



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:47 PM UTC

PDB ID : 2DQ0 / pdb_00002dq0
Title : Crystal structure of seryl-tRNA synthetase from *Pyrococcus horikoshii* complexed with a seryl-adenylate analog
Authors : Itoh, Y.; Sekine, S.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2006-05-18
Resolution : 2.60 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

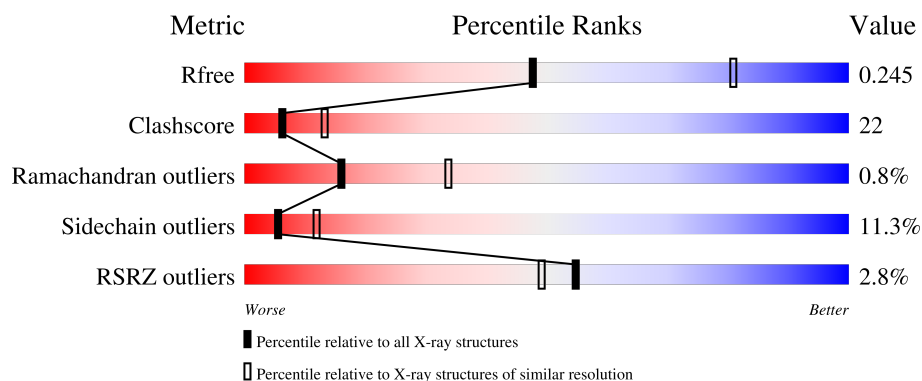
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	455	2% 53% 37% 7% ..
1	B	455	3% 54% 35% 9% .

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7650 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 Seryl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	447	Total	C	N	O	S	0	0	0
			3699	2376	645	670	8			
1	B	447	Total	C	N	O	S	0	0	0
			3699	2376	645	670	8			

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



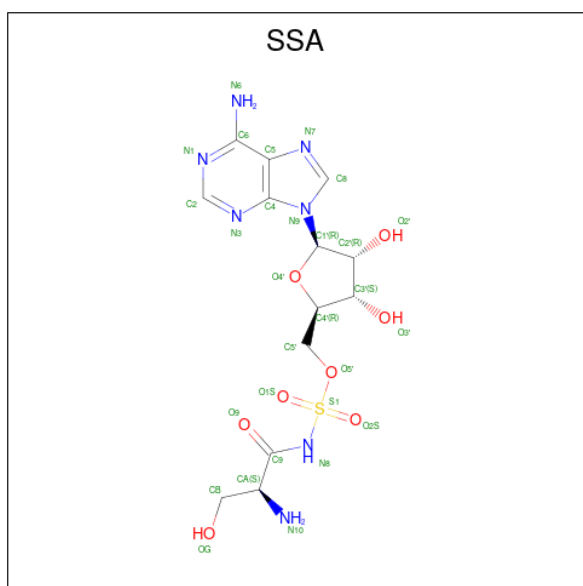
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 3 is 5'-O-(N-(L-SERYL)-SULFAMOYL)ADENOSINE (CCD ID: SSA) (formula: C₁₃H₁₉N₇O₈S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	
			29	13	7	8	1	0
3	B	1	Total	C	N	O	S	
			29	13	7	8	1	0

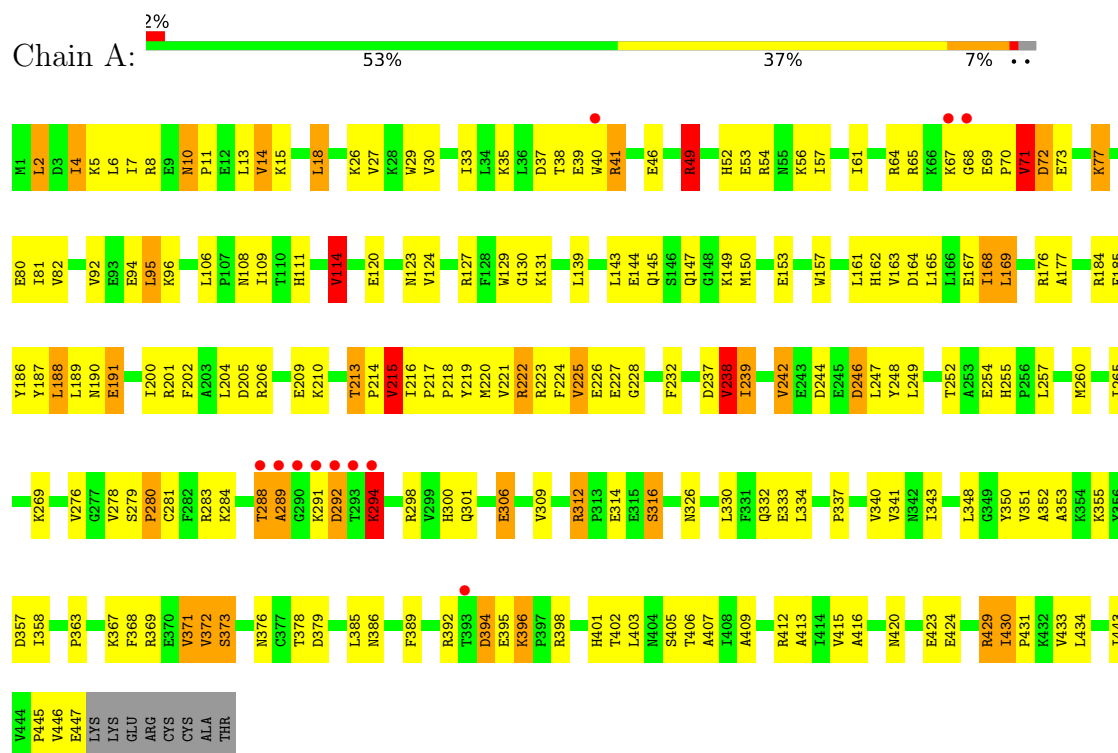
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	76	Total	O	0	0
			76	76		
4	B	83	Total	O	0	0
			83	83		

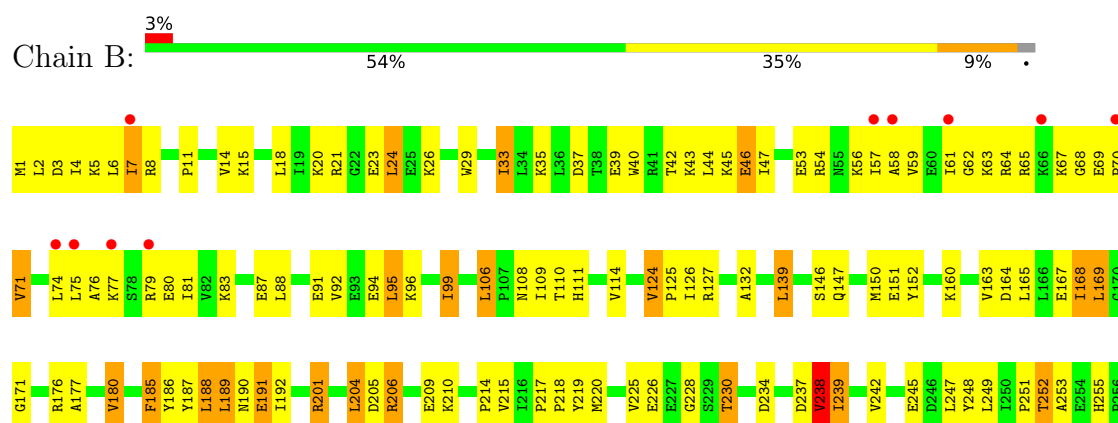
3 Residue-property plots [i](#)

