLU	N-CA-C	6.46	114.95	108.75
1	A	90	VAL	CB-CA-C	-5.73	104.63	111.97
1	A	209	VAL	N-CA-C	5.68	117.10	110.62
1	A	127	VAL	N-CA-C	5.64	117.33	109.55
1	A	212	ILE	N-CA-C	5.51	116.17	110.82
1	A	565	ASP	N-CA-C	-5.41	104.80	111.40
1	A	521	GLN	N-CA-C	-5.40	105.47	111.36
1	A	384	ILE	N-CA-C	5.40	115.61	110.53
1	A	710	GLU	N-CA-C	-5.33	106.46	113.12
1	A	319	PHE	N-CA-C	5.24	117.24	108.23
1	A	707	GLN	N-CA-C	-5.17	106.48	112.89
1	A	199	ARG	N-CA-C	-5.04	102.72	110.58

There are no chirality outliers.

There are no planarity outliers.

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	6399	0	6384	424	0
2	A	20	0	0	2	0
All	All	6419	0	6384	424	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 33.

All (424) 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:108:LEU:HA	1:A:141:MET:HE2	1.36	1.06
1:A:274:GLY:HA3	1:A:282:LYS:HZ1	1.21	1.01
1:A:79:MET:HE3	1:A:108:LEU:HD22	1.42	1.01
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
1:A:618:ILE:HD11	1:A:717:LEU:HD11	1.46	0.96
1:A:356:THR:HG23	1:A:359:ASN:H	1.36	0.85
1:A:644:PRO:HB2	1:A:647:GLU:HG2	1.57	0.85
1:A:563:MET:HA	1:A:563:MET:HE2	1.60	0.84
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:HB2	1:A:165:ARG:NH1	1.95	0.81
1:A:165:ARG:HB2	1:A:165:ARG:HH11	1.43	0.81
1:A:368:ALA:HA	1:A:387:MET:HE3	1.61	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:724:TRP:HA	1:A:763:MET:HE1	1.63	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:84:VAL:HA	1:A:87:MET:HE3	1.63	0.79
1:A:168:TYR:CE2	1:A:198:GLN:HG2	2.19	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD12	1:A:780:ILE:H	1.53	0.74
1:A:571:SER:HB3	1:A:574:VAL:HG12	1.70	0.73
1:A:689:MET:HE3	1:A:692:ILE:HB	1.69	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:189:MET:HE2	1:A:353:ALA:HB3	1.73	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: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:H	1:A:325:LYS:CE	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:N	1:A:518:ILE:HD12	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
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:552:GLU:HA	1:A:555:MET:HE3	1.76	0.67
1:A:315:ILE:H	1:A:315:ILE:HD12	1.60	0.67
1:A:749:LEU:O	1:A:753:GLN:HG3	1.95	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: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:189:MET:HE1	1:A:223:ILE:HG21	1.78	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:93:HIS:HD2	1:A:117:ASN:HD21	1.46	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:LYS:H	1:A:325:LYS:HE2	1.61	0.64
1:A:574:VAL:O	1:A:578:VAL:HG23	1.97	0.63
1:A:780:ILE:HD12	1:A:780:ILE:N	2.12	0.63
1:A:6:ASN:O	1:A:6:ASN:ND2	2.31	0.63
1:A:274:GLY:C	1:A:276:ASP:H	2.06	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:515:SER:HB2	1:A:518:ILE:HD13	1.80	0.63
1:A:571:SER:O	1:A:574:VAL:HG12	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:66:PHE:CE2	1:A:112:LEU:HB3	2.35	0.62
