



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:24 PM UTC

PDB ID : 1RF6 / pdb_00001rf6
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

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

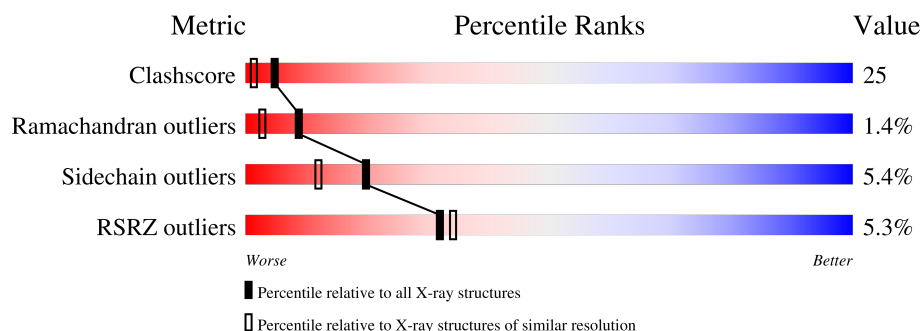
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (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 ≥ 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	4% 66% 30% .
1	B	427	4% 70% 26% ..
1	C	427	7% 58% 38% .
1	D	427	7% 63% 31% 5%

2 Entry composition [i](#)

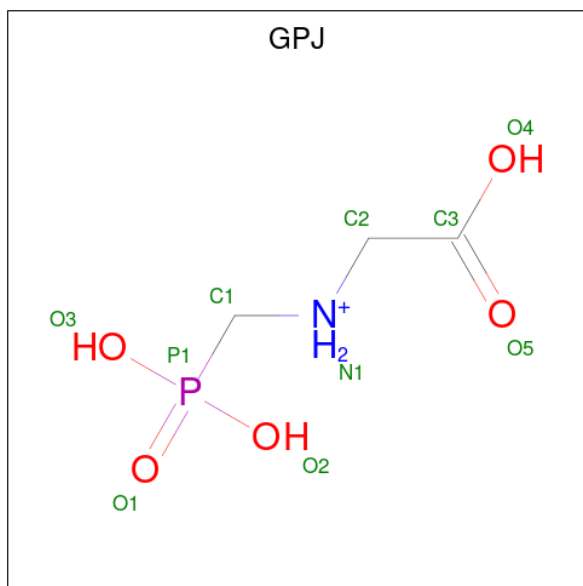
There are 4 unique types of molecules in this entry. The entry contains 13798 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: GPJ) (formula: C₃H₉NO₅P).



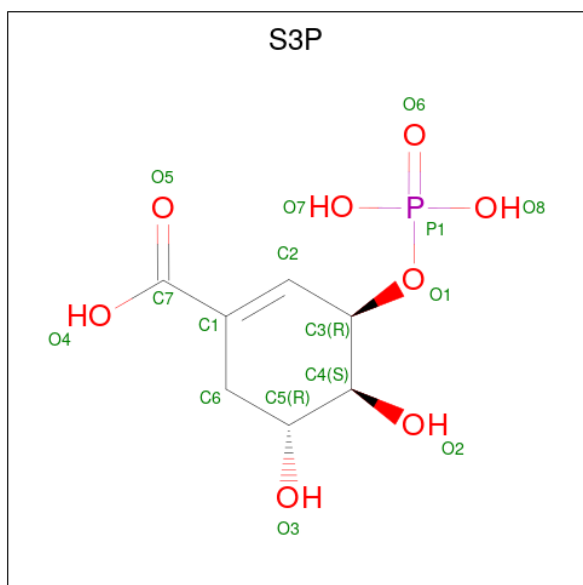
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			10	3	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			10	3	1	5	1		

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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 (CCD ID: 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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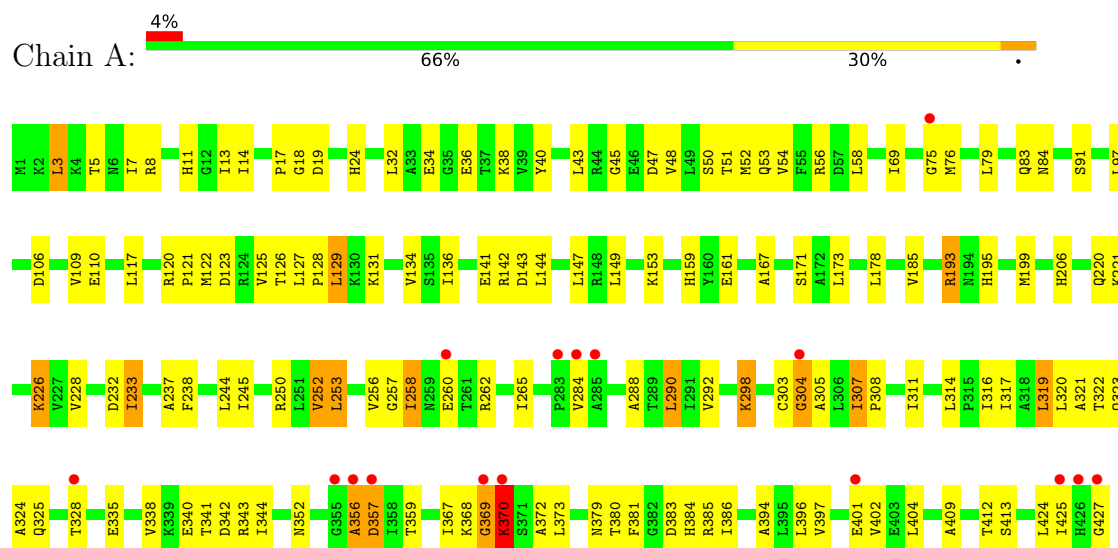
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	159	Total 159	O 159	0	0