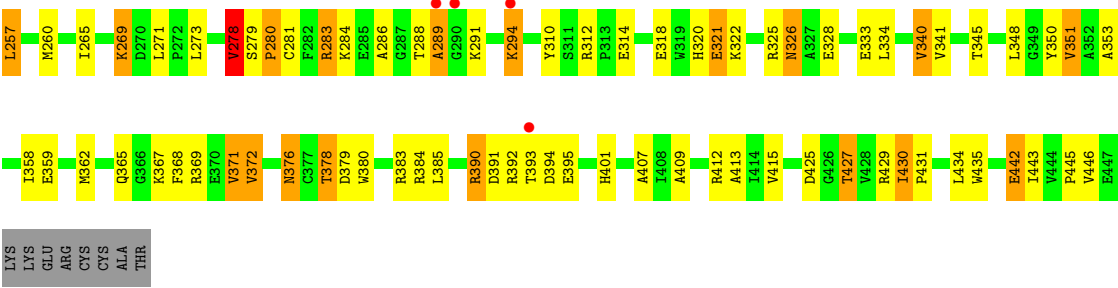
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Seryl-tRNA synthetase



• Molecule 1: Seryl-tRNA synthetase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	96.04Å 120.04Å 126.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.35 – 2.60 48.35 – 2.60	Depositor EDS
% Data completeness (in resolution range)	95.1 (48.35-2.60) 95.1 (48.35-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.46 (at 2.61Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.192 , 0.248 0.191 , 0.245	Depositor DCC
R_{free} test set	2180 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	52.9	Xtriage
Anisotropy	0.364	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 53.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7650	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% 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, SSA

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	0.61	0/3783	1.11	38/5109 (0.7%)
1	B	0.65	0/3783	1.15	30/5109 (0.6%)
All	All	0.63	0/7566	1.13	68/10218 (0.7%)

There are no bond length outliers.

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	124	VAL	N-CA-C	11.79	120.97	107.77
1	A	407	ALA	N-CA-C	-11.53	95.70	111.96
1	B	238	VAL	N-CA-C	10.85	121.23	112.12
1	A	350	TYR	N-CA-C	9.22	121.33	111.28
1	A	239	ILE	N-CA-C	8.69	121.10	108.58
1	A	294	LYS	N-CA-C	8.22	123.04	112.92
1	B	353	ALA	N-CA-C	-8.08	103.56	113.50
1	B	239	ILE	N-CA-C	7.91	120.24	108.54
1	B	280	PRO	N-CA-C	-7.68	99.90	111.57
1	A	348	LEU	N-CA-C	7.37	120.75	111.69
1	B	265	ILE	N-CA-C	-7.32	96.45	106.85
1	A	351	VAL	N-CA-C	7.08	117.87	110.72
1	B	395	GLU	N-CA-C	7.05	119.84	110.53
1	A	187	TYR	N-CA-C	-6.96	97.86	109.07
1	B	407	ALA	N-CA-C	-6.92	96.06	110.80
1	B	348	LEU	N-CA-C	6.87	118.42	111.07
1	B	350	TYR	N-CA-C	6.63	120.58	112.23
1	A	409	ALA	N-CA-C	-6.60	96.91	108.20
1	B	320	HIS	N-CA-C	-6.53	104.08	111.07
1	A	238	VAL	N-CA-C	6.42	117.52	112.12
1	B	409	ALA	N-CA-C	-6.40	97.25	108.20
1	B	294	LYS	N-CA-C	6.40	120.71	112.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	160	LYS	N-CA-C	6.32	118.68	110.53
1	A	280	PRO	N-CA-C	-6.30	101.75	111.13
1	A	124	VAL	N-CA-C	6.28	114.89	107.73
1	A	265	ILE	N-CA-C	-6.28	97.30	107.28
1	B	237	ASP	N-CA-C	6.22	120.07	112.23
1	A	309	VAL	N-CA-C	6.21	117.71	108.46
1	A	237	ASP	N-CA-C	6.07	120.89	112.45
1	A	353	ALA	N-CA-C	-6.07	104.95	112.90
1	A	77	LYS	N-CA-C	-6.00	104.83	111.36
1	A	216	ILE	N-CA-C	-5.98	101.20	107.60
1	A	130	GLY	N-CA-C	5.82	121.42	112.81
1	B	278	VAL	CB-CA-C	-5.82	101.95	110.62
1	A	316	SER	N-CA-C	5.79	117.27	111.07
1	B	20	LYS	N-CA-C	-5.79	104.88	111.07
1	B	376	ASN	N-CA-C	-5.78	98.99	108.41
1	A	367	LYS	N-CA-C	5.75	116.99	108.60
1	B	218	PRO	N-CA-C	-5.74	102.10	111.68
1	A	218	PRO	N-CA-C	-5.63	102.43	111.38
1	A	114	VAL	CA-C-N	5.56	125.51	119.78
1	A	114	VAL	C-N-CA	5.56	125.51	119.78
1	B	286	ALA	N-CA-C	5.51	117.29	111.28
1	B	326	ASN	N-CA-C	-5.51	105.18	111.07
1	A	71	VAL	N-CA-C	5.50	120.79	109.34
1	A	215	VAL	N-CA-C	5.50	115.62	108.35
1	B	341	VAL	N-CA-C	5.49	116.39	108.48
1	A	312	ARG	N-CA-C	-5.49	103.13	109.93
1	A	413	ALA	N-CA-C	-5.42	105.45	111.36
1	B	185	PHE	N-CA-C	-5.41	101.19	109.41
1	A	185	PHE	N-CA-C	-5.37	101.59	109.81
1	B	189	LEU	N-CA-C	5.36	117.82	109.52
1	B	413	ALA	N-CA-C	-5.34	105.63	111.82
1	A	49	ARG	N-CA-C	-5.33	105.47	111.28
1	B	362	MET	CA-C-N	5.23	124.68	119.24
1	B	362	MET	C-N-CA	5.23	124.68	119.24
1	A	246	ASP	N-CA-C	-5.22	102.34	109.71
1	A	244	ASP	N-CA-C	5.21	118.77	111.90
1	B	126	ILE	CB-CA-C	-5.20	105.21	110.93
1	A	279	SER	CA-C-N	-5.17	115.40	120.52
1	A	279	SER	C-N-CA	-5.17	115.40	120.52
1	A	306	GLU	N-CA-C	5.16	117.81	109.40
1	B	152	TYR	N-CA-C	5.15	115.33	108.38
1	B	367	LYS	N-CA-C	5.13	115.94	108.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	189	LEU	N-CA-C	5.12	117.46	109.52
1	A	429	ARG	CA-C-N	-5.12	118.33	123.04
1	A	429	ARG	C-N-CA	-5.12	118.33	123.04
1	A	352	ALA	N-CA-C	5.02	117.92	110.48

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	3699	0	3737	173	0
1	B	3699	0	3737	172	0
2	A	20	0	0	0	0
2	B	15	0	0	0	0
3	A	29	0	19	2	0
3	B	29	0	19	2	0
4	A	76	0	0	2	0
4	B	83	0	0	5	0
All	All	7650	0	7512	334	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 22.