1:A:313:VAL:HG11	1:A:337:ILE:CG2	2.28	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:8:MET:O	1:A:11:PRO:HD2	2.00	0.61
1:A:775:VAL:HG12	1:A:776:MET:HE2	1.81	0.61
1:A:358:GLN:O	1:A:362:ARG:HG3	2.01	0.60
1:A:435:GLY:HA2	1:A:483:ALA:O	2.01	0.60
1:A:738:ILE:HD13	1:A:738:ILE:O	2.01	0.60
1:A:226:GLN:HA	1:A:349:SER:HA	1.83	0.60
1:A:4:ILE:H	1:A:4:ILE:CD1	2.15	0.60
1:A:203:PHE:CE2	1:A:205:VAL:HG23	2.37	0.60
1:A:279:PHE:C	1:A:283:HIS:HB2	2.26	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:182:PHE:CZ	1:A:221:LEU:HD22	2.37	0.59
1:A:635:LEU:HD11	1:A:688:ILE:CD1	2.33	0.59
1:A:444:LEU:C	1:A:444:LEU:HD12	2.28	0.59
1:A:514:GLU:HB3	1:A:585:VAL:HG11	1.84	0.59
1:A:571:SER:CB	1:A:574:VAL:HG12	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:VAL:HB	1:A:180:LEU:HD11	1.84	0.58
1:A:727:HIS:HB2	1:A:763:MET:HE3	1.85	0.58
1:A:385:TYR:O	1:A:387:MET:HG3	2.04	0.58
1:A:70:ARG:HD2	1:A:86:LEU:HD21	1.85	0.58
1:A:411:MET:HB2	1:A:542:GLU:HB2	1.83	0.58
1:A:220:PRO:HG2	1:A:222:ILE:HD11	1.85	0.58
1:A:504:GLY:HA3	1:A:532:PRO:O	2.03	0.58
1:A:255:LYS:HZ1	1:A:638:ALA:HA	1.68	0.58
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:H	1:A:275:ILE:HD12	1.69	0.57
1:A:230:SER:OG	1:A:233:LEU:HD13	2.05	0.57
1:A:64:GLU:O	1:A:68:VAL:HG23	2.04	0.56
1:A:315:ILE:HG22	1:A:316:VAL:H	1.69	0.56
1:A:704:GLY:HA3	1:A:707:GLN:HE21	1.69	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: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:567:THR:HG23	1:A:568:PRO:HD3	1.86	0.56
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:519:ASP:HB2	1:A:537:PHE:CZ	2.41	0.56
1:A:563:MET:HA	1:A:563:MET:CE	2.36	0.56
1:A:704:GLY:CA	1:A:707:GLN:HE21	2.19	0.56
1:A:30:ARG:O	1:A:34:GLU:HB2	2.06	0.55
1:A:203:PHE:CE2	1:A:205:VAL:CG2	2.89	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: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:411:MET:O	1:A:414:LYS:HB3	2.06	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:431:PRO:HB3	1:A:476:GLN:O	2.06	0.55
1:A:434:VAL:CG2	1:A:482:ILE:HG12	2.37	0.55
1:A:164:LYS:O	1:A:165:ARG:C	2.49	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:GLY:CA	1:A:282:LYS:HZ1	2.08	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:518:ILE:N	1:A:518:ILE:CD1	2.70	0.54
1:A:38:ASP:O	1:A:42:LYS:HG3	2.08	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:138:ALA:HB2	1:A:174:TYR:CG	2.42	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:411:MET:HG2	1:A:415:PHE:HE1	1.72	0.54
1:A:246:ALA:O	1:A:249:ASP:HB3	2.08	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:97:ILE:HG13	1:A:387:MET:HE2	1.88	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
1:A:558:LEU:O	1:A:563:MET:HB2	2.08	0.53
1:A:516:ARG:O	1:A:517:ARG:C	2.51	0.53
1:A:27:ASP:O	1:A:30:ARG:HG2	2.09	0.53
