



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:00 AM UTC

PDB ID : 3IQM / pdb_00003iqm
Title : Active site mutants of B. subtilis SecA
Authors : Kim, D.; Hunt, J.F.
Deposited on : 2009-08-20
Resolution : 3.40 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

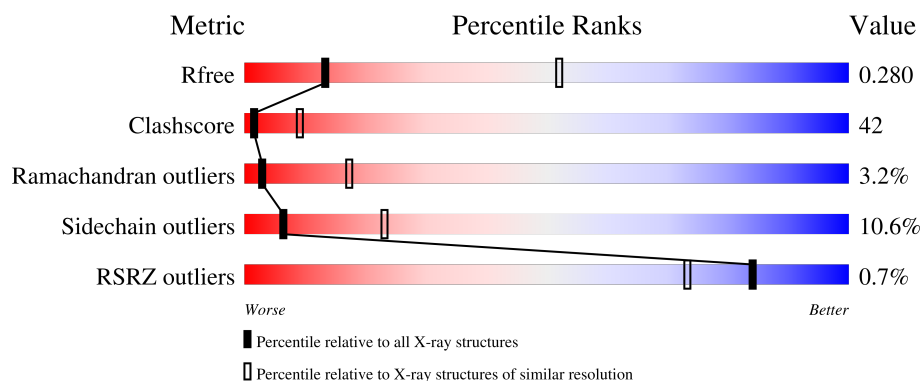
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	906	-	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6495 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	6401	4000	1118	1248	35	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	208	GLN	GLU	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
2	A	1	5	4	1	0	0

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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		
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		

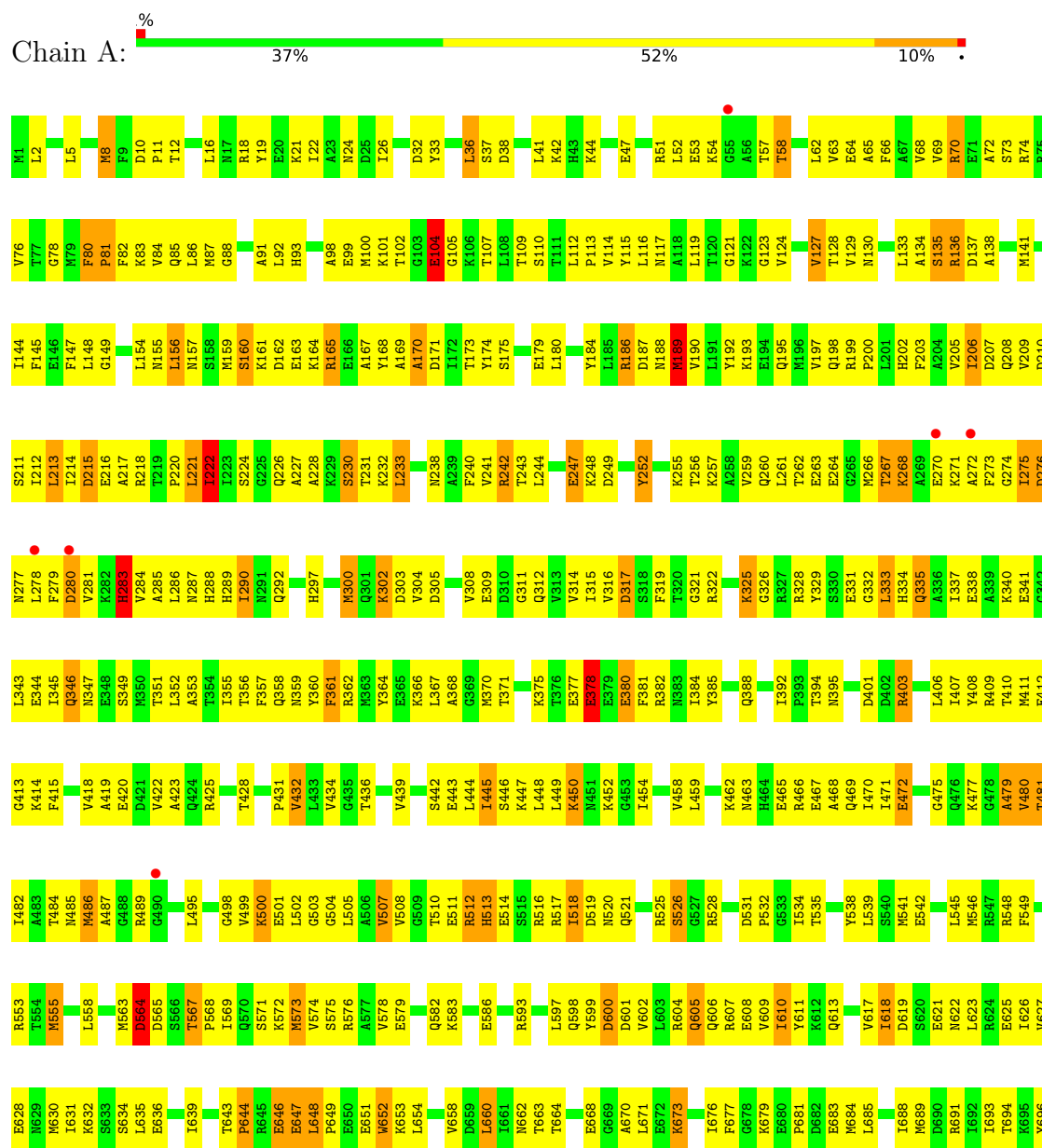
- Molecule 3 is water.

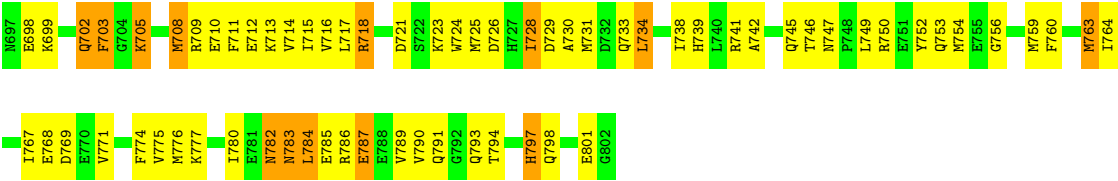
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	39	Total	O	0	0
			39	39		

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	130.14Å 130.14Å 153.95Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.98 – 3.40 19.98 – 3.40	Depositor EDS
% Data completeness (in resolution range)	79.5 (19.98-3.40) 88.5 (19.98-3.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.93 (at 3.39Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.209 , 0.267 0.224 , 0.280	Depositor DCC
R_{free} test set	937 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	95.6	Xtriage
Anisotropy	0.227	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 73.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.038 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6495	wwPDB-VP
Average B, all atoms (Å ²)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% 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	0.63	1/6491 (0.0%)	1.02	35/8731 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	573	MET	SD-CE	5.33	1.92	1.79