All (334) 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:378:THR:HG22	1:A:379:ASP:H	0.95	1.08
1:B:378:THR:CG2	1:B:379:ASP:H	1.68	1.07
1:B:61:ILE:HD12	1:B:74:LEU:HD22	1.37	1.06
1:B:358:ILE:HB	1:B:372:VAL:HG13	1.36	1.04
1:A:378:THR:HG22	1:A:379:ASP:N	1.77	0.97
1:B:321:GLU:HG3	1:B:325:ARG:HH21	1.28	0.95
1:A:378:THR:CG2	1:A:379:ASP:H	1.80	0.95
1:B:1:MET:H1	1:B:384:ARG:HH21	1.09	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:ILE:HB	1:A:372:VAL:HG13	1.49	0.93
1:A:67:LYS:HG2	1:A:68:GLY:H	1.33	0.89
1:A:8:ARG:HD3	1:A:37:ASP:OD2	1.73	0.88
1:B:378:THR:HG23	1:B:379:ASP:H	1.35	0.87
1:B:242:VAL:HG11	1:B:247:LEU:HB2	1.55	0.86
1:B:64:ARG:HB3	1:B:69:GLU:HA	1.57	0.85
1:A:294:LYS:H	1:A:294:LYS:HD2	1.41	0.85
1:A:430:ILE:CD1	1:A:434:LEU:HB2	2.08	0.83
1:A:343:ILE:HD12	1:A:355:LYS:HG2	1.60	0.82
1:B:378:THR:CG2	1:B:379:ASP:N	2.39	0.82
1:A:64:ARG:HB3	1:A:69:GLU:HA	1.60	0.82
1:B:110:THR:HB	1:B:114:VAL:HG21	1.60	0.81
1:B:242:VAL:CG1	1:B:247:LEU:HB2	2.10	0.80
1:B:87:GLU:O	1:B:91:GLU:HG3	1.81	0.80
1:A:430:ILE:HD11	1:A:434:LEU:HB2	1.64	0.80
1:B:43:LYS:O	1:B:47:ILE:HG12	1.82	0.79
1:B:7:ILE:HG12	1:B:33:ILE:HD11	1.66	0.78
1:A:52:HIS:NE2	1:A:56:LYS:HE3	1.99	0.78
1:A:238:VAL:HG22	1:A:239:ILE:HG13	1.65	0.78
1:B:378:THR:HG22	1:B:379:ASP:H	1.46	0.77
1:B:425:ASP:OD2	1:B:427:THR:HG23	1.85	0.77
1:B:365:GLN:HE22	1:B:369:ARG:HH21	1.34	0.76
1:A:225:VAL:HG11	1:B:180:VAL:HG22	1.68	0.76
1:B:47:ILE:HD11	1:B:88:LEU:HB3	1.68	0.75
1:A:2:LEU:HD23	1:A:106:LEU:HB2	1.67	0.74
1:A:222:ARG:HG3	1:A:246:ASP:OD1	1.87	0.74
1:A:372:VAL:HB	1:A:406:THR:HB	1.68	0.74
1:B:127:ARG:HB3	1:B:340:VAL:HG13	1.69	0.73
1:A:168:ILE:HD12	1:A:445:PRO:HB3	1.70	0.73
1:B:226:GLU:OE1	1:B:255:HIS:HD2	1.72	0.73
1:B:29:TRP:O	1:B:33:ILE:HG23	1.87	0.73
1:B:228:GLY:HA3	1:B:385:LEU:HD21	1.71	0.73
1:A:131:LYS:HE2	1:A:153:GLU:HB2	1.68	0.72
1:B:288:THR:HG21	1:B:291:LYS:HD2	1.71	0.72
1:A:210:LYS:HZ2	1:A:326:ASN:ND2	1.87	0.72
1:A:210:LYS:NZ	1:A:326:ASN:ND2	2.38	0.72
1:A:184:ARG:HH22	1:A:288:THR:HG23	1.53	0.71
1:A:40:TRP:HE1	1:A:96:LYS:HE3	1.54	0.71
1:A:343:ILE:HD11	1:A:357:ASP:CG	2.16	0.71
1:B:61:ILE:CD1	1:B:74:LEU:HD22	2.18	0.70
1:B:191:GLU:HG3	1:B:443:ILE:HG23	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:430:ILE:HD11	1:B:435:TRP:HD1	1.56	0.70
1:B:125:PRO:HG2	1:B:147:GLN:HE21	1.57	0.69
1:B:40:TRP:HE1	1:B:96:LYS:HE3	1.58	0.68
1:B:378:THR:HG22	1:B:379:ASP:N	2.06	0.68
1:A:191:GLU:HG3	1:A:443:ILE:HG23	1.75	0.68
1:B:40:TRP:HE1	1:B:96:LYS:CE	2.06	0.68
1:A:111:HIS:O	1:A:114:VAL:HG13	1.94	0.68
1:B:242:VAL:HG12	1:B:247:LEU:O	1.94	0.67
1:B:53:GLU:O	1:B:57:ILE:HG12	1.96	0.66
1:B:76:ALA:O	1:B:80:GLU:HG2	1.96	0.66
1:A:29:TRP:O	1:A:33:ILE:HG23	1.96	0.66
1:B:206:ARG:NH2	1:B:333:GLU:OE2	2.28	0.66
1:A:220:MET:HG2	1:A:249:LEU:HD23	1.78	0.65
1:B:205:ASP:O	1:B:209:GLU:HG3	1.97	0.65
1:A:123:ASN:HB3	1:A:341:VAL:HG11	1.78	0.65
1:B:321:GLU:CG	1:B:325:ARG:HH21	2.06	0.64
1:A:157:TRP:H	1:A:157:TRP:CD1	2.12	0.64
1:A:396:LYS:NZ	1:A:396:LYS:HA	2.12	0.64
1:B:318:GLU:O	1:B:322:LYS:HG3	1.96	0.64
1:A:4:ILE:O	1:A:7:ILE:HG13	1.98	0.64
1:A:37:ASP:O	1:A:41:ARG:HG2	1.98	0.64
1:A:228:GLY:HA3	1:A:385:LEU:HD21	1.78	0.64
1:A:190:ASN:HA	1:B:214:PRO:HG2	1.78	0.64
1:B:312:ARG:HH22	1:B:391:ASP:CG	2.06	0.63
1:A:2:LEU:HD23	1:A:106:LEU:CB	2.28	0.63
1:A:4:ILE:O	1:A:4:ILE:HD13	1.99	0.63
1:A:333:GLU:HB3	1:A:433:VAL:HG21	1.81	0.62
1:B:321:GLU:HG3	1:B:325:ARG:NH2	2.10	0.62
1:B:430:ILE:HD12	1:B:431:PRO:O	1.99	0.62
1:A:64:ARG:HH11	1:A:70:PRO:HD2	1.62	0.62
1:A:371:VAL:HG13	1:A:372:VAL:HG12	1.81	0.62
1:B:371:VAL:CG1	1:B:372:VAL:HG12	2.28	0.62
1:B:230:THR:HG21	1:B:234:ASP:OD2	1.99	0.62
1:B:273:LEU:HB2	1:B:310:TYR:HB2	1.81	0.62
1:A:162:HIS:CD2	1:A:415:VAL:HG12	2.35	0.62
1:A:26:LYS:HE2	1:A:29:TRP:CH2	2.35	0.62
1:A:226:GLU:OE1	1:A:255:HIS:HD2	1.83	0.61
1:A:446:VAL:O	1:A:447:GLU:HG3	2.01	0.61
1:B:69:GLU:N	1:B:70:PRO:HD3	2.16	0.61
1:B:164:ASP:O	1:B:168:ILE:HG23	2.01	0.60
1:A:260:MET:HE3	1:B:187:TYR:CD2	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:GLU:OE2	1:A:429:ARG:HD2	2.01	0.60
1:B:8:ARG:HD3	1:B:37:ASP:OD2	2.01	0.60
1:B:226:GLU:OE1	1:B:255:HIS:CD2	2.54	0.60
1:A:65:ARG:HA	1:A:69:GLU:CD	2.26	0.60
1:A:18:LEU:HD23	1:A:27:VAL:HA	1.84	0.59
1:A:40:TRP:CD1	1:A:92:VAL:HG13	2.37	0.59
1:B:1:MET:HE2	1:B:383:ARG:HB3	1.84	0.59
1:A:123:ASN:HB3	1:A:341:VAL:CG1	2.32	0.59
1:B:69:GLU:C	1:B:71:VAL:H	2.09	0.59
1:A:67:LYS:HG2	1:A:68:GLY:N	2.11	0.59
1:B:378:THR:HG23	1:B:379:ASP:N	2.11	0.59
1:A:294:LYS:H	1:A:294:LYS:CD	2.07	0.59
1:B:92:VAL:CG1	1:B:96:LYS:HE3	2.32	0.59
1:B:378:THR:O	1:B:401:HIS:HA	2.02	0.59
1:B:11:PRO:O	1:B:15:LYS:HG2	2.02	0.58
1:B:294:LYS:HE3	4:B:2089:HOH:O	2.02	0.58
1:B:238:VAL:HG22	1:B:239:ILE:HG13	1.85	0.58
1:B:67:LYS:HG2	1:B:68:GLY:H	1.69	0.58
1:A:49:ARG:HG3	1:A:49:ARG:HH11	1.68	0.58
1:A:225:VAL:HG11	1:B:180:VAL:CG2	2.32	0.58
1:A:7:ILE:HD12	1:A:7:ILE:C	2.29	0.58