1:A:244:LEU:HD12	1:A:268:LYS:HD2	1.91	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:101:LYS:O	1:A:104:GLU:HG2	2.09	0.52
1:A:308:VAL:HG13	1:A:343:LEU:HD12	1.91	0.52
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: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:131:GLU:OE2	1:A:156:LEU:HD22	2.10	0.52
1:A:502:LEU:HD12	1:A:502:LEU:N	2.24	0.52
1:A:106:LYS:O	1:A:370:MET:HE1	2.10	0.52
1:A:301:GLN:CB	1:A:304:VAL:HG12	2.39	0.52
1:A:643:THR:HA	1:A:652:TRP:CD1	2.45	0.52
1:A:680:GLU:HB3	1:A:681:PRO:HD2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:635:LEU:HD21	1:A:688:ILE:CG1	2.40	0.52
1:A:325:LYS:HD2	1:A:738:ILE:HG12	1.91	0.52
1:A:341:GLU:C	1:A:343:LEU:H	2.18	0.52
1:A:719:ALA:O	1:A:723:LYS:HG2	2.09	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:552:GLU:HG2	1:A:555:MET:HE3	1.93	0.51
1:A:368:ALA:HA	1:A:387:MET:CE	2.38	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:260:GLN:HG3	1:A:260:GLN:O	2.11	0.51
1:A:359:ASN:OD1	1:A:604:ARG:HD3	2.10	0.51
1:A:57:THR:OG1	1:A:60:ASP:OD1	2.29	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:524:GLY:C	1:A:526:SER:H	2.19	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:764:ILE:O	1:A:768:GLU:HG3	2.11	0.50
1:A:112:LEU:HB2	1:A:113:PRO:CD	2.42	0.50
1:A:724:TRP:CZ2	1:A:728:ILE:HD11	2.46	0.50
1:A:431:PRO:O	1:A:505:LEU:HD12	2.11	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:111:THR:CG2	1:A:141:MET:HG3	2.40	0.50
1:A:724:TRP:HA	1:A:763:MET:CE	2.36	0.50
1:A:189:MET:HE2	1:A:353:ALA:CB	2.39	0.50
1:A:218:ARG:HE	1:A:801:GLU:HG3	1.75	0.50
1:A:517:ARG:O	1:A:521:GLN:HG3	2.12	0.50
1:A:642:TYR:C	1:A:644:PRO:HD3	2.37	0.50
1:A:459:LEU:HD21	1:A:470:ILE:HG21	1.94	0.50
1:A:495:LEU:HD13	1:A:531:ASP:OD2	2.12	0.50
1:A:255:LYS:HD2	1:A:257:LYS:CE	2.41	0.49
1:A:77:THR:C	1:A:79:MET:H	2.21	0.49
1:A:352:LEU:HB3	1:A:725:MET:HE1	1.93	0.49
1:A:561:PHE:O	1:A:562:GLY:C	2.55	0.49
1:A:157:ASN:HB3	1:A:179:GLU:OE2	2.13	0.49
1:A:315:ILE:HD12	1:A:315:ILE:N	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:VAL:HB	1:A:180:LEU:CD1	2.42	0.49
1:A:168:TYR:CZ	1:A:198:GLN:HG2	2.47	0.49
1:A:710:GLU:O	1:A:714:VAL:HG23	2.12	0.49
1:A:723:LYS:C	1:A:763:MET:HE2	2.37	0.49
1:A:760:PHE:CZ	1:A:764:ILE:HD11	2.48	0.49
1:A:247:GLU:C	1:A:249:ASP:H	2.20	0.49
1:A:501:GLU:C	1:A:503:GLY:H	2.20	0.49
1:A:630:MET:HE3	1:A:771:VAL:HG11	1.95	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:750:ARG:HG3	1:A:754:MET:HE2	1.94	0.49
1:A:255:LYS:HD2	1:A:257:LYS:HE2	1.95	0.49
1:A:184:TYR:O	1:A:188:ASN:ND2	2.46	0.48
1:A:545:LEU:HG	1:A:549:PHE:CE2	2.48	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:262:THR:CG2	1:A:264:GLU:HG3	2.43	0.48
1:A:287:ASN:O	1:A:290:ILE:HG22	2.13	0.48
1:A:197:VAL:HG23	1:A:198:GLN:N	2.28	0.48
1:A:284:VAL:HG11	1:A:718:ARG:HD2	1.94	0.48
1:A:624:ARG:HG2	1:A:696:TYR:CE2	2.47	0.48