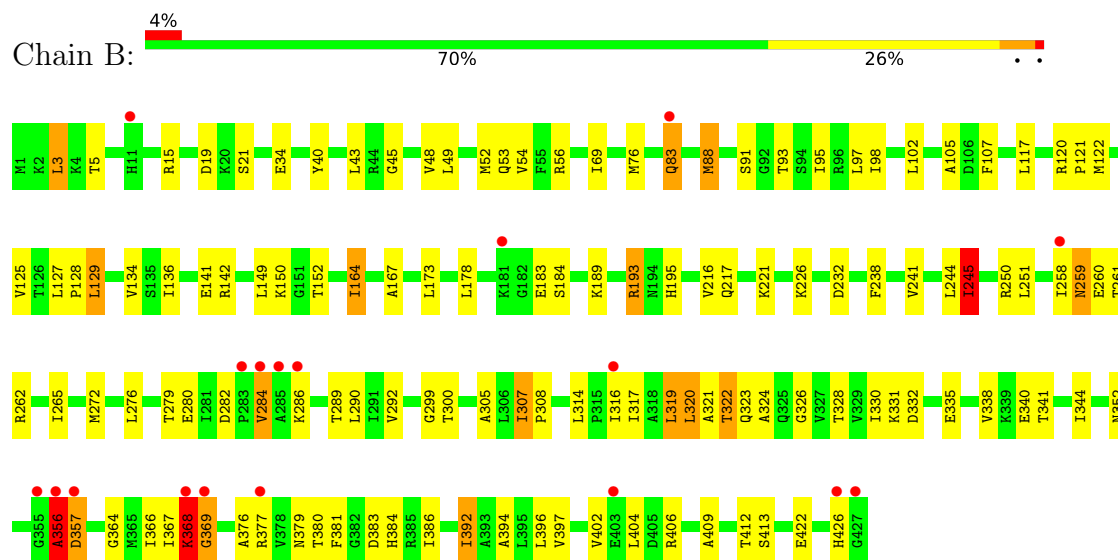
3 Residue-property plots

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

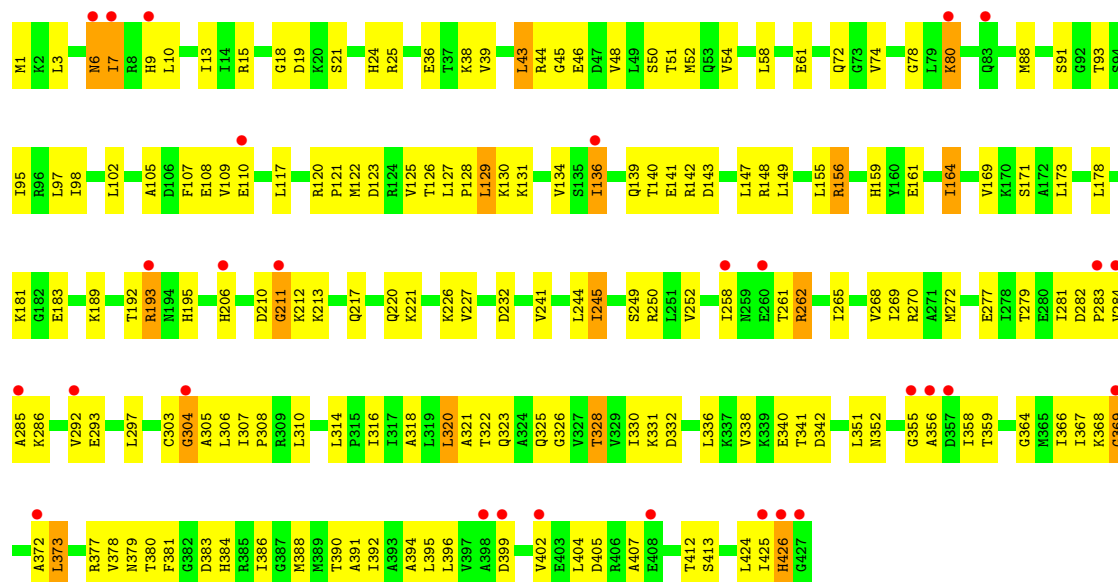


- Molecule 1: 5-enolpyruvylshikimate-3-phosphate synthase

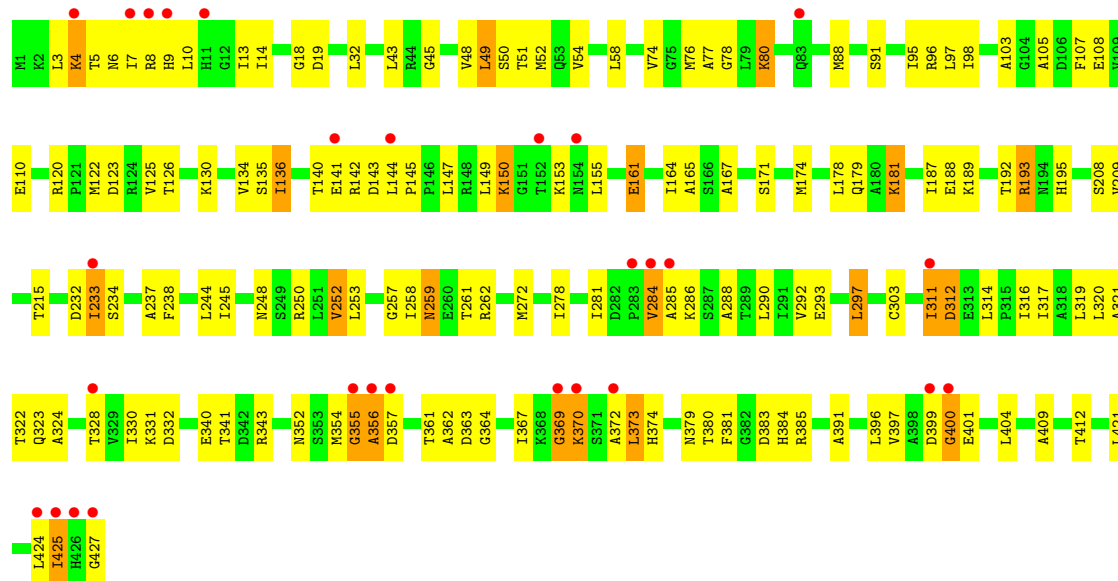


- Molecule 1: 5-enolpyruvylshikimate-3-phosphate synthase





• 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, α , β , γ	82.78Å 150.56Å 88.26Å 90.00° 91.20° 90.00°	Depositor
Resolution (Å)	10.00 – 1.90 10.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-1.90) 93.5 (10.00-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.03 (at 1.79Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.218 , 0.229 0.227 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	17.2	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.49 , 65.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.034 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13798	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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: 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	0.41	0/3252	0.94	12/4391 (0.3%)
1	B	0.41	0/3252	0.92	10/4391 (0.2%)
1	C	0.38	0/3252	0.90	9/4391 (0.2%)
1	D	0.37	0/3252	0.90	7/4391 (0.2%)
All	All	0.39	0/13008	0.91	38/17564 (0.2%)

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	369	GLY	N-CA-C	9.70	126.20	112.82
1	A	369	GLY	N-CA-C	9.10	127.50	112.85
1	B	91	SER	N-CA-C	7.87	120.88	108.67
1	C	91	SER	N-CA-C	7.33	120.21	108.41
1	C	245	ILE	N-CA-C	7.29	118.95	111.00
1	D	311	ILE	N-CA-C	-7.18	100.32	109.58
1	D	91	SER	N-CA-C	7.17	119.96	108.41
1	A	344	ILE	N-CA-C	-7.16	104.79	111.45
1	A	356	ALA	N-CA-C	6.91	125.51	110.80
1	C	189	LYS	N-CA-C	-6.81	103.94	111.36
1	A	91	SER	N-CA-C	6.56	119.54	107.99
1	A	372	ALA	N-CA-C	-6.51	98.66	109.46
1	D	18	GLY	N-CA-C	6.44	119.41	112.33
1	B	356	ALA	N-CA-C	6.42	124.47	110.80
1	B	368	LYS	N-CA-C	6.36	119.90	109.72
1	B	245	ILE	N-CA-C	6.29	118.25	111.58
1	C	18	GLY	N-CA-C	6.13	119.08	112.33
1	C	226	LYS	N-CA-C	-6.07	99.36	109.24
1	C	386	ILE	N-CA-C	-6.06	104.60	110.72
1	B	386	ILE	N-CA-C	-5.94	104.72	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	189	LYS	N-CA-C	-5.84	104.51	111.69
1	B	189	LYS	N-CA-C	-5.83	104.84	111.14
1	A	342	ASP	N-CA-C	-5.76	99.41	108.63
1	C	120	ARG	CA-C-N	5.75	125.94	119.90
1	C	120	ARG	C-N-CA	5.75	125.94	119.90
1	A	18	GLY	N-CA-C	5.61	118.50	112.33
1	A	120	ARG	CA-C-N	5.61	125.79	119.90
1	A	120	ARG	C-N-CA	5.61	125.79	119.90
1	A	307	ILE	CB-CA-C	-5.50	108.48	113.70
1	A	386	ILE	N-CA-C	-5.49	105.17	110.72
1	B	120	ARG	CA-C-N	5.34	125.60	119.83
1	B	120	ARG	C-N-CA	5.34	125.60	119.83
1	C	342	ASP	N-CA-C	-5.24	99.22	108.23
1	D	120	ARG	CA-C-N	5.24	125.00	119.76
1	D	120	ARG	C-N-CA	5.24	125.00	119.76
1	A	226	LYS	N-CA-C	-5.08	100.45	108.73
1	B	307	ILE	CB-CA-C	-5.05	108.90	113.70
1	B	344	ILE	N-CA-C	-5.05	106.15	110.74

