



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:55 PM UTC

PDB ID : 3WEF / pdb_00003wef
Title : Crystal structure of the human squalene synthase in complex with farnesyl thiopyrophosphate
Authors : Liu, C.I.; Jeng, W.Y.; Wang, A.H.J.
Deposited on : 2013-07-07
Resolution : 2.35 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:

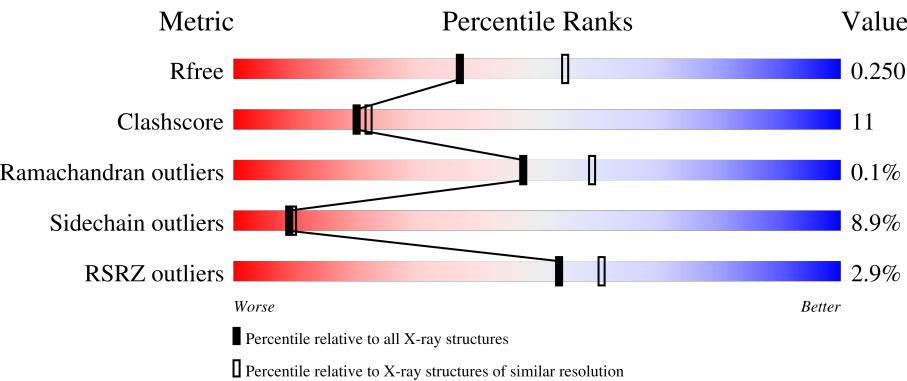
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	343	% 77% 16% • 5%
1	B	343	3% 73% 22% • •
1	C	343	4% 75% 20% • •
1	D	343	3% 74% 20% • •
1	E	343	3% 72% 20% • •

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Mol	Chain	Length	Quality of chain
1	F	343	3% 63% 26% • 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16505 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 Squalene synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	327	Total	C	N	O	S	0	0	0
			2650	1686	451	495	18			
1	B	333	Total	C	N	O	S	0	0	0
			2691	1711	459	503	18			
1	C	333	Total	C	N	O	S	0	0	0
			2690	1712	458	502	18			
1	D	329	Total	C	N	O	S	0	0	0
			2664	1695	453	498	18			
1	E	329	Total	C	N	O	S	0	0	0
			2658	1692	450	498	18			
1	F	322	Total	C	N	O	S	0	0	0
			2608	1659	442	489	18			

There are 18 discrepancies between the modelled and reference sequences:

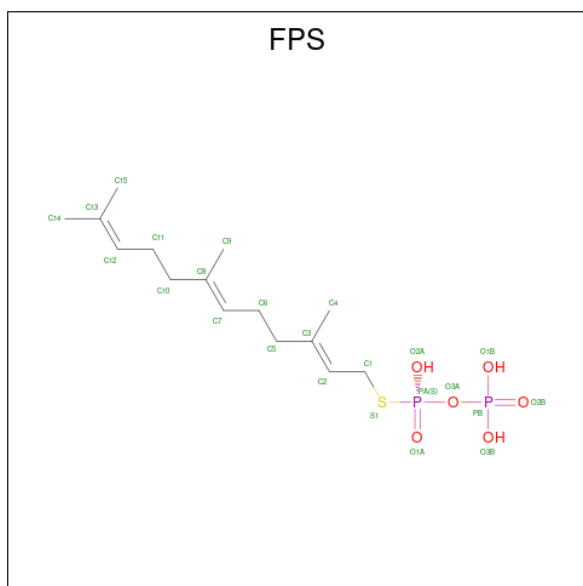
Chain	Residue	Modelled	Actual	Comment	Reference
A	28	GLY	-	expression tag	UNP P37268
A	29	SER	-	expression tag	UNP P37268
A	30	HIS	-	expression tag	UNP P37268
B	28	GLY	-	expression tag	UNP P37268
B	29	SER	-	expression tag	UNP P37268
B	30	HIS	-	expression tag	UNP P37268
C	28	GLY	-	expression tag	UNP P37268
C	29	SER	-	expression tag	UNP P37268
C	30	HIS	-	expression tag	UNP P37268
D	28	GLY	-	expression tag	UNP P37268
D	29	SER	-	expression tag	UNP P37268
D	30	HIS	-	expression tag	UNP P37268
E	28	GLY	-	expression tag	UNP P37268
E	29	SER	-	expression tag	UNP P37268
E	30	HIS	-	expression tag	UNP P37268
F	28	GLY	-	expression tag	UNP P37268
F	29	SER	-	expression tag	UNP P37268

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Chain	Residue	Modelled	Actual	Comment	Reference
F	30	HIS	-	expression tag	UNP P37268

- Molecule 2 is S-[(2E,6E)-3,7,11-TRIMETHYLDODECA-2,6,10-TRIENYL] TRIHYDRO-GEN THIODIPHOSPHATE (CCD ID: FPS) (formula: $C_{15}H_{28}O_6P_2S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	O	P	S	0	0
			24	15	6	2	1		
2	A	1	Total	C	O	P	S	0	0
			24	15	6	2	1		
2	B	1	Total	C	O	P	S	0	0
			24	15	6	2	1		
2	B	1	Total	C	O	P	S	0	0
			24	15	6	2	1		
2	C	1	Total	C	O	P	S	0	0
			24	15	6	2	1		
2	D	1	Total	C	O	P	S	0	0
			24	15	6	2	1		
2	E	1	Total	C	O	P	S	0	0
			24	15	6	2	1		
2	E	1	Total	C	O	P	S	0	0
			24	15	6	2	1		

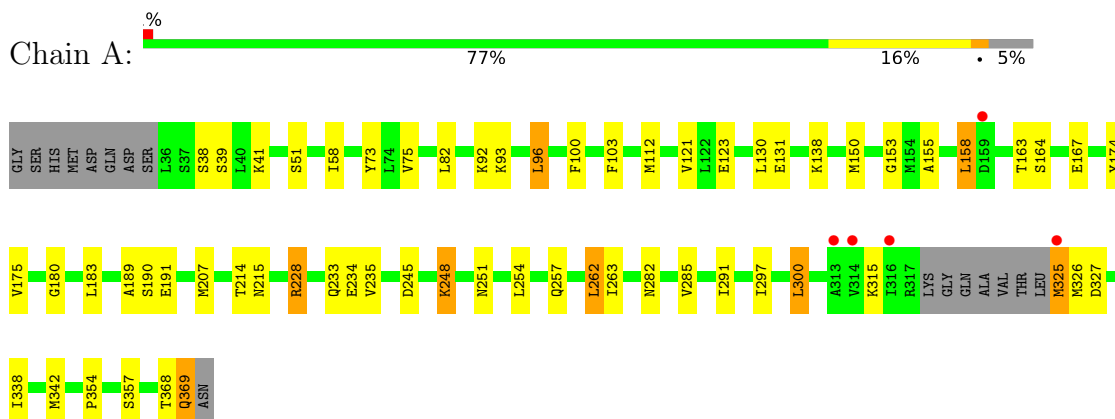
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	111	Total 111	O 111	0	0
3	B	75	Total 75	O 75	0	0
3	C	94	Total 94	O 94	0	0
3	D	22	Total 22	O 22	0	0
3	E	42	Total 42	O 42	0	0
3	F	8	Total 8	O 8	0	0

3 Residue-property plots [i](#)

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

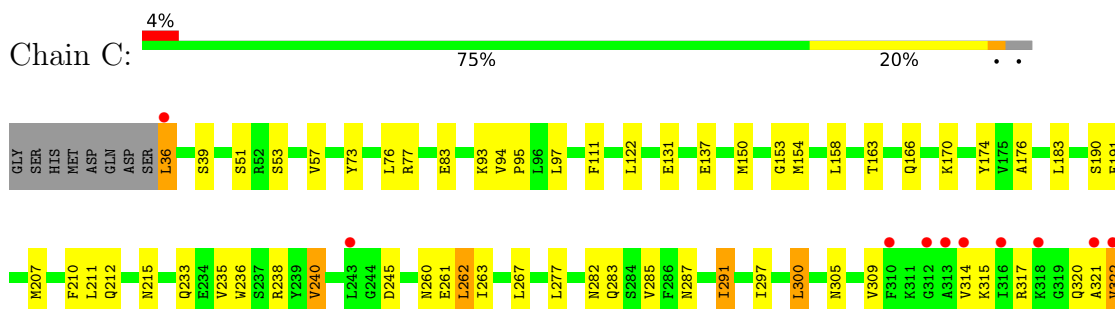
• Molecule 1: Squalene synthase



• Molecule 1: Squalene synthase

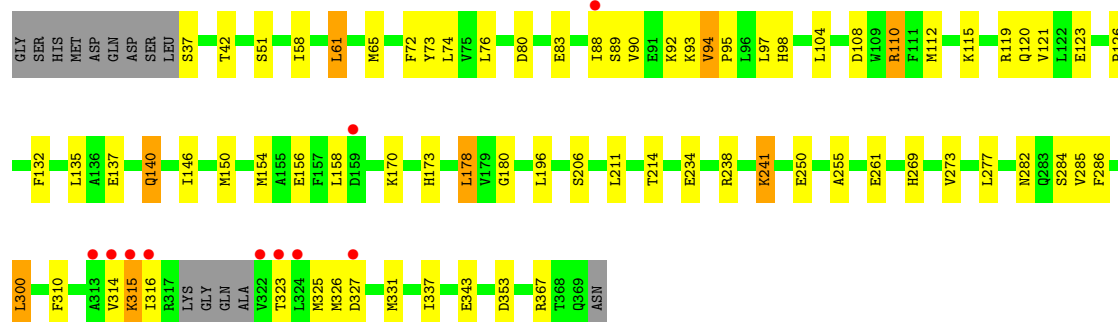
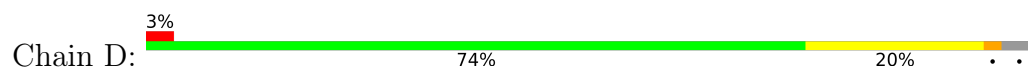