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	605	GLN	N-CA-C	-8.84	102.62	113.50
1	A	160	SER	N-CA-C	7.69	119.86	110.41
1	A	231	THR	N-CA-C	-7.55	104.53	113.21
1	A	378	GLU	N-CA-C	7.36	119.08	111.14
1	A	189	MET	N-CA-C	-7.26	104.94	114.31
1	A	576	ARG	N-CA-C	-6.44	105.41	113.20
1	A	212	ILE	N-CA-C	6.16	116.21	110.42
1	A	222	ILE	N-CA-C	6.12	115.89	108.06
1	A	432	VAL	N-CA-C	5.88	115.58	108.06
1	A	652	TRP	N-CA-C	-5.79	103.29	110.41
1	A	213	LEU	N-CA-C	5.77	118.52	111.82
1	A	477	LYS	N-CA-C	5.73	118.27	111.33
1	A	450	LYS	N-CA-C	-5.66	105.03	111.14
1	A	403	ARG	CA-C-N	5.65	125.56	119.85
1	A	403	ARG	C-N-CA	5.65	125.56	119.85
1	A	127	VAL	N-CA-C	5.59	116.62	108.58
1	A	206	ILE	N-CA-C	5.55	116.09	107.99
1	A	412	GLU	N-CA-C	-5.49	106.65	113.19
1	A	648	LEU	CA-C-N	5.46	126.67	119.84
1	A	648	LEU	C-N-CA	5.46	126.67	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	703	PHE	N-CA-C	5.38	119.10	112.54
1	A	80	PHE	CA-C-N	5.37	126.55	119.84
1	A	80	PHE	C-N-CA	5.37	126.55	119.84
1	A	793	GLN	N-CA-C	5.36	118.57	110.64
1	A	388	GLN	CA-C-N	-5.31	116.11	122.90
1	A	388	GLN	C-N-CA	-5.31	116.11	122.90
1	A	268	LYS	N-CA-C	-5.30	106.94	113.41
1	A	247	GLU	N-CA-C	-5.28	106.61	112.57
1	A	600	ASP	N-CA-C	-5.24	105.65	111.36
1	A	479	ALA	N-CA-C	5.23	117.93	110.24
1	A	791	GLN	N-CA-C	5.13	117.14	109.59
1	A	276	ASP	N-CA-C	5.13	117.28	111.02
1	A	272	ALA	N-CA-C	-5.12	105.59	111.07
1	A	283	HIS	N-CA-C	-5.09	106.23	112.90
1	A	337	ILE	N-CA-C	-5.08	105.46	111.00

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	6401	0	6384	543	0
2	A	55	0	0	4	0
3	A	39	0	0	7	0
All	All	6495	0	6384	543	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 42.

