



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 11, 2024 – 11:35 PM EDT

PDB ID : 1RF6  
Title : Structural Studies of Streptococcus pneumoniae EPSP Synthase in S3P-GLP Bound State  
Authors : Park, H.; Hilsenbeck, J.L.; Kim, H.J.; Shuttleworth, W.A.; Park, Y.H.; Evans, J.N.; Kang, C.  
Deposited on : 2003-11-07  
Resolution : 1.90 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](mailto: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>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

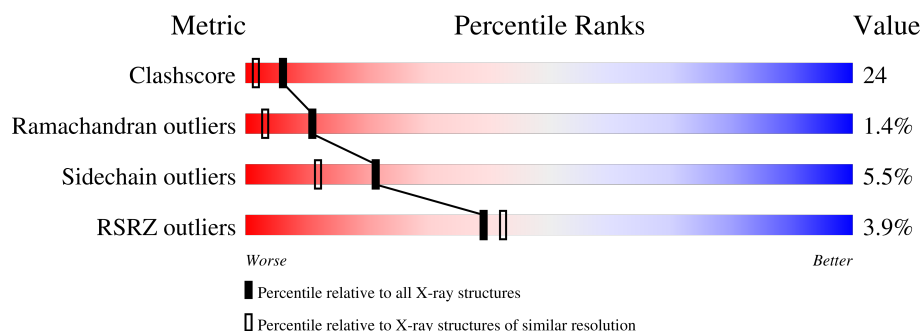
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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))
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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  $\geq 3$ , 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	427	<div> <div>2%</div> <div>67%</div> <div>30%</div> <div>.</div> </div>
1	B	427	<div> <div>3%</div> <div>71%</div> <div>26%</div> <div>.</div> </div>
1	C	427	<div> <div>5%</div> <div>61%</div> <div>35%</div> <div>.</div> </div>
1	D	427	<div> <div>6%</div> <div>65%</div> <div>31%</div> <div>.</div> </div>

## 2 Entry composition [i](#)

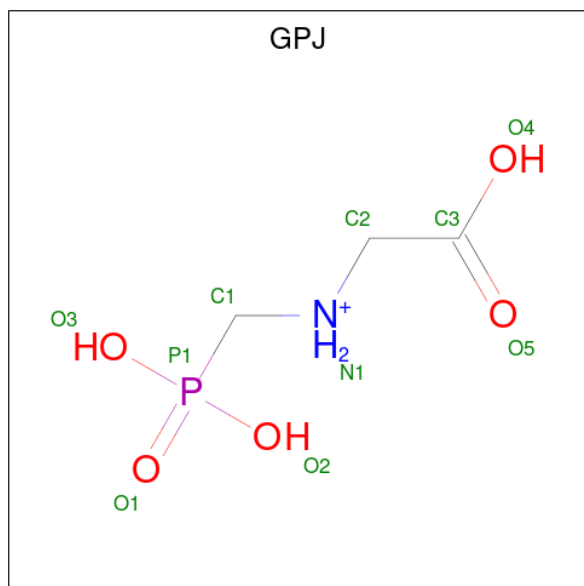
There are 4 unique types of molecules in this entry. The entry contains 13798 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 5-enolpyruvylshikimate-3-phosphate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	427	Total	C	N	O	S	0	0	0
			3212	2019	559	619	15			
1	B	427	Total	C	N	O	S	0	0	0
			3212	2019	559	619	15			
1	C	427	Total	C	N	O	S	0	0	0
			3212	2019	559	619	15			
1	D	427	Total	C	N	O	S	0	0	0
			3212	2019	559	619	15			

- Molecule 2 is GLYPHOSATE (three-letter code: GPJ) (formula: C<sub>3</sub>H<sub>9</sub>NO<sub>5</sub>P).



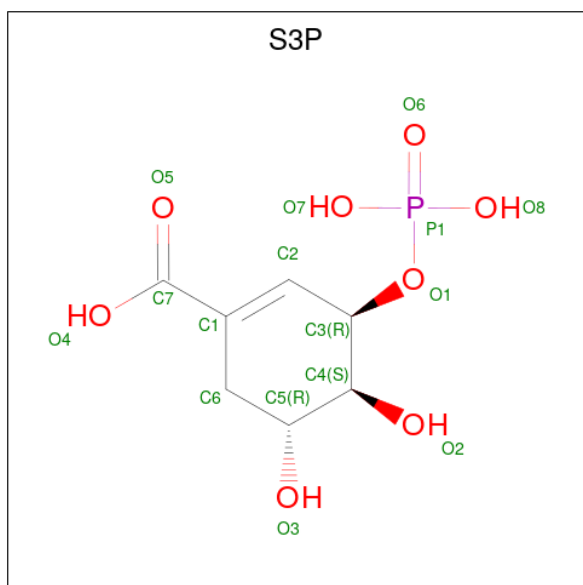
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			10	3	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			10	3	1	5	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			10	3	1	5	1		
2	D	1	Total	C	N	O	P	0	0
			10	3	1	5	1		

- Molecule 3 is SHIKIMATE-3-PHOSPHATE (three-letter code: S3P) (formula:  $C_7H_{11}O_8P$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			16	7	8	1		
3	B	1	Total	C	O	P	0	0
			16	7	8	1		
3	C	1	Total	C	O	P	0	0
			16	7	8	1		
3	D	1	Total	C	O	P	0	0
			16	7	8	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	263	Total	O	0	0
			263	263		
4	B	256	Total	O	0	0
			256	256		
4	C	168	Total	O	0	0
			168	168		

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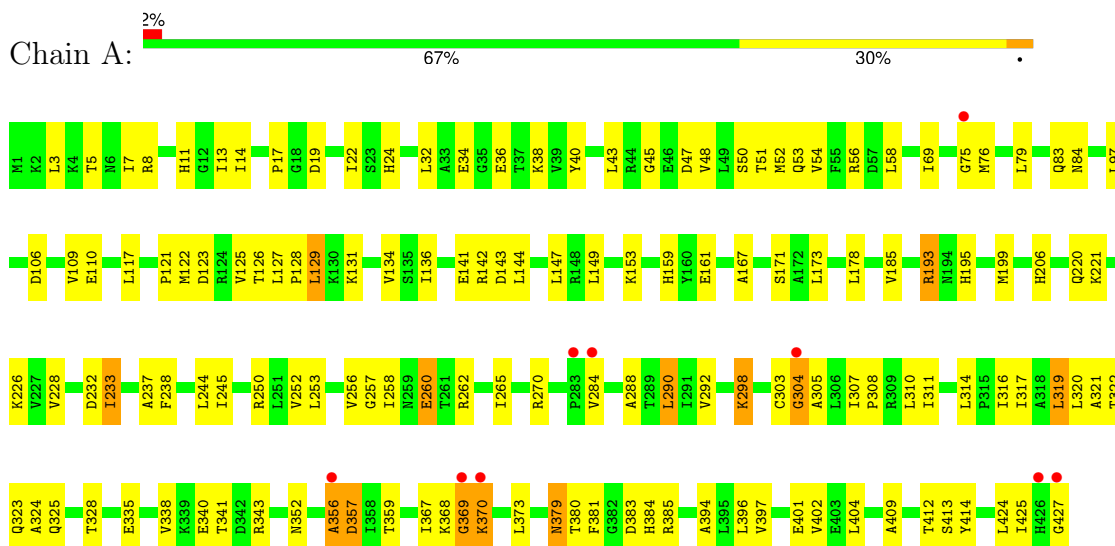
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	159	Total	O	0	0
			159	159		

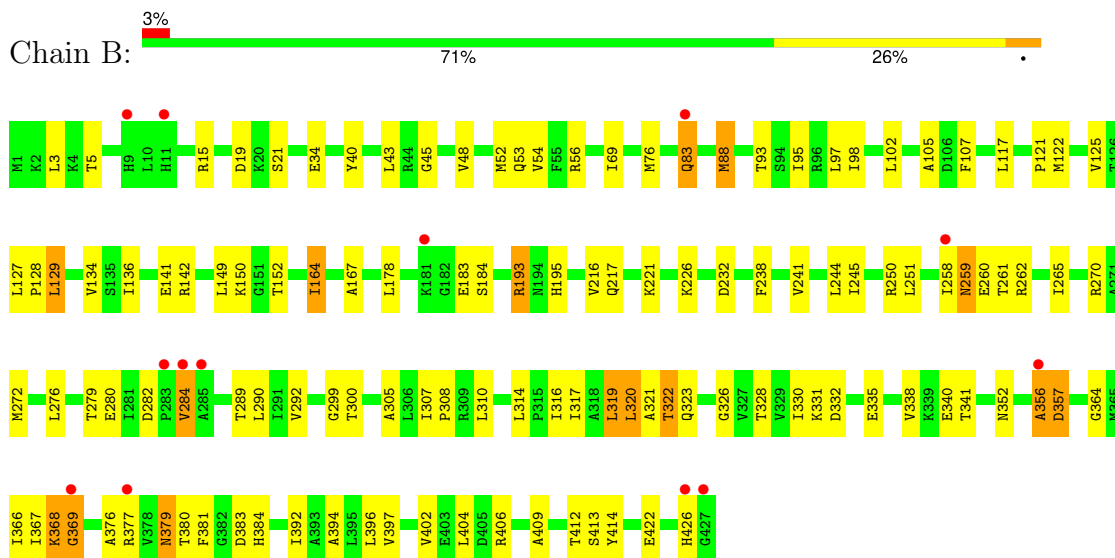
### 3 Residue-property plots

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: 5-enolpyruvylshikimate-3-phosphate synthase

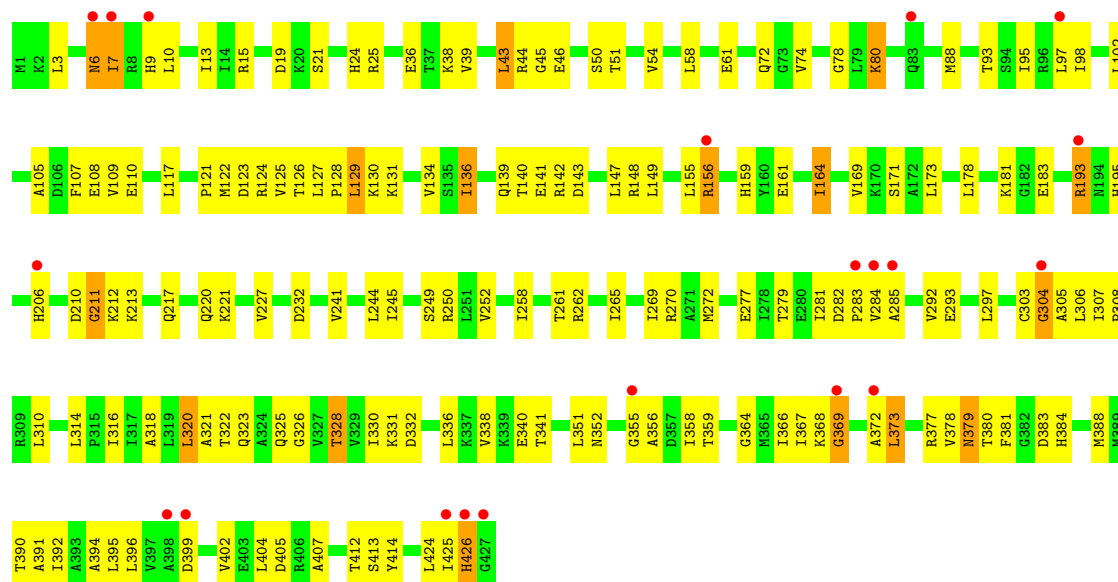


#### • Molecule 1: 5-enolpyruvylshikimate-3-phosphate synthase

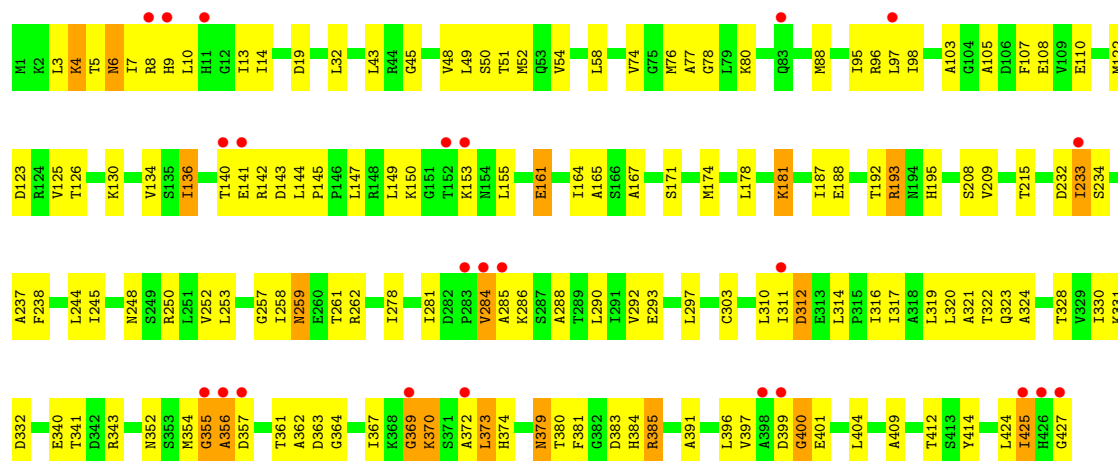


#### • Molecule 1: 5-enolpyruvylshikimate-3-phosphate synthase





• Molecule 1: 5-enolpyruvylshikimate-3-phosphate synthase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.78Å 150.56Å 88.26Å 90.00° 91.20° 90.00°	Depositor
Resolution (Å)	10.00 – 1.90 33.33 – 1.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-1.90) 94.1 (33.33-1.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.03 (at 1.79Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.218 , 0.229 0.222 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.2	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 59.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.034 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	13798	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: GPJ, S3P

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	0.33	0/3252	0.65	2/4391 (0.0%)
1	B	0.33	0/3252	0.64	0/4391
1	C	0.31	0/3252	0.60	0/4391
1	D	0.30	0/3252	0.60	1/4391 (0.0%)
All	All	0.32	0/13008	0.62	3/17564 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	369	GLY	N-CA-C	5.76	127.50	113.10
1	A	356	ALA	N-CA-C	5.37	125.51	111.00
1	D	369	GLY	N-CA-C	5.24	126.20	113.10

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	3212	0	3325	160	0
1	B	3212	0	3325	145	0
1	C	3212	0	3325	180	0
1	D	3212	0	3325	163	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	10	0	6	1	0
2	B	10	0	6	0	0
2	C	10	0	6	0	0
2	D	10	0	6	1	0
3	A	16	0	8	0	0
3	B	16	0	8	0	0
3	C	16	0	8	0	0
3	D	16	0	8	0	0
4	A	263	0	0	15	0
4	B	256	0	0	13	0
4	C	168	0	0	10	0
4	D	159	0	0	8	0
All	All	13798	0	13356	644	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 24.