• Molecule 1: Squalene synthase

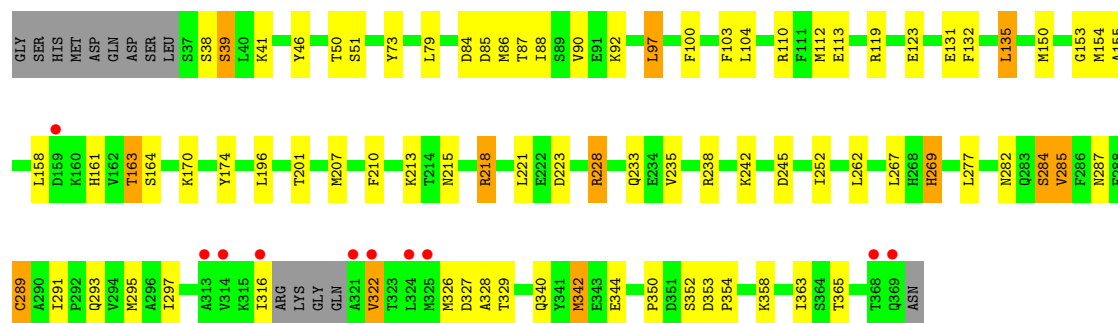




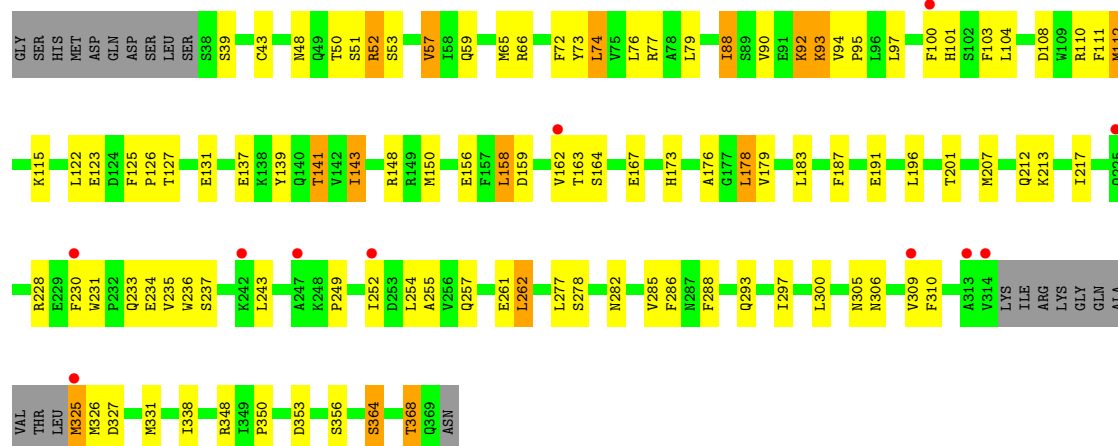
• Molecule 1: Squalene synthase



• Molecule 1: Squalene synthase



• Molecule 1: Squalene synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	85.89Å 153.75Å 91.61Å 90.00° 91.06° 90.00°	Depositor
Resolution (Å)	30.00 – 2.35 30.00 – 2.35	Depositor EDS
% Data completeness (in resolution range)	98.7 (30.00-2.35) 98.8 (30.00-2.35)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.18 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.190 , 0.257 0.184 , 0.250	Depositor DCC
R_{free} test set	4883 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	37.4	Xtriage
Anisotropy	0.450	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 51.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.034 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16505	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% 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: FPS

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	0.49	0/2704	1.00	2/3655 (0.1%)
1	B	0.45	0/2746	0.97	2/3713 (0.1%)
1	C	0.47	0/2745	0.99	3/3712 (0.1%)
1	D	0.41	0/2718	0.95	4/3675 (0.1%)
1	E	0.41	0/2712	0.97	5/3668 (0.1%)
1	F	0.39	0/2662	0.96	2/3600 (0.1%)
All	All	0.44	0/16287	0.97	18/22023 (0.1%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	317	ARG	N-CA-C	6.21	118.39	109.14
1	A	248	LYS	CA-C-N	5.89	127.20	119.84
1	A	248	LYS	C-N-CA	5.89	127.20	119.84
1	E	285	VAL	N-CA-C	-5.72	104.77	111.00
1	B	248	LYS	CA-C-N	5.62	125.29	119.56
1	B	248	LYS	C-N-CA	5.62	125.29	119.56
1	F	348	ARG	CA-C-N	-5.60	118.79	122.60
1	F	348	ARG	C-N-CA	-5.60	118.79	122.60
1	C	291	ILE	CA-C-N	-5.52	113.34	119.19
1	C	291	ILE	C-N-CA	-5.52	113.34	119.19
1	E	284	SER	CB-CA-C	-5.50	101.61	110.74
1	D	353	ASP	CA-C-N	5.39	125.73	119.47
1	D	353	ASP	C-N-CA	5.39	125.73	119.47
1	E	269	HIS	CA-C-N	5.35	123.61	120.24
1	E	269	HIS	C-N-CA	5.35	123.61	120.24
1	D	72	PHE	N-CA-C	-5.35	105.35	111.07
1	D	314	VAL	N-CA-C	5.13	116.19	109.21
1	E	289	CYS	N-CA-C	5.01	116.83	111.36

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	2650	0	2623	51	0
1	B	2691	0	2669	65	0
1	C	2690	0	2672	60	0
1	D	2664	0	2639	49	0
1	E	2658	0	2631	55	0
1	F	2608	0	2570	75	0
2	A	48	0	50	12	0
2	B	48	0	50	15	0
2	C	24	0	25	8	0
2	D	24	0	25	6	0
2	E	48	0	50	8	0
3	A	111	0	0	3	0
3	B	75	0	0	0	0
3	C	94	0	0	0	0
3	D	22	0	0	1	0
3	E	42	0	0	0	0
3	F	8	0	0	0	0
All	All	16505	0	16004	363	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 11.