All (543) 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:696:TYR:HA	1:A:699:LYS:HE2	1.36	1.04
1:A:436:THR:HG21	1:A:442:SER:HB3	1.45	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:LYS:HB2	1:A:165:ARG:NH2	1.83	0.93
1:A:409:ARG:HG2	1:A:564:ASP:HB3	1.52	0.91
1:A:325:LYS:H	1:A:325:LYS:HZ2	1.16	0.89
1:A:724:TRP:HA	1:A:763:MET:HE1	1.57	0.87
1:A:110:SER:O	1:A:114:VAL:HG12	1.77	0.85
1:A:249:ASP:HA	1:A:263:GLU:HG2	1.57	0.85
1:A:377:GLU:OE2	1:A:517:ARG:HD3	1.75	0.85
1:A:160:SER:OG	1:A:163:GLU:HG3	1.77	0.84
1:A:164:LYS:HB2	1:A:165:ARG:HH22	1.42	0.83
1:A:164:LYS:N	1:A:165:ARG:HH12	1.77	0.83
1:A:567:THR:HB	1:A:568:PRO:HD3	1.60	0.83
1:A:325:LYS:HB3	1:A:738:ILE:HA	1.62	0.81
1:A:261:LEU:HD22	1:A:777:LYS:NZ	1.95	0.81
1:A:157:ASN:HB3	1:A:179:GLU:OE2	1.81	0.81
1:A:112:LEU:H	1:A:112:LEU:HD12	1.44	0.81
1:A:782:ASN:HD22	1:A:783:ASN:H	1.27	0.80
1:A:510:THR:HG22	1:A:511:GLU:HG3	1.63	0.80
1:A:606:GLN:NE2	1:A:760:PHE:HB2	1.98	0.79
1:A:224:SER:HA	1:A:352:LEU:HG	1.65	0.79
1:A:623:LEU:HD22	1:A:713:LYS:HG2	1.65	0.79
1:A:608:GLU:HG2	3:A:979:HOH:O	1.81	0.78
1:A:332:GLY:C	1:A:335:GLN:HE22	1.89	0.78
1:A:275:ILE:HG21	1:A:278:LEU:HD12	1.64	0.78
1:A:516:ARG:NH1	1:A:583:LYS:HG2	1.99	0.78
1:A:164:LYS:H	1:A:165:ARG:HH12	1.33	0.77
1:A:128:THR:HG22	1:A:129:VAL:N	1.97	0.77
1:A:249:ASP:HB3	1:A:266:MET:HE2	1.67	0.76
1:A:286:LEU:O	1:A:290:ILE:HD13	1.86	0.76
1:A:333:LEU:HD23	1:A:333:LEU:O	1.86	0.75
1:A:713:LYS:HD2	1:A:786:ARG:NH2	2.01	0.75
1:A:361:PHE:O	1:A:367:LEU:HD22	1.88	0.74
1:A:644:PRO:HB2	1:A:647:GLU:HG2	1.70	0.74
1:A:406:LEU:HD12	1:A:538:TYR:CE1	2.24	0.73
1:A:356:THR:HG22	1:A:600:ASP:OD2	1.88	0.73
1:A:746:THR:HG21	1:A:750:ARG:HG2	1.69	0.73
1:A:705:LYS:HD3	1:A:705:LYS:H	1.53	0.72
1:A:425:ARG:NH2	1:A:534:ILE:HD13	2.05	0.72
1:A:425:ARG:O	1:A:428:THR:HG22	1.90	0.72
1:A:652:TRP:O	1:A:654:LEU:HD12	1.89	0.72
1:A:279:PHE:O	1:A:283:HIS:HB2	1.89	0.72
1:A:445:ILE:HD13	1:A:445:ILE:O	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:MET:HB2	1:A:542:GLU:HB2	1.70	0.72
1:A:114:VAL:HG23	1:A:124:VAL:HG11	1.71	0.71
1:A:70:ARG:HG3	1:A:86:LEU:HD21	1.71	0.71
1:A:622:ASN:HA	1:A:709:ARG:NH1	2.05	0.71
1:A:164:LYS:N	1:A:165:ARG:NH1	2.38	0.71
1:A:279:PHE:C	1:A:283:HIS:HB2	2.16	0.71
1:A:261:LEU:HD13	1:A:777:LYS:HD3	1.70	0.70
1:A:156:LEU:N	1:A:156:LEU:HD23	2.06	0.70
1:A:356:THR:HG23	1:A:359:ASN:H	1.57	0.70
1:A:635:LEU:HD11	1:A:688:ILE:HG21	1.73	0.70
1:A:425:ARG:HH22	1:A:534:ILE:HD13	1.56	0.70
1:A:763:MET:O	1:A:767:ILE:HG13	1.92	0.69
1:A:165:ARG:NH1	1:A:165:ARG:H	1.89	0.69
1:A:325:LYS:H	1:A:325:LYS:NZ	1.91	0.69
1:A:66:PHE:CE2	1:A:112:LEU:HB3	2.27	0.69
1:A:617:VAL:HG13	1:A:623:LEU:HD11	1.74	0.69
1:A:422:VAL:HG23	1:A:432:VAL:HG11	1.74	0.69
1:A:489:ARG:HH12	1:A:521:GLN:HB3	1.58	0.68
1:A:32:ASP:HB2	1:A:33:TYR:CE1	2.29	0.68
1:A:271:LYS:HD3	1:A:276:ASP:HB2	1.74	0.68
1:A:331:GLU:HG2	1:A:723:LYS:HD2	1.74	0.68
1:A:489:ARG:NH2	3:A:952:HOH:O	2.26	0.67
1:A:155:ASN:OD1	1:A:164:LYS:HE3	1.94	0.67
1:A:572:LYS:C	1:A:574:VAL:H	2.03	0.67
1:A:684:MET:O	1:A:688:ILE:HD12	1.95	0.67
1:A:93:HIS:CD2	1:A:117:ASN:HD21	2.12	0.67
1:A:68:VAL:HG12	1:A:148:LEU:HD11	1.75	0.67
1:A:230:SER:HB2	1:A:233:LEU:HD11	1.76	0.66
1:A:512:ARG:HB2	1:A:539:LEU:HD13	1.78	0.66
1:A:608:GLU:N	3:A:979:HOH:O	2.28	0.66
1:A:317:ASP:O	1:A:321:GLY:HA2	1.96	0.66
1:A:498:GLY:HA2	1:A:500:LYS:HE2	1.77	0.66
1:A:162:ASP:C	1:A:165:ARG:HH11	2.03	0.66
1:A:434:VAL:O	1:A:434:VAL:HG23	1.96	0.66
1:A:567:THR:HB	1:A:568:PRO:CD	2.24	0.66
1:A:572:LYS:O	1:A:574:VAL:N	2.26	0.66
1:A:767:ILE:O	1:A:771:VAL:HG23	1.95	0.65
1:A:407:ILE:H	1:A:407:ILE:HD12	1.61	0.65
1:A:210:ASP:OD1	1:A:211:SER:N	2.30	0.65
1:A:244:LEU:HD13	1:A:266:MET:HE1	1.79	0.65
1:A:199:ARG:HG2	1:A:200:PRO:HD2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:LEU:HD12	1:A:112:LEU:N	2.12	0.65
1:A:240:PHE:O	1:A:243:THR:HG22	1.97	0.65
1:A:498:GLY:CA	1:A:500:LYS:HE2	2.27	0.65
1:A:233:LEU:HD13	1:A:233:LEU:H	1.61	0.65
1:A:333:LEU:HD23	1:A:333:LEU:C	2.22	0.65
1:A:168:TYR:CE2	1:A:198:GLN:HG2	2.32	0.64
1:A:408:TYR:CD2	1:A:414:LYS:HA	2.32	0.64
1:A:517:ARG:O	1:A:520:ASN:N	2.30	0.64
1:A:84:VAL:HA	1:A:87:MET:HE3	1.78	0.64
1:A:215:ASP:O	1:A:218:ARG:HG3	1.98	0.64
1:A:226:GLN:HG2	1:A:349:SER:HB3	1.79	0.64
1:A:447:LYS:HA	1:A:450:LYS:HG3	1.79	0.64
1:A:72:ALA:CB	1:A:148:LEU:HD21	2.28	0.63
1:A:409:ARG:HH12	1:A:555:MET:HG2	1.63	0.63
1:A:264:GLU:HB3	1:A:268:LYS:HE3	1.80	0.63
1:A:128:THR:HB	1:A:134:ALA:HB2	1.81	0.63
1:A:322:ARG:HD3	1:A:741:ARG:NH2	2.14	0.63
1:A:10:ASP:N	1:A:11:PRO:HD2	2.13	0.62
1:A:168:TYR:CZ	1:A:198:GLN:HG2	2.34	0.62
1:A:164:LYS:HB2	1:A:165:ARG:CZ	2.30	0.62
1:A:545:LEU:C	1:A:545:LEU:HD12	2.24	0.62
1:A:325:LYS:HB2	1:A:325:LYS:HZ3	1.64	0.62
1:A:409:ARG:NH1	1:A:555:MET:HG2	2.14	0.62