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	150	0
1	C	3212	0	3325	189	0
1	D	3212	0	3325	175	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	670	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 25.

All (670) 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:A:52:MET:HE1	1:A:69:ILE:HD12	1.52	0.89
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:HD13	1:D:76:MET:HE1	1.62	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:D:4:LYS:H	1:D:4:LYS:HZ2	1.28	0.77
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:B:52:MET:HE1	1:B:69:ILE:HD12	1.66	0.74
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
1:C:1:MET:HE2	1:C:3:LEU:HD23	1.68	0.74
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:HZ2	1.33	0.74
1:A:325:GLN:NE2	1:A:370:LYS:HG3	2.03	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:361:THR:HG22	1:D:362:ALA:N	2.10	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:260:GLU:H	1:A:260:GLU:CD	2.04	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:N	1:A:245:ILE:HD12	2.11	0.66
1:A:245:ILE:HG23	4:A:1490:HOH:O	1.95	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:260:GLU:CD	1:B:260:GLU:H	2.04	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: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:A:83:GLN:CD	1:A:83:GLN:H	2.05	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:B:259:ASN:HD22	1:B:259:ASN:C	2.07	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:D:5:THR:HG22	1:D:6:ASN:N	2.14	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
1:D:328:THR:HG23	1:D:367:ILE:HB	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:C:149:LEU:C	1:C:149:LEU:HD13	2.27	0.60
1:D:379:ASN:HD22	1:D:379:ASN:C	2.07	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
1:D:9:HIS:HD2	1:D:10:LEU:N	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:C:6:ASN:O	1:C:7:ILE:O	2.22	0.58
1:D:76:MET:HE2	1:D:179:GLN:CG	2.33	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:B:272:MET:HE1	1:B:321:ALA:HA	1.86	0.57
1:C:125:VAL:O	1:C:129:LEU:HB2	2.04	0.57
1:C:258:ILE:HG12	1:C:258:ILE:O	2.03	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: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:D:4:LYS:HZ2	1:D:4:LYS:N	2.02	0.57
1:C:211:GLY:O	1:C:212:LYS:HB2	2.05	0.56
1:D:32:LEU:HD22	1:D:76:MET:HE3	1.87	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:A:127:LEU:C	1:A:127:LEU:HD23	2.30	0.56
1:D:126:THR:HA	1:D:136:ILE:HD12	1.87	0.56
1:A:338:VAL:HG22	1:A:338:VAL:O	2.04	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:B:250:ARG:C	1:B:251:LEU:HD12	2.31	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:D:49:LEU:HA	1:D:52:MET:HE3	1.90	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:B:127:LEU:HD23	1:B:127:LEU:C	2.33	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:272:MET:HE2	1:D:324:ALA:HB2	1.91	0.52
1:D:245:ILE:CD1	1:D:320:LEU:HA	2.27	0.52
1:B:88:MET:HE3	1:B:95:ILE:HA	1.91	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:149:LEU:HD23	1:A:149:LEU:C	2.35	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: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:C:424:LEU:C	1:C:426:HIS:H	2.17	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:195:HIS:HB3	1:A:199:MET:HE3	1.92	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:127:LEU:C	1:C:127:LEU:HD23	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:76:MET:HE2	1:D:179:GLN:HG2	1.93	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: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:C:425:ILE:O	1:C:425:ILE:HG22	2.10	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:A:83:GLN:CD	1:A:83:GLN:N	2.69	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:C:379:ASN:HD22	1:C:379:ASN:C	2.17	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:1:MET:HE2	1:C:3:LEU:CD2	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:THR:HG21	4:A:1467:HOH:O	2.12	0.49
1:B:316:ILE:HD12	1:B:316:ILE:C	2.38	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
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:149:LEU:C	1:B:149:LEU:HD23	2.39	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: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:B:272:MET:HE2	1:B:324:ALA:HB2	1.96	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:B:40:TYR:CE1	1:B:226:LYS:HG3	2.49	0.47
1:B:43:LEU:HD13	1:B:43:LEU:C	2.40	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:48:VAL:HG12	1:C:52:MET:HE2	1.96	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:4:LYS:H	1:D:4:LYS:HZ1	1.59	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: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:276:LEU:HD13	1:B:276:LEU:C	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:320:LEU:C	1:C:320:LEU:CD2	2.89	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: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
1:D:401:GLU:OE1	1:D:401:GLU:HA	2.15	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:C:320:LEU:HD23	1:C:320:LEU:C	2.42	0.45
1:C:355:GLY:O	1:C:356:ALA:HB3	2.14	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:C:123:ASP:HA	1:C:126:THR:HG1	1.81	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:D:5:THR:CG2	1:D:6:ASN:N	2.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:260:GLU:CD	1:A:260:GLU:N	2.72	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:B:259:ASN:ND2	1:B:259:ASN:C	2.74	0.44
1:D:145:PRO:HA	1:D:147:LEU:HD13	1.99	0.44
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:C:331:LYS:O	1:C:332:ASP:HB2	2.17	0.44
1:D:4:LYS:HZ2	1:D:4:LYS:HB2	1.82	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:B:258:ILE:HG22	1:B:286:LYS:C	2.43	0.44
1:B:368:LYS:O	1:B:369:GLY:O	2.36	0.43
1:C:192:THR:O	1:C:193:ARG:C	2.60	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:D:130:LYS:HZ2	1:D:135:SER:HA	1.82	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:272:MET:HE1	1:D:321:ALA:HA	2.00	0.43
1:D:370:LYS:HD2	1:D:370:LYS:HA	1.79	0.43
1:D:421:LEU:C	1:D:421:LEU:HD23	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:404:LEU:HD23	1:C:404:LEU:C	2.43	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:6:ASN:C	1:D:6:ASN:HD22	2.25	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:D:259:ASN:HD22	1:D:259:ASN:C	2.27	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
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: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:A:43:LEU:HD13	1:A:43:LEU:C	2.45	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:B:5:THR:OG1	1:B:397:VAL:HB	2.19	0.42
1:B:326:GLY:H	1:B:369:GLY:HA2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:245:ILE:HG23	1:C:396:LEU:HD21	2.02	0.42
1:C:268:VAL:CG1	1:C:272:MET:HE3	2.50	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
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: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:C:210:ASP:O	1:C:211:GLY:C	2.63	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:B:260:GLU:CD	1:B:260:GLU:N	2.75	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:394:ALA:HB2	1:B:402:VAL:HG11	2.02	0.41
1:C:330:ILE:O	1:C:364:GLY:HA3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:379:ASN:ND2	1:D:379:ASN:C	2.77	0.41
1:A:401:GLU:HG2	4:A:1610:HOH:O	2.20	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
1:C:21:SER:CB	1:C:193:ARG:HH21	2.28	0.40
1:D:32:LEU:HD22	1:D:76:MET:CE	2.49	0.40
1:D:354:MET:O	1:D:374:HIS:N	2.44	0.40
1:C:310:LEU:HD12	1:C:310:LEU:C	2.46	0.40
1:A:244:LEU:C	1:A:245:ILE:HD12	2.46	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 ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	425/427 (100%)	409 (96%)	12 (3%)	4 (1%)	14	6
1	B	425/427 (100%)	407 (96%)	13 (3%)	5 (1%)	10	4
1	C	425/427 (100%)	399 (94%)	18 (4%)	8 (2%)	6	1
1	D	425/427 (100%)	402 (95%)	16 (4%)	7 (2%)	7	2
All	All	1700/1708 (100%)	1617 (95%)	59 (4%)	24 (1%)	9	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
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%)	20	12
1	B	350/350 (100%)	329 (94%)	21 (6%)	17	9
1	C	350/350 (100%)	334 (95%)	16 (5%)	24	16
1	D	350/350 (100%)	330 (94%)	20 (6%)	18	11
All	All	1400/1400 (100%)	1324 (95%)	76 (5%)	20	12