All (363) 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:B:297:ILE:HD11	1:B:342:MET:CE	1.71	1.21
1:B:297:ILE:HD11	1:B:342:MET:HE1	1.15	1.15
1:C:83:GLU:HB2	1:C:154:MET:HE3	1.28	1.14
1:D:286:PHE:HE1	1:D:331:MET:CE	1.66	1.09
1:E:282:ASN:HD21	1:E:284:SER:HB2	0.96	1.08
1:E:282:ASN:ND2	1:E:284:SER:HB2	1.67	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:286:PHE:HE1	1:F:331:MET:HE2	1.17	1.04
1:D:83:GLU:HB2	1:D:154:MET:HE3	1.40	1.03
1:F:277:LEU:HB3	1:F:331:MET:HE1	1.41	1.02
1:D:277:LEU:HB3	1:D:331:MET:HE1	1.44	1.00
1:C:83:GLU:HB2	1:C:154:MET:CE	1.92	0.98
1:D:286:PHE:CE1	1:D:331:MET:CE	2.50	0.94
1:D:286:PHE:CE1	1:D:331:MET:HE2	2.01	0.94
1:F:286:PHE:CE1	1:F:331:MET:HE2	2.03	0.94
1:F:286:PHE:HE1	1:F:331:MET:CE	1.79	0.94
1:D:150:MET:HG2	1:D:178:LEU:HD21	1.49	0.92
1:F:50:THR:HG21	1:F:77:ARG:HG2	1.52	0.91
1:C:83:GLU:CB	1:C:154:MET:HE3	1.99	0.91
1:D:241:LYS:CE	1:D:241:LYS:HA	2.01	0.90
1:F:163:THR:HG23	1:F:164:SER:H	1.37	0.90
1:D:180:GLY:HA2	2:D:401:FPS:H152	1.51	0.89
1:D:51:SER:HB2	1:D:73:TYR:CZ	2.09	0.88
1:A:228:ARG:HG3	1:A:228:ARG:HH11	1.39	0.87
1:B:80:ASP:O	1:B:84:ASP:HB2	1.73	0.87
1:D:326:MET:HA	1:F:327:ASP:OD1	1.75	0.87
1:E:41:LYS:HA	1:F:368:THR:HG21	1.57	0.87
1:A:297:ILE:HD13	1:A:338:ILE:HG12	1.59	0.84
1:F:297:ILE:HD13	1:F:338:ILE:HG12	1.57	0.84
1:E:163:THR:CG2	1:E:164:SER:H	1.91	0.84
1:A:51:SER:HB2	1:A:73:TYR:CZ	2.13	0.84
1:F:213:LYS:O	1:F:217:ILE:HG12	1.79	0.82
1:F:65:MET:CE	1:F:187:PHE:HD1	1.91	0.82
1:D:132:PHE:O	1:D:140:GLN:NE2	2.13	0.81
1:E:322:VAL:HG13	1:E:326:MET:CE	2.11	0.81
1:B:282:ASN:HD22	1:B:285:VAL:H	1.29	0.80
1:B:51:SER:HB2	1:B:73:TYR:CZ	2.16	0.79
1:F:282:ASN:HD22	1:F:285:VAL:H	1.31	0.78
1:F:163:THR:HG23	1:F:164:SER:N	1.99	0.78
1:D:241:LYS:HA	1:D:241:LYS:HE3	1.65	0.78
1:B:50:THR:HG22	1:B:73:TYR:HE1	1.48	0.77
2:C:401:FPS:H91	2:C:401:FPS:H12	1.68	0.76
1:F:65:MET:HE1	1:F:187:PHE:CD1	2.20	0.76
2:E:402:FPS:H41	2:E:402:FPS:C7	2.16	0.75
1:B:297:ILE:CD1	1:B:342:MET:HE1	2.09	0.75
1:F:88:ILE:HG13	1:F:92:LYS:HD3	1.70	0.74
1:F:163:THR:CG2	1:F:164:SER:H	2.02	0.73
1:A:233:GLN:HE21	1:A:234:GLU:HG2	1.52	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:MET:CE	2:B:402:FPS:C4	2.66	0.73
1:F:101:HIS:CD2	1:F:148:ARG:HG3	2.24	0.72
1:F:176:ALA:HB2	1:F:212:GLN:HG2	1.70	0.72
1:E:322:VAL:HG13	1:E:326:MET:HE2	1.71	0.72
1:C:51:SER:HB2	1:C:73:TYR:CZ	2.24	0.72
1:A:138:LYS:HG2	1:A:189:ALA:HB1	1.70	0.72
1:A:180:GLY:HA2	2:A:401:FPS:H152	1.72	0.72
1:B:242:LYS:HE2	1:B:245:ASP:OD1	1.90	0.71
1:F:65:MET:HE1	1:F:187:PHE:HD1	1.53	0.71
1:B:50:THR:HG22	1:B:73:TYR:CE1	2.24	0.71
1:B:85:ASP:OD1	1:B:87:THR:HB	1.91	0.71
1:C:282:ASN:HD22	1:C:285:VAL:H	1.39	0.71
1:D:150:MET:CG	1:D:178:LEU:HD21	2.20	0.71
1:E:207:MET:HG2	2:E:401:FPS:H153	1.73	0.71
1:D:94:VAL:HG13	1:D:95:PRO:HD3	1.74	0.70
1:B:214:THR:HG23	1:B:300:LEU:HD13	1.73	0.69
1:B:297:ILE:HD11	1:B:342:MET:HE3	1.71	0.69
2:B:401:FPS:H12	2:B:401:FPS:H91	1.75	0.69
1:C:283:GLN:HE21	1:C:287:ASN:ND2	1.90	0.69
1:A:282:ASN:HD22	1:A:285:VAL:H	1.40	0.68
1:F:286:PHE:CE1	1:F:331:MET:CE	2.71	0.68
1:D:282:ASN:HD22	1:D:285:VAL:H	1.42	0.68
1:A:175:VAL:O	2:A:402:FPS:H51	1.94	0.68
1:D:83:GLU:HB2	1:D:154:MET:CE	2.22	0.68
1:E:97:LEU:HD21	1:E:155:ALA:HB2	1.76	0.67
1:E:163:THR:CG2	1:E:164:SER:N	2.55	0.67
1:E:282:ASN:HD22	1:E:285:VAL:H	1.40	0.67
1:A:325:MET:O	1:C:327:ASP:HB2	1.95	0.67
1:C:97:LEU:HD22	1:C:154:MET:HE2	1.77	0.66
1:F:350:PRO:HG2	1:F:353:ASP:HB2	1.76	0.66
1:F:65:MET:CE	1:F:187:PHE:CD1	2.76	0.66
1:D:286:PHE:CZ	1:D:331:MET:HE2	2.31	0.66
1:B:297:ILE:CD1	1:B:342:MET:CE	2.63	0.65
1:B:315:LYS:N	1:B:315:LYS:HD2	2.11	0.65
1:C:283:GLN:HE21	1:C:287:ASN:HD21	1.44	0.65
1:E:150:MET:HG2	1:E:174:TYR:O	1.97	0.65
1:A:58:ILE:HD11	2:A:402:FPS:H143	1.79	0.64
1:B:50:THR:CG2	1:B:73:TYR:HE1	2.09	0.64
1:E:322:VAL:CG1	1:E:326:MET:CE	2.75	0.64
2:E:402:FPS:H41	2:E:402:FPS:C8	2.28	0.64
1:A:369:GLN:HA	1:A:369:GLN:OE1	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:163:THR:HG22	1:E:164:SER:H	1.62	0.63
1:F:176:ALA:HB2	1:F:212:GLN:CG	2.27	0.63
1:B:45:LYS:O	1:B:49:GLN:HG3	1.99	0.63
1:C:260:ASN:HD21	1:C:305:ASN:HD22	1.46	0.63
1:E:163:THR:HG23	1:E:164:SER:N	2.14	0.63
1:B:315:LYS:HD2	1:B:315:LYS:H	1.63	0.63
1:A:180:GLY:CA	2:A:401:FPS:H152	2.29	0.62
1:F:100:PHE:HA	1:F:103:PHE:CD2	2.33	0.62
1:A:164:SER:HA	1:A:234:GLU:HG3	1.80	0.62
1:B:150:MET:HE3	2:B:402:FPS:H41	1.82	0.62
1:B:46:TYR:O	1:B:50:THR:HB	2.00	0.61
1:F:277:LEU:CB	1:F:331:MET:HE1	2.25	0.61
1:C:240:VAL:HG11	1:C:245:ASP:HB2	1.81	0.61
1:E:97:LEU:CD2	1:E:155:ALA:HB2	2.31	0.61
1:C:235:VAL:HA	1:C:238:ARG:HH21	1.66	0.60
1:E:163:THR:HG23	1:E:164:SER:H	1.62	0.60
1:F:139:TYR:O	1:F:143:ILE:HG23	2.00	0.60
1:F:163:THR:HG22	1:F:167:GLU:HG3	1.82	0.60
1:C:83:GLU:CG	1:C:154:MET:HE3	2.31	0.60
1:A:51:SER:HB2	1:A:73:TYR:OH	2.02	0.59
1:B:73:TYR:HB2	2:B:402:FPS:H152	1.83	0.59
1:B:50:THR:HG21	1:B:77:ARG:HG2	1.85	0.59
1:E:223:ASP:OD1	1:E:228:ARG:NH1	2.36	0.59
1:F:50:THR:CG2	1:F:77:ARG:HG2	2.30	0.59
1:D:83:GLU:CB	1:D:154:MET:HE3	2.25	0.58
1:C:320:GLN:HG2	1:C:321:ALA:H	1.68	0.58
1:E:50:THR:HG23	1:E:73:TYR:HE1	1.68	0.58
1:A:163:THR:C	1:A:234:GLU:HG3	2.28	0.58
1:C:322:VAL:HG13	1:C:340:GLN:HE22	1.69	0.58
1:F:112:MET:HA	1:F:123:GLU:HG2	1.86	0.57
2:B:401:FPS:H2	2:B:402:FPS:H101	1.85	0.57
1:B:154:MET:CE	2:B:402:FPS:H41	2.34	0.57
1:D:214:THR:HG23	1:D:300:LEU:HD13	1.87	0.57
1:F:325:MET:O	1:F:325:MET:HG3	2.05	0.57
1:F:39:SER:HB3	1:F:131:GLU:OE2	2.03	0.57