1:A:288:THR:HG21	1:A:298:ARG:HD3	1.87	0.57
1:A:184:ARG:HH22	1:A:288:THR:CG2	2.16	0.57
1:B:186:TYR:CD2	1:B:188:LEU:HD13	2.40	0.57
1:B:358:ILE:HB	1:B:372:VAL:CG1	2.23	0.57
1:B:376:ASN:ND2	1:B:378:THR:H	2.03	0.57
1:B:132:ALA:HB2	1:B:150:MET:HE2	1.85	0.56
1:A:169:LEU:HG	1:A:443:ILE:HG22	1.86	0.56
1:B:390:ARG:HD3	1:B:393:THR:HA	1.86	0.56
1:A:260:MET:O	1:B:176:ARG:HD3	2.04	0.56
1:B:4:ILE:HD12	1:B:99:ILE:HD12	1.87	0.56
1:B:95:LEU:O	1:B:99:ILE:HG23	2.06	0.56
1:B:127:ARG:NH2	1:B:328:GLU:OE2	2.37	0.56
1:A:176:ARG:HD3	1:B:260:MET:O	2.05	0.56
1:B:68:GLY:C	1:B:70:PRO:HD3	2.30	0.56
1:B:79:ARG:HH12	1:B:83:LYS:HD3	1.70	0.56
1:B:358:ILE:HD12	1:B:372:VAL:HG11	1.88	0.55
1:A:39:GLU:HG2	1:A:95:LEU:HD21	1.88	0.55
1:A:220:MET:HE3	1:B:185:PHE:HZ	1.70	0.55
1:A:376:ASN:HA	1:A:403:LEU:HG	1.87	0.55
1:A:127:ARG:HH11	1:A:127:ARG:HB2	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:288:THR:CG2	1:B:291:LYS:HD2	2.36	0.55
1:A:65:ARG:HA	1:A:69:GLU:OE2	2.07	0.55
1:B:65:ARG:O	1:B:65:ARG:HD3	2.06	0.55
1:A:249:LEU:HD21	1:B:249:LEU:HD11	1.88	0.55
1:A:222:ARG:HG3	1:A:246:ASP:CG	2.33	0.54
1:A:54:ARG:HG2	1:A:54:ARG:HH11	1.73	0.54
1:B:321:GLU:OE2	1:B:325:ARG:NH2	2.40	0.54
1:A:120:GLU:CD	1:A:120:GLU:H	2.15	0.54
1:A:161:LEU:HD13	1:A:294:LYS:NZ	2.23	0.54
1:B:242:VAL:HG13	1:B:245:GLU:HB2	1.88	0.54
1:B:371:VAL:HG12	1:B:372:VAL:HG12	1.90	0.54
1:B:40:TRP:HE1	1:B:96:LYS:CG	2.21	0.54
1:B:239:ILE:O	1:B:284:LYS:HE3	2.08	0.54
1:B:40:TRP:NE1	1:B:96:LYS:CG	2.71	0.54
1:B:392:ARG:HG2	1:B:392:ARG:HH11	1.73	0.54
1:B:368:PHE:O	1:B:369:ARG:HD2	2.08	0.53
1:A:412:ARG:O	1:A:415:VAL:HG22	2.08	0.53
1:A:108:ASN:HD22	1:A:109:ILE:H	1.55	0.53
1:B:7:ILE:C	1:B:7:ILE:HD12	2.34	0.53
1:A:191:GLU:HG3	1:A:443:ILE:CG2	2.39	0.53
1:B:54:ARG:HB2	1:B:81:ILE:HG21	1.90	0.53
1:B:371:VAL:HG13	1:B:372:VAL:HG12	1.90	0.53
1:A:5:LYS:HD2	1:A:8:ARG:HH11	1.74	0.52
1:A:157:TRP:CE2	1:A:424:GLU:HG2	2.44	0.52
1:A:13:LEU:C	1:A:13:LEU:HD13	2.34	0.52
1:A:69:GLU:N	1:A:70:PRO:HD3	2.23	0.52
1:B:427:THR:HG22	1:B:445:PRO:HD3	1.92	0.52
1:A:71:VAL:O	1:A:73:GLU:N	2.43	0.52
1:B:47:ILE:CD1	1:B:88:LEU:HB3	2.36	0.52
1:B:114:VAL:HG23	1:B:114:VAL:O	2.09	0.52
1:B:64:ARG:O	1:B:69:GLU:HB2	2.10	0.52
1:B:351:VAL:HB	1:B:380:TRP:CE3	2.44	0.52
1:A:64:ARG:O	1:A:69:GLU:HB2	2.10	0.52
1:A:168:ILE:CD1	1:A:445:PRO:HB3	2.40	0.52
1:A:412:ARG:HD2	3:A:1001:SSA:H2'	1.91	0.52
1:A:61:ILE:HG23	1:A:71:VAL:HG11	1.92	0.51
1:A:392:ARG:C	1:A:394:ASP:N	2.68	0.51
1:A:215:VAL:HB	1:B:189:LEU:HD23	1.91	0.51
1:A:157:TRP:CD2	1:A:424:GLU:HG2	2.45	0.51
1:B:24:LEU:H	1:B:24:LEU:HD22	1.74	0.51
1:A:186:TYR:CD2	1:A:188:LEU:HD13	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:GLU:OE1	3:A:1001:SSA:N10	2.44	0.51
1:B:43:LYS:HE2	1:B:91:GLU:CD	2.35	0.51
1:B:283:ARG:NH2	3:B:1002:SSA:O1S	2.43	0.51
1:A:226:GLU:OE1	1:A:255:HIS:CD2	2.63	0.51
1:B:390:ARG:HG3	1:B:392:ARG:O	2.10	0.51
1:A:15:LYS:HE2	1:A:30:VAL:HB	1.93	0.51
1:A:52:HIS:CD2	1:A:56:LYS:HE3	2.46	0.51
1:B:57:ILE:O	1:B:74:LEU:HD21	2.11	0.51
1:A:378:THR:CG2	1:A:379:ASP:N	2.50	0.50
1:B:23:GLU:HG3	1:B:26:LYS:HG2	1.93	0.50
1:B:65:ARG:HD3	1:B:65:ARG:C	2.35	0.50
1:B:5:LYS:NZ	4:B:2036:HOH:O	2.44	0.50
1:B:429:ARG:HG2	1:B:429:ARG:HH21	1.76	0.50
1:A:40:TRP:HE1	1:A:96:LYS:CE	2.23	0.50
1:A:210:LYS:NZ	1:A:326:ASN:HD22	2.07	0.50
1:A:392:ARG:C	1:A:394:ASP:H	2.18	0.50
1:A:169:LEU:HG	1:A:443:ILE:CG2	2.42	0.49
1:B:429:ARG:HA	1:B:442:GLU:HB2	1.94	0.49
1:A:65:ARG:O	1:A:65:ARG:HD3	2.12	0.49
1:A:177:ALA:CB	1:A:186:TYR:HA	2.42	0.49
1:A:127:ARG:NH1	4:A:2038:HOH:O	2.45	0.49
1:A:396:LYS:HA	1:A:396:LYS:HZ2	1.76	0.49
1:B:110:THR:CB	1:B:114:VAL:HG21	2.37	0.49
1:B:111:HIS:O	1:B:114:VAL:HG22	2.13	0.49
1:B:278:VAL:O	1:B:279:SER:HB3	2.12	0.49
1:A:386:ASN:C	1:A:386:ASN:HD22	2.20	0.49
1:B:269:LYS:HE2	1:B:269:LYS:N	2.28	0.48
1:A:206:ARG:HH21	1:A:333:GLU:CD	2.22	0.48
1:A:222:ARG:CG	1:A:246:ASP:OD1	2.58	0.48
1:B:58:ALA:O	1:B:61:ILE:HG22	2.13	0.48
1:B:392:ARG:C	1:B:394:ASP:H	2.21	0.47
1:A:57:ILE:HD12	1:A:81:ILE:CD1	2.44	0.47
1:A:163:VAL:HG21	1:A:294:LYS:HD2	1.96	0.47
1:A:373:SER:O	1:A:405:SER:HA	2.14	0.47
1:B:359:GLU:HB3	1:B:368:PHE:HB3	1.94	0.47
1:A:227:GLU:HB2	1:A:232:PHE:CE1	2.50	0.47
1:A:64:ARG:HD3	1:A:70:PRO:HD2	1.95	0.47
1:A:165:LEU:O	1:A:169:LEU:HB2	2.14	0.47
1:B:139:LEU:O	1:B:139:LEU:HD22	2.14	0.47
1:A:412:ARG:HA	1:A:415:VAL:HG22	1.96	0.47
1:B:251:PRO:O	1:B:283:ARG:NH1	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:LEU:HD21	1:B:278:VAL:HG21	1.97	0.47
1:B:201:ARG:HD2	1:B:201:ARG:HA	1.74	0.47
1:B:29:TRP:CE3	1:B:106:LEU:HD13	2.51	0.46
1:B:92:VAL:HG12	1:B:96:LYS:HE3	1.97	0.46
1:A:213:THR:HG22	1:B:190:ASN:HD21	1.79	0.46
1:A:220:MET:HE3	1:B:185:PHE:CZ	2.48	0.46
1:A:224:PHE:HA	1:A:227:GLU:HG2	1.98	0.46
1:A:205:ASP:O	1:A:209:GLU:HG3	2.16	0.46
1:B:29:TRP:HE3	1:B:106:LEU:HD13	1.79	0.46
1:B:171:GLY:HA3	1:B:192:ILE:CG1	2.45	0.46
1:B:238:VAL:CG2	1:B:239:ILE:HG13	2.46	0.46