1:A:309:GLU:N	3:A:953:HOH:O	2.32	0.62
1:A:475:GLY:O	1:A:499:VAL:HG21	2.00	0.62
1:A:516:ARG:HD3	1:A:586:GLU:OE2	2.00	0.62
1:A:210:ASP:HA	1:A:214:ILE:HD13	1.82	0.62
1:A:261:LEU:HD22	1:A:777:LYS:HZ1	1.64	0.62
1:A:138:ALA:HB2	1:A:174:TYR:CD2	2.34	0.61
1:A:499:VAL:HA	1:A:502:LEU:HD12	1.81	0.61
1:A:691:ARG:HA	1:A:694:THR:HG22	1.82	0.61
1:A:121:GLY:O	1:A:199:ARG:NH1	2.33	0.61
1:A:679:LYS:HE3	1:A:683:GLU:OE2	1.99	0.61
1:A:698:GLU:O	1:A:702:GLN:HB2	2.01	0.61
1:A:284:VAL:HG22	1:A:774:PHE:CE2	2.35	0.61
1:A:332:GLY:O	1:A:335:GLN:NE2	2.32	0.61
1:A:322:ARG:HD3	1:A:741:ARG:HH21	1.65	0.61
1:A:623:LEU:CD2	1:A:713:LYS:HG2	2.29	0.61
1:A:184:TYR:O	1:A:188:ASN:ND2	2.34	0.60
1:A:498:GLY:N	1:A:500:LYS:HE2	2.16	0.60
1:A:186:ARG:HG3	1:A:186:ARG:HH11	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:LYS:O	1:A:87:MET:HG3	2.02	0.60
1:A:114:VAL:HG23	1:A:124:VAL:CG1	2.32	0.60
1:A:315:ILE:HG22	1:A:316:VAL:H	1.65	0.60
1:A:444:LEU:O	1:A:448:LEU:HB2	2.01	0.60
1:A:495:LEU:HD12	1:A:531:ASP:CG	2.27	0.60
1:A:510:THR:CG2	1:A:511:GLU:HG3	2.31	0.60
1:A:159:MET:HE2	1:A:164:LYS:HG2	1.84	0.60
1:A:489:ARG:NH1	1:A:525:ARG:HH22	1.99	0.60
1:A:227:ALA:HB3	1:A:347:ASN:OD1	2.01	0.59
1:A:718:ARG:CZ	1:A:787:GLU:HB2	2.31	0.59
1:A:244:LEU:HB3	1:A:266:MET:HE1	1.85	0.59
1:A:623:LEU:HB3	1:A:712:GLU:OE1	2.02	0.59
1:A:137:ASP:HB3	1:A:174:TYR:HE2	1.65	0.59
1:A:702:GLN:HB3	1:A:703:PHE:HD1	1.68	0.59
1:A:760:PHE:O	1:A:764:ILE:HG12	2.03	0.59
1:A:401:ASP:OD1	1:A:403:ARG:NH1	2.36	0.59
1:A:425:ARG:NH1	1:A:534:ILE:HG21	2.18	0.59
1:A:623:LEU:HD23	1:A:712:GLU:CB	2.33	0.59
1:A:702:GLN:HB3	1:A:703:PHE:CD1	2.38	0.58
1:A:325:LYS:HZ2	1:A:325:LYS:N	1.94	0.58
1:A:459:LEU:HD13	1:A:487:ALA:HB3	1.84	0.58
1:A:26:ILE:HD11	1:A:63:VAL:HA	1.84	0.58
1:A:431:PRO:HG2	1:A:505:LEU:HA	1.86	0.58
1:A:189:MET:HE1	1:A:353:ALA:HB2	1.85	0.58
1:A:297:HIS:HD2	1:A:340:LYS:HD2	1.69	0.58
1:A:563:MET:C	1:A:565:ASP:H	2.12	0.58
1:A:128:THR:CG2	1:A:129:VAL:N	2.64	0.57
1:A:671:LEU:HD21	1:A:676:ILE:HD11	1.86	0.57
1:A:466:ARG:O	1:A:470:ILE:HG12	2.02	0.57
1:A:81:PRO:HA	1:A:85:GLN:OE1	2.05	0.57
1:A:228:ALA:C	1:A:230:SER:H	2.12	0.57
1:A:606:GLN:HE21	1:A:760:PHE:HB2	1.67	0.57
1:A:631:ILE:HD13	1:A:776:MET:HE2	1.87	0.57
1:A:175:SER:HB3	1:A:180:LEU:HD21	1.86	0.57
1:A:222:ILE:C	1:A:222:ILE:HD13	2.29	0.57
1:A:241:VAL:HA	1:A:244:LEU:CD1	2.35	0.57
1:A:484:THR:HG22	1:A:485:ASN:ND2	2.20	0.57
1:A:541:MET:HE3	1:A:555:MET:HG3	1.85	0.57
1:A:605:GLN:C	3:A:979:HOH:O	2.48	0.57
1:A:731:MET:C	1:A:733:GLN:H	2.13	0.57
1:A:780:ILE:HG23	1:A:784:LEU:HD23	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:VAL:HG13	1:A:195:GLN:HB2	1.86	0.57
1:A:207:ASP:O	1:A:208:GLN:HB2	2.04	0.57
1:A:434:VAL:HG12	1:A:508:VAL:CG1	2.35	0.56
1:A:660:LEU:O	1:A:664:THR:HG22	2.05	0.56
1:A:351:THR:C	1:A:352:LEU:HD23	2.30	0.56
1:A:613:GLN:O	1:A:617:VAL:HG23	2.06	0.56
1:A:717:LEU:O	1:A:721:ASP:HB2	2.04	0.56
1:A:138:ALA:HB2	1:A:174:TYR:CG	2.41	0.56
1:A:647:GLU:O	1:A:647:GLU:HG3	2.03	0.56
1:A:328:ARG:HD3	1:A:334:HIS:CD2	2.40	0.56
1:A:36:LEU:HD22	1:A:37:SER:N	2.21	0.56
1:A:115:TYR:CZ	1:A:119:LEU:HD21	2.40	0.56
1:A:72:ALA:O	1:A:76:VAL:HG23	2.06	0.55
1:A:187:ASP:OD1	1:A:197:VAL:HG12	2.05	0.55
1:A:192:TYR:CE2	1:A:786:ARG:HD2	2.41	0.55
1:A:58:THR:O	1:A:116:LEU:HD11	2.06	0.55
1:A:328:ARG:HG2	1:A:328:ARG:HH11	1.70	0.55
1:A:746:THR:HG22	1:A:747:ASN:H	1.72	0.55
1:A:335:GLN:HB2	1:A:345:ILE:HG23	1.88	0.55
1:A:507:VAL:CG1	1:A:535:THR:HG22	2.35	0.55
1:A:66:PHE:CG	1:A:112:LEU:HD23	2.42	0.55
1:A:280:ASP:O	1:A:284:VAL:HG23	2.07	0.55
1:A:326:GLY:HA2	2:A:908:SO4:S	2.47	0.55
1:A:517:ARG:O	1:A:519:ASP:N	2.39	0.55
1:A:648:LEU:HB3	1:A:651:GLU:HB2	1.88	0.55
1:A:670:ALA:C	1:A:691:ARG:HH12	2.14	0.55
1:A:380:GLU:OE1	1:A:593:ARG:NH1	2.30	0.55
1:A:159:MET:HE1	1:A:167:ALA:CB	2.37	0.55
1:A:681:PRO:HA	1:A:684:MET:HE3	1.87	0.55
1:A:715:ILE:CD1	1:A:771:VAL:HG13	2.37	0.55
1:A:221:LEU:HD13	1:A:357:PHE:CE2	2.42	0.55
1:A:252:TYR:O	1:A:256:THR:HA	2.07	0.55
1:A:708:MET:O	1:A:711:PHE:HB3	2.06	0.55
1:A:162:ASP:C	1:A:165:ARG:NH1	2.65	0.54
1:A:266:MET:O	1:A:270:GLU:HG3	2.06	0.54
1:A:498:GLY:H	1:A:500:LYS:HE2	1.72	0.54
1:A:114:VAL:HG11	1:A:145:PHE:HZ	1.72	0.54
1:A:160:SER:CB	1:A:163:GLU:HG3	2.38	0.54
1:A:147:PHE:HD2	1:A:148:LEU:HD22	1.73	0.54
1:A:377:GLU:CD	1:A:517:ARG:HD3	2.32	0.54
1:A:693:ILE:HG13	1:A:694:THR:N	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:MET:HE1	1:A:167:ALA:HB2	1.90	0.54
1:A:165:ARG:NH1	1:A:165:ARG:N	2.56	0.54
1:A:311:GLY:O	1:A:343:LEU:HD11	2.08	0.54
1:A:62:LEU:C	1:A:62:LEU:HD23	2.33	0.54
1:A:498:GLY:HA2	1:A:500:LYS:CE	2.37	0.54
1:A:541:MET:HE3	1:A:555:MET:CG	2.38	0.54
1:A:756:GLY:HA2	1:A:759:MET:HE3	1.90	0.54
1:A:136:ARG:HG2	1:A:136:ARG:HH11	1.72	0.54
