



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:08 AM UTC

PDB ID : 1M6N / pdb_00001m6n
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

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

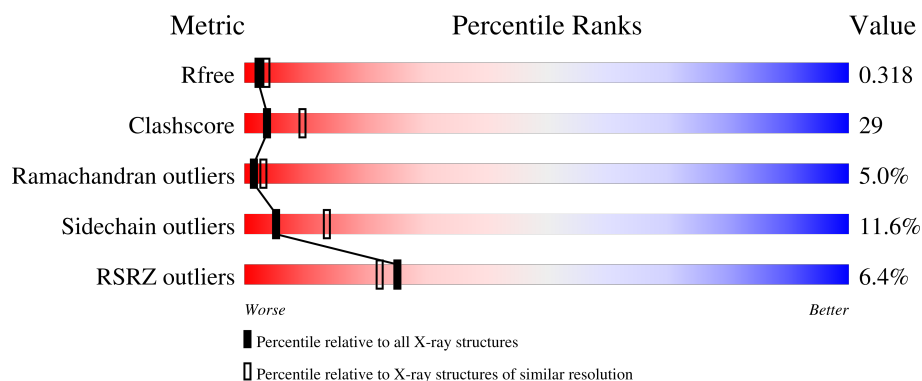
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 ≥ 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 (CCD ID: 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		
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		

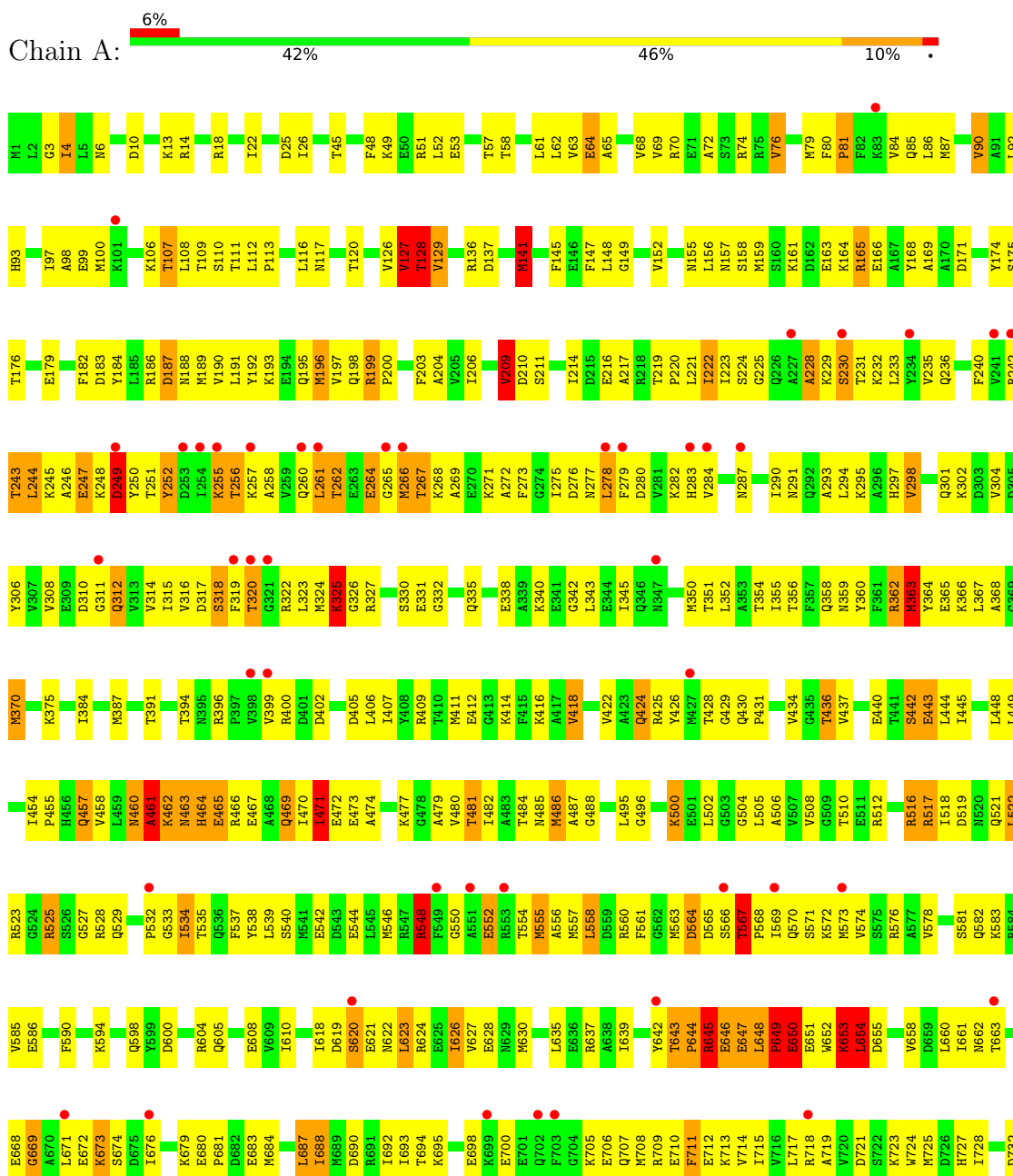
- Molecule 3 is water.