1:A:138:LYS:HB2	3:A:600:HOH:O	2.05	0.56
1:D:343:GLU:CD	1:D:367:ARG:HH21	2.13	0.56
1:A:215:ASN:ND2	3:A:579:HOH:O	2.37	0.56
1:E:39:SER:HB3	1:E:131:GLU:OE2	2.06	0.56
1:F:48:ASN:HD21	1:F:59:GLN:NE2	2.03	0.56
2:A:402:FPS:H42	2:A:402:FPS:O2A	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:PHE:HA	1:B:103:PHE:CD2	2.41	0.56
1:A:73:TYR:CD1	1:A:73:TYR:C	2.84	0.56
1:C:93:LYS:HG2	1:C:158:LEU:HD21	1.86	0.55
1:E:84:ASP:O	1:E:86:MET:HE2	2.07	0.55
1:F:173:HIS:CE1	1:F:178:LEU:HD13	2.42	0.55
1:E:132:PHE:O	1:E:135:LEU:HB2	2.07	0.55
1:C:297:ILE:HD13	1:C:338:ILE:HG12	1.89	0.55
1:F:51:SER:HB3	1:F:73:TYR:OH	2.06	0.55
1:F:137:GLU:O	1:F:141:THR:HG22	2.06	0.55
1:A:326:MET:HA	1:C:327:ASP:OD2	2.07	0.55
1:B:342:MET:HE2	1:B:342:MET:HA	1.88	0.55
1:C:207:MET:HB2	2:C:401:FPS:H153	1.88	0.55
1:D:241:LYS:HE3	1:D:241:LYS:CA	2.35	0.55
1:B:109:TRP:O	1:B:126:PRO:HD3	2.07	0.54
1:C:207:MET:CB	2:C:401:FPS:H153	2.38	0.54
1:C:343:GLU:OE1	1:C:367:ARG:NH2	2.41	0.54
1:E:46:TYR:O	1:E:50:THR:HG22	2.06	0.54
1:A:263:ILE:HG23	1:A:300:LEU:HG	1.89	0.54
1:C:235:VAL:HG11	1:C:262:LEU:HD13	1.90	0.54
1:E:213:LYS:NZ	1:E:269:HIS:HE1	2.06	0.54
1:F:235:VAL:HG11	1:F:262:LEU:HD13	1.89	0.54
1:A:163:THR:O	1:A:234:GLU:HG3	2.08	0.54
1:A:235:VAL:HG11	1:A:262:LEU:CD1	2.38	0.54
1:C:322:VAL:HG23	1:C:326:MET:HE2	1.89	0.54
1:F:277:LEU:C	1:F:331:MET:HE3	2.33	0.53
1:A:228:ARG:HH11	1:A:228:ARG:CG	2.18	0.53
1:D:286:PHE:HE1	1:D:331:MET:HE1	1.63	0.53
1:B:342:MET:HE2	1:B:342:MET:CA	2.39	0.53
1:C:342:MET:HE3	1:C:342:MET:HA	1.90	0.53
1:D:51:SER:HB2	1:D:73:TYR:OH	2.09	0.53
1:C:150:MET:HG3	1:C:174:TYR:O	2.09	0.53
1:F:353:ASP:O	1:F:356:SER:OG	2.26	0.53
1:B:195:PRO:O	1:B:199:GLU:HG3	2.09	0.53
1:F:231:TRP:HB2	1:F:243:LEU:HD11	1.90	0.53
2:C:401:FPS:H91	2:C:401:FPS:C12	2.38	0.52
1:E:293:GLN:O	1:E:297:ILE:HG12	2.09	0.52
1:C:283:GLN:NE2	1:C:287:ASN:HD21	2.07	0.52
1:E:350:PRO:HG2	1:E:353:ASP:HB2	1.90	0.52
1:A:228:ARG:HG3	1:A:228:ARG:NH1	2.15	0.52
1:E:235:VAL:HA	1:E:238:ARG:HH21	1.75	0.52
1:E:79:LEU:HG	1:E:154:MET:HE1	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:65:MET:HE3	1:F:187:PHE:HA	1.92	0.52
1:A:257:GLN:HG2	1:A:354:PRO:HD2	1.92	0.52
1:B:294:VAL:O	1:B:297:ILE:HG22	2.10	0.52
1:F:278:SER:HA	1:F:331:MET:HE3	1.92	0.51
1:A:207:MET:HB2	2:A:401:FPS:H153	1.91	0.51
1:F:325:MET:O	1:F:326:MET:HB3	2.10	0.51
1:A:326:MET:HE3	1:C:291:ILE:HD11	1.91	0.51
1:C:111:PHE:HB3	1:C:122:LEU:HB3	1.92	0.51
1:F:111:PHE:HB3	1:F:122:LEU:HB3	1.92	0.51
1:D:73:TYR:C	1:D:73:TYR:CD1	2.89	0.51
1:A:100:PHE:HA	1:A:103:PHE:CD2	2.46	0.51
1:F:72:PHE:O	1:F:76:LEU:HG	2.10	0.51
1:C:93:LYS:HE3	1:C:158:LEU:HD11	1.93	0.51
1:E:215:ASN:HA	1:E:218:ARG:NH1	2.26	0.51
1:C:39:SER:HB3	1:C:131:GLU:OE2	2.11	0.50
1:F:176:ALA:O	1:F:179:VAL:HB	2.11	0.50
1:E:210:PHE:CE2	1:E:297:ILE:HD13	2.47	0.50
1:F:79:LEU:HB2	1:F:100:PHE:CE2	2.46	0.50
1:A:368:THR:O	1:A:369:GLN:C	2.55	0.50
1:A:39:SER:HB3	1:A:131:GLU:OE2	2.12	0.50
1:C:215:ASN:HD22	2:C:401:FPS:H42	1.77	0.50
1:A:175:VAL:HB	2:A:402:FPS:H2	1.93	0.49
1:B:50:THR:HG23	1:B:77:ARG:HE	1.77	0.49
1:D:277:LEU:O	1:D:331:MET:HE3	2.12	0.49
1:F:217:ILE:CD1	1:F:262:LEU:HB3	2.42	0.49
1:F:163:THR:HA	1:F:233:GLN:HB3	1.94	0.49
1:B:342:MET:HE2	1:B:342:MET:N	2.27	0.49
1:E:153:GLY:HA3	1:E:174:TYR:CG	2.47	0.49
1:F:93:LYS:HG2	1:F:97:LEU:HD13	1.94	0.49
1:A:235:VAL:HG11	1:A:262:LEU:HD13	1.93	0.49
1:D:286:PHE:CE1	1:D:331:MET:HE1	2.39	0.49
1:E:110:ARG:HD2	1:E:112:MET:HE3	1.94	0.49
1:E:327:ASP:OD1	1:E:328:ALA:N	2.45	0.49
1:C:163:THR:HA	1:C:233:GLN:HG3	1.93	0.49
1:D:76:LEU:HD22	1:D:150:MET:SD	2.53	0.49
1:D:90:VAL:O	1:D:94:VAL:HG12	2.13	0.49
1:D:238:ARG:NH2	1:D:261:GLU:OE2	2.47	0.48
1:D:315:LYS:O	1:D:315:LYS:HG2	2.12	0.48
1:C:51:SER:HB2	1:C:73:TYR:OH	2.13	0.48
1:A:82:LEU:O	1:A:93:LYS:HD2	2.13	0.48
1:C:233:GLN:HA	1:C:236:TRP:NE1	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:150:MET:O	1:E:154:MET:HG3	2.14	0.48
2:B:401:FPS:H12	2:B:401:FPS:C9	2.42	0.48
1:D:170:LYS:HB2	1:D:170:LYS:HE3	1.58	0.48
1:F:207:MET:HG3	1:F:293:GLN:NE2	2.28	0.48
1:F:48:ASN:HD21	1:F:59:GLN:HE22	1.61	0.48
1:F:110:ARG:NH1	1:F:123:GLU:O	2.42	0.48
2:C:401:FPS:H12	2:C:401:FPS:C9	2.40	0.48
1:B:52:ARG:HG2	2:B:401:FPS:O1B	2.14	0.48
1:D:110:ARG:HB3	1:D:126:PRO:HD3	1.96	0.47
1:C:83:GLU:OE2	1:C:154:MET:HG2	2.14	0.47
1:A:58:ILE:HD11	2:A:402:FPS:C14	2.45	0.47
1:A:369:GLN:OE1	1:C:36:LEU:HD11	2.14	0.47
1:B:289:CYS:SG	2:B:401:FPS:H141	2.55	0.47
1:A:245:ASP:HB3	1:A:251:ASN:HD22	1.80	0.47
1:B:73:TYR:CD1	1:B:73:TYR:C	2.92	0.47
1:B:154:MET:HE2	2:B:402:FPS:C4	2.44	0.47
1:E:51:SER:HB2	1:E:73:TYR:CZ	2.48	0.47
1:E:353:ASP:HA	1:E:354:PRO:HD3	1.75	0.47
1:B:220:TYR:CZ	1:B:246:PHE:HB2	2.49	0.47
1:B:320:GLN:HE21	1:B:321:ALA:H	1.62	0.47
1:A:112:MET:SD	1:A:123:GLU:HG2	2.55	0.46
1:E:207:MET:HE1	1:E:277:LEU:HD21	1.97	0.46
1:A:327:ASP:OD2	1:B:326:MET:HA	2.15	0.46
1:C:176:ALA:HB2	1:C:212:GLN:HE21	1.80	0.46
1:D:180:GLY:CA	2:D:401:FPS:H152	2.33	0.46
1:E:289:CYS:SG	2:E:401:FPS:H141	2.56	0.46
1:A:150:MET:HG3	1:A:174:TYR:O	2.16	0.46
1:B:119:ARG:O	1:B:123:GLU:HG3	2.15	0.46
1:B:323:THR:CG2	1:B:340:GLN:HG2	2.46	0.46
1:E:170:LYS:HE2	1:E:174:TYR:CE2	2.51	0.46
2:A:401:FPS:H51	2:A:402:FPS:H7	1.98	0.46
1:C:325:MET:HE3	1:C:325:MET:HA	1.98	0.46
1:E:100:PHE:HA	1:E:103:PHE:CD2	2.50	0.46
1:A:214:THR:HG23	1:A:300:LEU:HD13	1.97	0.46
1:A:257:GLN:HG2	1:A:354:PRO:CD	2.46	0.46
1:B:255:ALA:HB1	1:B:310:PHE:CZ	2.51	0.46
1:B:297:ILE:CD1	1:B:342:MET:HE3	2.41	0.46