1:A:325:LYS:N	1:A:325:LYS:HD3	2.23	0.54
1:A:312:GLN:OE1	1:A:346:GLN:HB2	2.08	0.54
1:A:410:THR:OG1	1:A:413:GLY:HA3	2.07	0.54
1:A:443:GLU:O	1:A:446:SER:HB3	2.08	0.54
1:A:230:SER:C	1:A:232:LYS:H	2.15	0.53
1:A:569:ILE:HG23	1:A:569:ILE:O	2.06	0.53
1:A:160:SER:C	1:A:162:ASP:H	2.16	0.53
1:A:343:LEU:HD23	1:A:344:GLU:N	2.23	0.53
1:A:99:GLU:HA	1:A:371:THR:O	2.08	0.53
1:A:517:ARG:HA	1:A:520:ASN:HB2	1.90	0.53
1:A:718:ARG:NE	1:A:787:GLU:HB2	2.24	0.53
1:A:286:LEU:C	1:A:290:ILE:HD13	2.33	0.53
1:A:85:GLN:O	1:A:109:THR:HG23	2.08	0.53
1:A:53:GLU:OE2	1:A:53:GLU:N	2.40	0.53
1:A:193:LYS:HD2	1:A:619:ASP:HB2	1.91	0.53
1:A:214:ILE:HG23	1:A:593:ARG:CZ	2.39	0.53
1:A:128:THR:HG22	1:A:129:VAL:H	1.68	0.53
1:A:100:MET:HG2	1:A:392:ILE:HB	1.91	0.53
1:A:261:LEU:HD23	1:A:663:THR:HA	1.90	0.53
1:A:267:THR:HA	1:A:270:GLU:OE2	2.09	0.53
1:A:302:LYS:O	1:A:304:VAL:N	2.34	0.53
1:A:432:VAL:HG13	1:A:480:VAL:HA	1.90	0.53
1:A:599:TYR:CE2	1:A:749:LEU:HA	2.44	0.53
1:A:32:ASP:OD1	1:A:32:ASP:N	2.40	0.53
1:A:241:VAL:HA	1:A:244:LEU:HD12	1.91	0.52
1:A:708:MET:HE2	1:A:711:PHE:HD2	1.72	0.52
1:A:715:ILE:HD12	1:A:716:VAL:N	2.24	0.52
1:A:186:ARG:HG3	1:A:186:ARG:NH1	2.23	0.52
1:A:38:ASP:O	1:A:42:LYS:HG3	2.09	0.52
1:A:448:LEU:HD23	1:A:448:LEU:O	2.08	0.52
1:A:623:LEU:HD23	1:A:712:GLU:HB2	1.91	0.52
1:A:135:SER:O	1:A:136:ARG:C	2.53	0.52
1:A:355:ILE:HG22	1:A:607:ARG:CZ	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:ARG:CG	1:A:200:PRO:HD2	2.40	0.52
1:A:724:TRP:CA	1:A:763:MET:HE1	2.37	0.52
1:A:721:ASP:O	1:A:725:MET:HG2	2.10	0.52
1:A:88:GLY:O	1:A:92:LEU:HG	2.10	0.51
1:A:98:ALA:HB1	1:A:100:MET:HE2	1.92	0.51
1:A:358:GLN:CB	1:A:597:LEU:HD13	2.40	0.51
1:A:712:GLU:O	1:A:715:ILE:HG13	2.10	0.51
1:A:789:VAL:HG12	1:A:789:VAL:O	2.10	0.51
1:A:63:VAL:HG23	1:A:64:GLU:H	1.75	0.51
1:A:76:VAL:HG11	1:A:144:ILE:HD13	1.91	0.51
1:A:285:ALA:O	1:A:289:HIS:HB2	2.11	0.51
1:A:423:ALA:HA	1:A:454:ILE:CD1	2.40	0.51
1:A:528:ARG:CZ	1:A:528:ARG:HB3	2.40	0.51
1:A:21:LYS:O	1:A:24:ASN:N	2.42	0.51
1:A:434:VAL:HG22	1:A:481:THR:O	2.11	0.51
1:A:286:LEU:O	1:A:289:HIS:N	2.39	0.51
1:A:442:SER:O	1:A:445:ILE:HG22	2.10	0.51
1:A:623:LEU:HD23	1:A:712:GLU:HB3	1.93	0.51
1:A:165:ARG:H	1:A:165:ARG:HH11	1.56	0.51
1:A:632:LYS:HB2	1:A:689:MET:SD	2.51	0.51
1:A:203:PHE:CE2	1:A:205:VAL:HG23	2.45	0.51
1:A:325:LYS:CB	1:A:738:ILE:HA	2.38	0.51
1:A:439:VAL:O	1:A:443:GLU:HG2	2.10	0.51
1:A:261:LEU:HD22	1:A:777:LYS:HZ2	1.74	0.51
1:A:351:THR:O	1:A:352:LEU:HD23	2.11	0.51
1:A:355:ILE:HG22	1:A:607:ARG:NE	2.26	0.51
1:A:738:ILE:HD12	1:A:742:ALA:HB2	1.92	0.51
1:A:114:VAL:CG1	1:A:145:PHE:HZ	2.24	0.51
1:A:203:PHE:CE1	1:A:366:LYS:HE3	2.46	0.51
1:A:210:ASP:HB2	1:A:517:ARG:NH2	2.26	0.51
1:A:627:VAL:CG1	1:A:775:VAL:HG11	2.41	0.51
1:A:724:TRP:HA	1:A:763:MET:CE	2.33	0.51
1:A:785:GLU:O	1:A:787:GLU:HG2	2.11	0.51
1:A:244:LEU:HD13	1:A:266:MET:CE	2.40	0.50
1:A:222:ILE:O	1:A:797:HIS:HD2	1.93	0.50
1:A:714:VAL:HG12	1:A:786:ARG:HA	1.93	0.50
1:A:639:ILE:CD1	1:A:685:LEU:HA	2.41	0.50
1:A:252:TYR:OH	1:A:660:LEU:HB2	2.11	0.50
1:A:309:GLU:C	1:A:311:GLY:H	2.19	0.50
1:A:356:THR:O	1:A:357:PHE:C	2.54	0.50
1:A:545:LEU:HD12	1:A:546:MET:N	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:601:ASP:HA	1:A:604:ARG:HG2	1.92	0.50
1:A:434:VAL:HG12	1:A:508:VAL:HG13	1.91	0.50
1:A:449:LEU:HA	1:A:452:LYS:HB2	1.92	0.50
1:A:241:VAL:C	1:A:243:THR:H	2.19	0.50
1:A:518:ILE:HG22	1:A:518:ILE:O	2.12	0.50
1:A:598:GLN:O	1:A:601:ASP:HB2	2.12	0.50
1:A:710:GLU:HG3	1:A:784:LEU:HD12	1.93	0.50
1:A:714:VAL:HG23	1:A:715:ILE:N	2.25	0.50
1:A:274:GLY:O	1:A:276:ASP:N	2.44	0.50
1:A:517:ARG:O	1:A:518:ILE:C	2.55	0.50
1:A:541:MET:SD	1:A:546:MET:HE3	2.51	0.50
1:A:362:ARG:HH21	1:A:597:LEU:HD11	1.76	0.49
1:A:489:ARG:NH2	2:A:902:SO4:S	2.85	0.49
1:A:160:SER:OG	1:A:163:GLU:CG	2.54	0.49
1:A:789:VAL:O	1:A:790:VAL:HG13	2.13	0.49
1:A:261:LEU:CD2	1:A:663:THR:HA	2.43	0.49
1:A:175:SER:CB	1:A:180:LEU:HD21	2.42	0.49
1:A:220:PRO:O	1:A:798:GLN:HG3	2.13	0.49
1:A:267:THR:O	1:A:271:LYS:HE3	2.12	0.49
1:A:62:LEU:HA	1:A:116:LEU:HD22	1.93	0.49
1:A:286:LEU:HD22	1:A:290:ILE:HD11	1.94	0.49
1:A:328:ARG:HG2	1:A:328:ARG:NH1	2.27	0.49
1:A:507:VAL:HG13	1:A:535:THR:HA	1.95	0.49
1:A:93:HIS:CD2	1:A:366:LYS:NZ	2.81	0.49
1:A:631:ILE:HD11	1:A:775:VAL:HG21	1.95	0.49
1:A:213:LEU:HD13	1:A:385:TYR:CE1	2.48	0.48
1:A:302:LYS:HG3	1:A:341:GLU:OE2	2.13	0.48
1:A:73:SER:HA	1:A:144:ILE:HD12	1.94	0.48
1:A:380:GLU:OE2	1:A:384:ILE:HD12	2.12	0.48
1:A:418:VAL:HG22	1:A:538:TYR:CD2	2.48	0.48
1:A:673:LYS:HB2	1:A:673:LYS:NZ	2.28	0.48
1:A:715:ILE:HD12	1:A:715:ILE:C	2.38	0.48
1:A:248:LYS:HG3	3:A:966:HOH:O	2.13	0.48
1:A:558:LEU:HD23	1:A:563:MET:HB2	1.95	0.48
1:A:631:ILE:HD13	1:A:776:MET:CE	2.42	0.48
1:A:643:THR:HA	1:A:652:TRP:CD1	2.48	0.48