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	58	LEU
1	A	79	LEU
1	A	117	LEU
1	A	129	LEU
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	252	VAL
1	A	253	LEU
1	A	258	ILE
1	A	290	LEU
1	A	298	LYS
1	A	319	LEU
1	A	370	LYS
1	A	404	LEU
1	B	3	LEU
1	B	49	LEU
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	173	LEU
1	B	178	LEU
1	B	193	ARG
1	B	245	ILE
1	B	259	ASN

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Mol	Chain	Res	Type
1	B	290	LEU
1	B	319	LEU
1	B	320	LEU
1	B	322	THR
1	B	368	LYS
1	B	392	ILE
1	B	404	LEU
1	C	43	LEU
1	C	46	GLU
1	C	58	LEU
1	C	80	LYS
1	C	117	LEU
1	C	129	LEU
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	262	ARG
1	C	286	LYS
1	C	320	LEU
1	C	328	THR
1	D	4	LYS
1	D	49	LEU
1	D	80	LYS
1	D	110	GLU
1	D	136	ILE
1	D	150	LYS
1	D	161	GLU
1	D	181	LYS
1	D	193	ARG
1	D	233	ILE
1	D	252	VAL
1	D	259	ASN
1	D	290	LEU
1	D	297	LEU
1	D	314	LEU
1	D	319	LEU
1	D	357	ASP
1	D	404	LEU
1	D	412	THR

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Mol	Chain	Res	Type
1	D	425	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	24	HIS
1	A	53	GLN
1	A	72	GLN
1	A	84	ASN
1	A	139	GLN
1	A	159	HIS
1	A	195	HIS
1	A	202	GLN
1	A	220	GLN
1	A	323	GLN
1	A	325	GLN
1	A	345	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	195	HIS
1	B	201	GLN
1	B	248	ASN
1	B	255	ASN
1	B	259	ASN
1	B	323	GLN
1	B	345	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	179	GLN

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Mol	Chain	Res	Type
1	C	202	GLN
1	C	217	GLN
1	C	220	GLN
1	C	254	GLN
1	C	345	GLN
1	C	379	ASN
1	C	384	HIS
1	C	411	ASN
1	D	6	ASN
1	D	9	HIS
1	D	24	HIS
1	D	53	GLN
1	D	84	ASN
1	D	139	GLN
1	D	154	ASN
1	D	195	HIS
1	D	202	GLN
1	D	259	ASN
1	D	325	GLN
1	D	345	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 oligosaccharides 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
3	S3P	B	1529	-	15,16,16	2.54	5 (33%)	21,24,24	1.16	1 (4%)
2	GPJ	C	1628	-	9,9,9	1.84	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	D	1728	-	9,9,9	1.68	2 (22%)	9,12,12	1.26	1 (11%)
3	S3P	D	1729	-	15,16,16	2.57	6 (40%)	21,24,24	1.23	2 (9%)
2	GPJ	A	1428	-	9,9,9	1.72	2 (22%)	9,12,12	1.45	1 (11%)
2	GPJ	B	1528	-	9,9,9	1.74	2 (22%)	9,12,12	1.34	1 (11%)
3	S3P	A	1429	-	15,16,16	2.50	6 (40%)	21,24,24	1.20	2 (9%)

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	S3P	B	1529	-	-	0/9/25/25	0/1/1/1
2	GPJ	C	1628	-	-	0/7/7/7	-
3	S3P	C	1629	-	-	0/9/25/25	0/1/1/1
2	GPJ	D	1728	-	-	0/7/7/7	-
3	S3P	D	1729	-	-	0/9/25/25	0/1/1/1
2	GPJ	A	1428	-	-	0/7/7/7	-
2	GPJ	B	1528	-	-	0/7/7/7	-
3	S3P	A	1429	-	-	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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.