1:A:389:PHE:HD1	1:A:398:ARG:O	1.99	0.46
1:A:164:ASP:O	1:A:168:ILE:HG23	2.15	0.46
1:A:40:TRP:HD1	1:A:92:VAL:HG13	1.79	0.46
1:A:372:VAL:HG23	1:A:373:SER:N	2.32	0.46
1:B:125:PRO:HG2	1:B:147:GLN:NE2	2.27	0.46
1:A:389:PHE:CD1	1:A:398:ARG:O	2.68	0.45
1:A:363:PRO:HG2	1:A:420:ASN:HA	1.98	0.45
1:A:41:ARG:HB3	1:A:41:ARG:CZ	2.45	0.45
1:A:242:VAL:HG13	1:A:247:LEU:O	2.17	0.45
1:A:415:VAL:HG23	1:A:416:ALA:N	2.31	0.45
1:B:206:ARG:HH21	1:B:333:GLU:CD	2.24	0.45
1:A:219:TYR:CE2	1:A:280:PRO:HD2	2.52	0.45
1:B:61:ILE:HD12	1:B:74:LEU:CD2	2.26	0.45
1:B:392:ARG:C	1:B:394:ASP:N	2.74	0.45
1:B:39:GLU:HG2	1:B:95:LEU:HD21	1.97	0.45
1:B:40:TRP:NE1	1:B:96:LYS:HG2	2.32	0.45
1:B:191:GLU:HG3	1:B:443:ILE:CG2	2.45	0.45
1:A:394:ASP:O	1:A:395:GLU:HB3	2.17	0.45
1:A:386:ASN:C	1:A:386:ASN:ND2	2.74	0.45
1:B:430:ILE:CD1	1:B:434:LEU:HB2	2.47	0.45
1:A:446:VAL:C	1:A:447:GLU:HG3	2.41	0.45
1:B:228:GLY:HA3	1:B:385:LEU:CD2	2.42	0.45
1:B:288:THR:O	1:B:289:ALA:HB2	2.17	0.45
1:B:110:THR:HB	1:B:114:VAL:CG2	2.40	0.44
1:B:257:LEU:HD12	1:B:257:LEU:HA	1.83	0.44
1:A:392:ARG:HG3	1:A:394:ASP:H	1.82	0.44
1:B:61:ILE:HB	1:B:74:LEU:CD2	2.47	0.44
1:B:69:GLU:C	1:B:71:VAL:N	2.75	0.44
1:A:200:ILE:O	1:A:204:LEU:HB2	2.17	0.44
1:A:147:GLN:O	1:A:149:LYS:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:ILE:HD12	1:A:372:VAL:HG11	2.00	0.44
1:B:252:THR:HA	1:B:281:CYS:SG	2.57	0.44
1:A:276:VAL:HA	1:A:306:GLU:O	2.17	0.44
1:A:288:THR:OG1	1:A:291:LYS:HG3	2.17	0.44
1:B:312:ARG:NH2	1:B:391:ASP:OD1	2.51	0.44
1:A:288:THR:OG1	1:A:289:ALA:N	2.51	0.44
1:B:230:THR:HG23	4:B:2039:HOH:O	2.17	0.44
1:A:11:PRO:HA	1:A:14:VAL:CG1	2.48	0.44
1:A:139:LEU:HD13	1:A:143:LEU:HD12	1.98	0.44
1:A:157:TRP:CD1	1:A:424:GLU:HG2	2.53	0.44
1:A:157:TRP:CG	1:A:424:GLU:HG2	2.53	0.44
1:A:314:GLU:CD	1:A:314:GLU:H	2.26	0.44
1:B:108:ASN:HD22	1:B:109:ILE:H	1.66	0.44
1:B:146:SER:O	1:B:147:GLN:HB2	2.16	0.44
1:B:171:GLY:HA3	1:B:192:ILE:HG13	2.00	0.43
1:A:368:PHE:O	1:A:369:ARG:HD2	2.18	0.43
1:A:57:ILE:HD12	1:A:81:ILE:HD12	2.01	0.43
1:B:4:ILE:O	1:B:8:ARG:HG3	2.19	0.43
1:A:201:ARG:HD2	1:A:201:ARG:HA	1.89	0.43
1:B:427:THR:HG22	1:B:445:PRO:CD	2.48	0.43
1:A:150:MET:CE	1:A:337:PRO:HB2	2.49	0.43
1:B:294:LYS:CE	4:B:2089:HOH:O	2.65	0.43
1:A:223:ARG:HB2	1:A:248:TYR:CE1	2.54	0.43
1:A:269:LYS:HD2	1:A:269:LYS:HA	1.85	0.43
1:A:312:ARG:HB3	1:A:314:GLU:OE2	2.19	0.43
1:B:124:VAL:HA	1:B:125:PRO:HD2	1.95	0.43
1:A:61:ILE:HG23	1:A:71:VAL:CG1	2.49	0.42
1:A:294:LYS:HD2	1:A:294:LYS:N	2.18	0.42
1:B:177:ALA:CB	1:B:186:TYR:HA	2.48	0.42
1:A:281:CYS:O	1:A:301:GLN:HA	2.19	0.42
1:B:253:ALA:O	1:B:257:LEU:HB2	2.19	0.42
1:A:210:LYS:HZ3	1:A:326:ASN:ND2	2.15	0.42
1:A:77:LYS:HA	1:A:80:GLU:HG2	2.01	0.42
1:A:129:TRP:CD2	1:A:332:GLN:HG2	2.54	0.42
1:B:40:TRP:NE1	1:B:96:LYS:HG3	2.35	0.42
1:A:145:GLN:HG3	4:A:2012:HOH:O	2.20	0.42
1:B:21:ARG:HA	1:B:345:THR:HB	2.02	0.42
1:B:220:MET:HA	1:B:248:TYR:O	2.19	0.42
1:A:378:THR:O	1:A:401:HIS:HA	2.20	0.42
1:A:4:ILE:CD1	1:A:8:ARG:HG3	2.50	0.42
1:B:79:ARG:NH1	1:B:80:GLU:OE1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:THR:C	1:A:403:LEU:HD12	2.45	0.41
1:A:11:PRO:O	1:A:14:VAL:HG13	2.20	0.41
1:A:316:SER:HB2	1:A:403:LEU:HD11	2.02	0.41
1:B:191:GLU:CD	1:B:191:GLU:H	2.26	0.41
1:B:314:GLU:H	1:B:314:GLU:CD	2.28	0.41
1:B:429:ARG:HG2	1:B:429:ARG:NH2	2.35	0.41
1:A:430:ILE:HA	1:A:431:PRO:HD3	1.90	0.41
1:B:15:LYS:HA	1:B:18:LEU:HD12	2.02	0.41
1:A:94:GLU:HG3	1:A:95:LEU:N	2.35	0.41
1:A:214:PRO:HA	1:A:276:VAL:HG13	2.02	0.41
1:B:3:ASP:O	1:B:6:LEU:HB3	2.20	0.41
1:B:56:LYS:O	1:B:59:VAL:HG12	2.21	0.41
1:B:219:TYR:CZ	1:B:280:PRO:HD2	2.56	0.41
1:A:29:TRP:HE3	1:A:106:LEU:HD21	1.85	0.41
1:B:62:GLY:O	1:B:65:ARG:HB3	2.19	0.41
1:B:210:LYS:HD3	1:B:326:ASN:ND2	2.36	0.41
1:A:6:LEU:HD22	1:A:6:LEU:O	2.21	0.41
1:B:63:LYS:HE3	1:B:63:LYS:HB3	1.80	0.41
1:B:58:ALA:C	1:B:61:ILE:HG22	2.45	0.41
1:B:412:ARG:HD2	3:B:1002:SSA:H2'	2.03	0.41
1:A:10:ASN:OD1	1:A:13:LEU:HB2	2.21	0.41
1:A:202:PHE:CE2	1:A:330:LEU:HD22	2.56	0.41
1:A:222:ARG:O	1:A:225:VAL:HG13	2.20	0.41
1:A:396:LYS:HD3	1:A:396:LYS:C	2.45	0.41
1:B:165:LEU:O	1:B:169:LEU:HD22	2.21	0.41
1:B:430:ILE:HD11	1:B:435:TRP:CD1	2.43	0.41
1:A:11:PRO:O	1:A:15:LYS:HG3	2.21	0.41
1:A:71:VAL:O	1:A:72:ASP:C	2.64	0.41
1:A:108:ASN:HD22	1:A:109:ILE:N	2.17	0.41
1:B:83:LYS:O	1:B:87:GLU:HG2	2.21	0.41
1:B:365:GLN:HE21	1:B:365:GLN:HB3	1.65	0.40
1:B:46:GLU:HB3	1:B:88:LEU:HD13	2.03	0.40
1:B:79:ARG:NE	4:B:2026:HOH:O	2.54	0.40
1:B:168:ILE:O	1:B:446:VAL:HG22	2.21	0.40
1:A:191:GLU:CD	1:A:191:GLU:H	2.29	0.40
1:A:221:VAL:HG21	1:A:225:VAL:HG22	2.03	0.40
1:A:284:LYS:O	1:A:300:HIS:HE1	2.04	0.40
1:A:161:LEU:HD23	1:A:161:LEU:HA	1.95	0.40
1:B:42:THR:O	1:B:45:LYS:HB3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	445/455 (98%)	416 (94%)	24 (5%)	5 (1%)	11	25
1	B	445/455 (98%)	423 (95%)	20 (4%)	2 (0%)	30	51
All	All	890/910 (98%)	839 (94%)	44 (5%)	7 (1%)	16	34