1:A:738:ILE:HD13	1:A:738:ILE:C	2.38	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:727:HIS:CB	1:A:763:MET:HE1	2.44	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:377:GLU:CD	1:A:517:ARG:HH11	2.22	0.47
1:A:400:ARG:HE	1:A:535:THR:HG21	1.79	0.47
1:A:676:ILE:HG23	1:A:684:MET:HG2	1.96	0.47
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:780:ILE:H	1:A:780:ILE:CD1	2.23	0.46
1:A:399:VAL:HG12	1:A:399:VAL:O	2.16	0.46
1:A:52:LEU:HG	1:A:61:LEU:HD11	1.97	0.46
1:A:66:PHE:CD2	1:A:112:LEU:HB3	2.51	0.46
1:A:168:TYR:CD2	1:A:198:GLN:HA	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:ARG:NH1	1:A:534:ILE:HD11	2.31	0.46
1:A:19:TYR:O	1:A:87:MET:HG2	2.15	0.46
1:A:406:LEU:HD12	1:A:538:TYR:CE1	2.50	0.46
1:A:426:TYR:CD2	1:A:454:ILE:HG23	2.51	0.46
1:A:788:GLU:HG2	1:A:790:VAL:H	1.81	0.46
1:A:436:THR:HB	1:A:441:THR:HB	1.97	0.46
1:A:727:HIS:HB2	1:A:763:MET:HE1	1.98	0.46
1:A:354:THR:CG2	1:A:355:ILE:N	2.79	0.46
1:A:545:LEU:HG	1:A:549:PHE:CZ	2.51	0.45
1:A:563:MET:C	1:A:565:ASP:H	2.23	0.45
1:A:608:GLU:O	1:A:612:LYS:HB3	2.16	0.45
1:A:165:ARG:HG3	1:A:197:VAL:HA	1.97	0.45
1:A:327:ARG:HD2	1:A:755:GLU:OE1	2.15	0.45
1:A:402:ASP:HA	1:A:535:THR:OG1	2.16	0.45
1:A:518:ILE:CD1	1:A:518:ILE:H	2.29	0.45
1:A:48:PHE:CE1	1:A:68:VAL:HG21	2.52	0.45
1:A:400:ARG:NH1	1:A:400:ARG:HB3	2.31	0.45
1:A:610:ILE:HG13	1:A:724:TRP:CE3	2.51	0.45
1:A:120:THR:HB	1:A:122:LYS:HG3	1.98	0.45
1:A:335:GLN:HA	1:A:338:GLU:OE1	2.17	0.45
1:A:190:VAL:HG11	1:A:196:MET:HG3	1.99	0.45
1:A:618:ILE:HD12	1:A:717:LEU:HD21	1.98	0.45
1:A:721:ASP:O	1:A:725:MET:HG2	2.16	0.45
1:A:406:LEU:HG	1:A:536:GLN:NE2	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:22:ILE:O	1:A:26:ILE:HG13	2.16	0.44
1:A:274:GLY:C	1:A:276:ASP:N	2.74	0.44
1:A:385:TYR:O	1:A:386:ASN:C	2.60	0.44
1:A:618:ILE:CD1	1:A:717:LEU:HD11	2.34	0.44
1:A:693:ILE:N	1:A:693:ILE:HD12	2.32	0.44
1:A:486:MET:HE2	1:A:521:GLN:HB3	1.99	0.44
1:A:459:LEU:HD21	1:A:470:ILE:CG2	2.48	0.44
1:A:507:VAL:CG1	1:A:535:THR:HG22	2.47	0.44
1:A:671:LEU:HA	1:A:691:ARG:HH12	1.82	0.44
1:A:711:PHE:HD1	1:A:784:LEU:HD11	1.82	0.44
1:A:255:LYS:NZ	1:A:638:ALA:HA	2.32	0.44
1:A:325:LYS:H	1:A:325:LYS:HE3	1.80	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:627:VAL:O	1:A:628:GLU:C	2.59	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:ILE:HD13	1:A:799:PRO:CD	2.48	0.44
1:A:486:MET:HE1	1:A:525:ARG:HE	1.81	0.44
1:A:626:ILE:HG22	1:A:630:MET:HE2	1.99	0.44
1:A:630:MET:CE	1:A:771:VAL:HG11	2.48	0.44
1:A:676:ILE:CG2	1:A:684:MET:SD	3.06	0.44
1:A:320:THR:O	1:A:321:GLY:C	2.60	0.44
1:A:326:GLY:HA3	1:A:737:GLY:HA3	1.99	0.44
1:A:718:ARG:HG2	1:A:718:ARG:HH11	1.83	0.44
1:A:251:THR:HG21	1:A:298:VAL:HG11	1.99	0.43
1:A:275:ILE:HG22	1:A:275:ILE:O	2.18	0.43
1:A:360:TYR:C	1:A:362:ARG:H	2.26	0.43
1:A:434:VAL:O	1:A:434:VAL:HG23	2.18	0.43
1:A:774:PHE:O	1:A:778:ALA:HB3	2.18	0.43