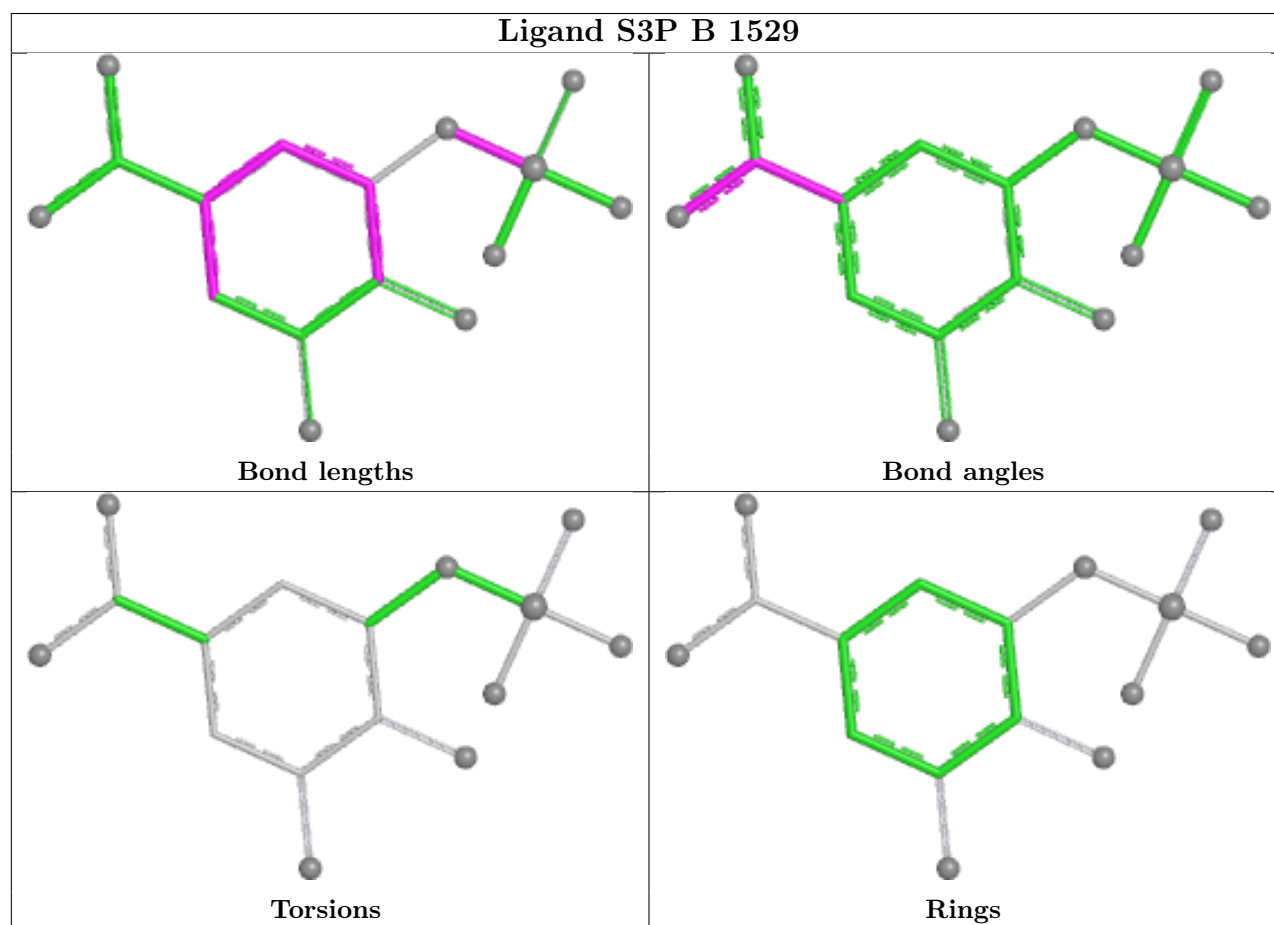
There are no torsion outliers.

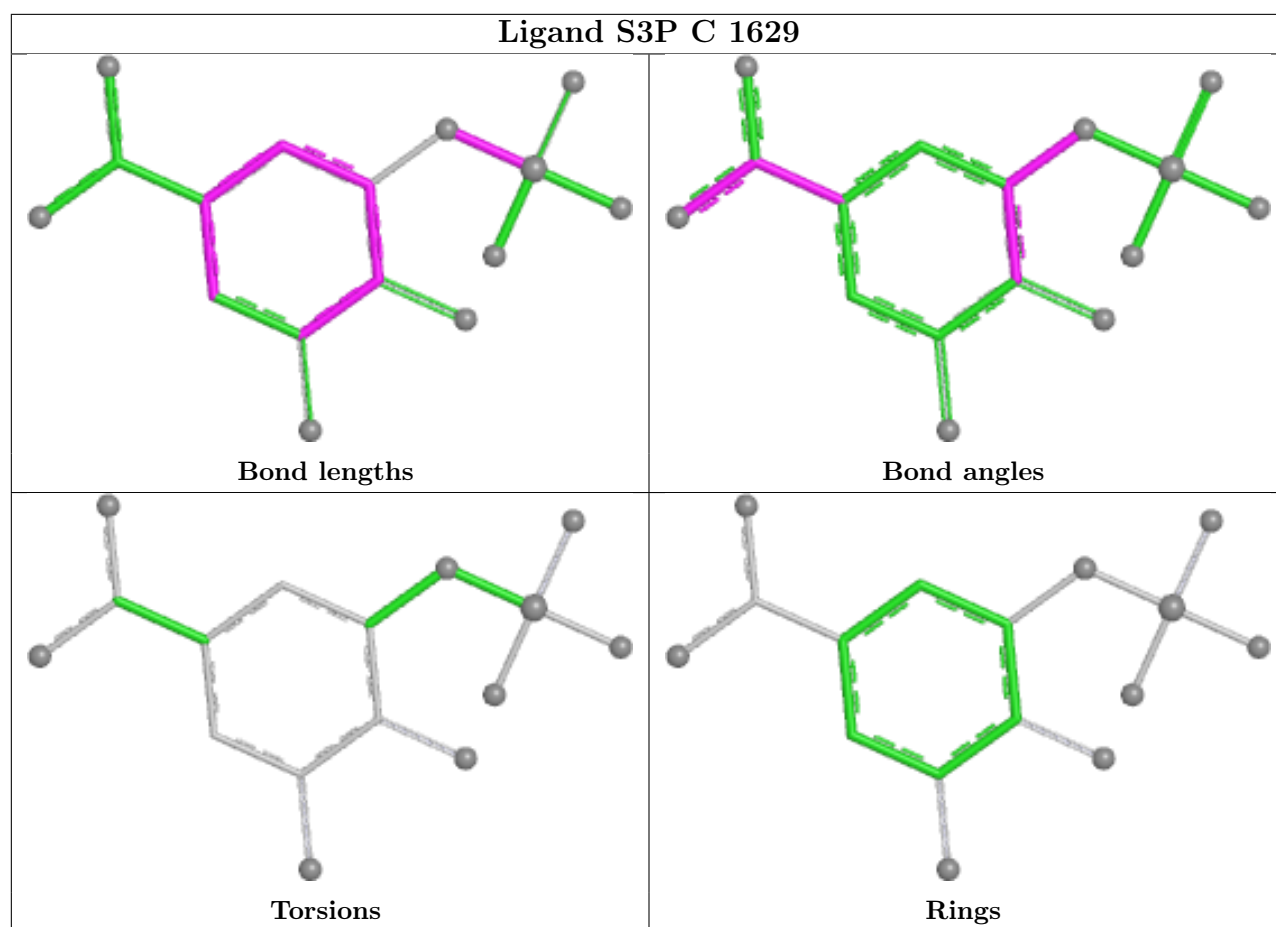
There are no ring outliers.