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	71	VAL
1	A	72	ASP
1	B	289	ALA
1	A	289	ALA
1	A	394	ASP
1	B	71	VAL
1	A	292	ASP

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	398/405 (98%)	357 (90%)	41 (10%)	7	15
1	B	398/405 (98%)	349 (88%)	49 (12%)	4	9
All	All	796/810 (98%)	706 (89%)	90 (11%)	5	12

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	4	ILE
1	A	10	ASN
1	A	14	VAL
1	A	18	LEU
1	A	35	LYS
1	A	38	THR
1	A	41	ARG
1	A	46	GLU
1	A	49	ARG
1	A	53	GLU
1	A	82	VAL
1	A	95	LEU
1	A	114	VAL
1	A	144	GLU
1	A	167	GLU
1	A	168	ILE
1	A	169	LEU
1	A	188	LEU
1	A	191	GLU
1	A	213	THR
1	A	215	VAL
1	A	217	PRO
1	A	222	ARG
1	A	225	VAL
1	A	238	VAL
1	A	242	VAL
1	A	252	THR
1	A	257	LEU
1	A	278	VAL
1	A	283	ARG
1	A	288	THR
1	A	292	ASP
1	A	294	LYS
1	A	334	LEU
1	A	340	VAL
1	A	371	VAL
1	A	372	VAL
1	A	373	SER
1	A	396	LYS
1	A	430	ILE
1	B	2	LEU
1	B	7	ILE