All (644) 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:321:ALA:HB1	1:A:328:THR:HG21	1.19	1.18
1:C:378:VAL:HG11	1:C:390:THR:HG21	1.25	1.15
1:D:321:ALA:HB1	1:D:328:THR:HG21	1.18	1.12
1:A:233:ILE:H	1:A:233:ILE:HD12	1.12	1.09
1:D:233:ILE:HD12	1:D:233:ILE:H	1.15	1.05
1:B:43:LEU:HD13	1:B:45:GLY:H	1.23	1.04
1:A:245:ILE:HD11	1:A:320:LEU:HD12	1.41	1.02
1:C:43:LEU:HD22	1:C:45:GLY:H	1.22	1.02
1:C:352:ASN:HA	1:C:356:ALA:HA	1.40	1.00
1:D:245:ILE:HD11	1:D:320:LEU:HA	1.44	1.00
1:B:193:ARG:CZ	1:B:262:ARG:HE	1.77	0.97
1:A:256:VAL:HG11	1:A:290:LEU:HD22	1.47	0.94
1:C:321:ALA:HB1	1:C:328:THR:HG21	1.50	0.94
1:D:321:ALA:CB	1:D:328:THR:HG21	2.00	0.92
1:A:43:LEU:HD13	1:A:45:GLY:H	1.32	0.92
1:D:244:LEU:HG	1:D:292:VAL:HG21	1.52	0.92
1:A:321:ALA:CB	1:A:328:THR:HG21	2.00	0.90
1:D:4:LYS:NZ	1:D:4:LYS:H	1.69	0.90
1:D:355:GLY:HA3	1:D:373:LEU:HD23	1.52	0.90
1:B:245:ILE:HG23	1:B:396:LEU:HD21	1.52	0.89
1:B:88:MET:HG2	1:B:95:ILE:HB	1.54	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:352:ASN:HA	1:B:356:ALA:HA	1.56	0.88
1:D:208:SER:HB3	1:D:215:THR:CG2	2.04	0.87
1:A:380:THR:HG21	1:A:409:ALA:HB3	1.56	0.85
1:A:233:ILE:H	1:A:233:ILE:CD1	1.90	0.84
1:C:21:SER:HB3	1:C:193:ARG:NH2	1.93	0.84
1:D:233:ILE:H	1:D:233:ILE:CD1	1.91	0.83
1:A:244:LEU:HG	1:A:292:VAL:HG21	1.61	0.82
1:D:379:ASN:HD22	1:D:380:THR:N	1.78	0.81
1:A:106:ASP:HB2	1:A:153:LYS:HE2	1.62	0.81
1:A:245:ILE:HG21	1:A:323:GLN:HG3	1.61	0.81
1:B:380:THR:HG22	1:B:383:ASP:H	1.46	0.81
1:D:4:LYS:H	1:D:4:LYS:HZ1	1.28	0.81
1:D:380:THR:HG21	1:D:409:ALA:HB3	1.63	0.81
1:A:373:LEU:HB2	4:A:1667:HOH:O	1.80	0.80
1:D:32:LEU:HD22	1:D:76:MET:HE3	1.61	0.80
1:B:193:ARG:HH11	1:B:262:ARG:HH21	1.30	0.79
1:B:322:THR:HG22	1:B:323:GLN:HE21	1.46	0.79
1:A:352:ASN:HA	1:A:356:ALA:HA	1.65	0.79
1:B:76:MET:H	1:B:221:LYS:NZ	1.81	0.79
1:D:245:ILE:CG2	1:D:323:GLN:HG3	2.13	0.79
1:A:3:LEU:HB2	1:A:402:VAL:HG13	1.64	0.78
1:C:206:HIS:H	1:C:220:GLN:HE22	1.30	0.78
1:C:43:LEU:HD22	1:C:45:GLY:N	1.97	0.78
1:B:34:GLU:OE2	1:B:221:LYS:HE2	1.83	0.77
1:A:328:THR:CG2	1:A:367:ILE:HB	2.14	0.77
1:D:13:ILE:HG12	1:D:252:VAL:HG11	1.67	0.77
1:B:338:VAL:O	1:B:338:VAL:HG22	1.85	0.77
1:C:13:ILE:HG12	1:C:252:VAL:HG21	1.66	0.76
1:D:245:ILE:CG2	1:D:396:LEU:HD11	2.16	0.76
1:D:245:ILE:HG21	1:D:396:LEU:HD11	1.67	0.76
1:B:384:HIS:HB3	1:B:412:THR:HG22	1.68	0.75
1:B:379:ASN:HD22	1:B:381:PHE:H	1.32	0.75
1:B:380:THR:HG23	1:B:383:ASP:O	1.86	0.75
1:D:13:ILE:HG12	1:D:252:VAL:CG1	2.17	0.75
1:A:379:ASN:HD22	1:A:381:PHE:H	1.32	0.75
1:B:244:LEU:HG	1:B:292:VAL:HG21	1.67	0.75
1:D:245:ILE:HG21	1:D:323:GLN:HG3	1.68	0.75
1:C:13:ILE:HG12	1:C:252:VAL:CG2	2.16	0.74
1:C:394:ALA:HB1	1:C:402:VAL:HG11	1.67	0.74
1:D:181:LYS:HD3	1:D:181:LYS:N	2.02	0.74
1:D:5:THR:HG23	1:D:397:VAL:HB	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:258:ILE:HG22	1:D:258:ILE:O	1.85	0.74
1:D:311:ILE:O	1:D:312:ASP:HB2	1.86	0.74
1:B:76:MET:H	1:B:221:LYS:HZ1	1.33	0.74
1:A:325:GLN:NE2	1:A:370:LYS:HG3	2.03	0.73
1:C:181:LYS:HD2	1:C:181:LYS:N	2.03	0.73
1:D:96:ARG:HG3	1:D:125:VAL:HG11	1.70	0.73
1:D:259:ASN:HD22	1:D:261:THR:H	1.35	0.73
1:A:13:ILE:HA	1:A:252:VAL:HG13	1.68	0.73
1:B:380:THR:HB	4:B:1719:HOH:O	1.88	0.73
1:C:183:GLU:HB2	1:C:217:GLN:HE22	1.53	0.73
1:A:245:ILE:HD11	1:A:320:LEU:CD1	2.16	0.73
1:A:237:ALA:HB1	1:A:316:ILE:CD1	2.18	0.73
1:B:245:ILE:HG13	1:B:323:GLN:HG3	1.70	0.73
1:A:195:HIS:HB3	1:A:199:MET:CE	2.19	0.73
1:B:43:LEU:HD13	1:B:45:GLY:N	2.01	0.73
1:A:321:ALA:HB1	1:A:328:THR:CG2	2.11	0.73
1:A:343:ARG:NH2	1:A:385:ARG:HG3	2.03	0.73
1:D:379:ASN:ND2	1:D:381:PHE:H	1.86	0.73
1:A:206:HIS:H	1:A:220:GLN:HE22	1.37	0.72
1:B:83:GLN:HG3	4:B:1635:HOH:O	1.88	0.72
1:B:322:THR:CG2	1:B:323:GLN:HE21	2.01	0.72
1:D:136:ILE:HG23	1:D:149:LEU:HD13	1.71	0.72
1:A:245:ILE:CG2	1:A:323:GLN:HG3	2.19	0.72
1:B:328:THR:OG1	1:B:367:ILE:HB	1.89	0.72
1:A:324:ALA:O	1:A:369:GLY:HA3	1.90	0.72
1:C:245:ILE:HG23	1:C:396:LEU:HD11	1.70	0.72
1:C:384:HIS:HB3	1:C:412:THR:HG22	1.72	0.72
1:D:321:ALA:HB1	1:D:328:THR:CG2	2.09	0.72
1:D:352:ASN:HA	1:D:356:ALA:HA	1.71	0.72
1:C:297:LEU:HD13	1:C:320:LEU:HD21	1.70	0.72
1:D:328:THR:CG2	1:D:367:ILE:HB	2.19	0.72
1:A:394:ALA:HB1	1:A:402:VAL:HG11	1.72	0.71
1:D:181:LYS:HD3	1:D:181:LYS:H	1.53	0.71
1:D:324:ALA:O	1:D:369:GLY:HA3	1.90	0.71
1:B:19:ASP:HA	1:B:232:ASP:HB2	1.72	0.71
1:C:121:PRO:HD2	1:C:338:VAL:HG13	1.73	0.71
1:C:193:ARG:NH1	1:C:195:HIS:HB2	2.05	0.71
1:B:352:ASN:HA	1:B:356:ALA:CA	2.21	0.71
1:D:237:ALA:HB1	1:D:316:ILE:CD1	2.20	0.71
1:A:256:VAL:HG12	1:A:288:ALA:O	1.90	0.71
1:D:13:ILE:HA	1:D:252:VAL:HG13	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:21:SER:HB3	1:C:193:ARG:HH21	1.56	0.71
1:C:328:THR:HG23	1:C:367:ILE:HB	1.73	0.70
1:A:380:THR:HG21	1:A:409:ALA:CB	2.21	0.70
1:C:394:ALA:CB	1:C:402:VAL:HG11	2.22	0.70
1:A:245:ILE:HG21	1:A:396:LEU:HD11	1.74	0.70
1:B:43:LEU:CD1	1:B:45:GLY:H	2.03	0.70
1:A:384:HIS:HB3	1:A:412:THR:HG22	1.74	0.70
1:A:394:ALA:CB	1:A:402:VAL:HG11	2.22	0.70
1:A:316:ILE:HG23	4:A:1444:HOH:O	1.92	0.69
1:B:125:VAL:HG22	1:B:129:LEU:HD22	1.74	0.69
1:D:19:ASP:HA	1:D:232:ASP:HB2	1.74	0.69
1:D:237:ALA:HB1	1:D:316:ILE:HD11	1.73	0.69
1:A:380:THR:HG22	1:A:383:ASP:H	1.58	0.69
1:A:341:THR:HG23	1:A:383:ASP:HB2	1.75	0.69
1:B:121:PRO:HD2	1:B:338:VAL:HG23	1.74	0.69
1:A:357:ASP:OD2	1:A:368:LYS:HB3	1.92	0.69
1:C:355:GLY:HA3	1:C:373:LEU:HD12	1.75	0.68
1:B:300:THR:H	1:B:328:THR:HG22	1.58	0.68
1:D:195:HIS:HE1	1:D:262:ARG:HH11	1.39	0.68
1:C:321:ALA:HB1	1:C:328:THR:CG2	2.23	0.68
1:A:307:ILE:O	1:A:311:ILE:HG23	1.94	0.68
1:C:80:LYS:HE3	1:C:80:LYS:HA	1.76	0.68
1:C:338:VAL:HG12	1:C:338:VAL:O	1.93	0.67
1:A:237:ALA:HB1	1:A:316:ILE:HD11	1.75	0.67
1:C:341:THR:HG23	1:C:383:ASP:HB2	1.76	0.67
1:D:361:THR:HG22	1:D:362:ALA:N	2.10	0.67
1:D:142:ARG:HB2	1:D:144:LEU:CD1	2.25	0.67
1:D:341:THR:HG23	1:D:383:ASP:HB2	1.75	0.67
1:A:352:ASN:HA	1:A:356:ALA:CA	2.24	0.67
1:D:140:THR:HG22	1:D:141:GLU:N	2.10	0.67
1:A:253:LEU:N	1:A:253:LEU:HD22	2.10	0.66
1:B:380:THR:HG21	1:B:409:ALA:HB3	1.77	0.66
1:A:322:THR:HB	4:A:1454:HOH:O	1.96	0.66
1:D:140:THR:HG22	1:D:141:GLU:H	1.61	0.66
1:B:316:ILE:HD12	1:B:317:ILE:N	2.10	0.66
1:A:245:ILE:HG23	4:A:1490:HOH:O	1.95	0.66
1:A:245:ILE:N	1:A:245:ILE:HD12	2.11	0.66
1:B:279:THR:HG23	1:B:289:THR:HB	1.77	0.66
1:D:164:ILE:HD12	1:D:165:ALA:H	1.59	0.66
1:C:3:LEU:HD13	1:C:391:ALA:HA	1.78	0.65
1:D:316:ILE:HG23	4:D:1732:HOH:O	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:244:LEU:HG	1:B:292:VAL:CG2	2.26	0.65
1:B:366:ILE:HG22	1:B:368:LYS:HD2	1.79	0.65
1:C:9:HIS:HB2	4:C:1773:HOH:O	1.95	0.65
1:C:245:ILE:HG13	1:C:323:GLN:HG3	1.76	0.65
1:D:281:ILE:HD13	1:D:288:ALA:HB2	1.78	0.65
1:B:238:PHE:CD2	1:B:316:ILE:HG21	2.32	0.65
1:A:385:ARG:HD2	2:A:1428:GPJ:O5	1.96	0.65
1:C:379:ASN:HD22	1:C:380:THR:N	1.95	0.65
1:D:278:ILE:HG22	1:D:281:ILE:HD11	1.77	0.64
1:C:321:ALA:CB	1:C:328:THR:HG21	2.26	0.64
1:B:259:ASN:HD22	1:B:261:THR:H	1.45	0.64
1:A:19:ASP:HA	1:A:232:ASP:HB2	1.78	0.64
1:A:52:MET:HE3	1:A:69:ILE:HD12	1.79	0.64
1:C:378:VAL:HG11	1:C:390:THR:CG2	2.16	0.64
1:C:39:VAL:HG13	1:C:227:VAL:HG23	1.80	0.64
1:A:195:HIS:HE1	1:A:262:ARG:HH11	1.46	0.64