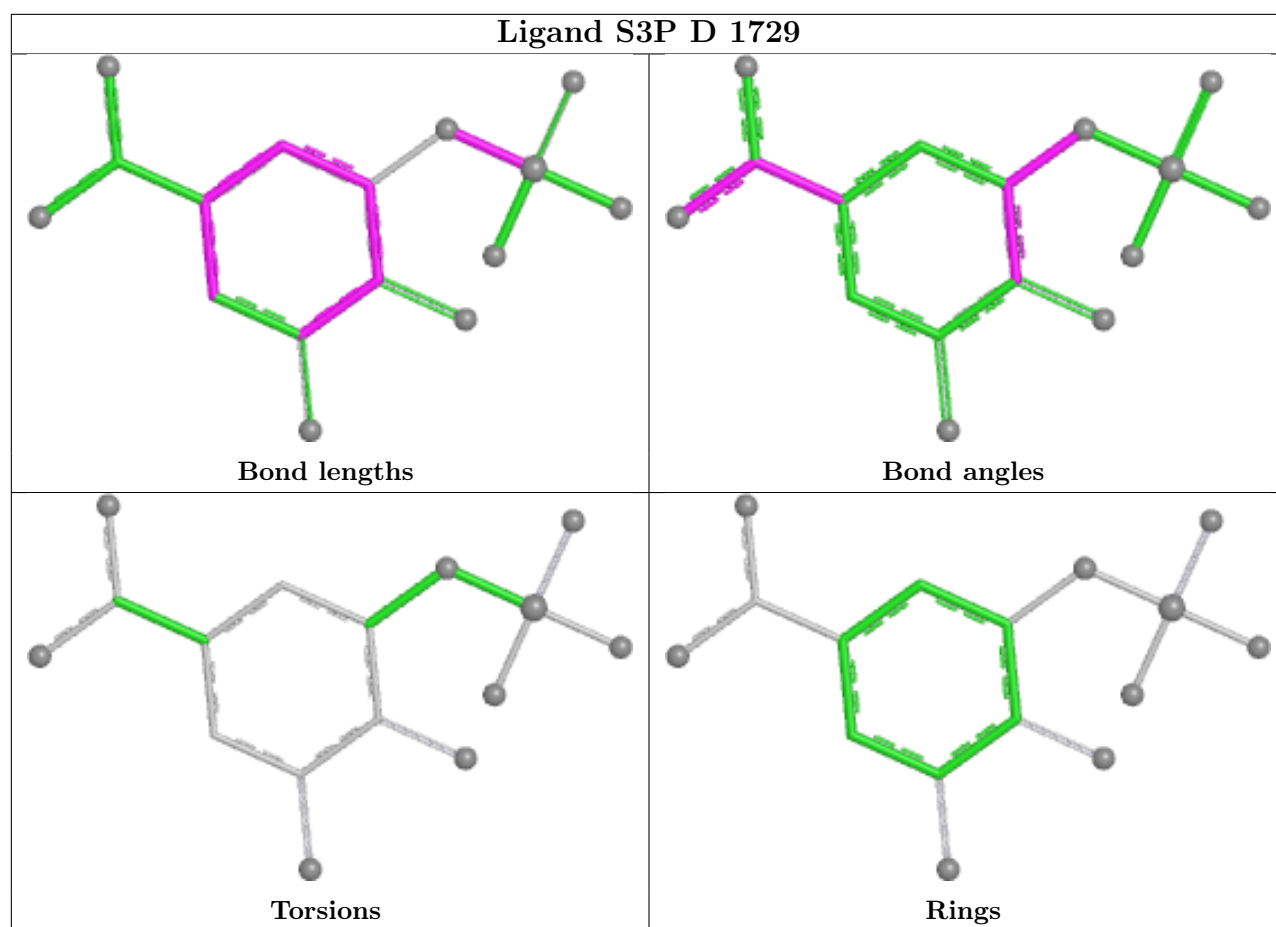
2 monomers are involved in 2 short contacts:

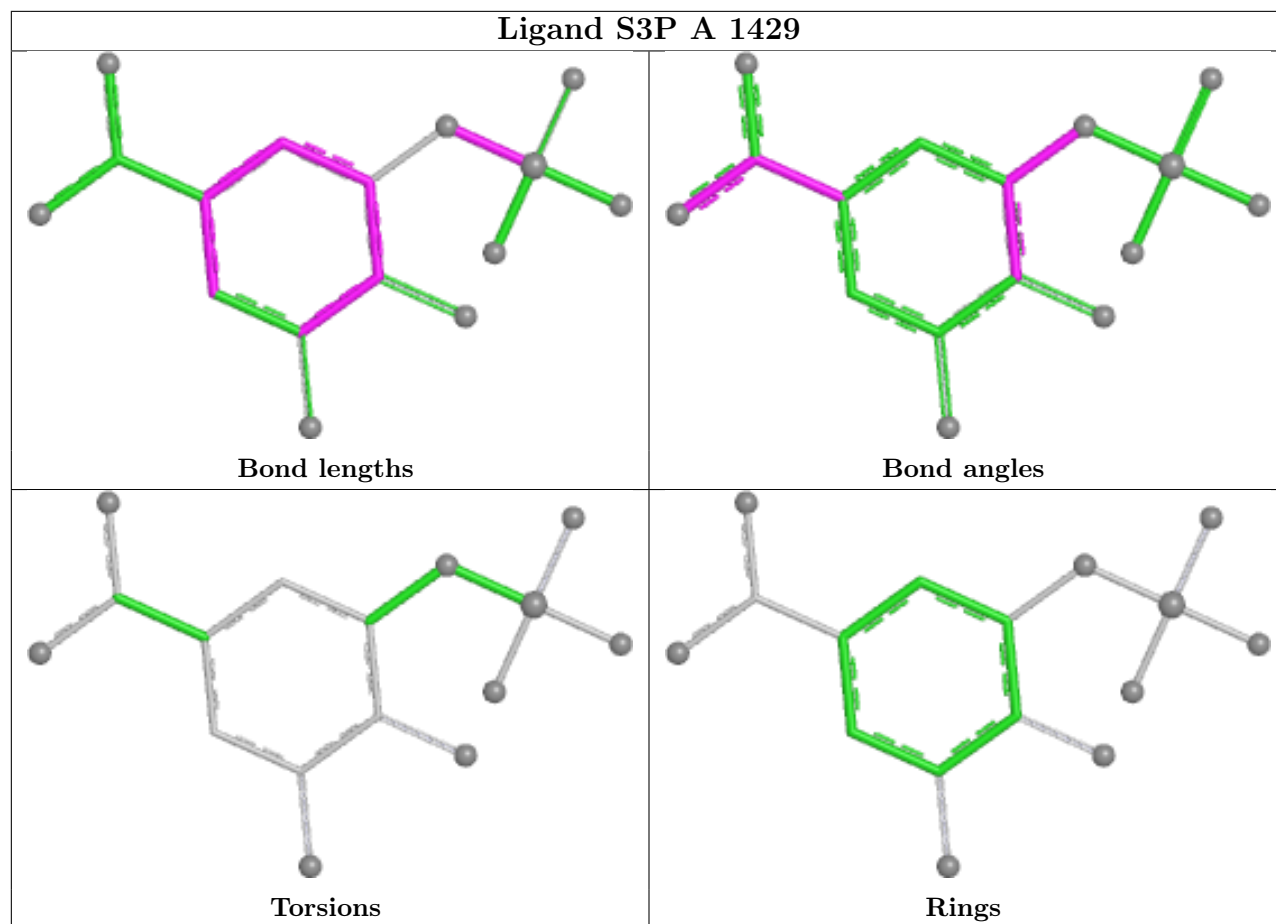
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1728	GPJ	1	0
2	A	1428	GPJ	1	0