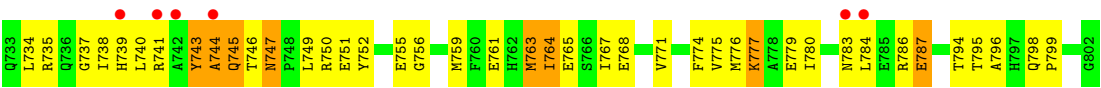
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	45	Total	O	0	0
			45	45		

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





4 Data and refinement statistics

Property	Value	Source
Space group	P 31 1 2	Depositor
Cell constants a, b, c, α , β , γ	130.83Å 130.83Å 150.35Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.24 – 2.70 45.24 – 2.70	Depositor EDS
% Data completeness (in resolution range)	80.4 (45.24-2.70) 90.4 (45.24-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	74.8	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 103.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	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 ²)	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.*

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	0.76	2/6492 (0.0%)	1.22	64/8731 (0.7%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	141	MET	SD-CE	-5.58	1.65	1.79
1	A	196	MET	SD-CE	5.25	1.92	1.79

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	707	GLN	N-CA-C	-9.10	101.27	111.82
1	A	247	GLU	N-CA-C	-8.76	102.51	113.02
1	A	249	ASP	N-CA-C	-8.61	92.46	110.80
1	A	621	GLU	N-CA-C	-8.29	101.29	111.40
1	A	320	THR	N-CA-C	-8.13	103.95	114.04
1	A	127	VAL	N-CA-C	7.99	120.11	108.53
1	A	298	VAL	N-CA-C	7.77	117.83	110.53
1	A	272	ALA	N-CA-C	-7.76	103.92	113.15
1	A	620	SER	N-CA-C	7.64	121.43	107.99
1	A	264	GLU	N-CA-C	-7.58	102.61	111.03
1	A	18	ARG	N-CA-C	-7.03	102.68	111.11
1	A	250	TYR	N-CA-C	6.92	120.76	109.76
1	A	209	VAL	CB-CA-C	-6.88	102.86	112.14
1	A	693	ILE	N-CA-C	-6.46	104.04	110.30
1	A	747	ASN	CA-C-N	6.40	127.83	119.84
1	A	747	ASN	C-N-CA	6.40	127.83	119.84
1	A	522	LEU	N-CA-C	-6.23	104.18	110.97
1	A	267	THR	N-CA-C	-6.23	103.60	112.13
1	A	648	LEU	CA-C-N	6.20	127.59	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	648	LEU	C-N-CA	6.20	127.59	119.84
1	A	623	LEU	N-CA-C	6.20	117.70	111.07
1	A	171	ASP	N-CA-C	-6.11	105.09	112.54
1	A	209	VAL	N-CA-C	6.07	116.81	110.62
1	A	461	ALA	N-CA-C	6.04	123.67	110.80
1	A	222	ILE	CB-CA-C	-6.03	101.54	110.82
1	A	711	PHE	N-CA-C	-6.01	104.64	111.07
1	A	525	ARG	N-CA-C	6.00	120.14	112.34
1	A	747	ASN	N-CA-C	-6.00	100.54	109.42
1	A	363	MET	N-CA-C	5.92	119.77	112.54
1	A	310	ASP	N-CA-C	-5.90	105.94	113.01
1	A	550	GLY	N-CA-C	-5.88	105.43	115.08
1	A	126	VAL	N-CA-C	-5.85	99.32	107.80
1	A	152	VAL	N-CA-C	5.75	116.90	107.24
1	A	477	LYS	N-CA-C	5.69	117.16	111.07
1	A	199	ARG	N-CA-C	-5.69	101.40	110.10
1	A	384	ILE	N-CA-C	5.68	118.19	111.09
1	A	590	PHE	N-CA-C	-5.60	105.09	111.14
1	A	22	ILE	N-CA-C	5.60	115.79	110.42
1	A	555	MET	N-CA-C	-5.59	106.16	112.87
1	A	255	LYS	N-CA-C	5.52	120.52	113.18
1	A	783	ASN	N-CA-C	5.52	117.72	108.73
1	A	471	ILE	N-CA-C	5.49	116.22	110.62
1	A	331	GLU	N-CA-C	5.46	119.23	112.24
1	A	516	ARG	N-CA-C	-5.46	105.23	111.07
1	A	626	ILE	CB-CA-C	-5.44	104.89	112.02
1	A	266	MET	N-CA-C	-5.44	106.65	113.72
1	A	643	THR	CA-C-N	5.39	126.58	119.84
1	A	643	THR	C-N-CA	5.39	126.58	119.84
1	A	779	GLU	N-CA-C	5.39	117.68	108.90
1	A	129	VAL	N-CA-C	5.39	117.83	111.09
1	A	365	GLU	N-CA-C	-5.38	105.52	111.71
1	A	437	VAL	N-CA-C	-5.35	108.62	113.71
1	A	692	ILE	N-CA-C	-5.34	104.29	111.44
1	A	128	THR	N-CA-C	5.25	117.17	109.24
1	A	777	LYS	N-CA-C	5.22	119.51	113.20
1	A	25	ASP	N-CA-C	-5.19	105.70	111.36
1	A	243	THR	N-CA-C	-5.19	99.75	110.80
1	A	705	LYS	N-CA-C	5.18	117.60	111.33
1	A	76	VAL	N-CA-C	5.15	118.34	111.44
1	A	90	VAL	CB-CA-C	-5.15	105.38	111.97
1	A	375	LYS	CA-C-N	5.11	127.44	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	375	LYS	C-N-CA	5.11	127.44	120.54
1	A	362	ARG	N-CA-C	-5.08	106.91	113.01
1	A	228	ALA	N-CA-C	5.05	121.56	110.80