1:A:258:ILE:HG23	1:A:258:ILE:O	1.97	0.64
1:C:352:ASN:HA	1:C:356:ALA:CA	2.24	0.64
1:D:208:SER:HB3	1:D:215:THR:HG23	1.79	0.64
1:B:88:MET:HG2	1:B:95:ILE:CB	2.28	0.64
1:C:284:VAL:HG23	1:C:285:ALA:N	2.13	0.64
1:B:259:ASN:ND2	1:B:261:THR:H	1.96	0.63
1:C:164:ILE:HD13	1:C:164:ILE:H	1.64	0.63
1:D:244:LEU:HG	1:D:292:VAL:CG2	2.27	0.63
1:A:233:ILE:HD12	1:A:233:ILE:N	1.98	0.63
1:B:193:ARG:NH1	1:B:262:ARG:HH21	1.96	0.63
1:B:195:HIS:HE1	1:B:262:ARG:CZ	2.10	0.63
1:D:5:THR:HG22	1:D:6:ASN:N	2.14	0.62
1:C:284:VAL:HG23	1:C:285:ALA:H	1.62	0.62
1:D:259:ASN:ND2	1:D:261:THR:H	1.96	0.62
1:D:340:GLU:OE2	1:D:384:HIS:HE1	1.81	0.62
1:B:134:VAL:HG12	1:B:136:ILE:HG13	1.81	0.62
1:B:121:PRO:HD2	1:B:338:VAL:CG2	2.28	0.62
1:A:233:ILE:HG13	1:A:257:GLY:O	1.99	0.62
1:C:245:ILE:CG2	1:C:396:LEU:HD11	2.30	0.62
1:C:388:MET:O	1:C:392:ILE:HD13	1.99	0.62
1:A:43:LEU:CD1	1:A:45:GLY:H	2.10	0.62
1:C:221:LYS:HD2	1:C:221:LYS:N	2.14	0.62
1:C:392:ILE:O	1:C:395:LEU:HB2	2.00	0.62
1:C:169:VAL:O	1:C:173:LEU:HD13	1.98	0.62
1:C:241:VAL:HG21	1:C:316:ILE:HG13	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:328:THR:HG23	1:D:367:ILE:HB	1.81	0.62
1:C:379:ASN:ND2	1:C:381:PHE:H	1.98	0.61
1:C:391:ALA:O	1:C:395:LEU:HD13	2.00	0.61
1:A:260:GLU:H	1:A:260:GLU:CD	2.04	0.61
1:C:272:MET:SD	1:C:320:LEU:HD22	2.40	0.61
1:A:195:HIS:CE1	1:A:262:ARG:HH11	2.18	0.61
1:A:380:THR:HG23	1:A:383:ASP:O	2.00	0.61
1:B:262:ARG:CZ	4:B:1563:HOH:O	2.49	0.61
1:A:325:GLN:HE22	1:A:370:LYS:HG3	1.64	0.61
1:B:307:ILE:HB	1:B:308:PRO:HD3	1.82	0.61
1:C:139:GLN:O	1:C:140:THR:HB	1.99	0.61
1:B:380:THR:HG22	1:B:383:ASP:N	2.16	0.61
1:C:3:LEU:HB2	1:C:402:VAL:HG13	1.83	0.61
1:D:54:VAL:O	1:D:58:LEU:HD13	2.01	0.61
1:C:378:VAL:CG1	1:C:390:THR:HG21	2.16	0.61
1:A:121:PRO:HD2	1:A:338:VAL:CG2	2.31	0.61
1:B:245:ILE:CG2	1:B:396:LEU:HD21	2.28	0.61
1:B:260:GLU:CD	1:B:260:GLU:H	2.04	0.61
1:D:142:ARG:HB2	1:D:144:LEU:HD11	1.81	0.61
1:C:36:GLU:OE1	1:C:38:LYS:HE3	2.00	0.60
1:B:394:ALA:HB1	1:B:402:VAL:HG11	1.83	0.60
1:C:307:ILE:HB	1:C:308:PRO:HD3	1.82	0.60
1:D:355:GLY:HA3	1:D:373:LEU:CD2	2.28	0.60
1:A:244:LEU:HG	1:A:292:VAL:CG2	2.29	0.60
1:A:316:ILE:HG13	1:A:317:ILE:N	2.16	0.60
1:B:193:ARG:NH1	1:B:262:ARG:HE	1.97	0.60
1:D:380:THR:HG22	1:D:383:ASP:H	1.66	0.60
1:B:394:ALA:CB	1:B:402:VAL:HG11	2.31	0.60
1:A:323:GLN:HG2	4:A:1454:HOH:O	2.01	0.60
1:B:280:GLU:HG2	4:B:1613:HOH:O	2.01	0.60
1:C:380:THR:HG23	1:C:404:LEU:HD21	1.83	0.60
1:C:88:MET:HG3	1:C:95:ILE:HB	1.83	0.60
1:C:136:ILE:HG23	1:C:149:LEU:HD23	1.84	0.60
1:A:13:ILE:HG12	1:A:252:VAL:CG1	2.32	0.59
1:A:7:ILE:HD11	1:A:425:ILE:HG23	1.83	0.59
1:C:134:VAL:HG12	1:C:136:ILE:HG13	1.84	0.59
1:B:258:ILE:HG12	1:B:258:ILE:O	2.01	0.59
1:C:338:VAL:HG12	4:C:1643:HOH:O	2.02	0.59
1:A:34:GLU:OE1	1:A:221:LYS:HD2	2.03	0.59
1:B:379:ASN:ND2	1:B:381:PHE:H	1.99	0.59
1:C:303:CYS:O	1:C:304:GLY:O	2.20	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:9:HIS:HD2	1:D:10:LEU:N	2.01	0.59
1:D:161:GLU:HG3	4:D:1875:HOH:O	2.03	0.59
1:A:24:HIS:HD2	1:A:51:THR:OG1	1.86	0.59
1:B:136:ILE:HG12	1:B:149:LEU:HG	1.84	0.59
1:C:10:LEU:HB2	1:C:249:SER:OG	2.03	0.59
1:D:297:LEU:N	1:D:297:LEU:HD22	2.18	0.59
1:A:13:ILE:HG12	1:A:252:VAL:HG11	1.85	0.58
1:A:83:GLN:CD	1:A:83:GLN:H	2.05	0.58
1:C:181:LYS:HD2	1:C:181:LYS:H	1.67	0.58
1:D:281:ILE:HD13	1:D:288:ALA:CB	2.33	0.58
1:A:43:LEU:HD12	1:A:48:VAL:CG2	2.33	0.58
1:B:21:SER:HB2	1:B:262:ARG:NH2	2.18	0.58
1:C:258:ILE:HG12	1:C:258:ILE:O	2.03	0.58
1:D:126:THR:O	1:D:130:LYS:HB2	2.03	0.58
1:A:75:GLY:HA3	4:A:1520:HOH:O	2.03	0.58
1:A:122:MET:O	1:A:125:VAL:HG12	2.04	0.58
1:C:250:ARG:HH21	1:C:250:ARG:HG3	1.68	0.58
1:D:380:THR:HG21	1:D:409:ALA:CB	2.31	0.58
1:D:245:ILE:HG23	1:D:323:GLN:HG3	1.84	0.58
1:D:372:ALA:O	1:D:373:LEU:HB2	2.04	0.58
1:B:259:ASN:HD22	1:B:259:ASN:C	2.07	0.58
1:C:6:ASN:O	1:C:7:ILE:O	2.22	0.58
1:A:43:LEU:HD13	1:A:45:GLY:N	2.12	0.57
1:B:19:ASP:HA	1:B:232:ASP:CB	2.34	0.57
1:C:125:VAL:O	1:C:129:LEU:HB2	2.04	0.57
1:C:326:GLY:H	1:C:369:GLY:HA2	1.69	0.57
1:D:233:ILE:HD12	1:D:233:ILE:N	2.01	0.57
1:D:253:LEU:N	1:D:253:LEU:HD22	2.19	0.57
1:A:338:VAL:HG22	1:A:338:VAL:O	2.04	0.57
1:A:379:ASN:ND2	1:A:381:PHE:H	2.02	0.57
1:D:174:MET:O	1:D:178:LEU:HD13	2.04	0.57
1:A:32:LEU:O	1:A:75:GLY:O	2.21	0.57
1:B:152:THR:HG21	4:B:1768:HOH:O	2.04	0.57
1:C:281:ILE:O	1:C:283:PRO:HD3	2.04	0.57
1:C:211:GLY:O	1:C:212:LYS:HB2	2.05	0.56
1:B:265:ILE:HD12	1:B:316:ILE:HD11	1.87	0.56
1:C:122:MET:HB2	1:C:143:ASP:O	2.05	0.56
1:C:193:ARG:HH12	1:C:195:HIS:HB2	1.67	0.56
1:D:80:LYS:HB3	1:D:80:LYS:NZ	2.21	0.56
1:D:322:THR:HG22	1:D:323:GLN:NE2	2.21	0.56
1:C:24:HIS:HD2	1:C:51:THR:OG1	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:377:ARG:HD2	1:C:405:ASP:OD2	2.06	0.56
1:D:126:THR:HA	1:D:136:ILE:HD12	1.87	0.56
1:A:308:PRO:HA	1:A:311:ILE:HG23	1.86	0.56
1:C:210:ASP:O	1:C:213:LYS:HG2	2.05	0.56
1:D:195:HIS:CE1	1:D:262:ARG:HH11	2.23	0.55
1:A:265:ILE:HD12	1:A:316:ILE:HD11	1.88	0.55
1:A:298:LYS:HE2	4:A:1621:HOH:O	2.05	0.55
1:B:193:ARG:HH11	1:B:262:ARG:NH2	2.03	0.55
1:C:44:ARG:HG2	1:C:44:ARG:HH11	1.70	0.55
1:A:40:TYR:HE1	1:A:226:LYS:HG3	1.71	0.55
1:B:164:ILE:HD13	1:B:164:ILE:H	1.71	0.55
1:D:95:ILE:HD11	1:D:147:LEU:HD22	1.87	0.55
1:D:234:SER:HB3	1:D:385:ARG:NH1	2.21	0.55
1:C:149:LEU:C	1:C:149:LEU:HD13	2.27	0.55
1:D:379:ASN:HD22	1:D:379:ASN:C	2.07	0.55
1:B:88:MET:CG	1:B:95:ILE:HB	2.34	0.55
1:C:372:ALA:O	1:C:373:LEU:HB2	2.06	0.55
1:D:322:THR:HG22	1:D:323:GLN:HE21	1.71	0.55
1:D:380:THR:HG23	1:D:383:ASP:O	2.06	0.54
1:B:193:ARG:NH1	1:B:262:ARG:NH2	2.56	0.54
1:C:39:VAL:HG22	1:C:227:VAL:CG2	2.38	0.54
1:D:311:ILE:O	1:D:312:ASP:CB	2.56	0.54
1:A:122:MET:HG3	1:A:147:LEU:HD11	1.89	0.54
1:B:3:LEU:HB2	1:B:402:VAL:HG13	1.89	0.54
1:C:61:GLU:OE2	1:C:72:GLN:HG2	2.06	0.54
1:A:36:GLU:OE2	1:A:38:LYS:HE2	2.08	0.54
1:C:15:ARG:HB3	1:C:15:ARG:HH11	1.73	0.53
1:C:338:VAL:O	1:C:338:VAL:CG1	2.56	0.53
1:D:49:LEU:HD12	1:D:52:MET:CE	2.39	0.53
1:A:380:THR:HG22	1:A:383:ASP:N	2.23	0.53
1:B:422:GLU:HG2	4:B:1721:HOH:O	2.08	0.53
1:D:303:CYS:HB2	1:D:332:ASP:OD1	2.09	0.53
1:C:355:GLY:HA3	1:C:373:LEU:CD1	2.38	0.53
1:C:140:THR:HG22	1:C:141:GLU:N	2.23	0.53
1:B:238:PHE:CE2	1:B:316:ILE:HG21	2.43	0.53
1:C:305:ALA:O	1:C:308:PRO:HD2	2.09	0.53
1:B:338:VAL:O	1:B:338:VAL:CG2	2.57	0.53
1:C:380:THR:CG2	1:C:404:LEU:HD21	2.38	0.53
1:D:278:ILE:CG2	1:D:281:ILE:HD11	2.39	0.53
1:B:183:GLU:HG3	1:B:217:GLN:NE2	2.24	0.53
1:B:380:THR:CG2	1:B:383:ASP:O	2.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:25:ARG:NE	1:C:193:ARG:HH12	2.05	0.53
1:A:305:ALA:N	4:A:1658:HOH:O	2.41	0.53
1:C:320:LEU:O	1:C:320:LEU:HD23	2.09	0.53
1:B:21:SER:HB2	1:B:262:ARG:HH22	1.72	0.52
1:B:368:LYS:HD3	1:B:368:LYS:N	2.23	0.52
1:D:285:ALA:O	1:D:286:LYS:HB2	2.08	0.52
1:A:43:LEU:HD12	1:A:48:VAL:HG23	1.89	0.52
1:D:181:LYS:H	1:D:181:LYS:CD	2.16	0.52
1:D:245:ILE:CD1	1:D:320:LEU:HA	2.27	0.52
1:D:3:LEU:HD23	1:D:391:ALA:HA	1.92	0.52
1:D:54:VAL:HG11	1:D:98:ILE:HD13	1.90	0.52
1:A:359:THR:OG1	1:C:368:LYS:HE3	2.10	0.52
1:A:328:THR:HG22	1:A:367:ILE:HB	1.92	0.52
1:D:193:ARG:HD2	4:D:1778:HOH:O	2.09	0.52
1:A:245:ILE:CG2	1:A:396:LEU:HD11	2.38	0.52