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Mol	Chain	Res	Type
1	B	14	VAL
1	B	24	LEU
1	B	33	ILE
1	B	35	LYS
1	B	44	LEU
1	B	46	GLU
1	B	75	LEU
1	B	77	LYS
1	B	94	GLU
1	B	95	LEU
1	B	99	ILE
1	B	106	LEU
1	B	139	LEU
1	B	151	GLU
1	B	163	VAL
1	B	167	GLU
1	B	168	ILE
1	B	169	LEU
1	B	180	VAL
1	B	188	LEU
1	B	191	GLU
1	B	201	ARG
1	B	204	LEU
1	B	206	ARG
1	B	215	VAL
1	B	217	PRO
1	B	225	VAL
1	B	230	THR
1	B	238	VAL
1	B	252	THR
1	B	257	LEU
1	B	269	LYS
1	B	271	LEU
1	B	278	VAL
1	B	283	ARG
1	B	321	GLU
1	B	334	LEU
1	B	340	VAL
1	B	351	VAL
1	B	371	VAL
1	B	372	VAL
1	B	378	THR

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Mol	Chain	Res	Type
1	B	390	ARG
1	B	415	VAL
1	B	427	THR
1	B	430	ILE
1	B	442	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	10	ASN
1	A	108	ASN
1	A	190	ASN
1	A	255	HIS
1	A	263	ASN
1	A	307	GLN
1	A	326	ASN
1	A	332	GLN
1	A	386	ASN
1	B	90	ASN
1	B	108	ASN
1	B	145	GLN
1	B	147	GLN
1	B	190	ASN
1	B	255	HIS
1	B	263	ASN
1	B	307	GLN
1	B	326	ASN
1	B	332	GLN
1	B	365	GLN
1	B	376	ASN
1	B	386	ASN
1	B	420	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](#)

9 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	2005	-	4,4,4	0.45	0	6,6,6	0.12	0
2	SO4	A	2003	-	4,4,4	0.38	0	6,6,6	0.17	0
2	SO4	A	2007	-	4,4,4	0.42	0	6,6,6	0.08	0
2	SO4	B	2006	-	4,4,4	0.40	0	6,6,6	0.14	0
2	SO4	B	2004	-	4,4,4	0.36	0	6,6,6	0.15	0
2	SO4	B	2002	-	4,4,4	0.37	0	6,6,6	0.15	0
3	SSA	A	1001	-	30,31,31	1.28	2 (6%)	41,46,46	0.78	1 (2%)
2	SO4	A	2001	-	4,4,4	0.34	0	6,6,6	0.09	0
3	SSA	B	1002	-	30,31,31	1.15	2 (6%)	41,46,46	0.81	1 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SSA	B	1002	-	-	1/20/37/37	0/3/3/3
3	SSA	A	1001	-	-	0/20/37/37	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	SSA	O2S-S1	4.35	1.46	1.42
3	B	1002	SSA	O1S-S1	4.11	1.46	1.42
3	A	1001	SSA	O1S-S1	4.10	1.46	1.42
3	B	1002	SSA	O2S-S1	3.94	1.45	1.42

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1002	SSA	O5'-C5'-C4'	2.75	112.47	107.57
3	A	1001	SSA	O5'-C5'-C4'	2.40	111.84	107.57

There are no chirality outliers.

All (1) torsion outliers are listed below:

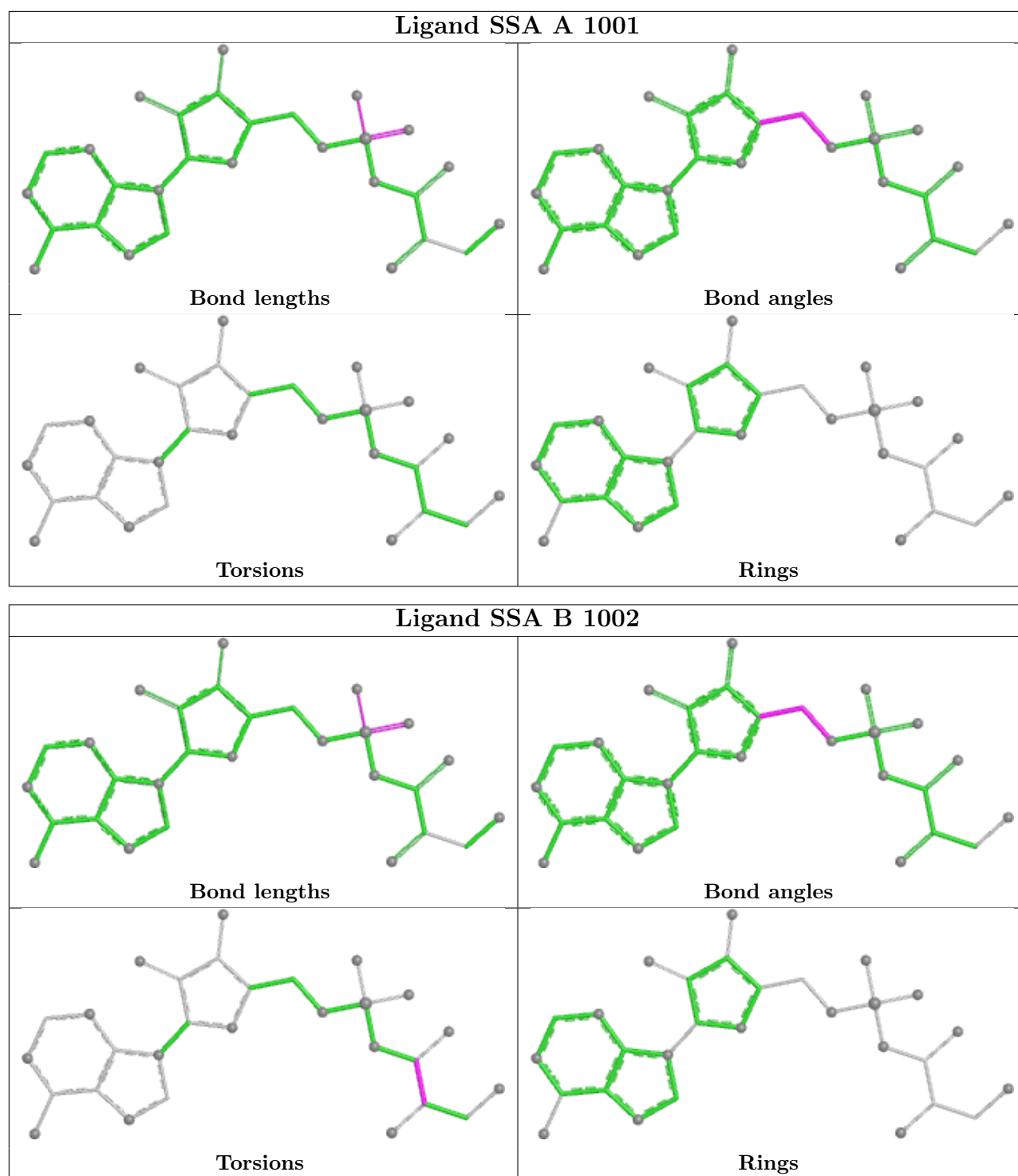
Mol	Chain	Res	Type	Atoms
3	B	1002	SSA	O9-C9-CA-N10