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	6402	0	6382	371	0
2	A	35	0	0	2	0
3	A	45	0	0	4	0
All	All	6482	0	6382	371	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 29.

All (371) 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:756:GLY:HA2	1:A:759:MET:HE3	1.47	0.94
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:108:LEU:HA	1:A:141:MET:HE3	1.60	0.81
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:724:TRP:HA	1:A:763:MET:HE2	1.66	0.78
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:301:GLN:HB2	1:A:304:VAL:CG1	2.17	0.75
1:A:727:HIS:CB	1:A:763:MET:HE3	2.17	0.75
1:A:727:HIS:HB2	1:A:763:MET:HE3	1.68	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:681:PRO:HA	1:A:684:MET:HE3	1.67	0.74
1:A:261:LEU:HD22	1:A:777:LYS:HZ1	1.53	0.74
1:A:724:TRP:HE3	1:A:763:MET:HE1	1.52	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:368:ALA:HA	1:A:387:MET:HE3	1.72	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:552:GLU:HA	1:A:555:MET:HE3	1.73	0.71
1:A:724:TRP:HA	1:A:763:MET:CE	2.20	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:98:ALA:HB1	1:A:100:MET:HE2	1.74	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:352:LEU:HD22	1:A:725:MET:HE3	1.75	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
1:A:630:MET:HE1	1:A:771:VAL:HG21	1.76	0.67
1:A:186:ARG:HA	1:A:189:MET:HE3	1.74	0.67
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:679:LYS:O	1:A:684:MET:HE2	1.97	0.65
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:724:TRP:CE3	1:A:763:MET:HE1	2.33	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:744:ALA:C	1:A:746:THR:H	2.07	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
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:563:MET:C	1:A:565:ASP:H	2.11	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:LEU:HD11	1:A:370:MET:HE3	1.85	0.58
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:734:LEU:HD23	1:A:759:MET:HE1	1.85	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:649:PRO:C	1:A:651:GLU:H	2.12	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: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:630:MET:HE2	1:A:771:VAL:HG11	1.88	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:VAL:CG2	1:A:482:ILE:HG12	2.38	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:251:THR:HA	1:A:257:LYS:O	2.08	0.53
1:A:271:LYS:C	1:A:273:PHE:H	2.15	0.53
1:A:654:LEU:HD12	1:A:654:LEU:H	1.73	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:222:ILE:HG23	1:A:351:THR:HG23	1.90	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:222:ILE:HG22	1:A:223:ILE:N	2.23	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:248:LYS:C	1:A:262:THR:HG21	2.35	0.52
1:A:278:LEU:HB2	1:A:282:LYS:HG2	1.91	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:738:ILE:C	1:A:740:LEU:H	2.17	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:311:GLY:C	1:A:312:GLN:HG2	2.33	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:84:VAL:HA	1:A:87:MET:HE3	1.93	0.51
1:A:137:ASP:O	1:A:141:MET:HB2	2.10	0.51
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:429:GLY:C	1:A:502:LEU:HD13	2.37	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:741:ARG:HD3	1:A:741:ARG:C	2.36	0.50
1:A:210:ASP:O	1:A:214:ILE:HB	2.12	0.50
1:A:72:ALA:O	1:A:76:VAL:HG23	2.12	0.49
1:A:569:ILE:HG22	1:A:570:GLN:N	2.26	0.49
1:A:623:LEU:HD23	1:A:712:GLU:HB3	1.93	0.49
1:A:653:LYS:HD2	1:A:653:LYS:C	2.37	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: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: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:563:MET:C	1:A:565:ASP:N	2.71	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