1:A:195:HIS:HB3	1:A:199:MET:HE3	1.91	0.52
1:A:75:GLY:O	4:A:1537:HOH:O	2.18	0.51
1:C:93:THR:O	1:C:97:LEU:HG	2.09	0.51
1:D:361:THR:CG2	1:D:362:ALA:N	2.73	0.51
1:A:328:THR:HG23	1:A:367:ILE:HB	1.91	0.51
1:B:384:HIS:HB3	1:B:412:THR:CG2	2.38	0.51
1:C:340:GLU:OE2	1:C:384:HIS:HE1	1.94	0.51
1:C:404:LEU:HD22	1:C:407:ALA:HB2	1.92	0.51
1:A:127:LEU:C	1:A:127:LEU:HD23	2.30	0.51
1:B:262:ARG:HD2	4:B:1643:HOH:O	2.09	0.51
1:D:245:ILE:HG22	1:D:396:LEU:HD11	1.91	0.51
1:A:50:SER:O	1:A:54:VAL:HG23	2.10	0.51
1:A:228:VAL:HG23	1:A:228:VAL:O	2.10	0.51
1:A:284:VAL:HG22	1:B:284:VAL:HA	1.91	0.51
1:B:40:TYR:HE1	1:B:226:LYS:HG3	1.76	0.51
1:C:284:VAL:HG12	1:D:284:VAL:HA	1.92	0.51
1:D:5:THR:HG22	1:D:6:ASN:H	1.76	0.51
1:D:19:ASP:HA	1:D:232:ASP:CB	2.39	0.51
1:A:167:ALA:CB	1:A:193:ARG:HG2	2.40	0.51
1:A:237:ALA:HB1	1:A:316:ILE:HD13	1.91	0.51
1:B:193:ARG:NH1	1:B:262:ARG:NE	2.58	0.51
1:C:425:ILE:O	1:C:425:ILE:HG22	2.10	0.51
1:B:245:ILE:HD13	1:B:320:LEU:HD23	1.92	0.51
1:C:250:ARG:HG3	4:C:1732:HOH:O	2.10	0.51
1:D:8:ARG:HG3	1:D:8:ARG:HH11	1.76	0.51
1:B:250:ARG:C	1:B:251:LEU:HD12	2.31	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340:GLU:OE2	1:B:384:HIS:HE1	1.94	0.51
1:C:156:ARG:NH2	1:C:159:HIS:HD2	2.09	0.50
1:D:385:ARG:HD2	2:D:1728:GPJ:O5	2.11	0.50
1:A:11:HIS:HB2	1:A:427:GLY:OXT	2.11	0.50
1:C:25:ARG:CZ	1:C:193:ARG:NH1	2.74	0.50
1:C:282:ASP:OD1	1:C:284:VAL:HG22	2.12	0.50
1:A:19:ASP:HA	1:A:232:ASP:CB	2.42	0.50
1:B:321:ALA:HB1	1:B:328:THR:OG1	2.11	0.50
1:D:105:ALA:HB1	1:D:107:PHE:CZ	2.46	0.50
1:D:122:MET:HB2	1:D:143:ASP:O	2.10	0.50
1:D:233:ILE:CD1	1:D:233:ILE:N	2.70	0.50
1:D:343:ARG:NH2	1:D:385:ARG:HG3	2.25	0.50
1:C:105:ALA:HB1	1:C:107:PHE:CZ	2.46	0.50
1:B:316:ILE:HG23	4:B:1544:HOH:O	2.12	0.50
1:A:384:HIS:HD2	1:A:413:SER:OG	1.95	0.50
1:A:245:ILE:HG21	1:A:396:LEU:CD1	2.42	0.49
1:B:262:ARG:HG3	1:B:262:ARG:NH1	2.28	0.49
1:C:25:ARG:CZ	1:C:193:ARG:NH2	2.75	0.49
1:C:193:ARG:NH2	1:C:195:HIS:ND1	2.60	0.49
1:D:97:LEU:HD22	1:D:171:SER:HB2	1.94	0.49
1:A:53:GLN:NE2	1:A:56:ARG:HE	2.11	0.49
1:B:15:ARG:HH11	1:B:15:ARG:HB3	1.77	0.49
1:B:121:PRO:CD	1:B:338:VAL:HG23	2.40	0.49
1:D:130:LYS:HD2	1:D:134:VAL:O	2.12	0.49
1:A:159:HIS:CD2	1:A:185:VAL:HG22	2.48	0.49
1:A:142:ARG:HB2	1:A:144:LEU:HD11	1.95	0.49
1:B:93:THR:O	1:B:97:LEU:HG	2.13	0.49
1:B:43:LEU:HD12	1:B:48:VAL:CG2	2.41	0.49
1:B:245:ILE:CG2	1:B:396:LEU:HD11	2.42	0.49
1:C:122:MET:O	1:C:126:THR:HG23	2.13	0.49
1:D:13:ILE:HG12	1:D:252:VAL:HG13	1.93	0.49
1:A:412:THR:HG21	4:A:1467:HOH:O	2.12	0.49
1:D:7:ILE:CD1	1:D:425:ILE:HD13	2.42	0.49
1:D:9:HIS:CD2	1:D:10:LEU:N	2.80	0.49
1:A:24:HIS:CD2	1:A:51:THR:OG1	2.65	0.48
1:B:193:ARG:CZ	1:B:262:ARG:NE	2.62	0.48
1:C:206:HIS:HE1	4:C:1764:HOH:O	1.95	0.48
1:D:380:THR:HG22	1:D:383:ASP:N	2.27	0.48
1:B:238:PHE:CE2	1:B:316:ILE:CG2	2.96	0.48
1:C:19:ASP:HA	1:C:232:ASP:HB2	1.95	0.48
1:C:270:ARG:HG3	1:C:270:ARG:HH11	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:TYR:CE1	1:A:226:LYS:HG3	2.47	0.48
1:B:164:ILE:HD13	1:B:164:ILE:N	2.27	0.48
1:C:140:THR:HG22	1:C:142:ARG:H	1.79	0.48
1:B:244:LEU:CD2	1:B:292:VAL:HG23	2.44	0.48
1:C:195:HIS:HE1	1:C:262:ARG:HD2	1.78	0.48
1:B:127:LEU:HD23	1:B:127:LEU:C	2.33	0.48
1:B:376:ALA:O	1:B:402:VAL:HA	2.13	0.48
1:C:97:LEU:HD22	1:C:171:SER:HB2	1.95	0.48
1:C:277:GLU:HG2	1:C:279:THR:HG23	1.96	0.48
1:C:305:ALA:N	4:C:1636:HOH:O	2.46	0.48
1:D:5:THR:HG22	1:D:397:VAL:O	2.13	0.48
1:D:7:ILE:HD11	1:D:425:ILE:HD13	1.94	0.48
1:D:245:ILE:HD11	1:D:320:LEU:HD12	1.95	0.48
1:A:343:ARG:HH22	1:A:385:ARG:HG3	1.75	0.48
1:B:251:LEU:HD12	1:B:251:LEU:N	2.29	0.48
1:B:167:ALA:CB	1:B:193:ARG:HG2	2.44	0.48
1:C:252:VAL:O	1:C:252:VAL:HG23	2.13	0.48
1:A:47:ASP:OD2	1:A:412:THR:OG1	2.31	0.48
1:B:195:HIS:HD2	4:B:1553:HOH:O	1.97	0.48
1:A:167:ALA:HB2	1:A:193:ARG:HG2	1.96	0.47
1:A:245:ILE:N	1:A:245:ILE:CD1	2.77	0.47
1:B:262:ARG:NH1	4:B:1563:HOH:O	2.47	0.47
1:B:279:THR:HG23	1:B:280:GLU:HG3	1.95	0.47
1:C:355:GLY:O	1:C:356:ALA:HB3	2.14	0.47
1:C:121:PRO:CD	1:C:338:VAL:HG13	2.43	0.47
1:D:233:ILE:HG13	1:D:257:GLY:O	2.13	0.47
1:D:361:THR:HG22	1:D:362:ALA:H	1.79	0.47
1:B:122:MET:O	1:B:125:VAL:HG12	2.14	0.47
1:B:262:ARG:HG3	1:B:262:ARG:HH11	1.79	0.47
1:C:110:GLU:HG3	4:C:1778:HOH:O	2.14	0.47
1:C:412:THR:HG21	4:C:1663:HOH:O	2.13	0.47
1:D:48:VAL:O	1:D:51:THR:HG22	2.15	0.47
1:D:140:THR:CG2	1:D:141:GLU:H	2.28	0.47
1:D:341:THR:CG2	1:D:383:ASP:HB2	2.43	0.47
1:A:52:MET:CE	1:A:69:ILE:HD12	2.44	0.47
1:A:149:LEU:HD23	1:A:149:LEU:C	2.35	0.47
1:A:298:LYS:HD3	1:A:298:LYS:N	2.30	0.47
1:B:335:GLU:O	1:B:338:VAL:HG12	2.13	0.47
1:C:164:ILE:HD13	1:C:164:ILE:N	2.29	0.47
1:C:325:GLN:HB2	4:C:1757:HOH:O	2.13	0.47
1:A:335:GLU:O	1:A:338:VAL:HG12	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:TYR:CE1	1:B:226:LYS:HG3	2.49	0.47
1:B:134:VAL:HG11	1:B:136:ILE:HD11	1.97	0.47
1:C:7:ILE:HG21	1:C:395:LEU:HG	1.97	0.47
1:C:424:LEU:C	1:C:426:HIS:H	2.17	0.47
1:D:188:GLU:HG2	4:D:1792:HOH:O	2.14	0.47
1:D:355:GLY:O	1:D:356:ALA:HB3	2.15	0.47
1:B:184:SER:HB2	1:B:216:VAL:HG13	1.96	0.47
1:D:401:GLU:OE1	1:D:401:GLU:HA	2.15	0.47
1:C:304:GLY:O	1:C:306:LEU:N	2.43	0.47
1:A:144:LEU:HD12	1:A:144:LEU:N	2.30	0.46
1:C:368:LYS:O	1:C:369:GLY:O	2.33	0.46
1:C:127:LEU:C	1:C:127:LEU:HD23	2.35	0.46
1:C:404:LEU:HD23	1:C:405:ASP:N	2.30	0.46
1:D:140:THR:CG2	1:D:141:GLU:N	2.78	0.46
1:A:83:GLN:NE2	1:A:84:ASN:H	2.13	0.46
1:C:384:HIS:HD2	1:C:413:SER:OG	1.98	0.46
1:D:77:ALA:HA	4:D:1816:HOH:O	2.14	0.46
1:C:127:LEU:HB3	1:C:128:PRO:CD	2.45	0.46
1:D:259:ASN:HD22	1:D:261:THR:N	2.10	0.46
1:A:303:CYS:O	1:A:304:GLY:O	2.33	0.46
1:D:161:GLU:HG2	1:D:187:ILE:HB	1.97	0.46
1:A:394:ALA:HB2	1:A:402:VAL:HG11	1.97	0.46
1:A:396:LEU:HB2	4:A:1667:HOH:O	2.15	0.46
1:D:134:VAL:CG1	1:D:149:LEU:HD11	2.46	0.46
1:A:5:THR:OG1	1:A:397:VAL:HB	2.16	0.46
1:A:304:GLY:O	1:A:305:ALA:HB3	2.16	0.46
1:C:122:MET:HG3	1:C:147:LEU:HD11	1.98	0.46
1:C:284:VAL:CG1	1:D:284:VAL:HG22	2.46	0.46
1:D:292:VAL:HG22	1:D:293:GLU:N	2.30	0.46
1:A:53:GLN:NE2	1:A:56:ARG:HH21	2.14	0.46
1:A:238:PHE:CE2	1:A:316:ILE:CG2	2.98	0.46
1:B:380:THR:HG21	1:B:409:ALA:CB	2.44	0.46
1:C:13:ILE:HA	1:C:252:VAL:CG2	2.46	0.46
1:C:181:LYS:N	1:C:181:LYS:CD	2.76	0.46
1:C:244:LEU:HG	1:C:292:VAL:CG1	2.46	0.46
1:B:245:ILE:CD1	1:B:320:LEU:HD23	2.45	0.45
1:B:272:MET:SD	1:B:320:LEU:HD13	2.56	0.45
1:D:4:LYS:HB2	1:D:4:LYS:HZ2	1.80	0.45
1:B:15:ARG:HB3	1:B:15:ARG:NH1	2.31	0.45
1:C:7:ILE:O	1:C:7:ILE:HG23	2.15	0.45
1:D:134:VAL:HG12	1:D:136:ILE:HG12	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:GLN:CD	1:A:83:GLN:N	2.69	0.45
1:A:233:ILE:CG1	1:A:257:GLY:O	2.62	0.45
1:B:127:LEU:HB3	1:B:128:PRO:CD	2.46	0.45
1:B:241:VAL:HG22	1:B:320:LEU:HG	1.99	0.45
1:C:297:LEU:HD13	1:C:320:LEU:CD2	2.42	0.45
1:D:379:ASN:HD22	1:D:381:PHE:H	1.64	0.45
1:A:265:ILE:CD1	1:A:316:ILE:HD11	2.46	0.45
1:D:331:LYS:O	1:D:332:ASP:HB2	2.16	0.45
1:D:427:GLY:HA2	4:D:1777:HOH:O	2.17	0.45
1:B:43:LEU:HD12	1:B:48:VAL:HG23	1.99	0.45
1:C:7:ILE:HG22	1:C:395:LEU:O	2.17	0.45
1:C:25:ARG:CZ	1:C:193:ARG:CZ	2.94	0.45
1:D:330:ILE:O	1:D:364:GLY:HA3	2.16	0.45
1:B:53:GLN:HE21	1:B:56:ARG:HH21	1.65	0.45