1:A:746:THR:HG22	1:A:747:ASN:N	2.28	0.48
1:A:164:LYS:HB3	1:A:197:VAL:HG21	1.94	0.48
1:A:222:ILE:CG1	1:A:351:THR:HG23	2.44	0.48
1:A:377:GLU:OE2	1:A:517:ARG:CD	2.55	0.48
1:A:463:ASN:ND2	1:A:465:GLU:HB2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:514:GLU:CD	1:A:514:GLU:H	2.21	0.48
1:A:169:ALA:O	1:A:170:ALA:C	2.57	0.48
1:A:504:GLY:HA3	1:A:532:PRO:O	2.13	0.48
1:A:572:LYS:C	1:A:574:VAL:N	2.71	0.48
1:A:764:ILE:O	1:A:768:GLU:HG3	2.12	0.48
1:A:679:LYS:HE3	1:A:683:GLU:CD	2.38	0.48
1:A:128:THR:HG21	1:A:133:LEU:HB3	1.95	0.48
1:A:458:VAL:HG12	1:A:459:LEU:N	2.29	0.48
1:A:467:GLU:O	1:A:471:ILE:HG12	2.13	0.48
1:A:147:PHE:C	1:A:149:GLY:H	2.21	0.48
1:A:154:LEU:O	1:A:167:ALA:HB1	2.14	0.48
1:A:155:ASN:C	1:A:156:LEU:HD23	2.39	0.48
1:A:512:ARG:HG3	1:A:512:ARG:HH11	1.78	0.48
1:A:643:THR:HA	1:A:652:TRP:NE1	2.28	0.48
1:A:676:ILE:HG23	1:A:684:MET:SD	2.54	0.48
1:A:36:LEU:HD13	1:A:37:SER:O	2.13	0.47
1:A:110:SER:HB3	1:A:370:MET:HE1	1.96	0.47
1:A:513:HIS:CD2	1:A:514:GLU:OE1	2.67	0.47
1:A:575:SER:O	1:A:578:VAL:HG12	2.14	0.47
1:A:214:ILE:N	1:A:214:ILE:HD12	2.29	0.47
1:A:408:TYR:O	1:A:541:MET:N	2.48	0.47
1:A:693:ILE:HG13	1:A:694:THR:H	1.78	0.47
1:A:325:LYS:H	1:A:325:LYS:HD3	1.79	0.47
1:A:507:VAL:O	1:A:535:THR:HA	2.15	0.47
1:A:749:LEU:O	1:A:753:GLN:HG3	2.14	0.47
1:A:243:THR:O	1:A:244:LEU:HD23	2.14	0.47
1:A:335:GLN:CD	1:A:335:GLN:H	2.22	0.47
1:A:414:LYS:HG3	1:A:415:PHE:N	2.30	0.47
1:A:582:GLN:O	1:A:586:GLU:HG3	2.15	0.47
1:A:144:ILE:O	1:A:148:LEU:HD23	2.15	0.47
1:A:431:PRO:CB	1:A:479:ALA:HB3	2.45	0.47
1:A:485:ASN:O	1:A:486:MET:HB2	2.14	0.47
1:A:8:MET:O	1:A:11:PRO:HD2	2.15	0.47
1:A:419:ALA:CB	1:A:448:LEU:HD22	2.45	0.47
1:A:626:ILE:HG22	1:A:630:MET:HE2	1.97	0.47
1:A:41:LEU:O	1:A:44:LYS:N	2.42	0.46
1:A:634:SER:OG	1:A:769:ASP:OD1	2.30	0.46
1:A:238:ASN:O	1:A:242:ARG:HB2	2.15	0.46
1:A:505:LEU:HB3	1:A:526:SER:OG	2.14	0.46
1:A:92:LEU:HB2	1:A:113:PRO:HG3	1.97	0.46
1:A:107:THR:HG22	1:A:141:MET:HE3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:VAL:HG13	1:A:198:GLN:N	2.30	0.46
1:A:262:THR:HG23	1:A:663:THR:HG22	1.97	0.46
1:A:676:ILE:CG2	1:A:684:MET:SD	3.03	0.46
1:A:699:LYS:HE3	1:A:776:MET:SD	2.55	0.46
1:A:84:VAL:O	1:A:87:MET:HB2	2.16	0.46
1:A:68:VAL:CG1	1:A:148:LEU:HD11	2.44	0.46
1:A:630:MET:CE	1:A:771:VAL:HG11	2.44	0.46
1:A:381:PHE:O	1:A:382:ARG:C	2.58	0.46
1:A:462:LYS:HG3	1:A:466:ARG:NH1	2.31	0.46
1:A:571:SER:O	1:A:574:VAL:HG12	2.15	0.46
1:A:63:VAL:HG23	1:A:64:GLU:N	2.31	0.46
1:A:284:VAL:HG22	1:A:774:PHE:HE2	1.80	0.46
1:A:708:MET:HE2	1:A:711:PHE:CD2	2.50	0.46
1:A:358:GLN:HB2	1:A:597:LEU:HD13	1.98	0.46
1:A:495:LEU:CD1	1:A:531:ASP:CG	2.89	0.46
1:A:161:LYS:NZ	1:A:195:GLN:HG2	2.30	0.46
1:A:255:LYS:HG3	1:A:255:LYS:O	2.15	0.46
1:A:286:LEU:O	1:A:287:ASN:C	2.59	0.45
1:A:70:ARG:CZ	1:A:80:PHE:CZ	2.99	0.45
1:A:325:LYS:H	1:A:325:LYS:CD	2.30	0.45
1:A:407:ILE:HD12	1:A:407:ILE:N	2.31	0.45
1:A:627:VAL:HA	1:A:630:MET:HE3	1.98	0.45
1:A:410:THR:HG23	2:A:906:SO4:O2	2.17	0.45
1:A:66:PHE:CD2	1:A:112:LEU:HB3	2.52	0.45
1:A:252:TYR:HB3	1:A:257:LYS:H	1.80	0.45
1:A:703:PHE:CD1	1:A:703:PHE:N	2.85	0.45
1:A:233:LEU:HD13	1:A:233:LEU:N	2.29	0.45
1:A:338:GLU:CD	1:A:345:ILE:HA	2.41	0.45
1:A:52:LEU:C	1:A:54:LYS:H	2.25	0.45
1:A:643:THR:N	1:A:644:PRO:HD3	2.32	0.45
1:A:136:ARG:HG2	1:A:136:ARG:NH1	2.31	0.44
1:A:267:THR:HA	1:A:270:GLU:CD	2.41	0.44
1:A:325:LYS:NZ	1:A:325:LYS:HB2	2.27	0.44
1:A:214:ILE:HG22	1:A:215:ASP:N	2.31	0.44
1:A:286:LEU:O	1:A:290:ILE:N	2.50	0.44
1:A:563:MET:O	1:A:565:ASP:N	2.49	0.44
1:A:114:VAL:CG1	1:A:145:PHE:CZ	3.01	0.44
1:A:133:LEU:HD23	1:A:133:LEU:HA	1.82	0.44
1:A:203:PHE:CE2	1:A:205:VAL:CG2	3.00	0.44
1:A:407:ILE:O	1:A:569:ILE:HG22	2.17	0.44
1:A:746:THR:HG21	1:A:750:ARG:CG	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:ASN:OD1	1:A:130:ASN:C	2.59	0.44
1:A:315:ILE:HG22	1:A:316:VAL:N	2.31	0.44
1:A:341:GLU:C	1:A:343:LEU:H	2.25	0.44
1:A:360:TYR:C	1:A:362:ARG:H	2.25	0.44
1:A:112:LEU:H	1:A:112:LEU:CD1	2.22	0.44
1:A:333:LEU:C	1:A:333:LEU:CD2	2.90	0.44
1:A:21:LYS:O	1:A:22:ILE:C	2.61	0.44
1:A:36:LEU:HD22	1:A:37:SER:H	1.83	0.44
1:A:489:ARG:NH1	1:A:525:ARG:NH2	2.65	0.44
1:A:252:TYR:HD2	1:A:255:LYS:HB3	1.83	0.44
1:A:375:LYS:HA	1:A:378:GLU:HB2	1.99	0.44
1:A:414:LYS:CG	1:A:415:PHE:N	2.81	0.44
1:A:489:ARG:NH1	1:A:521:GLN:HB3	2.27	0.44
1:A:610:ILE:HG22	1:A:611:TYR:HD1	1.82	0.44
1:A:128:THR:CG2	1:A:129:VAL:H	2.26	0.44
1:A:643:THR:HB	1:A:652:TRP:CZ2	2.53	0.44
1:A:500:LYS:H	1:A:500:LYS:HG3	1.58	0.43
1:A:70:ARG:HD3	1:A:86:LEU:HD11	1.99	0.43
1:A:420:GLU:O	1:A:423:ALA:HB3	2.17	0.43
1:A:545:LEU:HD13	1:A:549:PHE:CE2	2.53	0.43
1:A:605:GLN:O	1:A:609:VAL:HG23	2.18	0.43
1:A:114:VAL:HG13	1:A:145:PHE:CZ	2.53	0.43
1:A:513:HIS:HD2	1:A:514:GLU:OE1	2.01	0.43