1:A:108:LEU:CA	1:A:141:MET:HE3	2.39	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: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: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:743:TYR:C	1:A:745:GLN:H	2.22	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:163:GLU:O	1:A:166:GLU:HB3	2.14	0.47
1:A:426:TYR:C	1:A:428:THR:H	2.23	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:424:GLN:HG2	1:A:425:ARG:N	2.30	0.46
1:A:727:HIS:CB	1:A:763:MET:CE	2.92	0.46
1:A:287:ASN:OD1	1:A:291:ASN:ND2	2.49	0.46
1:A:359:ASN:O	1:A:363:MET:HE3	2.15	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:62:LEU:HA	1:A:116:LEU:HD22	1.98	0.46
1:A:107:THR:O	1:A:110:SER:OG	2.28	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:100:MET:HE3	1:A:106:LYS:HG2	1.99	0.45
1:A:268:LYS:HA	1:A:271:LYS:CD	2.47	0.45
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:516:ARG:O	1:A:517:ARG:C	2.59	0.45
1:A:642:TYR:C	1:A:644:PRO:HD3	2.40	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:681:PRO:CA	1:A:684:MET:HE3	2.44	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:363:MET:HE1	3:A:1115:HOH:O	2.16	0.44
1:A:695:LYS:HD3	1:A:776:MET:HE3	1.98	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:644:PRO:O	1:A:645:ARG:C	2.60	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:744:ALA:C	1:A:746:THR:N	2.72	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:668:GLU:O	1:A:669:GLY:C	2.59	0.43
1:A:279:PHE:O	1:A:283:HIS:CB	2.61	0.43
1:A:571:SER:O	1:A:572:LYS:C	2.61	0.43
1:A:653:LYS:C	1:A:655:ASP:H	2.26	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:271:LYS:C	1:A:273:PHE:N	2.77	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:147:PHE:C	1:A:149:GLY:H	2.27	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:486:MET:HE1	1:A:525:ARG:NE	2.34	0.43
1:A:256:THR:HG22	1:A:295:LYS:HE3	2.01	0.43
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:688:ILE:HD13	1:A:688:ILE:C	2.44	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:62:LEU:C	1:A:62:LEU:HD23	2.43	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:486:MET:HE2	1:A:486:MET:HB3	1.89	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:3:GLY:O	1:A:4:ILE:C	2.63	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:504:GLY:HA3	1:A:532:PRO:O	2.19	0.42
1:A:672:GLU:O	1:A:673:LYS:C	2.62	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:106:LYS:O	1:A:370:MET:HE1	2.20	0.41
1:A:267:THR:C	1:A:269:ALA:N	2.78	0.41
1:A:306:TYR:HB2	1:A:314:VAL:O	2.19	0.41
1:A:660:LEU:O	1:A:661:ILE:C	2.62	0.41
1:A:368:ALA:CA	1:A:387:MET:HE3	2.46	0.41
1:A:394:THR:HG22	1:A:396:ARG:O	2.20	0.41
1:A:268:LYS:HG2	1:A:271:LYS:HZ2	1.83	0.41
1:A:462:LYS:O	1:A:463:ASN:C	2.64	0.41
1:A:315:ILE:HG22	1:A:316:VAL:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:460:ASN:OD1	1:A:460:ASN:N	2.53	0.41
1:A:554:THR:C	1:A:556:ALA:N	2.78	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: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:522:LEU:O	1:A:523:ARG:C	2.63	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
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:627:VAL:O	1:A:628:GLU:C	2.63	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:671:LEU:O	1:A:672:GLU:HG3	2.21	0.40
1:A:743:TYR:C	1:A:743:TYR:CD1	2.99	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%)	1 3

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
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

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Mol	Chain	Res	Type
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%)	609 (88%)	80 (12%)	5 13