1:C:215:ASN:ND2	2:C:401:FPS:C4	2.79	0.46
1:E:207:MET:HG2	2:E:401:FPS:C15	2.43	0.46
1:B:180:GLY:HA2	2:B:401:FPS:H152	1.98	0.45
1:E:207:MET:HE1	1:E:277:LEU:CD2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:THR:CG2	1:B:73:TYR:CE1	2.94	0.45
1:F:233:GLN:O	1:F:237:SER:HB3	2.16	0.45
1:A:245:ASP:O	1:A:248:LYS:HG2	2.16	0.45
1:B:323:THR:HG23	1:B:340:GLN:HG2	1.98	0.45
1:F:277:LEU:C	1:F:331:MET:CE	2.89	0.45
1:F:255:ALA:HB1	1:F:310:PHE:CZ	2.52	0.45
1:B:220:TYR:OH	1:B:243:LEU:O	2.28	0.45
2:B:401:FPS:H91	2:B:401:FPS:C12	2.46	0.45
1:C:260:ASN:HD21	1:C:305:ASN:ND2	2.13	0.45
1:F:163:THR:CG2	1:F:167:GLU:HG3	2.47	0.45
1:C:153:GLY:HA3	1:C:174:TYR:CG	2.51	0.45
1:A:326:MET:HE3	1:C:291:ILE:CD1	2.47	0.45
1:C:94:VAL:HB	1:C:95:PRO:HD3	1.99	0.45
1:F:57:VAL:HG13	1:F:288:PHE:HD2	1.81	0.45
1:F:93:LYS:HD2	1:F:158:LEU:HD21	1.99	0.45
1:A:342:MET:HE2	1:A:342:MET:HB2	1.54	0.45
1:B:163:THR:HA	1:B:233:GLN:HB3	1.99	0.45
1:C:153:GLY:HA3	1:C:174:TYR:CD1	2.52	0.45
1:D:269:HIS:O	1:D:273:VAL:HG23	2.17	0.45
2:D:401:FPS:C12	2:D:401:FPS:H91	2.46	0.45
1:D:323:THR:HG23	1:D:337:ILE:HG12	1.98	0.45
1:E:163:THR:HA	1:E:233:GLN:HB3	1.99	0.45
1:F:236:TRP:CD1	1:F:243:LEU:HD12	2.52	0.45
1:D:316:ILE:HG13	1:D:316:ILE:O	2.16	0.44
1:F:125:PHE:N	1:F:126:PRO:CD	2.81	0.44
1:F:297:ILE:CD1	1:F:338:ILE:HG12	2.39	0.44
1:B:121:VAL:HG22	1:B:128:ILE:HD11	1.99	0.44
1:B:53:SER:HB2	2:B:401:FPS:O2A	2.17	0.44
1:E:170:LYS:HE2	1:E:174:TYR:CZ	2.51	0.44
1:F:306:ASN:O	1:F:309:VAL:HG22	2.17	0.44
1:B:150:MET:HE3	1:B:154:MET:HE3	2.00	0.44
1:B:320:GLN:HG3	1:B:321:ALA:N	2.33	0.44
1:B:291:ILE:HD11	1:C:326:MET:HG3	1.98	0.44
1:B:154:MET:HE1	2:B:402:FPS:C4	2.44	0.44
2:E:402:FPS:C7	2:E:402:FPS:C4	2.92	0.44
1:F:286:PHE:HE1	1:F:331:MET:HE1	1.76	0.44
1:C:235:VAL:HG11	1:C:262:LEU:CD1	2.48	0.44
1:F:364:SER:O	1:F:368:THR:HG23	2.18	0.44
2:A:401:FPS:H91	2:A:401:FPS:H12	1.98	0.44
1:C:322:VAL:HG13	1:C:340:GLN:NE2	2.32	0.44
1:D:170:LYS:O	1:D:173:HIS:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:119:ARG:O	1:E:123:GLU:HG3	2.18	0.44
1:A:190:SER:O	1:A:191:GLU:HB2	2.18	0.43
1:B:105:TYR:O	1:B:107:PRO:HD3	2.18	0.43
1:D:58:ILE:HA	1:D:61:LEU:HD22	2.01	0.43
1:D:65:MET:HE1	1:D:285:VAL:HG23	2.00	0.43
1:E:289:CYS:SG	2:E:401:FPS:C14	3.06	0.43
1:E:242:LYS:O	1:E:245:ASP:HB2	2.17	0.43
1:E:110:ARG:HH11	1:E:112:MET:HE3	1.84	0.43
1:D:323:THR:HG22	1:D:323:THR:O	2.17	0.43
1:E:85:ASP:HB3	1:E:88:ILE:HD12	2.00	0.43
1:A:326:MET:HE1	3:A:541:HOH:O	2.18	0.43
1:B:153:GLY:HA3	1:B:174:TYR:CD1	2.53	0.43
1:F:249:PRO:O	1:F:252:ILE:HG12	2.19	0.43
1:B:219:ASP:O	1:B:220:TYR:C	2.61	0.43
1:C:215:ASN:ND2	2:C:401:FPS:H43	2.34	0.43
1:E:170:LYS:HD2	1:E:170:LYS:HA	1.86	0.43
1:E:215:ASN:HA	1:E:218:ARG:HH11	1.84	0.43
1:F:94:VAL:HB	1:F:95:PRO:HD3	2.01	0.43
1:D:343:GLU:OE2	1:D:367:ARG:NE	2.48	0.42
2:A:401:FPS:H2	2:A:402:FPS:H101	2.02	0.42
1:B:101:HIS:O	1:B:104:LEU:HB2	2.19	0.42
1:C:210:PHE:CE2	1:C:297:ILE:HG13	2.54	0.42
2:D:401:FPS:H91	2:D:401:FPS:H12	2.01	0.42
1:B:315:LYS:N	1:B:315:LYS:CD	2.78	0.42
1:C:309:VAL:HG22	1:C:314:VAL:HG21	2.02	0.42
1:F:43:CYS:O	1:F:74:LEU:HD21	2.19	0.42
1:B:50:THR:CG2	1:B:77:ARG:HG2	2.49	0.42
1:D:326:MET:HA	1:F:327:ASP:CG	2.43	0.42
1:C:233:GLN:HA	1:C:236:TRP:CD1	2.54	0.42
1:C:263:ILE:HG23	1:C:300:LEU:HG	2.02	0.42
1:E:322:VAL:HB	1:E:340:GLN:NE2	2.33	0.42
1:C:77:ARG:HD3	1:C:77:ARG:HA	1.66	0.42
2:D:401:FPS:H142	3:D:505:HOH:O	2.19	0.42
1:E:342:MET:HE2	1:E:363:ILE:HG12	2.02	0.42
2:E:401:FPS:H93	2:E:402:FPS:H142	2.00	0.42
1:B:142:VAL:O	1:B:146:ILE:HG12	2.19	0.42
1:B:236:TRP:CD1	1:B:243:LEU:HD13	2.55	0.42
1:C:240:VAL:CG1	1:C:245:ASP:HB2	2.48	0.42
1:C:190:SER:O	1:C:191:GLU:HB2	2.19	0.42
1:F:282:ASN:ND2	1:F:285:VAL:HG23	2.35	0.42
1:D:115:LYS:HD2	1:D:115:LYS:HA	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:119:ARG:O	1:D:123:GLU:HG3	2.20	0.42
1:F:108:ASP:OD1	1:F:108:ASP:C	2.63	0.42
2:D:401:FPS:H12	2:D:401:FPS:C9	2.51	0.41
1:F:52:ARG:HH11	1:F:53:SER:H	1.67	0.41
1:A:163:THR:HA	1:A:233:GLN:HG3	2.02	0.41
1:B:154:MET:HE2	2:B:402:FPS:H43	2.03	0.41
1:C:328:ALA:HB1	1:C:334:VAL:HG22	2.02	0.41
1:E:158:LEU:HD23	1:E:158:LEU:HA	1.92	0.41
1:F:207:MET:HE1	1:F:277:LEU:CD2	2.50	0.41
1:A:155:ALA:HA	1:A:158:LEU:HD22	2.01	0.41
1:E:287:ASN:O	1:E:291:ILE:HD12	2.20	0.41
1:F:162:VAL:HG21	1:F:230:PHE:O	2.20	0.41
1:A:92:LYS:O	1:A:96:LEU:HD22	2.21	0.41
1:A:153:GLY:HA3	1:A:174:TYR:CG	2.56	0.41
1:A:207:MET:CB	2:A:401:FPS:H153	2.51	0.41
1:B:314:VAL:HG13	1:B:315:LYS:HD2	2.02	0.41
1:C:238:ARG:NH2	1:C:261:GLU:OE2	2.54	0.41
1:C:267:LEU:HD22	1:C:342:MET:HE1	2.02	0.41
1:D:150:MET:HE2	1:D:150:MET:HB3	1.80	0.41
1:D:255:ALA:HB1	1:D:310:PHE:CZ	2.56	0.41
1:D:282:ASN:ND2	1:D:284:SER:OG	2.54	0.41
1:F:79:LEU:HD13	1:F:100:PHE:CG	2.56	0.41
1:B:82:LEU:HD13	1:B:122:LEU:HD13	2.03	0.41
1:C:97:LEU:CD2	1:C:154:MET:HE2	2.48	0.40
1:C:353:ASP:HA	1:C:354:PRO:HD3	1.80	0.40
1:B:190:SER:O	1:B:191:GLU:HB2	2.21	0.40
1:D:277:LEU:HB3	1:D:331:MET:CE	2.32	0.40
1:D:327:ASP:OD2	1:E:327:ASP:N	2.48	0.40
1:F:163:THR:CG2	1:F:164:SER:N	2.64	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	323/343 (94%)	316 (98%)	7 (2%)	0	100	100
1	B	331/343 (96%)	326 (98%)	5 (2%)	0	100	100
1	C	331/343 (96%)	321 (97%)	9 (3%)	1 (0%)	36	43
1	D	325/343 (95%)	312 (96%)	13 (4%)	0	100	100
1	E	325/343 (95%)	314 (97%)	11 (3%)	0	100	100
1	F	318/343 (93%)	298 (94%)	19 (6%)	1 (0%)	36	43
All	All	1953/2058 (95%)	1887 (97%)	64 (3%)	2 (0%)	48	59