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, 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	427/427 (100%)	-0.01	16 (3%) 45 48	9, 15, 27, 46	0
1	B	427/427 (100%)	0.01	18 (4%) 40 43	8, 15, 29, 50	0
1	C	427/427 (100%)	0.36	29 (6%) 23 24	12, 21, 36, 59	0
1	D	427/427 (100%)	0.42	28 (6%) 24 26	11, 21, 35, 56	0
All	All	1708/1708 (100%)	0.19	91 (5%) 32 34	8, 18, 34, 59	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	356	ALA	9.7
1	A	356	ALA	8.8
1	D	355	GLY	7.9
1	B	369	GLY	7.7
1	C	427	GLY	6.9
1	C	355	GLY	6.6
1	D	427	GLY	6.1
1	C	369	GLY	6.0
1	C	426	HIS	5.9
1	A	75	GLY	5.7
1	B	427	GLY	5.4
1	D	284	VAL	5.3
1	B	426	HIS	5.1
1	B	284	VAL	5.0
1	A	304	GLY	4.8
1	A	284	VAL	4.8
1	C	9	HIS	4.7
1	C	304	GLY	4.7
1	A	427	GLY	4.6
1	C	284	VAL	4.5
1	D	356	ALA	4.5

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Mol	Chain	Res	Type	RSRZ
1	D	9	HIS	4.5
1	D	425	ILE	4.4
1	C	211	GLY	4.3
1	C	285	ALA	4.2
1	A	426	HIS	4.1
1	D	372	ALA	4.1
1	D	285	ALA	4.0
1	B	11	HIS	3.9
1	A	370	LYS	3.9
1	C	193	ARG	3.9
1	B	285	ALA	3.8
1	C	206	HIS	3.8
1	A	369	GLY	3.7
1	C	398	ALA	3.7
1	B	357	ASP	3.6
1	D	369	GLY	3.6
1	D	11	HIS	3.6
1	C	283	PRO	3.4
1	C	6	ASN	3.4
1	D	357	ASP	3.3
1	C	372	ALA	3.3
1	A	355	GLY	3.3
1	D	399	ASP	3.2
1	B	377	ARG	3.2
1	C	425	ILE	3.1
1	A	283	PRO	3.1
1	A	357	ASP	3.0
1	B	283	PRO	3.0
1	B	83	GLN	3.0
1	D	370	LYS	2.9
1	B	355	GLY	2.9
1	B	403	GLU	2.8
1	D	400	GLY	2.8
1	D	233	ILE	2.6
1	B	258	ILE	2.6
1	C	399	ASP	2.5
1	D	144	LEU	2.5
1	D	424	LEU	2.5
1	A	285	ALA	2.5
1	C	356	ALA	2.5
1	C	83	GLN	2.5
1	A	260	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	152	THR	2.5
1	B	316	ILE	2.5
1	D	83	GLN	2.5
1	B	368	LYS	2.4
1	C	408	GLU	2.4
1	C	136	ILE	2.3
1	D	328	THR	2.3
1	D	4	LYS	2.3
1	C	402	VAL	2.3
1	C	258	ILE	2.3
1	D	426	HIS	2.3
1	C	7	ILE	2.2
1	D	7	ILE	2.2
1	D	311	ILE	2.2
1	D	154	ASN	2.2
1	A	401	GLU	2.2
1	C	110	GLU	2.2
1	D	283	PRO	2.1
1	A	425	ILE	2.1
1	C	292	VAL	2.1
1	D	8	ARG	2.1
1	B	181	LYS	2.1
1	C	80	LYS	2.1
1	C	357	ASP	2.1
1	B	286	LYS	2.0
1	C	260	GLU	2.0
1	D	141	GLU	2.0
1	A	328	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

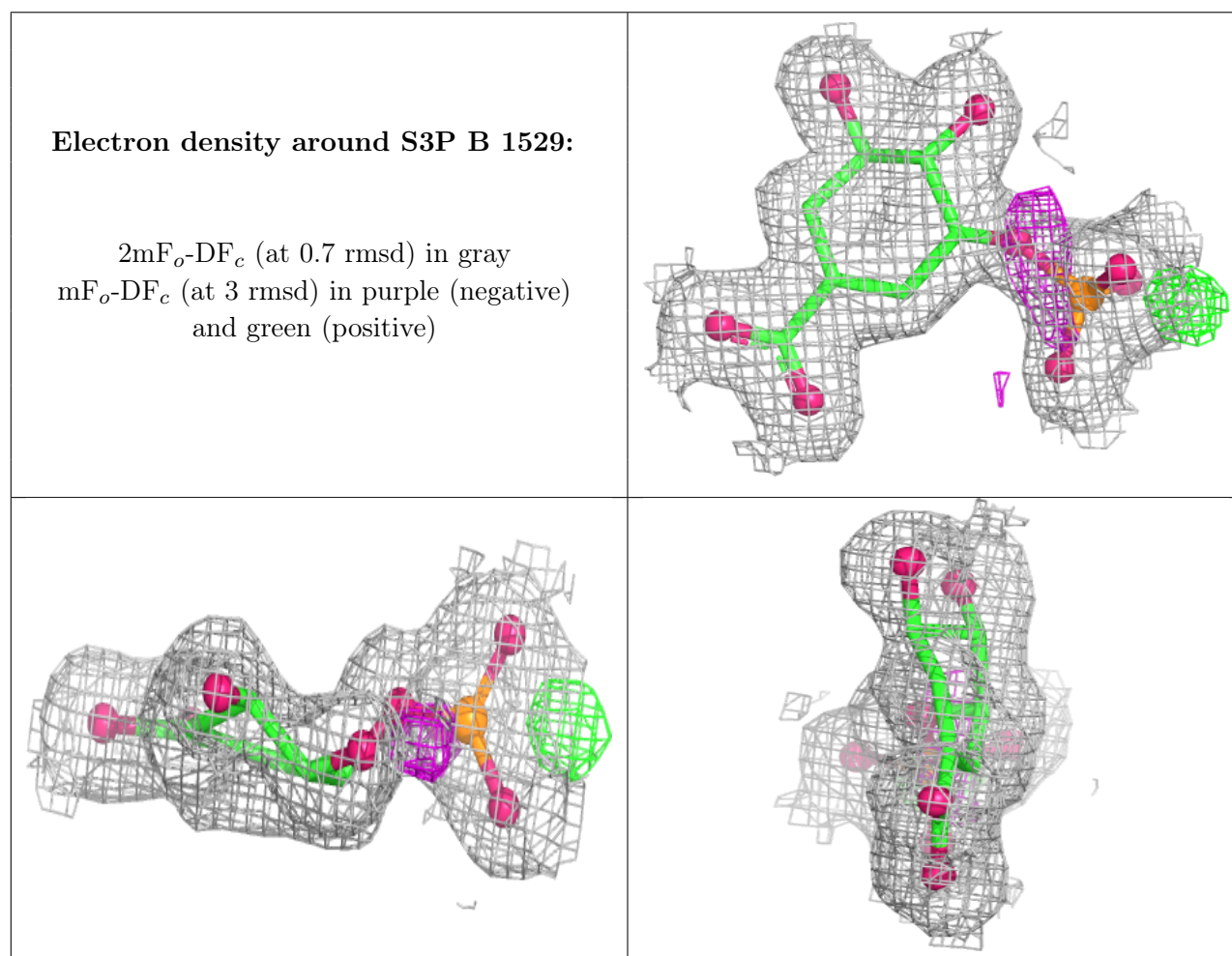
6.4 Ligands [i](#)