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	ARG
1	A	58	THR
1	A	64	GLU
1	A	81	PRO
1	A	97	ILE
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	165	ARG
1	A	187	ASP
1	A	190	VAL
1	A	191	LEU
1	A	209	VAL
1	A	211	SER
1	A	247	GLU
1	A	249	ASP
1	A	252	TYR
1	A	262	THR
1	A	277	ASN
1	A	280	ASP
1	A	318	SER

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Mol	Chain	Res	Type
1	A	325	LYS
1	A	330	SER
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	418	VAL
1	A	424	GLN
1	A	436	THR
1	A	442	SER
1	A	443	GLU
1	A	457	GLN
1	A	460	ASN
1	A	462	LYS
1	A	464	HIS
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	517	ARG
1	A	534	ILE
1	A	539	LEU
1	A	548	ARG
1	A	552	GLU
1	A	558	LEU
1	A	560	ARG
1	A	566	SER
1	A	567	THR
1	A	573	MET
1	A	618	ILE
1	A	619	ASP
1	A	645	ARG
1	A	649	PRO
1	A	650	GLU
1	A	653	LYS
1	A	654	LEU

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Mol	Chain	Res	Type
1	A	674	SER
1	A	687	LEU
1	A	688	ILE
1	A	690	ASP
1	A	706	GLU
1	A	717	LEU
1	A	728	ILE
1	A	743	TYR
1	A	745	GLN
1	A	747	ASN
1	A	749	LEU
1	A	763	MET
1	A	764	ILE
1	A	787	GLU

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

Mol	Chain	Res	Type
1	A	6	ASN
1	A	93	HIS
1	A	178	ASN
1	A	287	ASN
1	A	291	ASN
1	A	335	GLN
1	A	395	ASN
1	A	463	ASN
1	A	469	GLN
1	A	485	ASN
1	A	513	HIS
1	A	570	GLN
1	A	589	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 [i](#)

There are no oligosaccharides 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	1002	-	4,4,4	0.29	0	6,6,6	0.18	0
2	SO4	A	1006	-	4,4,4	0.33	0	6,6,6	0.37	0
2	SO4	A	1003	-	4,4,4	0.26	0	6,6,6	0.27	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
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

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 ⓘ

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	802/802 (100%)	0.33	51 (6%)	25 22	35, 92, 168, 207	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	260	GLN	4.2
1	A	549	PHE	4.0
1	A	261	LEU	4.0
1	A	254	ILE	3.8
1	A	620	SER	3.8
1	A	253	ASP	3.6
1	A	784	LEU	3.5
1	A	101	LYS	3.4
1	A	739	HIS	3.4
1	A	279	PHE	3.3
1	A	249	ASP	3.2
1	A	718	ARG	3.1
1	A	241	VAL	2.9
1	A	278	LEU	2.8
1	A	320	THR	2.8
1	A	551	ALA	2.8
1	A	676	ILE	2.8
1	A	566	SER	2.7
1	A	242	ARG	2.7
1	A	319	PHE	2.6
1	A	532	PRO	2.6
1	A	283	HIS	2.6
1	A	311	GLY	2.6
1	A	742	ALA	2.6
1	A	569	ILE	2.5
1	A	703	PHE	2.5
1	A	287	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	227	ALA	2.5
1	A	744	ALA	2.5
1	A	230	SER	2.4
1	A	642	TYR	2.3
1	A	783	ASN	2.3
1	A	257	LYS	2.3
1	A	284	VAL	2.3
1	A	255	LYS	2.3
1	A	265	GLY	2.3
1	A	671	LEU	2.3
1	A	321	GLY	2.3
1	A	398	VAL	2.3
1	A	83	LYS	2.2
1	A	573	MET	2.2
1	A	347	ASN	2.2
1	A	702	GLN	2.2
1	A	427	MET	2.2
1	A	266	MET	2.2
1	A	399	VAL	2.2
1	A	741	ARG	2.1
1	A	234	TYR	2.1
1	A	699	LYS	2.1
1	A	663	THR	2.0
1	A	553	ARG	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($\text{\AA}^2$)	Q<0.9
2	SO4	A	1007	5/5	0.76	0.13	107,112,116,130	0
2	SO4	A	1005	5/5	0.85	0.13	111,114,117,118	0
2	SO4	A	1003	5/5	0.86	0.13	95,96,110,111	0
2	SO4	A	1006	5/5	0.92	0.09	78,93,98,100	0
2	SO4	A	1004	5/5	0.92	0.07	75,76,83,105	0
2	SO4	A	1002	5/5	0.93	0.14	93,99,108,110	0
2	SO4	A	1001	5/5	0.97	0.05	46,63,71,78	0

6.5 Other polymers [i](#)

There are no such residues in this entry.