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	315	LYS
1	F	66	ARG

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	292/305 (96%)	274 (94%)	18 (6%)	16	19
1	B	296/305 (97%)	270 (91%)	26 (9%)	9	10
1	C	296/305 (97%)	278 (94%)	18 (6%)	17	20
1	D	294/305 (96%)	260 (88%)	34 (12%)	5	5
1	E	293/305 (96%)	265 (90%)	28 (10%)	8	7
1	F	287/305 (94%)	254 (88%)	33 (12%)	5	5
All	All	1758/1830 (96%)	1601 (91%)	157 (9%)	9	10

All (157) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	SER
1	A	41	LYS
1	A	75	VAL

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Mol	Chain	Res	Type
1	A	96	LEU
1	A	121	VAL
1	A	130	LEU
1	A	158	LEU
1	A	167	GLU
1	A	183	LEU
1	A	228	ARG
1	A	254	LEU
1	A	262	LEU
1	A	291	ILE
1	A	300	LEU
1	A	315	LYS
1	A	325	MET
1	A	357	SER
1	A	369	GLN
1	B	41	LYS
1	B	50	THR
1	B	52	ARG
1	B	76	LEU
1	B	82	LEU
1	B	87	THR
1	B	90	VAL
1	B	104	LEU
1	B	115	LYS
1	B	121	VAL
1	B	159	ASP
1	B	160	LYS
1	B	175	VAL
1	B	184	SER
1	B	186	LEU
1	B	233	GLN
1	B	234	GLU
1	B	300	LEU
1	B	315	LYS
1	B	317	ARG
1	B	322	VAL
1	B	324	LEU
1	B	357	SER
1	B	358	LYS
1	B	361	GLN
1	B	367	ARG
1	C	36	LEU

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Mol	Chain	Res	Type
1	C	53	SER
1	C	57	VAL
1	C	76	LEU
1	C	137	GLU
1	C	166	GLN
1	C	170	LYS
1	C	183	LEU
1	C	211	LEU
1	C	240	VAL
1	C	262	LEU
1	C	277	LEU
1	C	300	LEU
1	C	322	VAL
1	C	342	MET
1	C	351	ASP
1	C	365	THR
1	C	368	THR
1	D	37	SER
1	D	42	THR
1	D	61	LEU
1	D	74	LEU
1	D	80	ASP
1	D	88	ILE
1	D	89	SER
1	D	92	LYS
1	D	93	LYS
1	D	94	VAL
1	D	97	LEU
1	D	98	HIS
1	D	104	LEU
1	D	108	ASP
1	D	110	ARG
1	D	112	MET
1	D	120	GLN
1	D	121	VAL
1	D	135	LEU
1	D	137	GLU
1	D	140	GLN
1	D	146	ILE
1	D	156	GLU
1	D	158	LEU
1	D	178	LEU

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Mol	Chain	Res	Type
1	D	196	LEU
1	D	206	SER
1	D	211	LEU
1	D	234	GLU
1	D	241	LYS
1	D	250	GLU
1	D	300	LEU
1	D	315	LYS
1	D	325	MET
1	E	38	SER
1	E	39	SER
1	E	87	THR
1	E	90	VAL
1	E	92	LYS
1	E	97	LEU
1	E	104	LEU
1	E	113	GLU
1	E	135	LEU
1	E	161	HIS
1	E	163	THR
1	E	196	LEU
1	E	201	THR
1	E	218	ARG
1	E	221	LEU
1	E	228	ARG
1	E	252	ILE
1	E	262	LEU
1	E	267	LEU
1	E	295	MET
1	E	316	ILE
1	E	322	VAL
1	E	329	THR
1	E	342	MET
1	E	344	GLU
1	E	352	SER
1	E	358	LYS
1	E	365	THR
1	F	52	ARG
1	F	57	VAL
1	F	74	LEU
1	F	88	ILE
1	F	90	VAL

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Mol	Chain	Res	Type
1	F	92	LYS
1	F	93	LYS
1	F	104	LEU
1	F	112	MET
1	F	115	LYS
1	F	127	THR
1	F	141	THR
1	F	143	ILE
1	F	150	MET
1	F	156	GLU
1	F	158	LEU
1	F	159	ASP
1	F	178	LEU
1	F	183	LEU
1	F	191	GLU
1	F	196	LEU
1	F	201	THR
1	F	228	ARG
1	F	234	GLU
1	F	254	LEU
1	F	257	GLN
1	F	261	GLU
1	F	262	LEU
1	F	300	LEU
1	F	305	ASN
1	F	325	MET
1	F	364	SER
1	F	368	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	215	ASN
1	A	233	GLN
1	A	251	ASN
1	A	282	ASN
1	B	48	ASN
1	B	59	GLN
1	B	101	HIS
1	B	161	HIS
1	B	224	GLN
1	B	282	ASN

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Mol	Chain	Res	Type
1	B	308	GLN
1	B	320	GLN
1	C	98	HIS
1	C	101	HIS
1	C	106	GLN
1	C	140	GLN
1	C	212	GLN
1	C	215	ASN
1	C	251	ASN
1	C	257	GLN
1	C	282	ASN
1	C	287	ASN
1	C	293	GLN
1	C	305	ASN
1	C	308	GLN
1	D	166	GLN
1	D	212	GLN
1	D	215	ASN
1	D	224	GLN
1	D	251	ASN
1	D	282	ASN
1	D	287	ASN
1	D	293	GLN
1	D	307	GLN
1	E	48	ASN
1	E	49	GLN
1	E	59	GLN
1	E	67	ASN
1	E	98	HIS
1	E	212	GLN
1	E	215	ASN
1	E	260	ASN
1	E	268	HIS
1	E	269	HIS
1	E	282	ASN
1	E	293	GLN
1	E	305	ASN
1	E	307	GLN
1	E	347	HIS
1	E	361	GLN
1	F	49	GLN
1	F	59	GLN

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Mol	Chain	Res	Type
1	F	98	HIS
1	F	134	ASN
1	F	140	GLN
1	F	282	ASN
1	F	283	GLN
1	F	293	GLN
1	F	305	ASN
1	F	306	ASN

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$
2	FPS	E	402	-	20,23,23	2.63	8 (40%)	24,31,31	1.72	5 (20%)
2	FPS	B	401	-	20,23,23	2.63	9 (45%)	24,31,31	1.56	7 (29%)
2	FPS	A	401	-	20,23,23	2.63	9 (45%)	24,31,31	1.60	5 (20%)
2	FPS	E	401	-	20,23,23	2.66	9 (45%)	24,31,31	1.60	6 (25%)
2	FPS	A	402	-	20,23,23	2.65	9 (45%)	24,31,31	1.18	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FPS	D	401	-	20,23,23	2.66	8 (40%)	24,31,31	1.65	5 (20%)
2	FPS	C	401	-	20,23,23	2.65	8 (40%)	24,31,31	1.89	6 (25%)
2	FPS	B	402	-	20,23,23	2.62	9 (45%)	24,31,31	1.62	6 (25%)

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	FPS	E	402	-	-	2/19/25/25	-
2	FPS	B	401	-	-	2/19/25/25	-
2	FPS	A	401	-	-	0/19/25/25	-
2	FPS	E	401	-	-	1/19/25/25	-
2	FPS	A	402	-	-	7/19/25/25	-
2	FPS	D	401	-	-	0/19/25/25	-
2	FPS	C	401	-	-	1/19/25/25	-
2	FPS	B	402	-	-	5/19/25/25	-