1:B:319:LEU:HD12	1:B:392:ILE:HG23	1.98	0.45
1:D:372:ALA:O	1:D:373:LEU:CB	2.64	0.45
1:B:105:ALA:HB1	1:B:107:PHE:CZ	2.51	0.45
1:B:282:ASP:OD1	1:B:284:VAL:HB	2.17	0.45
1:A:129:LEU:HD12	1:A:129:LEU:HA	1.87	0.45
1:C:98:ILE:O	1:C:102:LEU:HD13	2.16	0.45
1:C:123:ASP:HA	1:C:126:THR:OG1	2.17	0.45
1:A:121:PRO:HD2	1:A:338:VAL:HG23	1.97	0.45
1:A:307:ILE:HG12	4:A:1658:HOH:O	2.17	0.45
1:A:53:GLN:HE21	1:A:56:ARG:HH21	1.63	0.45
1:A:185:VAL:O	1:A:185:VAL:HG23	2.17	0.45
1:B:384:HIS:HD2	1:B:413:SER:OG	2.00	0.45
1:C:250:ARG:HH21	1:C:250:ARG:CG	2.30	0.45
1:C:379:ASN:HD22	1:C:379:ASN:C	2.17	0.45
1:D:5:THR:CG2	1:D:6:ASN:N	2.80	0.45
1:D:74:VAL:O	1:D:78:GLY:HA3	2.16	0.45
1:C:244:LEU:HG	1:C:292:VAL:HG11	1.98	0.44
1:D:355:GLY:N	4:D:1865:HOH:O	2.50	0.44
1:A:43:LEU:HD12	1:A:48:VAL:HG21	1.99	0.44
1:C:74:VAL:O	1:C:78:GLY:HA3	2.17	0.44
1:C:359:THR:OG1	1:C:366:ILE:HB	2.17	0.44
1:D:316:ILE:HG13	1:D:317:ILE:N	2.31	0.44
1:B:142:ARG:HD2	4:B:1709:HOH:O	2.17	0.44
1:B:341:THR:HG23	1:B:383:ASP:HB2	1.99	0.44
1:C:136:ILE:CG2	1:C:149:LEU:HD23	2.47	0.44
1:A:17:PRO:HB2	1:A:43:LEU:HD23	2.00	0.44
1:D:145:PRO:HA	1:D:147:LEU:HD13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:167:ALA:CB	1:D:193:ARG:HG2	2.48	0.44
1:A:34:GLU:HG2	1:A:75:GLY:HA2	2.00	0.44
1:A:325:GLN:NE2	1:A:370:LYS:CG	2.75	0.44
1:B:149:LEU:HD23	1:B:150:LYS:N	2.32	0.44
1:B:316:ILE:HD12	1:B:316:ILE:C	2.38	0.44
1:C:331:LYS:O	1:C:332:ASP:HB2	2.17	0.44
1:D:258:ILE:O	1:D:258:ILE:CG2	2.58	0.44
1:D:361:THR:CG2	1:D:362:ALA:H	2.31	0.44
1:A:134:VAL:HG11	1:A:136:ILE:HD11	2.00	0.44
1:C:136:ILE:HA	1:C:148:ARG:O	2.18	0.44
1:D:9:HIS:CD2	1:D:248:ASN:O	2.70	0.44
1:D:48:VAL:O	1:D:51:THR:CG2	2.66	0.44
1:D:50:SER:O	1:D:54:VAL:HG23	2.17	0.44
1:A:8:ARG:HH11	1:A:8:ARG:HG3	1.82	0.44
1:A:22:ILE:HA	1:A:199:MET:HE1	2.00	0.43
1:B:368:LYS:O	1:B:369:GLY:O	2.36	0.43
1:D:88:MET:HG3	1:D:95:ILE:HB	2.00	0.43
1:A:340:GLU:OE2	1:A:384:HIS:HE1	2.01	0.43
1:B:149:LEU:HD23	1:B:149:LEU:C	2.39	0.43
1:C:24:HIS:CD2	1:C:51:THR:OG1	2.69	0.43
1:C:25:ARG:NH1	1:C:193:ARG:NH2	2.66	0.43
1:D:370:LYS:HD2	1:D:370:LYS:HA	1.79	0.43
1:B:319:LEU:O	1:B:322:THR:HB	2.17	0.43
1:B:379:ASN:HD22	1:B:381:PHE:N	2.07	0.43
1:A:142:ARG:HB2	1:A:144:LEU:CD1	2.48	0.43
1:A:253:LEU:N	1:A:253:LEU:CD2	2.79	0.43
1:B:53:GLN:NE2	1:B:56:ARG:HH21	2.16	0.43
1:D:233:ILE:CG1	1:D:257:GLY:O	2.66	0.43
1:B:299:GLY:HA2	1:B:328:THR:CG2	2.48	0.43
1:C:326:GLY:O	1:C:369:GLY:N	2.51	0.43
1:C:412:THR:HG23	4:C:1686:HOH:O	2.19	0.43
1:C:25:ARG:NH2	1:C:193:ARG:CZ	2.82	0.43
1:D:43:LEU:HG	1:D:45:GLY:H	1.83	0.43
1:A:379:ASN:HD22	1:A:381:PHE:N	2.09	0.43
1:D:153:LYS:H	1:D:153:LYS:HG2	1.64	0.43
1:B:305:ALA:O	1:B:308:PRO:HD2	2.18	0.42
1:A:134:VAL:HG12	1:A:136:ILE:HG13	2.00	0.42
1:C:284:VAL:CG2	1:C:285:ALA:H	2.31	0.42
1:A:314:LEU:HD23	1:A:314:LEU:HA	1.89	0.42
1:C:102:LEU:HD23	1:C:109:VAL:HG21	2.01	0.42
1:C:139:GLN:O	1:C:140:THR:CB	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:209:VAL:HG23	1:D:209:VAL:O	2.19	0.42
1:D:215:THR:HG22	4:D:1768:HOH:O	2.18	0.42
1:B:43:LEU:HD13	1:B:43:LEU:C	2.40	0.42
1:B:53:GLN:NE2	1:B:56:ARG:HE	2.16	0.42
1:B:167:ALA:HB2	1:B:193:ARG:HG2	2.01	0.42
1:C:38:LYS:N	1:C:38:LYS:HD2	2.34	0.42
1:D:250:ARG:HA	1:D:292:VAL:O	2.20	0.42
1:A:131:LYS:HB3	1:A:131:LYS:HE2	1.83	0.42
1:A:401:GLU:HB2	4:A:1610:HOH:O	2.19	0.42
1:C:128:PRO:O	1:C:131:LYS:HB2	2.20	0.42
1:D:14:ILE:HD11	1:D:424:LEU:CD1	2.50	0.42
1:D:144:LEU:N	1:D:144:LEU:HD12	2.34	0.42
1:A:144:LEU:N	1:A:144:LEU:CD1	2.83	0.42
1:C:318:ALA:O	1:C:322:THR:HG23	2.20	0.42
1:D:399:ASP:OD1	1:D:400:GLY:N	2.53	0.42
1:C:15:ARG:HB3	1:C:15:ARG:NH1	2.35	0.42
1:C:140:THR:CG2	1:C:141:GLU:N	2.83	0.42
1:C:210:ASP:HB3	1:C:213:LYS:CG	2.49	0.42
1:C:292:VAL:CG1	1:C:293:GLU:N	2.82	0.42
1:D:4:LYS:HZ1	1:D:4:LYS:N	2.07	0.42
1:B:5:THR:OG1	1:B:397:VAL:HB	2.19	0.42
1:B:52:MET:HE3	1:B:69:ILE:HD12	2.02	0.42
1:B:326:GLY:H	1:B:369:GLY:HA2	1.85	0.42
1:C:245:ILE:HG23	1:C:396:LEU:HD21	2.02	0.42
1:D:49:LEU:HD12	1:D:52:MET:HE3	2.02	0.42
1:B:127:LEU:HB3	1:B:128:PRO:HD3	2.00	0.42
1:B:406:ARG:HG2	4:B:1719:HOH:O	2.18	0.42
1:C:351:LEU:HB2	1:C:358:ILE:HD12	2.01	0.42
1:A:123:ASP:HA	1:A:126:THR:OG1	2.21	0.41
1:A:127:LEU:HB3	1:A:128:PRO:CD	2.49	0.41
1:A:356:ALA:HB1	1:A:357:ASP:H	1.45	0.41
1:C:136:ILE:HD12	1:C:136:ILE:N	2.34	0.41
1:C:193:ARG:HA	1:C:261:THR:OG1	2.20	0.41
1:C:284:VAL:CG2	1:C:285:ALA:N	2.82	0.41
1:A:14:ILE:HG12	1:A:424:LEU:HD21	2.02	0.41
1:A:121:PRO:CD	1:A:338:VAL:CG2	2.98	0.41
1:A:319:LEU:HD22	4:A:1454:HOH:O	2.20	0.41
1:B:356:ALA:HB1	1:B:357:ASP:H	1.50	0.41
1:C:13:ILE:HG23	1:C:252:VAL:HG23	2.03	0.41
1:C:21:SER:HB3	1:C:193:ARG:HH22	1.79	0.41
1:C:108:GLU:HA	1:C:149:LEU:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:195:HIS:HD2	4:C:1676:HOH:O	2.02	0.41
1:D:7:ILE:HD12	1:D:7:ILE:HA	1.95	0.41
1:B:52:MET:CE	1:B:69:ILE:HD12	2.50	0.41
1:C:25:ARG:NH1	1:C:193:ARG:HH22	2.19	0.41
1:C:126:THR:O	1:C:130:LYS:HG3	2.21	0.41
1:D:331:LYS:HA	1:D:363:ASP:O	2.20	0.41
1:A:109:VAL:HG22	1:A:110:GLU:N	2.35	0.41
1:B:279:THR:OG1	1:B:280:GLU:N	2.54	0.41
1:C:265:ILE:O	1:C:269:ILE:HG13	2.20	0.41
1:C:272:MET:SD	1:C:320:LEU:CD2	3.08	0.41
1:C:314:LEU:HD13	1:C:336:LEU:HD11	2.03	0.41
1:A:53:GLN:HE22	1:A:56:ARG:HE	1.68	0.41
1:B:54:VAL:HG11	1:B:98:ILE:HD13	2.02	0.41
1:A:245:ILE:CG2	1:A:396:LEU:CD1	2.99	0.41
1:C:6:ASN:O	1:C:7:ILE:HG22	2.20	0.41
1:C:352:ASN:OD1	1:C:356:ALA:HA	2.21	0.41
1:D:167:ALA:HB2	1:D:192:THR:HB	2.03	0.41
1:C:25:ARG:NH2	1:C:193:ARG:NH1	2.68	0.41
1:D:108:GLU:HA	1:D:149:LEU:O	2.21	0.41
1:D:238:PHE:CE2	1:D:316:ILE:CG2	3.04	0.41
1:B:276:LEU:HD13	1:B:276:LEU:C	2.41	0.41
1:B:394:ALA:HB2	1:B:402:VAL:HG11	2.02	0.41
1:C:320:LEU:CD2	1:C:320:LEU:C	2.89	0.41
1:C:330:ILE:O	1:C:364:GLY:HA3	2.19	0.41
1:A:260:GLU:CD	1:A:260:GLU:N	2.72	0.41
1:A:401:GLU:HG2	4:A:1610:HOH:O	2.20	0.41
1:C:320:LEU:HD23	1:C:320:LEU:C	2.42	0.41
1:D:103:ALA:CB	1:D:155:LEU:HD11	2.51	0.41
1:D:149:LEU:HD12	1:D:150:LYS:H	1.86	0.41
1:D:164:ILE:CD1	1:D:165:ALA:H	2.28	0.41
1:A:122:MET:HB2	1:A:143:ASP:O	2.21	0.41
1:C:221:LYS:N	1:C:221:LYS:CD	2.84	0.41
1:A:97:LEU:HD22	1:A:171:SER:HB2	2.03	0.40
1:A:250:ARG:HA	1:A:292:VAL:O	2.21	0.40
1:A:328:THR:HG23	1:A:328:THR:O	2.21	0.40
1:C:155:LEU:H	1:C:181:LYS:NZ	2.20	0.40
1:C:193:ARG:CZ	1:C:195:HIS:HB2	2.49	0.40
1:D:123:ASP:HA	1:D:126:THR:OG1	2.21	0.40
1:B:330:ILE:O	1:B:364:GLY:HA3	2.20	0.40
1:B:331:LYS:O	1:B:332:ASP:HB2	2.21	0.40
1:B:377:ARG:NH1	4:B:1723:HOH:O	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:21:SER:CB	1:C:193:ARG:HH21	2.28	0.40
1:D:354:MET:O	1:D:374:HIS:N	2.44	0.40
1:A:384:HIS:CD2	1:A:413:SER:OG	2.74	0.40
1:B:21:SER:CB	1:B:262:ARG:NH2	2.84	0.40
1:B:314:LEU:HD23	1:B:314:LEU:HA	1.85	0.40
1:C:44:ARG:HH11	1:C:44:ARG:CG	2.33	0.40
1:C:50:SER:O	1:C:54:VAL:HG23	2.21	0.40
1:D:155:LEU:O	1:D:181:LYS:HE2	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	425/427 (100%)	409 (96%)	12 (3%)	4 (1%)	17	7
1	B	425/427 (100%)	407 (96%)	13 (3%)	5 (1%)	13	4
1	C	425/427 (100%)	399 (94%)	18 (4%)	8 (2%)	8	1
1	D	425/427 (100%)	402 (95%)	16 (4%)	7 (2%)	9	2
All	All	1700/1708 (100%)	1617 (95%)	59 (4%)	24 (1%)	11	3