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	SSA	2	0
3	B	1002	SSA	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	447/455 (98%)	-0.25	11 (2%) 58 52	32, 54, 99, 156	0
1	B	447/455 (98%)	-0.32	14 (3%) 51 45	30, 50, 108, 156	0
All	All	894/910 (98%)	-0.28	25 (2%) 55 49	30, 52, 106, 156	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	289	ALA	5.0
1	B	289	ALA	4.8
1	B	294	LYS	3.8
1	B	75	LEU	3.5
1	A	293	THR	3.3
1	A	292	ASP	3.1
1	B	290	GLY	3.1
1	B	70	PRO	3.0
1	A	290	GLY	2.9
1	A	288	THR	2.9
1	A	294	LYS	2.8
1	B	66	LYS	2.7
1	B	57	ILE	2.7
1	A	68	GLY	2.6
1	A	393	THR	2.4
1	A	291	LYS	2.4
1	B	393	THR	2.3
1	A	40	TRP	2.3
1	B	79	ARG	2.2
1	B	58	ALA	2.1
1	A	67	LYS	2.1
1	B	77	LYS	2.1
1	B	61	ILE	2.1
1	B	7	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	74	LEU	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

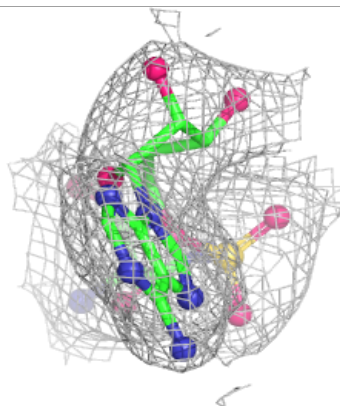
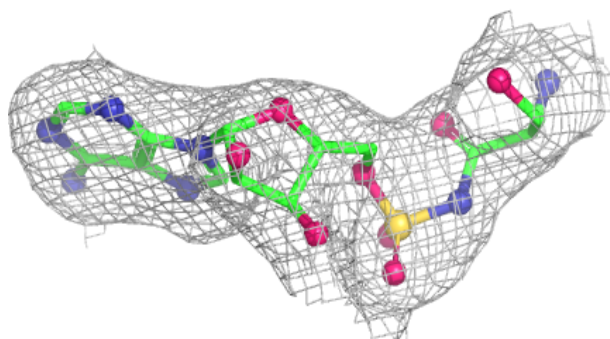
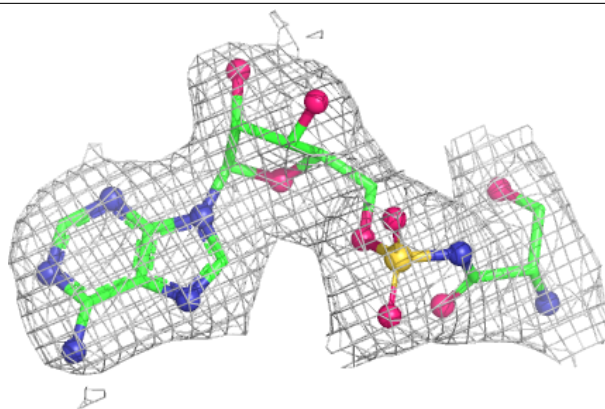
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	B	2006	5/5	0.80	0.15	117,121,124,129	0
2	SO4	A	2005	5/5	0.85	0.12	103,107,110,112	0
2	SO4	A	2003	5/5	0.86	0.13	105,107,107,108	0
2	SO4	B	2002	5/5	0.93	0.09	74,74,79,86	0
2	SO4	A	2007	5/5	0.93	0.17	66,77,80,83	0
2	SO4	B	2004	5/5	0.94	0.07	95,98,100,102	0
2	SO4	A	2001	5/5	0.96	0.10	65,71,78,82	0
3	SSA	A	1001	29/29	0.98	0.05	26,40,47,52	0
3	SSA	B	1002	29/29	0.98	0.05	30,37,45,47	0

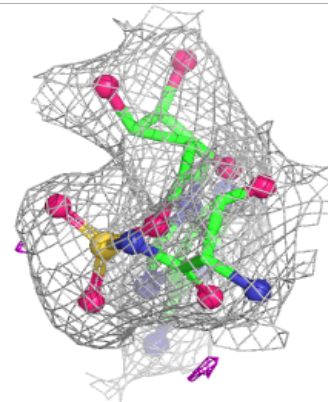
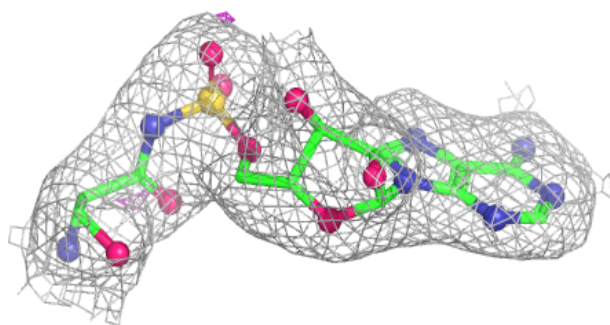
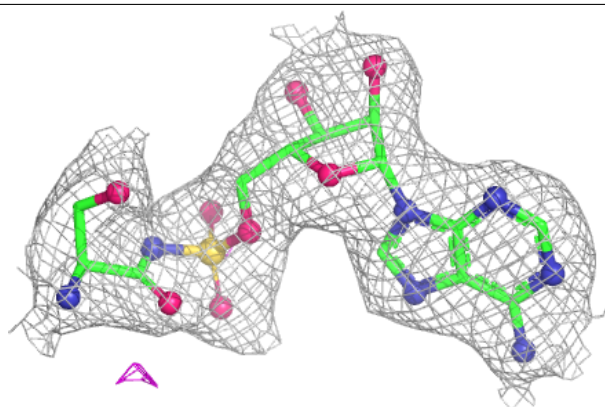
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around SSA A 1001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around SSA B 1002:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.