1:A:160:SER:OG	1:A:163:GLU:HG3	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:192:TYR:CE2	1:A:786:ARG:HD2	2.53	0.43
1:A:380:GLU:OE1	1:A:593:ARG:NH1	2.50	0.43
1:A:97:ILE:CD1	1:A:387:MET:HE2	2.49	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:708:MET:HE3	1:A:708:MET:HA	2.00	0.43
1:A:62:LEU:HD23	1:A:66:PHE:CD1	2.53	0.43
1:A:102:THR:HG21	1:A:525:ARG:NH1	2.33	0.43
1:A:125:HIS:HA	1:A:173:THR:O	2.18	0.43
1:A:279:PHE:CA	1:A:283:HIS:HB2	2.49	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:328:ARG:HH22	1:A:346:GLN:CB	2.30	0.43
1:A:377:GLU:CG	1:A:517:ARG:HD3	2.49	0.43
1:A:567:THR:HG23	1:A:568:PRO:CD	2.47	0.43
1:A:723:LYS:HD3	1:A:723:LYS:N	2.34	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:341:GLU:C	1:A:343:LEU:N	2.76	0.43
1:A:572:LYS:HE2	1:A:576:ARG:NH2	2.34	0.43
1:A:48:PHE:CZ	1:A:68:VAL:HG21	2.54	0.43
1:A:235:VAL:HG23	1:A:236:GLN:N	2.33	0.43
1:A:237:ALA:O	1:A:241:VAL:HG23	2.19	0.43
1:A:631:ILE:CD1	1:A:776:MET:HE3	2.49	0.43
1:A:704:GLY:H	1:A:707:GLN:HE21	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:VAL:CG1	1:A:369:GLY:HA3	2.49	0.43
1:A:573:MET:HE3	1:A:576:ARG:NH1	2.33	0.43
1:A:607:ARG:O	1:A:611:TYR:HB2	2.19	0.43
1:A:246:ALA:C	1:A:248:LYS:N	2.77	0.42
1:A:17:ASN:O	1:A:18:ARG:C	2.61	0.42
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:317:ASP:O	1:A:318:SER:C	2.62	0.42
1:A:102:THR:HG21	1:A:525:ARG:HH11	1.85	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:41:LEU:O	1:A:44:LYS:HB2	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:70:ARG:HG2	1:A:80:PHE:CE1	2.54	0.42
1:A:127:VAL:HG13	1:A:206:ILE:HA	2.01	0.42
1:A:222:ILE:HG23	1:A:351:THR:HG23	2.01	0.42
1:A:523:ARG:HH11	1:A:523:ARG:HG3	1.85	0.42
1:A:96:ASN:HB3	1:A:388:GLN:O	2.20	0.42
1:A:97:ILE:HD12	1:A:387:MET:CB	2.49	0.42
1:A:127:VAL:CG1	1:A:206:ILE:HG12	2.49	0.42
1:A:128:THR:O	1:A:176:THR:HA	2.19	0.42
1:A:276:ASP:HB3	1:A:277:ASN:H	1.57	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:220:PRO:O	1:A:798:GLN:HG3	2.20	0.41
1:A:462:LYS:HD3	1:A:462:LYS:H	1.84	0.41
1:A:449:LEU:HD11	1:A:482:ILE:HD11	2.01	0.41
1:A:623:LEU:O	1:A:627:VAL:HG23	2.20	0.41
1:A:45:THR:O	1:A:49:LYS:HG3	2.20	0.41
1:A:203:PHE:CE1	1:A:366:LYS:HG2	2.56	0.41
1:A:430:GLN:HE21	1:A:504:GLY:H	1.68	0.41
1:A:193:LYS:HD2	1:A:619:ASP:HB2	2.03	0.41
1:A:226:GLN:HG2	1:A:227:ALA:H	1.84	0.41
1:A:543:ASP:C	1:A:545:LEU:N	2.76	0.41
1:A:711:PHE:CD1	1:A:784:LEU:HD11	2.56	0.41
1:A:6:ASN:ND2	1:A:6:ASN:C	2.78	0.41
1:A:398:VAL:HG12	1:A:400:ARG:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:GLN:HE21	1:A:469:GLN:HB3	1.67	0.41
1:A:651:GLU:N	1:A:651:GLU:CD	2.79	0.41
1:A:723:LYS:C	1:A:763:MET:CE	2.94	0.41
1:A:213:LEU:HD23	1:A:213:LEU:HA	1.86	0.41
1:A:319:PHE:C	1:A:320:THR:HG23	2.45	0.41
1:A:355:ILE:HG12	1:A:356:THR:N	2.35	0.41
1:A:462:LYS:H	1:A:462:LYS:CD	2.34	0.41
1:A:627:VAL:O	1:A:630:MET:N	2.46	0.41