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	76	MET
1	A	304	GLY
1	B	356	ALA
1	B	357	ASP
1	C	7	ILE
1	C	304	GLY
1	C	369	GLY

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Mol	Chain	Res	Type
1	A	357	ASP
1	A	370	LYS
1	B	369	GLY
1	C	211	GLY
1	D	370	LYS
1	D	400	GLY
1	B	284	VAL
1	B	426	HIS
1	C	6	ASN
1	C	399	ASP
1	C	426	HIS
1	D	312	ASP
1	D	373	LEU
1	C	373	LEU
1	D	356	ALA
1	D	284	VAL
1	D	355	GLY

### 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	350/350 (100%)	331 (95%)	19 (5%)	22	13
1	B	350/350 (100%)	330 (94%)	20 (6%)	20	11
1	C	350/350 (100%)	332 (95%)	18 (5%)	24	14
1	D	350/350 (100%)	330 (94%)	20 (6%)	20	11
All	All	1400/1400 (100%)	1323 (94%)	77 (6%)	21	12

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	LEU
1	A	79	LEU
1	A	117	LEU
1	A	129	LEU

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Mol	Chain	Res	Type
1	A	141	GLU
1	A	161	GLU
1	A	173	LEU
1	A	178	LEU
1	A	193	ARG
1	A	233	ILE
1	A	260	GLU
1	A	270	ARG
1	A	290	LEU
1	A	298	LYS
1	A	310	LEU
1	A	319	LEU
1	A	379	ASN
1	A	404	LEU
1	A	414	TYR
1	B	83	GLN
1	B	88	MET
1	B	102	LEU
1	B	117	LEU
1	B	129	LEU
1	B	141	GLU
1	B	164	ILE
1	B	178	LEU
1	B	193	ARG
1	B	259	ASN
1	B	270	ARG
1	B	290	LEU
1	B	310	LEU
1	B	319	LEU
1	B	320	LEU
1	B	322	THR
1	B	368	LYS
1	B	379	ASN
1	B	404	LEU
1	B	414	TYR
1	C	43	LEU
1	C	46	GLU
1	C	58	LEU
1	C	80	LYS
1	C	117	LEU
1	C	124	ARG
1	C	129	LEU

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Mol	Chain	Res	Type
1	C	136	ILE
1	C	156	ARG
1	C	161	GLU
1	C	164	ILE
1	C	178	LEU
1	C	193	ARG
1	C	310	LEU
1	C	320	LEU
1	C	328	THR
1	C	379	ASN
1	C	414	TYR
1	D	4	LYS
1	D	6	ASN
1	D	110	GLU
1	D	136	ILE
1	D	161	GLU
1	D	181	LYS
1	D	193	ARG
1	D	233	ILE
1	D	259	ASN
1	D	290	LEU
1	D	310	LEU
1	D	314	LEU
1	D	319	LEU
1	D	357	ASP
1	D	379	ASN
1	D	385	ARG
1	D	404	LEU
1	D	412	THR
1	D	414	TYR
1	D	425	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	9	HIS
1	A	24	HIS
1	A	53	GLN
1	A	72	GLN
1	A	83	GLN
1	A	84	ASN

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Mol	Chain	Res	Type
1	A	159	HIS
1	A	195	HIS
1	A	220	GLN
1	A	325	GLN
1	A	379	ASN
1	A	384	HIS
1	B	6	ASN
1	B	11	HIS
1	B	24	HIS
1	B	53	GLN
1	B	84	ASN
1	B	139	GLN
1	B	159	HIS
1	B	195	HIS
1	B	259	ASN
1	B	323	GLN
1	B	379	ASN
1	B	384	HIS
1	C	24	HIS
1	C	53	GLN
1	C	84	ASN
1	C	90	ASN
1	C	139	GLN
1	C	159	HIS
1	C	201	GLN
1	C	202	GLN
1	C	217	GLN
1	C	220	GLN
1	C	379	ASN
1	C	384	HIS
1	C	411	ASN
1	D	6	ASN
1	D	9	HIS
1	D	53	GLN
1	D	84	ASN
1	D	90	ASN
1	D	195	HIS
1	D	202	GLN
1	D	259	ASN
1	D	323	GLN
1	D	379	ASN
1	D	384	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

8 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	GPJ	D	1728	-	9,9,9	1.68	2 (22%)	9,12,12	1.26	1 (11%)
3	S3P	C	1629	-	15,16,16	2.44	6 (40%)	21,24,24	1.24	2 (9%)
2	GPJ	C	1628	-	9,9,9	1.84	2 (22%)	9,12,12	1.26	1 (11%)
2	GPJ	A	1428	-	9,9,9	1.72	2 (22%)	9,12,12	1.45	1 (11%)
3	S3P	A	1429	-	15,16,16	2.50	6 (40%)	21,24,24	1.20	2 (9%)
3	S3P	D	1729	-	15,16,16	2.57	6 (40%)	21,24,24	1.23	2 (9%)
2	GPJ	B	1528	-	9,9,9	1.74	2 (22%)	9,12,12	1.34	1 (11%)
3	S3P	B	1529	-	15,16,16	2.54	5 (33%)	21,24,24	1.16	1 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GPJ	D	1728	-	-	0/7/7/7	-
3	S3P	C	1629	-	-	0/9/25/25	0/1/1/1
2	GPJ	C	1628	-	-	0/7/7/7	-
2	GPJ	A	1428	-	-	0/7/7/7	-
3	S3P	A	1429	-	-	0/9/25/25	0/1/1/1
3	S3P	D	1729	-	-	0/9/25/25	0/1/1/1
2	GPJ	B	1528	-	-	0/7/7/7	-
3	S3P	B	1529	-	-	0/9/25/25	0/1/1/1

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1729	S3P	P1-O1	6.13	1.70	1.59
3	B	1529	S3P	P1-O1	5.89	1.69	1.59
3	A	1429	S3P	P1-O1	5.79	1.69	1.59
3	C	1629	S3P	P1-O1	5.58	1.69	1.59
3	B	1529	S3P	C2-C1	4.29	1.43	1.33
3	D	1729	S3P	C2-C1	4.22	1.43	1.33
3	A	1429	S3P	C2-C1	4.15	1.42	1.33
3	C	1629	S3P	C2-C1	4.09	1.42	1.33
3	B	1529	S3P	C4-C3	3.84	1.59	1.52
2	C	1628	GPJ	P1-O2	-3.74	1.46	1.55
3	D	1729	S3P	C4-C3	3.66	1.58	1.52
3	C	1629	S3P	C4-C3	3.57	1.58	1.52
3	A	1429	S3P	C4-C3	3.55	1.58	1.52
2	A	1428	GPJ	P1-O2	-3.54	1.47	1.55
2	D	1728	GPJ	P1-O2	-3.52	1.47	1.55
2	B	1528	GPJ	P1-O2	-3.48	1.47	1.55
3	D	1729	S3P	C3-C2	3.20	1.54	1.50
3	C	1629	S3P	C6-C1	-3.07	1.46	1.51
3	A	1429	S3P	C6-C1	-3.05	1.46	1.51
3	D	1729	S3P	C6-C1	-3.02	1.46	1.51
2	C	1628	GPJ	P1-C1	-3.01	1.75	1.81
3	B	1529	S3P	C3-C2	3.01	1.54	1.50
3	A	1429	S3P	C3-C2	2.98	1.54	1.50
3	B	1529	S3P	C6-C1	-2.85	1.46	1.51
3	C	1629	S3P	C3-C2	2.70	1.53	1.50
2	A	1428	GPJ	P1-C1	-2.60	1.76	1.81
2	D	1728	GPJ	P1-C1	-2.51	1.76	1.81
2	B	1528	GPJ	P1-C1	-2.43	1.76	1.81
3	A	1429	S3P	C5-C4	2.39	1.56	1.52
3	C	1629	S3P	C5-C4	2.36	1.56	1.52
3	D	1729	S3P	C5-C4	2.23	1.55	1.52



All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1729	S3P	O5-C7-C1	-2.87	116.61	121.64
3	C	1629	S3P	O5-C7-C1	-2.80	116.73	121.64
3	A	1429	S3P	O5-C7-C1	-2.72	116.87	121.64
2	A	1428	GPJ	O2-P1-C1	-2.72	100.78	106.78
2	B	1528	GPJ	O2-P1-C1	-2.57	101.12	106.78
3	B	1529	S3P	O5-C7-C1	-2.45	117.34	121.64
3	D	1729	S3P	O1-C3-C4	2.34	111.46	106.80
2	C	1628	GPJ	O2-P1-C1	-2.32	101.65	106.78
3	C	1629	S3P	O1-C3-C4	2.23	111.24	106.80
2	D	1728	GPJ	O2-P1-C1	-2.19	101.94	106.78
3	A	1429	S3P	O1-C3-C4	2.05	110.90	106.80

There are no chirality outliers.

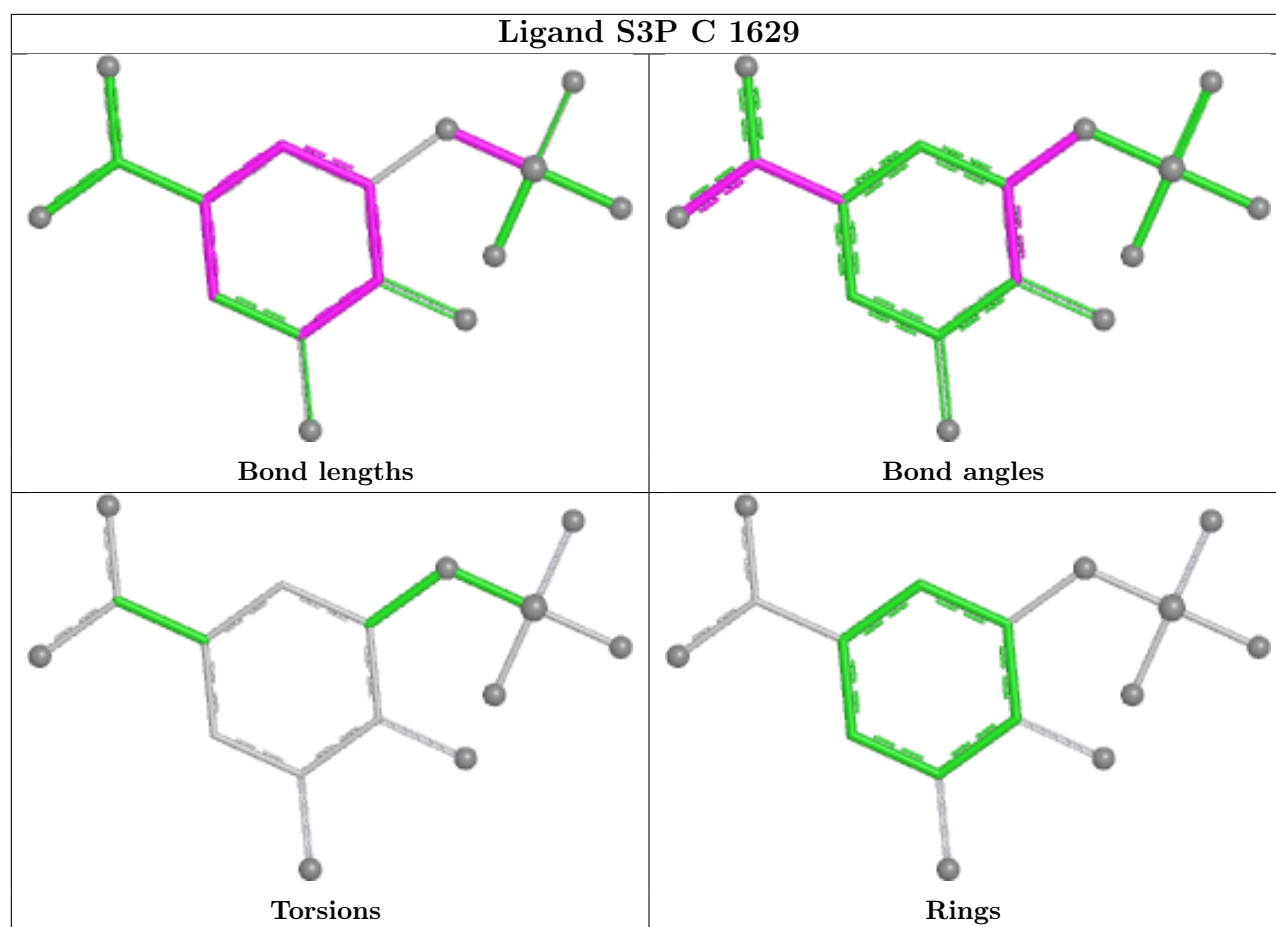
There are no torsion outliers.