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	401	FPS	PA-O1A	7.22	1.62	1.46
2	A	401	FPS	PA-O1A	7.14	1.62	1.46
2	E	402	FPS	PA-O1A	7.10	1.62	1.46
2	B	402	FPS	PA-O1A	7.02	1.62	1.46
2	D	401	FPS	PA-O1A	7.01	1.62	1.46
2	C	401	FPS	PA-O1A	7.00	1.62	1.46
2	A	402	FPS	PA-O1A	6.97	1.61	1.46
2	B	401	FPS	PA-O1A	6.78	1.61	1.46
2	A	402	FPS	PB-O2B	3.87	1.62	1.50
2	B	401	FPS	PB-O2B	3.85	1.62	1.50
2	E	402	FPS	C11-C12	-3.83	1.38	1.50
2	E	402	FPS	PB-O2B	3.81	1.62	1.50
2	C	401	FPS	PB-O2B	3.77	1.62	1.50
2	D	401	FPS	PB-O2B	3.76	1.62	1.50
2	C	401	FPS	C6-C7	-3.74	1.39	1.50
2	A	402	FPS	C6-C7	-3.71	1.39	1.50
2	A	401	FPS	C6-C7	-3.71	1.39	1.50
2	A	401	FPS	PB-O2B	3.70	1.62	1.50
2	B	402	FPS	PB-O2B	3.69	1.61	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	402	FPS	C11-C12	-3.65	1.39	1.50
2	B	402	FPS	C6-C7	-3.65	1.39	1.50
2	B	402	FPS	C11-C12	-3.65	1.39	1.50
2	D	401	FPS	C6-C7	-3.64	1.39	1.50
2	E	401	FPS	C11-C12	-3.62	1.39	1.50
2	D	401	FPS	C11-C12	-3.61	1.39	1.50
2	E	401	FPS	C6-C7	-3.59	1.39	1.50
2	E	401	FPS	PB-O2B	3.57	1.61	1.50
2	E	402	FPS	C6-C7	-3.57	1.39	1.50
2	A	401	FPS	C11-C12	-3.57	1.39	1.50
2	B	401	FPS	C6-C7	-3.54	1.39	1.50
2	B	401	FPS	C11-C12	-3.46	1.40	1.50
2	C	401	FPS	C11-C12	-3.42	1.40	1.50
2	D	401	FPS	PA-O2A	-3.36	1.48	1.56
2	B	402	FPS	PA-O2A	-3.35	1.48	1.56
2	C	401	FPS	C2-C3	3.33	1.40	1.33
2	B	401	FPS	PA-O2A	-3.21	1.48	1.56
2	A	402	FPS	PA-O2A	-3.20	1.48	1.56
2	E	401	FPS	PA-O2A	-3.19	1.48	1.56
2	A	402	FPS	C2-C3	3.09	1.40	1.33
2	C	401	FPS	PA-O2A	-3.06	1.49	1.56
2	E	402	FPS	PA-O2A	-3.04	1.49	1.56
2	D	401	FPS	C2-C3	3.03	1.40	1.33
2	A	401	FPS	PA-O2A	-3.02	1.49	1.56
2	D	401	FPS	C7-C8	2.98	1.39	1.33
2	B	401	FPS	C7-C8	2.98	1.39	1.33
2	E	402	FPS	C7-C8	2.97	1.39	1.33
2	B	401	FPS	C2-C3	2.97	1.39	1.33
2	C	401	FPS	C7-C8	2.89	1.39	1.33
2	E	401	FPS	C7-C8	2.87	1.39	1.33
2	E	401	FPS	C2-C3	2.87	1.39	1.33
2	B	402	FPS	C7-C8	2.87	1.39	1.33
2	A	401	FPS	C7-C8	2.82	1.39	1.33
2	B	402	FPS	C2-C3	2.82	1.39	1.33
2	A	402	FPS	C7-C8	2.82	1.39	1.33
2	C	401	FPS	C12-C13	2.79	1.40	1.32
2	A	401	FPS	C2-C3	2.76	1.39	1.33
2	E	402	FPS	C2-C3	2.66	1.39	1.33
2	B	401	FPS	C12-C13	2.61	1.40	1.32
2	A	401	FPS	C12-C13	2.51	1.40	1.32
2	E	401	FPS	C12-C13	2.51	1.40	1.32
2	D	401	FPS	C12-C13	2.44	1.39	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	402	FPS	C12-C13	2.34	1.39	1.32
2	B	402	FPS	C12-C13	2.32	1.39	1.32
2	E	402	FPS	C12-C13	2.17	1.39	1.32
2	E	401	FPS	PB-O3B	2.09	1.62	1.54
2	B	402	FPS	PB-O3B	2.09	1.62	1.54
2	A	402	FPS	PB-O3B	2.08	1.62	1.54
2	A	401	FPS	PB-O3B	2.05	1.62	1.54
2	B	401	FPS	PB-O3B	2.04	1.62	1.54

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	FPS	C6-C7-C8	4.99	139.04	127.62
2	E	402	FPS	C4-C3-C5	4.65	123.30	115.23
2	C	401	FPS	C9-C8-C7	-4.13	113.02	123.63
2	D	401	FPS	C4-C3-C5	3.74	121.72	115.23
2	A	401	FPS	C4-C3-C5	3.57	121.42	115.23
2	C	401	FPS	O1B-PB-O3A	3.31	115.74	104.64
2	E	401	FPS	C4-C3-C5	3.20	120.78	115.23
2	E	402	FPS	O2A-PA-O3A	3.15	115.79	107.27
2	B	401	FPS	C4-C3-C5	2.99	120.42	115.23
2	B	402	FPS	O1B-PB-O3A	2.98	114.63	104.64
2	B	402	FPS	C4-C3-C2	-2.97	116.00	123.63
2	E	402	FPS	O1B-PB-O3A	2.96	114.56	104.64
2	D	401	FPS	O1B-PB-O3A	2.91	114.38	104.64
2	A	402	FPS	O1B-PB-O3A	2.86	114.22	104.64
2	C	401	FPS	C10-C8-C7	2.84	127.55	121.17
2	A	401	FPS	C9-C8-C7	-2.81	116.41	123.63
2	B	402	FPS	C4-C3-C5	2.80	120.09	115.23
2	A	401	FPS	O1B-PB-O3A	2.80	114.01	104.64
2	E	401	FPS	C9-C8-C10	2.79	120.07	115.23
2	D	401	FPS	O2A-PA-O3A	2.74	114.67	107.27
2	C	401	FPS	O2A-PA-O3A	2.73	114.65	107.27
2	E	401	FPS	C9-C8-C7	-2.71	116.66	123.63
2	D	401	FPS	C9-C8-C7	-2.70	116.70	123.63
2	E	402	FPS	C4-C3-C2	-2.64	116.83	123.63
2	E	401	FPS	O1B-PB-O3A	2.63	113.47	104.64
2	B	402	FPS	O2A-PA-O3A	2.61	114.34	107.27
2	B	401	FPS	C9-C8-C10	2.60	119.74	115.23
2	B	402	FPS	C14-C13-C12	-2.58	114.92	122.66
2	B	401	FPS	C14-C13-C12	-2.58	114.93	122.66
2	E	402	FPS	C15-C13-C14	2.56	120.49	114.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	FPS	C9-C8-C10	2.54	119.64	115.23
2	A	401	FPS	C9-C8-C10	2.51	119.59	115.23
2	B	401	FPS	C9-C8-C7	-2.51	117.18	123.63
2	B	402	FPS	C15-C13-C14	2.45	120.22	114.59
2	C	401	FPS	C9-C8-C10	2.41	119.42	115.23
2	E	401	FPS	O2A-PA-O3A	2.38	113.70	107.27
2	B	401	FPS	O1B-PB-O3A	2.26	112.22	104.64
2	A	402	FPS	C9-C8-C10	2.24	119.12	115.23
2	E	401	FPS	C14-C13-C12	-2.11	116.34	122.66
2	B	401	FPS	C6-C7-C8	2.09	132.41	127.62
2	B	401	FPS	C11-C12-C13	2.08	134.59	127.64
2	A	401	FPS	C6-C7-C8	2.06	132.35	127.62

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	402	FPS	PA-O3A-PB-O1B
2	B	401	FPS	PA-O3A-PB-O1B
2	E	402	FPS	C4-C3-C5-C6
2	E	402	FPS	C2-C3-C5-C6
2	A	402	FPS	C3-C5-C6-C7
2	B	402	FPS	C3-C5-C6-C7
2	A	402	FPS	C8-C10-C11-C12
2	A	402	FPS	C11-C10-C8-C9
2	A	402	FPS	C11-C10-C8-C7
2	B	402	FPS	PA-O3A-PB-O1B
2	B	402	FPS	PB-O3A-PA-O2A
2	E	401	FPS	PA-O3A-PB-O2B
2	B	402	FPS	C11-C10-C8-C9
2	A	402	FPS	PA-O3A-PB-O2B
2	A	402	FPS	PA-O3A-PB-O3B
2	B	401	FPS	PA-O3A-PB-O3B
2	C	401	FPS	C3-C5-C6-C7
2	B	402	FPS	PB-O3A-PA-O1A

There are no ring outliers.

8 monomers are involved in 49 short contacts:

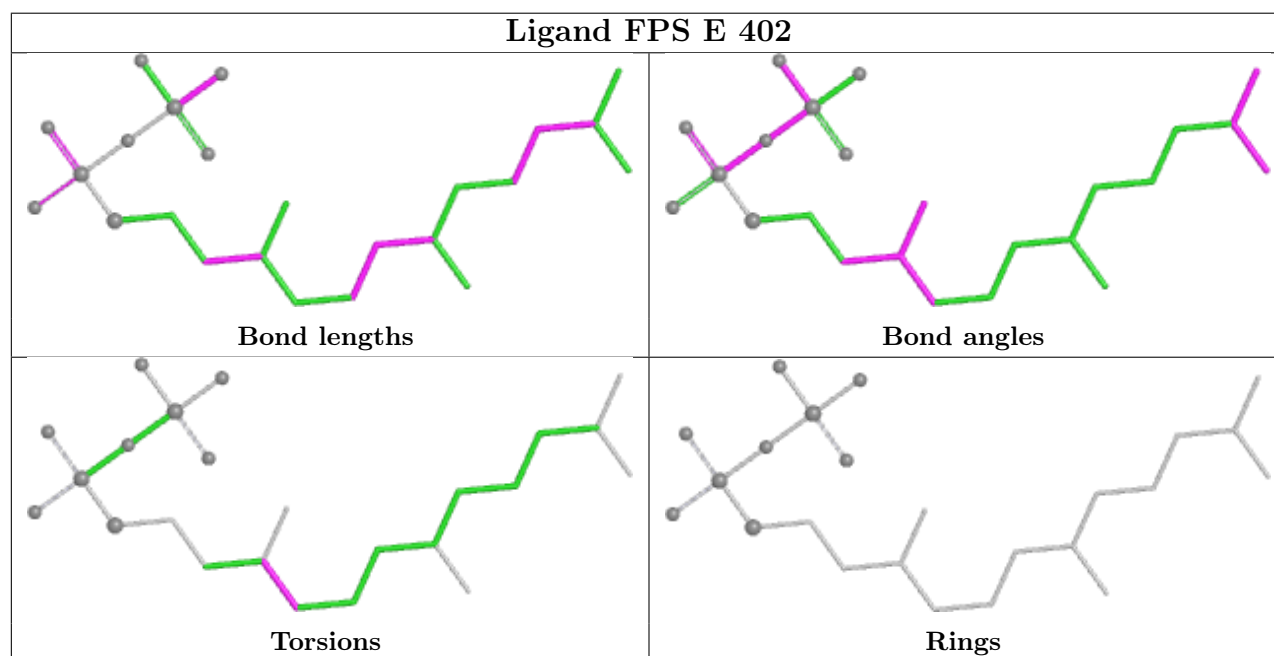
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	402	FPS	4	0