1:A:657:LEU:O	1:A:660:LEU:N	2.54	0.41
1:A:64:GLU:O	1:A:67:ALA:HB3	2.22	0.41
1:A:151:THR:HB	1:A:171:ASP:H	1.86	0.41
1:A:222:ILE:HD13	1:A:799:PRO:HD3	2.01	0.41
1:A:497:GLU:C	1:A:499:VAL:N	2.79	0.41
1:A:800:GLN:HG2	1:A:801:GLU:N	2.36	0.41
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:626:ILE:O	1:A:630:MET:HG3	2.21	0.40
1:A:12:THR:O	1:A:16:LEU:HD12	2.22	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:727:HIS:CB	1:A:763:MET:CE	2.99	0.40
1:A:106:LYS:HE3	2:A:901:SO4:S	2.61	0.40
1:A:126:VAL:O	1:A:126:VAL:HG12	2.21	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:609:VAL:O	1:A:613:GLN:HB3	2.21	0.40
1:A:79:MET:CE	1:A:108:LEU:HD22	2.31	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
1:A:708:MET:HE2	1:A:711:PHE:HB3	2.03	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	800/841 (95%)	680 (85%)	94 (12%)	26 (3%)	3	19

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%)	636 (92%)	53 (8%)	12	37

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	THR
1	A	81	PRO
1	A	97	ILE
1	A	120	THR
1	A	136	ARG
1	A	139	GLU
1	A	141	MET
1	A	151	THR
1	A	158	SER
1	A	165	ARG
1	A	187	ASP
1	A	190	VAL
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	271	LYS
1	A	286	LEU
1	A	315	ILE
1	A	325	LYS
1	A	343	LEU
1	A	363	MET
1	A	377	GLU
1	A	388	GLN
1	A	391	THR
1	A	457	GLN
1	A	462	LYS
1	A	469	GLN
1	A	470	ILE
1	A	484	THR
1	A	501	GLU
1	A	548	ARG
1	A	560	ARG
1	A	563	MET
1	A	567	THR
1	A	573	MET

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Mol	Chain	Res	Type
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
1	A	741	ARG
1	A	746	THR
1	A	747	ASN
1	A	749	LEU
1	A	763	MET
1	A	780	ILE
1	A	785	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	43	HIS
1	A	93	HIS
1	A	157	ASN
1	A	226	GLN
1	A	236	GLN
1	A	277	ASN
1	A	287	ASN
1	A	289	HIS
1	A	291	ASN
1	A	297	HIS
1	A	334	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
1	A	753	GLN
1	A	782	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	902	-	4,4,4	0.42	0	6,6,6	0.10	0
2	SO4	A	904	-	4,4,4	0.38	0	6,6,6	0.09	0
2	SO4	A	901	-	4,4,4	0.36	0	6,6,6	0.10	0
2	SO4	A	903	-	4,4,4	0.39	0	6,6,6	0.07	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 [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, 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%)	-0.12	11 (1%) 73 55	47, 97, 146, 177	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	261	LEU	3.2
1	A	55	GLY	2.6
1	A	567	THR	2.6
1	A	252	TYR	2.5
1	A	281	VAL	2.5
1	A	646	GLU	2.3
1	A	227	ALA	2.2
1	A	566	SER	2.1
1	A	244	LEU	2.1
1	A	746	THR	2.1
1	A	260	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SO4	A	903	5/5	0.68	0.13	171,172,177,179	0
2	SO4	A	904	5/5	0.83	0.14	159,164,168,172	1
2	SO4	A	902	5/5	0.91	0.09	107,116,122,123	0
2	SO4	A	901	5/5	0.98	0.05	66,77,82,84	0

6.5 Other polymers [i](#)

There are no such residues in this entry.