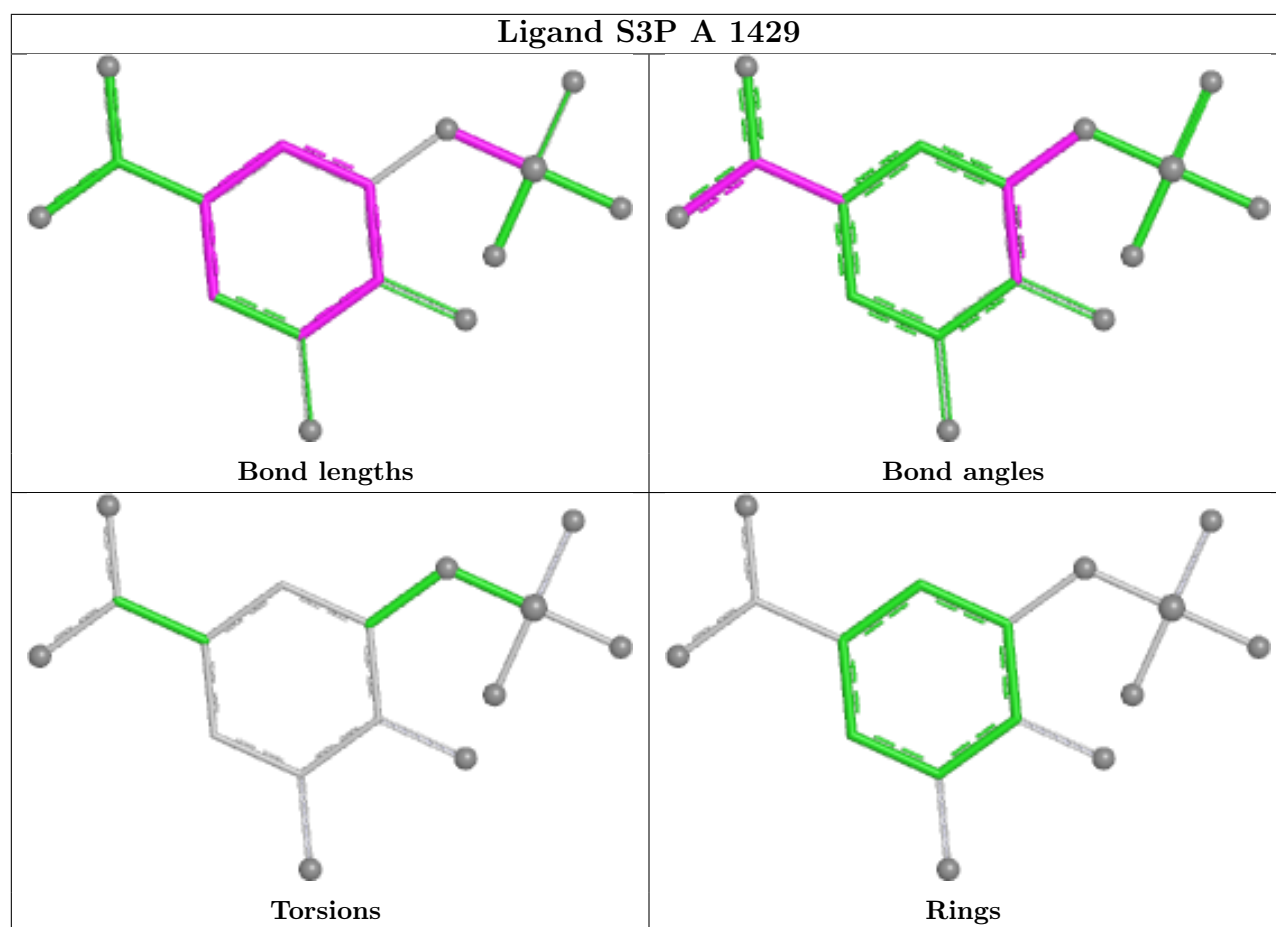
There are no ring outliers.

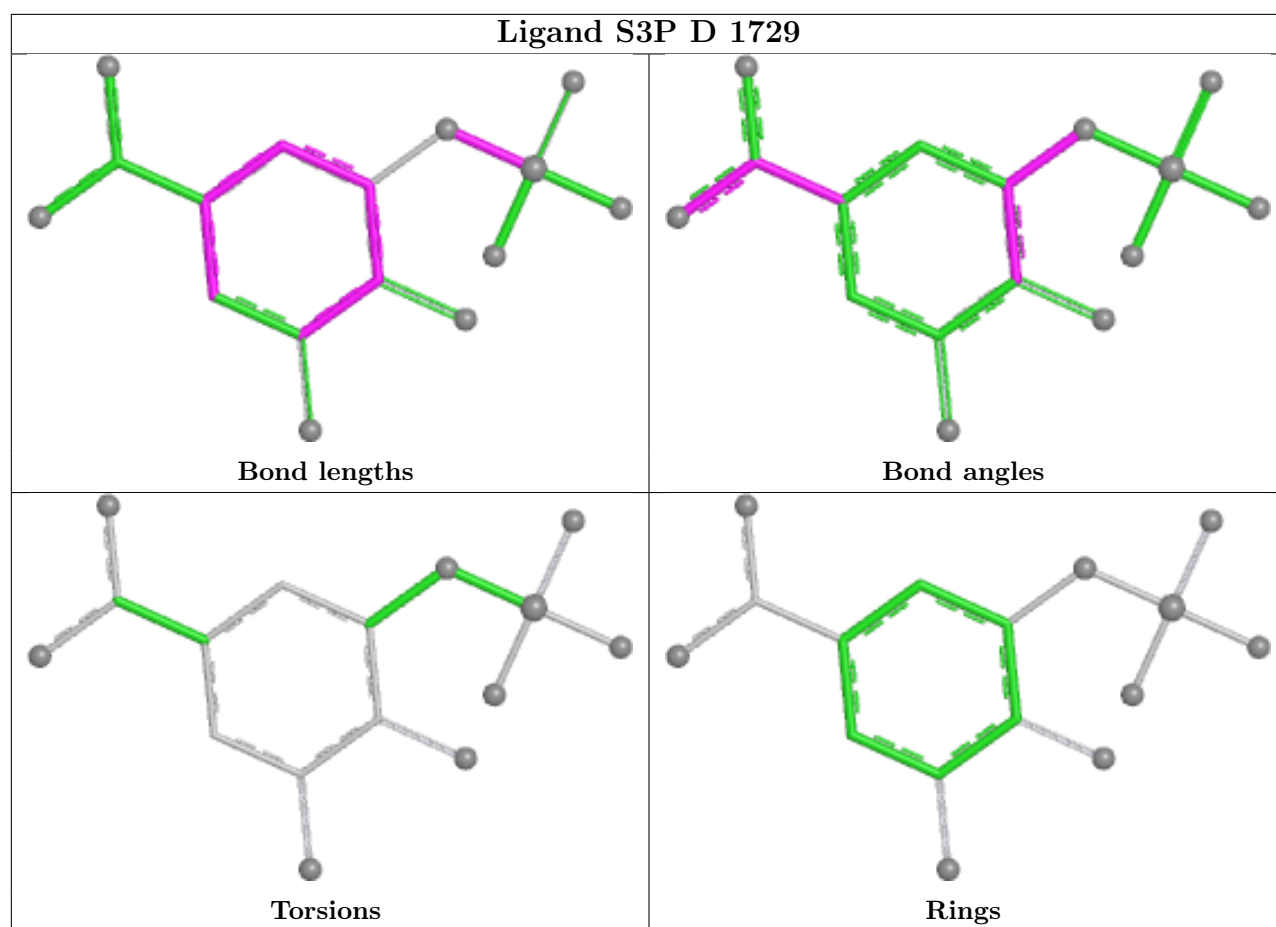
2 monomers are involved in 2 short contacts:

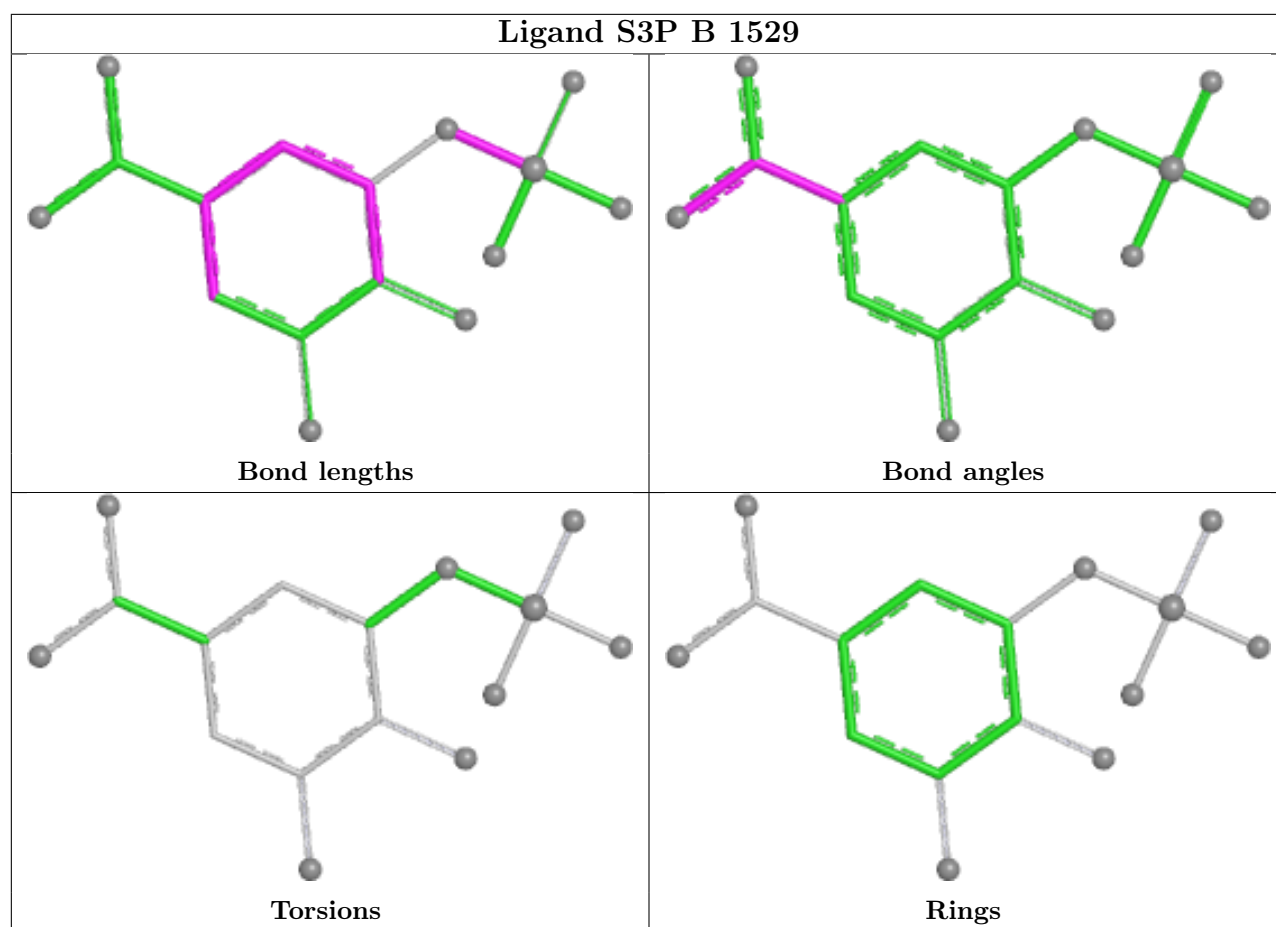
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1728	GPJ	1	0
2	A	1428	GPJ	1	0