1:A:724:TRP:CZ2	1:A:728:ILE:HD13	2.53	0.43
1:A:300:MET:HE2	1:A:305:ASP:HB3	2.00	0.43
1:A:636:GLU:HG3	1:A:685:LEU:HD22	2.00	0.43
1:A:747:ASN:HD21	1:A:749:LEU:HB3	1.84	0.43
1:A:797:HIS:N	1:A:797:HIS:CD2	2.85	0.43
1:A:168:TYR:CD2	1:A:198:GLN:HA	2.53	0.43
1:A:708:MET:O	1:A:711:PHE:N	2.49	0.43
1:A:286:LEU:CD2	1:A:290:ILE:HD11	2.49	0.43
1:A:367:LEU:HD12	1:A:368:ALA:H	1.84	0.43
1:A:252:TYR:CD2	1:A:255:LYS:HB3	2.53	0.43
1:A:600:ASP:C	1:A:602:VAL:N	2.76	0.43
1:A:408:TYR:CE2	1:A:414:LYS:HA	2.54	0.43
1:A:279:PHE:O	1:A:280:ASP:C	2.62	0.43
1:A:315:ILE:HD12	1:A:329:TYR:CE1	2.53	0.43
1:A:436:THR:CG2	1:A:484:THR:HA	2.48	0.43
1:A:653:LYS:O	1:A:653:LYS:HG3	2.19	0.43
1:A:76:VAL:CB	1:A:144:ILE:HD13	2.49	0.42
1:A:82:PHE:O	1:A:85:GLN:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:647:GLU:O	1:A:647:GLU:CG	2.64	0.42
1:A:19:TYR:CE1	1:A:91:ALA:HA	2.53	0.42
1:A:70:ARG:CZ	1:A:80:PHE:CE2	3.02	0.42
1:A:84:VAL:HG13	1:A:392:ILE:HG22	2.01	0.42
1:A:123:GLY:O	1:A:202:HIS:HB3	2.19	0.42
1:A:358:GLN:HB3	1:A:597:LEU:HD13	2.01	0.42
1:A:571:SER:OG	1:A:574:VAL:HG12	2.18	0.42
1:A:41:LEU:HD11	1:A:68:VAL:HG13	2.01	0.42
1:A:213:LEU:HD23	1:A:213:LEU:HA	1.76	0.42
1:A:434:VAL:HA	1:A:508:VAL:HG13	2.01	0.42
1:A:558:LEU:HD23	1:A:558:LEU:O	2.19	0.42
1:A:65:ALA:O	1:A:69:VAL:HG23	2.19	0.42
1:A:214:ILE:HG23	1:A:593:ARG:NH1	2.34	0.42
1:A:309:GLU:C	1:A:311:GLY:N	2.78	0.42
1:A:325:LYS:N	1:A:325:LYS:CD	2.82	0.42
1:A:621:GLU:HA	3:A:987:HOH:O	2.19	0.42
1:A:33:TYR:CD1	1:A:33:TYR:N	2.88	0.42
1:A:169:ALA:O	1:A:199:ARG:NH2	2.53	0.42
1:A:314:VAL:HG12	1:A:315:ILE:O	2.20	0.42
1:A:360:TYR:CE2	1:A:364:TYR:HE1	2.37	0.42
1:A:469:GLN:HA	1:A:472:GLU:HG3	2.01	0.42
1:A:481:THR:C	1:A:482:ILE:HD12	2.44	0.42
1:A:74:ARG:O	1:A:78:GLY:HA2	2.20	0.42
1:A:76:VAL:CG1	1:A:144:ILE:HD13	2.49	0.42
1:A:104:GLU:HB3	1:A:105:GLY:H	1.65	0.42
1:A:290:ILE:N	1:A:290:ILE:CD1	2.82	0.42
1:A:375:LYS:HE3	1:A:378:GLU:OE1	2.20	0.42
1:A:774:PHE:C	1:A:776:MET:N	2.74	0.42
1:A:160:SER:C	1:A:162:ASP:N	2.78	0.42
1:A:696:TYR:HD2	1:A:699:LYS:HD2	1.85	0.42
1:A:745:GLN:HG2	1:A:746:THR:N	2.34	0.42
1:A:128:THR:HG21	1:A:133:LEU:CB	2.50	0.41
1:A:284:VAL:O	1:A:288:HIS:HB3	2.20	0.41
1:A:503:GLY:O	1:A:532:PRO:HG2	2.19	0.41
1:A:567:THR:HA	2:A:906:SO4:O1	2.20	0.41
1:A:723:LYS:O	1:A:726:ASP:HB3	2.20	0.41
1:A:752:TYR:O	1:A:753:GLN:C	2.63	0.41
1:A:10:ASP:N	1:A:11:PRO:CD	2.83	0.41
1:A:292:GLN:NE2	1:A:333:LEU:HB2	2.35	0.41
1:A:325:LYS:HG2	1:A:738:ILE:CD1	2.50	0.41
1:A:394:THR:O	1:A:395:ASN:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:501:GLU:C	1:A:503:GLY:N	2.77	0.41
1:A:782:ASN:ND2	1:A:783:ASN:H	2.06	0.41
1:A:277:ASN:HD22	1:A:277:ASN:HA	1.65	0.41
1:A:731:MET:C	1:A:733:GLN:N	2.77	0.41
1:A:308:VAL:HG13	1:A:343:LEU:HD12	2.03	0.41
1:A:66:PHE:CD1	1:A:112:LEU:HD23	2.55	0.41
1:A:76:VAL:HB	1:A:144:ILE:CD1	2.50	0.41
1:A:630:MET:HE3	1:A:771:VAL:HG11	2.00	0.41
1:A:651:GLU:N	1:A:651:GLU:CD	2.78	0.41
1:A:18:ARG:O	1:A:21:LYS:N	2.53	0.41
1:A:215:ASP:C	1:A:217:ALA:H	2.29	0.41
1:A:241:VAL:C	1:A:243:THR:N	2.78	0.41
1:A:411:MET:C	1:A:413:GLY:H	2.28	0.41
1:A:423:ALA:HA	1:A:454:ILE:HD11	2.01	0.41
1:A:423:ALA:HA	1:A:454:ILE:HD13	2.01	0.41
1:A:93:HIS:CD2	1:A:366:LYS:HZ2	2.39	0.41
1:A:370:MET:HE2	1:A:370:MET:HB3	1.82	0.41
1:A:715:ILE:HD11	1:A:771:VAL:HG13	2.01	0.41
1:A:5:LEU:HG	1:A:5:LEU:O	2.20	0.41
1:A:100:MET:O	1:A:101:LYS:C	2.63	0.41
1:A:316:VAL:O	1:A:316:VAL:HG13	2.21	0.41
1:A:468:ALA:O	1:A:472:GLU:HG2	2.21	0.41
1:A:513:HIS:CD2	1:A:514:GLU:CD	2.99	0.41
1:A:47:GLU:O	1:A:51:ARG:HG3	2.21	0.41
1:A:92:LEU:HD21	1:A:98:ALA:HB3	2.02	0.41
1:A:93:HIS:HD2	1:A:366:LYS:NZ	2.19	0.41
1:A:112:LEU:HB2	1:A:113:PRO:HD3	2.01	0.41
1:A:512:ARG:HH11	1:A:512:ARG:CG	2.34	0.41
1:A:627:VAL:HG11	1:A:775:VAL:HG11	2.03	0.41
1:A:628:GLU:O	1:A:631:ILE:N	2.53	0.41
1:A:696:TYR:HA	1:A:699:LYS:CE	2.26	0.41
1:A:76:VAL:HB	1:A:144:ILE:HD13	2.03	0.41
1:A:190:VAL:O	1:A:618:ILE:HD11	2.21	0.41
1:A:462:LYS:HB3	1:A:466:ARG:HD3	2.03	0.41
1:A:539:LEU:HD11	1:A:545:LEU:HD21	2.03	0.41
1:A:214:ILE:HD11	1:A:381:PHE:CZ	2.56	0.40
1:A:355:ILE:O	1:A:355:ILE:HG13	2.20	0.40
1:A:425:ARG:HH22	1:A:534:ILE:CD1	2.28	0.40
1:A:482:ILE:HD12	1:A:482:ILE:N	2.36	0.40
1:A:658:VAL:HG12	1:A:662:ASN:ND2	2.37	0.40
1:A:70:ARG:NH1	1:A:80:PHE:CE2	2.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:713:LYS:HD2	1:A:786:ARG:HH21	1.84	0.40
1:A:115:TYR:O	1:A:119:LEU:HG	2.21	0.40
1:A:127:VAL:HG13	1:A:206:ILE:HG23	2.04	0.40
1:A:729:ASP:O	1:A:733:GLN:HB2	2.20	0.40
1:A:730:ALA:O	1:A:734:LEU:HD23	2.22	0.40
1:A:230:SER:C	1:A:232:LYS:N	2.80	0.40
1:A:360:TYR:O	1:A:362:ARG:N	2.54	0.40
1:A:775:VAL:HG23	1:A:776:MET:HG2	2.02	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%)	643 (80%)	131 (16%)	26 (3%)	3	17