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

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

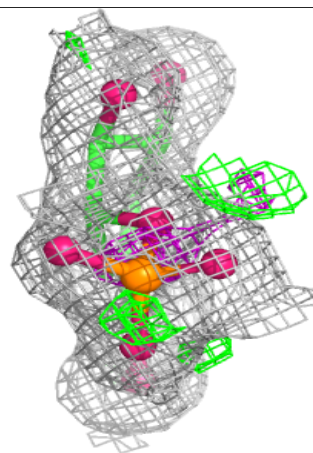
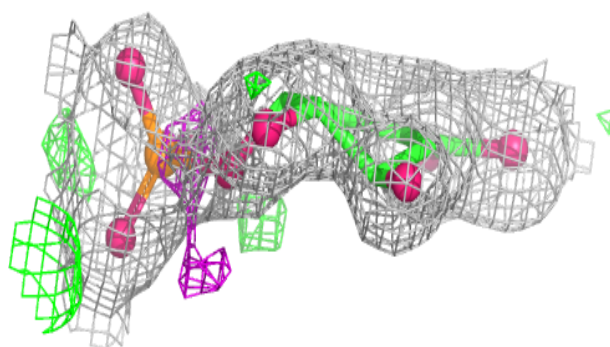
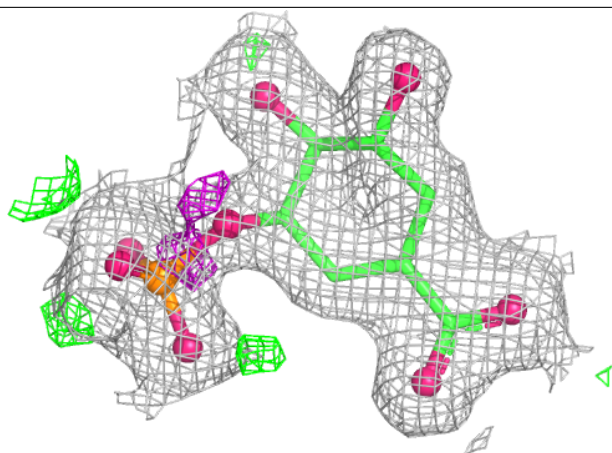
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	S3P	B	1529	16/16	0.92	0.07	10,14,21,21	0
3	S3P	D	1729	16/16	0.92	0.07	18,22,28,30	0
3	S3P	C	1629	16/16	0.93	0.08	16,18,27,29	0
3	S3P	A	1429	16/16	0.94	0.07	12,17,22,23	0
2	GPJ	D	1728	10/10	0.95	0.08	15,18,19,20	0
2	GPJ	C	1628	10/10	0.96	0.06	14,16,17,18	0
2	GPJ	A	1428	10/10	0.96	0.06	9,11,14,14	0
2	GPJ	B	1528	10/10	0.97	0.05	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.



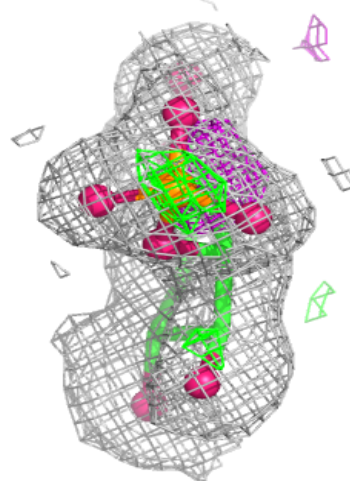
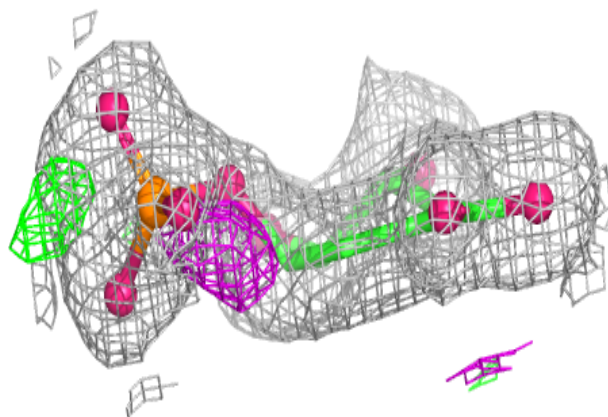
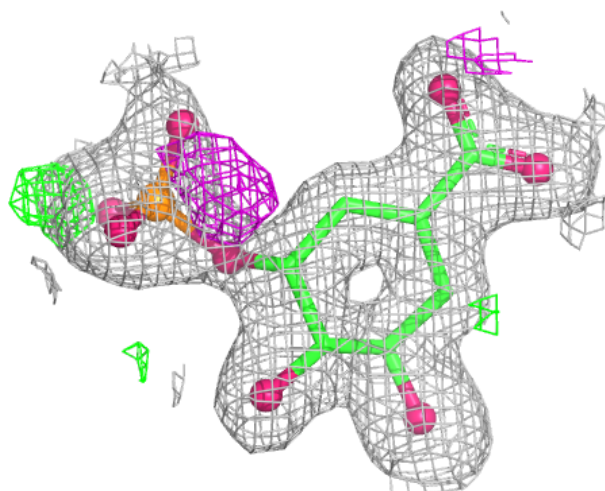
Electron density around S3P D 1729:

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



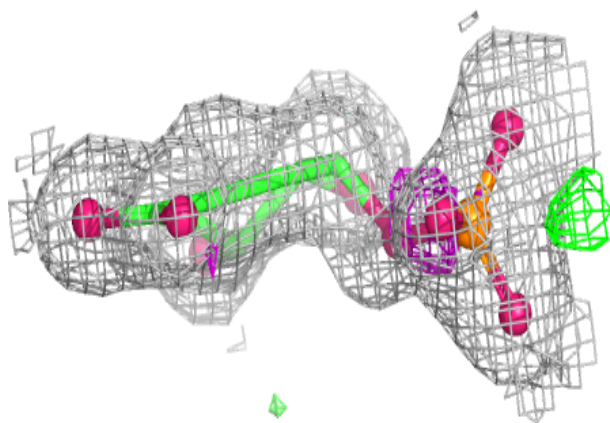
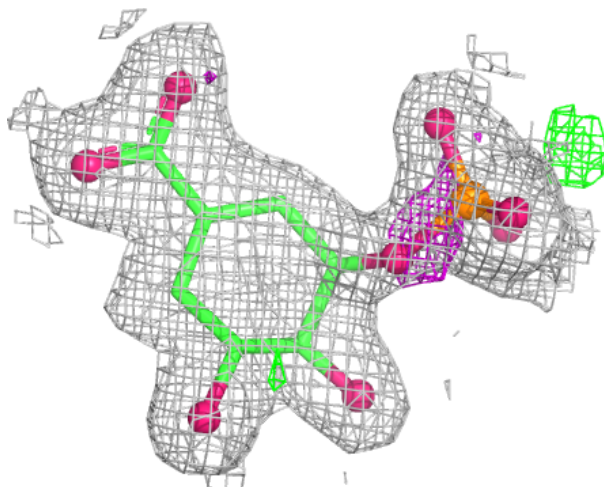
Electron density around S3P C 1629:

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



Electron density around S3P 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.