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 [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 ⓘ

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	427/427 (100%)	0.01	9 (2%) 63 66	9, 15, 27, 46	0
1	B	427/427 (100%)	0.01	13 (3%) 50 53	8, 15, 29, 50	0
1	C	427/427 (100%)	0.25	20 (4%) 31 34	12, 21, 36, 59	0
1	D	427/427 (100%)	0.31	24 (5%) 24 27	11, 21, 35, 56	0
All	All	1708/1708 (100%)	0.15	66 (3%) 39 42	8, 18, 34, 59	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	427	GLY	10.1
1	A	356	ALA	7.5
1	B	356	ALA	7.5
1	C	426	HIS	7.4
1	C	427	GLY	7.2
1	B	427	GLY	6.1
1	A	284	VAL	5.5
1	D	284	VAL	5.5
1	D	425	ILE	5.4
1	C	369	GLY	5.3
1	B	284	VAL	5.3
1	B	369	GLY	5.0
1	C	9	HIS	5.0
1	C	284	VAL	5.0
1	B	426	HIS	4.9
1	C	283	PRO	4.7
1	A	426	HIS	4.6
1	C	355	GLY	4.6
1	D	356	ALA	4.6
1	B	285	ALA	4.2
1	C	425	ILE	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	426	HIS	3.9
1	D	355	GLY	3.7
1	D	9	HIS	3.7
1	D	285	ALA	3.7
1	D	399	ASP	3.6
1	A	427	GLY	3.6
1	C	399	ASP	3.4
1	B	283	PRO	3.4
1	D	152	THR	3.3
1	D	8	ARG	3.3
1	A	283	PRO	3.3
1	C	7	ILE	3.3
1	C	304	GLY	3.1
1	D	311	ILE	3.1
1	D	153	LYS	3.1
1	C	193	ARG	2.9
1	C	206	HIS	2.9
1	D	83	GLN	2.8
1	D	372	ALA	2.7
1	C	398	ALA	2.6
1	D	11	HIS	2.6
1	A	369	GLY	2.6
1	C	6	ASN	2.6
1	C	285	ALA	2.5
1	C	372	ALA	2.5
1	D	141	GLU	2.5
1	D	398	ALA	2.5
1	A	370	LYS	2.5
1	D	233	ILE	2.5
1	A	304	GLY	2.4
1	B	11	HIS	2.4
1	D	283	PRO	2.4
1	D	369	GLY	2.4
1	B	377	ARG	2.3
1	C	97	LEU	2.3
1	D	357	ASP	2.3
1	A	75	GLY	2.2
1	B	83	GLN	2.2
1	C	83	GLN	2.2
1	B	181	LYS	2.1
1	B	258	ILE	2.1
1	D	140	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	9	HIS	2.0
1	C	156	ARG	2.0
1	D	97	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 monosaccharides 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, 95<sup>th</sup> 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.

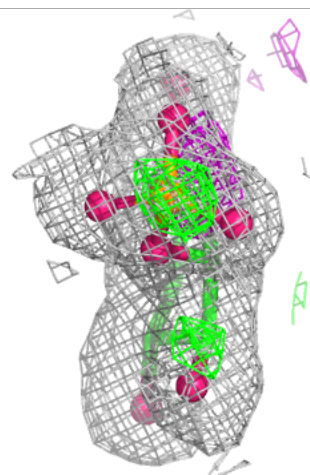
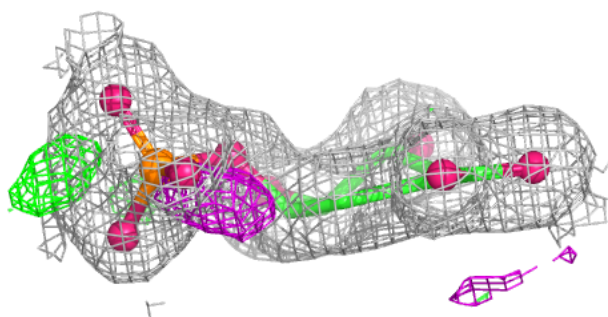
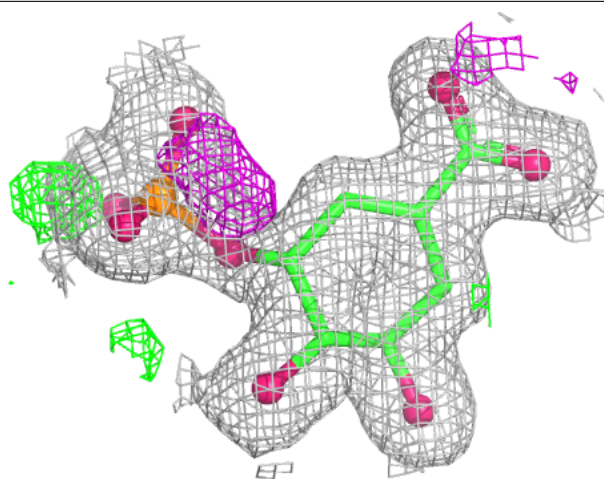
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	S3P	C	1629	16/16	0.93	0.14	16,18,27,29	0
3	S3P	D	1729	16/16	0.93	0.13	18,22,28,30	0
3	S3P	A	1429	16/16	0.94	0.13	12,17,22,23	0
2	GPJ	D	1728	10/10	0.95	0.13	15,18,19,20	0
3	S3P	B	1529	16/16	0.95	0.13	10,14,21,21	0
2	GPJ	C	1628	10/10	0.97	0.13	14,16,17,18	0
2	GPJ	A	1428	10/10	0.97	0.13	9,11,14,14	0
2	GPJ	B	1528	10/10	0.98	0.11	9,10,11,12	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.



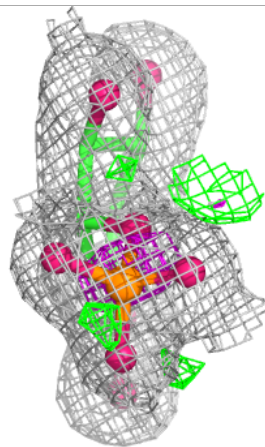
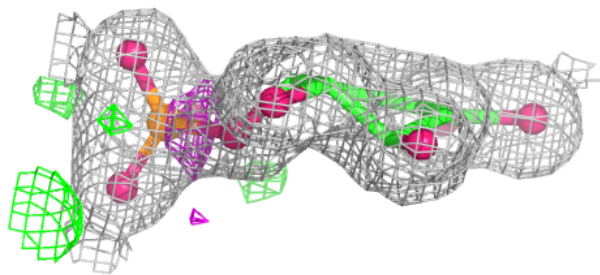
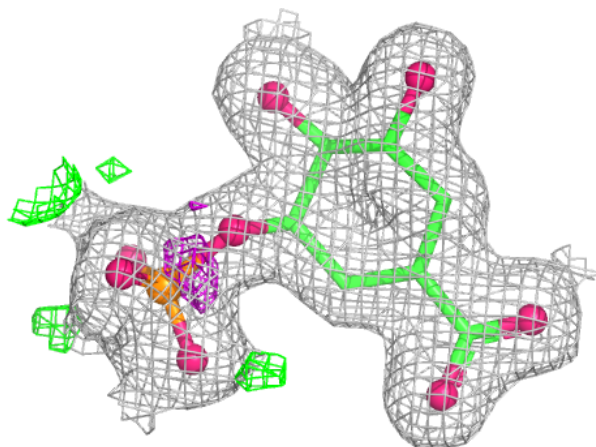
**Electron density around S3P C 1629:**

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



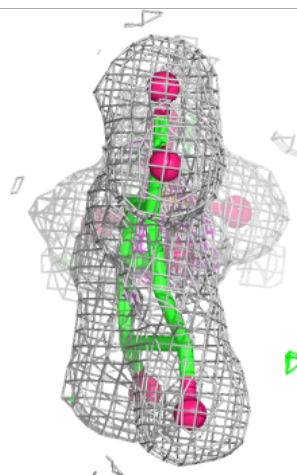
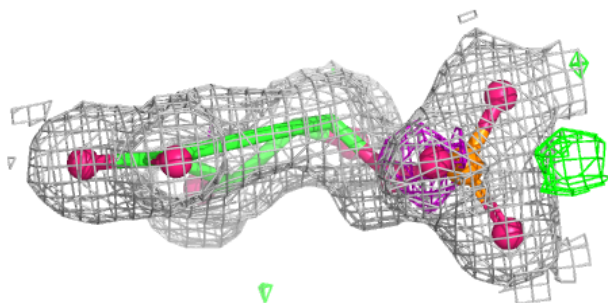
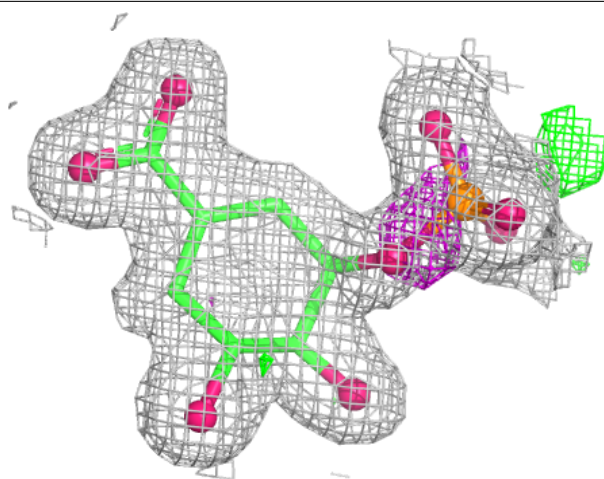
**Electron density around S3P D 1729:**

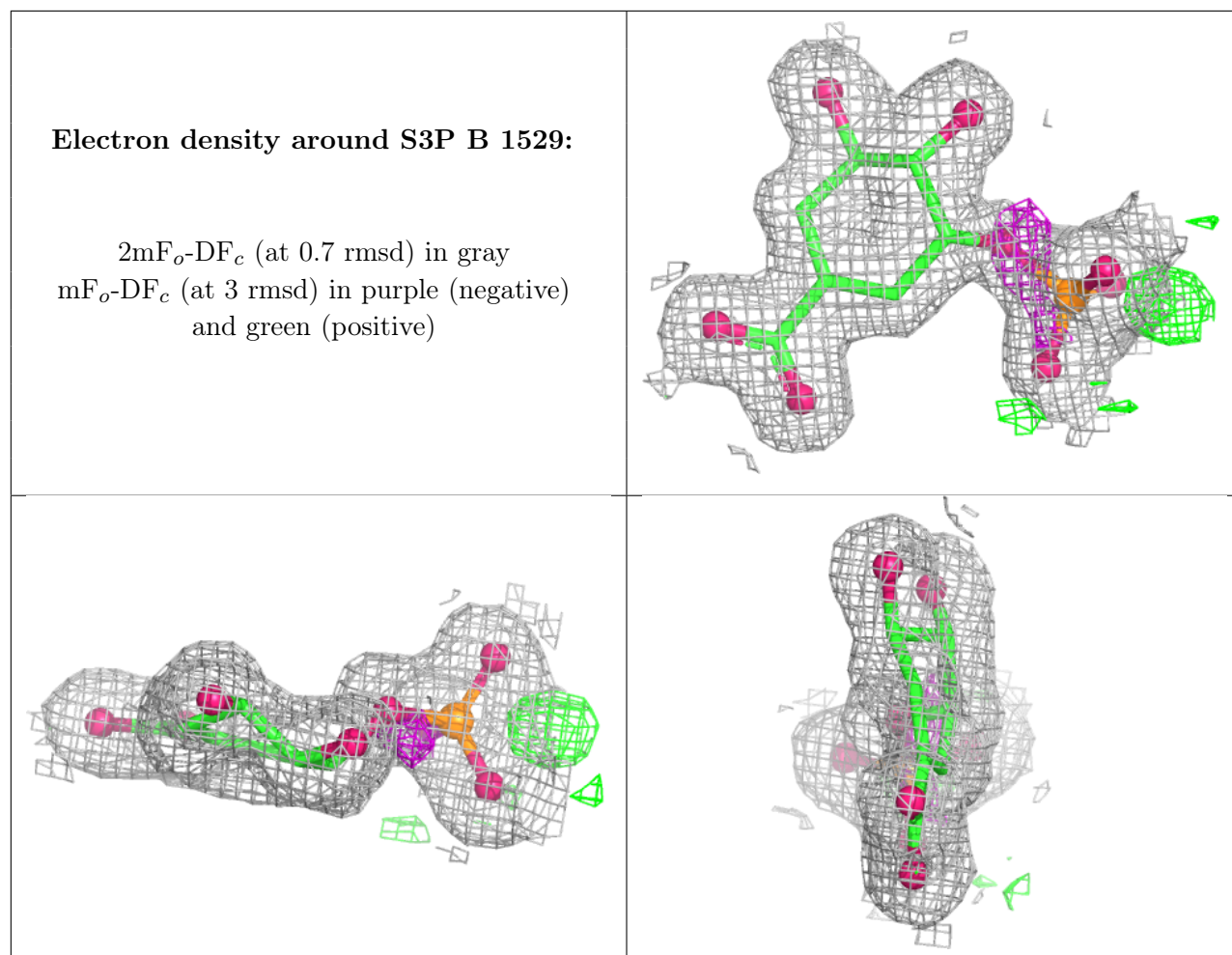
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around S3P A 1429:**

$2mF_o-DF_c$  (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.