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	259	VAL
1	A	280	ASP
1	A	302	LYS
1	A	303	ASP
1	A	319	PHE
1	A	564	ASP
1	A	573	MET
1	A	646	GLU
1	A	649	PRO
1	A	170	ALA
1	A	275	ILE
1	A	361	PHE
1	A	668	GLU

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Mol	Chain	Res	Type
1	A	480	VAL
1	A	518	ILE
1	A	135	SER
1	A	215	ASP
1	A	230	SER
1	A	281	VAL
1	A	567	THR
1	A	754	MET
1	A	81	PRO
1	A	104	GLU
1	A	216	GLU
1	A	677	PHE
1	A	644	PRO

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%)	616 (89%)	73 (11%)	6	23

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	8	MET
1	A	12	THR
1	A	16	LEU
1	A	36	LEU
1	A	57	THR
1	A	58	THR
1	A	70	ARG
1	A	102	THR
1	A	104	GLU
1	A	136	ARG
1	A	156	LEU
1	A	165	ARG

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Mol	Chain	Res	Type
1	A	171	ASP
1	A	173	THR
1	A	186	ARG
1	A	189	MET
1	A	209	VAL
1	A	221	LEU
1	A	222	ILE
1	A	233	LEU
1	A	242	ARG
1	A	247	GLU
1	A	252	TYR
1	A	260	GLN
1	A	267	THR
1	A	273	PHE
1	A	283	HIS
1	A	290	ILE
1	A	300	MET
1	A	317	ASP
1	A	325	LYS
1	A	333	LEU
1	A	335	GLN
1	A	346	GLN
1	A	378	GLU
1	A	380	GLU
1	A	445	ILE
1	A	472	GLU
1	A	481	THR
1	A	486	MET
1	A	500	LYS
1	A	507	VAL
1	A	512	ARG
1	A	513	HIS
1	A	526	SER
1	A	548	ARG
1	A	553	ARG
1	A	555	MET
1	A	564	ASP
1	A	579	GLU
1	A	610	ILE
1	A	618	ILE
1	A	625	GLU
1	A	646	GLU

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Mol	Chain	Res	Type
1	A	647	GLU
1	A	660	LEU
1	A	673	LYS
1	A	702	GLN
1	A	705	LYS
1	A	708	MET
1	A	718	ARG
1	A	728	ILE
1	A	734	LEU
1	A	739	HIS
1	A	763	MET
1	A	782	ASN
1	A	783	ASN
1	A	784	LEU
1	A	787	GLU
1	A	794	THR
1	A	797	HIS
1	A	801	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	43	HIS
1	A	93	HIS
1	A	96	ASN
1	A	236	GLN
1	A	277	ASN
1	A	283	HIS
1	A	289	HIS
1	A	292	GLN
1	A	346	GLN
1	A	388	GLN
1	A	395	ASN
1	A	457	GLN
1	A	463	ASN
1	A	464	HIS
1	A	476	GLN
1	A	485	ASN
1	A	513	HIS
1	A	697	ASN
1	A	707	GLN
1	A	747	ASN

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Mol	Chain	Res	Type
1	A	782	ASN
1	A	783	ASN
1	A	797	HIS

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](#)

11 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	908	-	4,4,4	0.36	0	6,6,6	0.06	0
2	SO4	A	903	-	4,4,4	0.37	0	6,6,6	0.09	0
2	SO4	A	909	-	4,4,4	0.35	0	6,6,6	0.16	0
2	SO4	A	905	-	4,4,4	0.39	0	6,6,6	0.13	0
2	SO4	A	901	-	4,4,4	0.38	0	6,6,6	0.09	0
2	SO4	A	904	-	4,4,4	0.34	0	6,6,6	0.07	0
2	SO4	A	910	-	4,4,4	0.32	0	6,6,6	0.09	0
2	SO4	A	902	-	4,4,4	0.24	0	6,6,6	0.15	0
2	SO4	A	907	-	4,4,4	0.31	0	6,6,6	0.16	0
2	SO4	A	911	-	4,4,4	0.35	0	6,6,6	0.09	0
2	SO4	A	906	-	4,4,4	0.41	0	6,6,6	0.14	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.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	908	SO4	1	0
2	A	902	SO4	1	0
2	A	906	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	802/802 (100%)	-0.26	6 (0%) 84 73	58, 100, 146, 179	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	270	GLU	3.0
1	A	490	GLY	2.9
1	A	272	ALA	2.1
1	A	280	ASP	2.1
1	A	55	GLY	2.0
1	A	278	LEU	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	908	5/5	0.59	0.20	180,181,187,187	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	A	907	5/5	0.60	0.22	161,162,166,167	0
2	SO4	A	909	5/5	0.83	0.15	113,117,124,130	1
2	SO4	A	904	5/5	0.84	0.09	118,119,123,123	0
2	SO4	A	910	5/5	0.86	0.11	137,143,146,146	0
2	SO4	A	903	5/5	0.90	0.08	113,114,121,121	0
2	SO4	A	911	5/5	0.90	0.08	129,130,137,138	0
2	SO4	A	906	5/5	0.92	0.10	94,104,110,114	0
2	SO4	A	905	5/5	0.94	0.08	115,118,131,131	0
2	SO4	A	902	5/5	0.95	0.07	85,90,94,99	0
2	SO4	A	901	5/5	0.96	0.05	75,86,89,89	0

6.5 Other polymers [i](#)

There are no such residues in this entry.