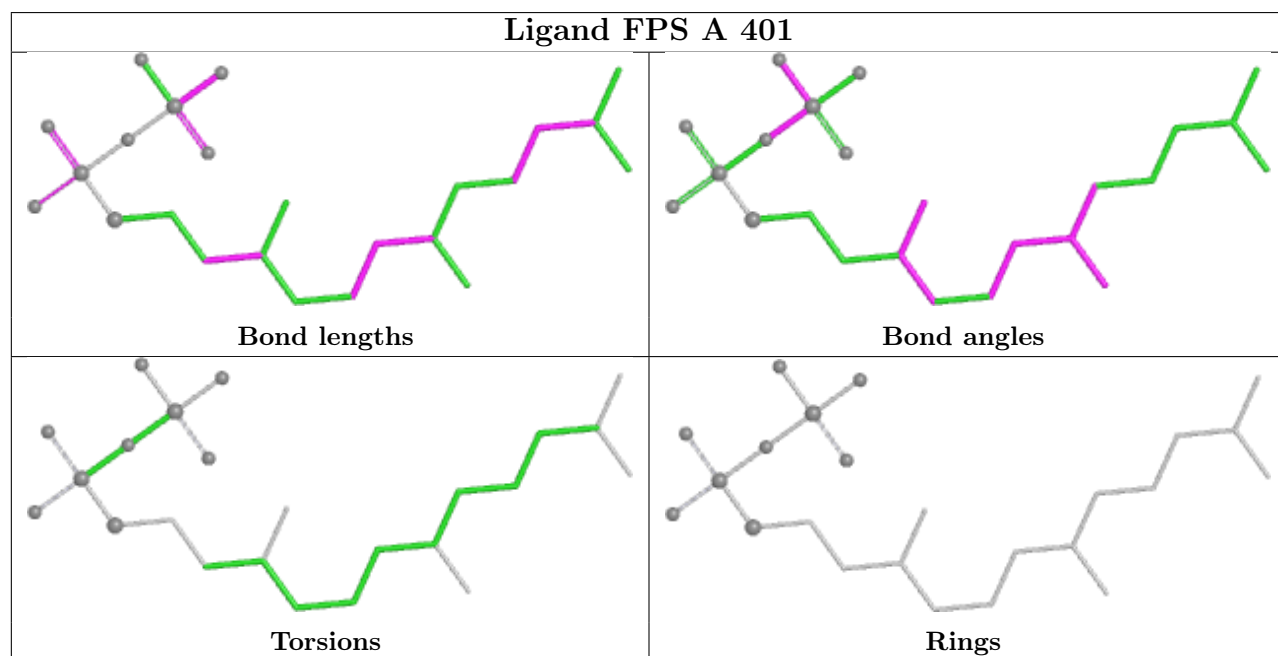
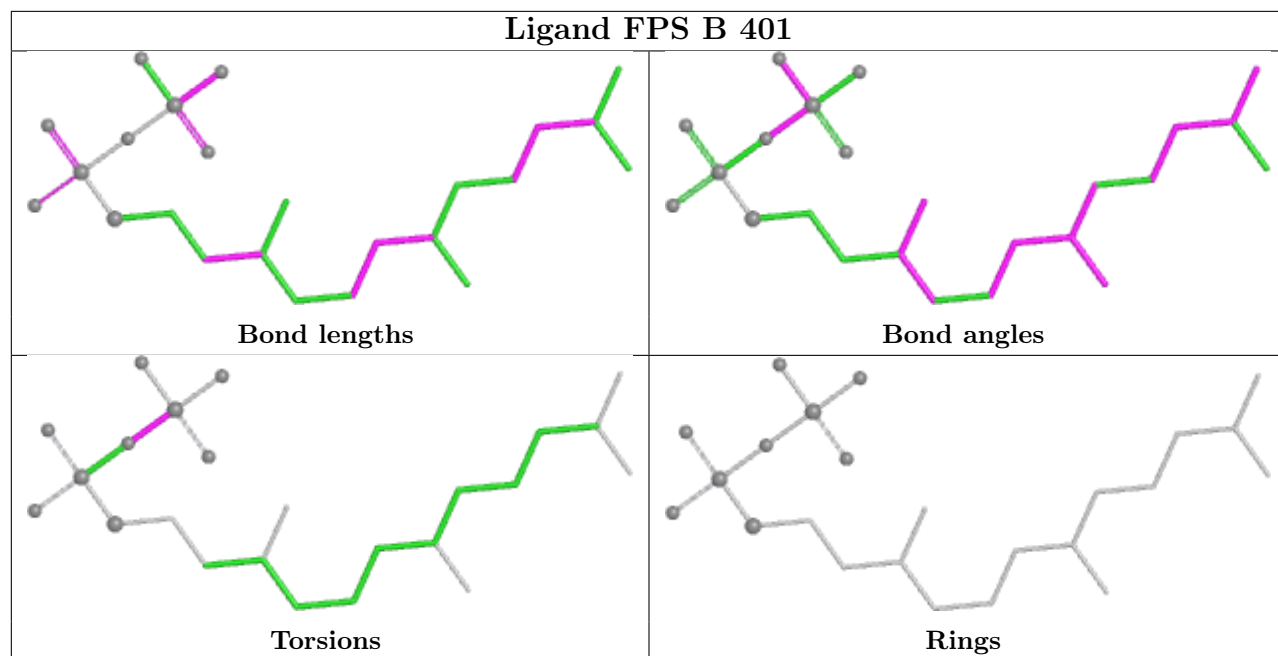
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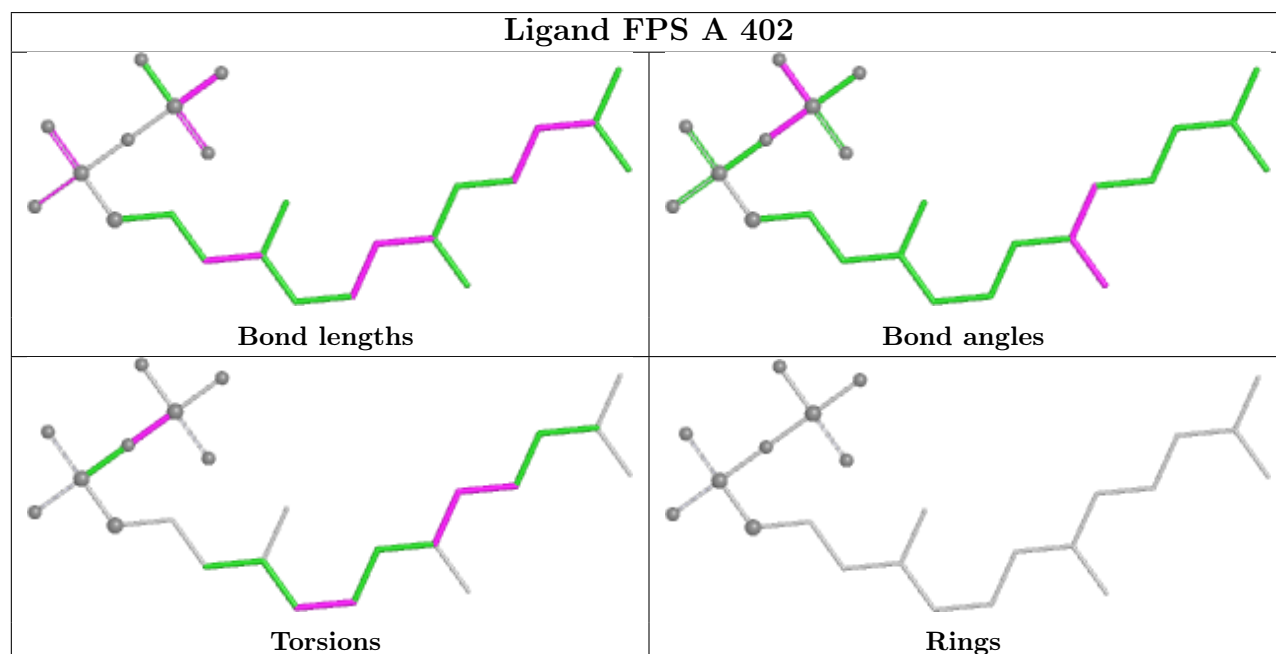
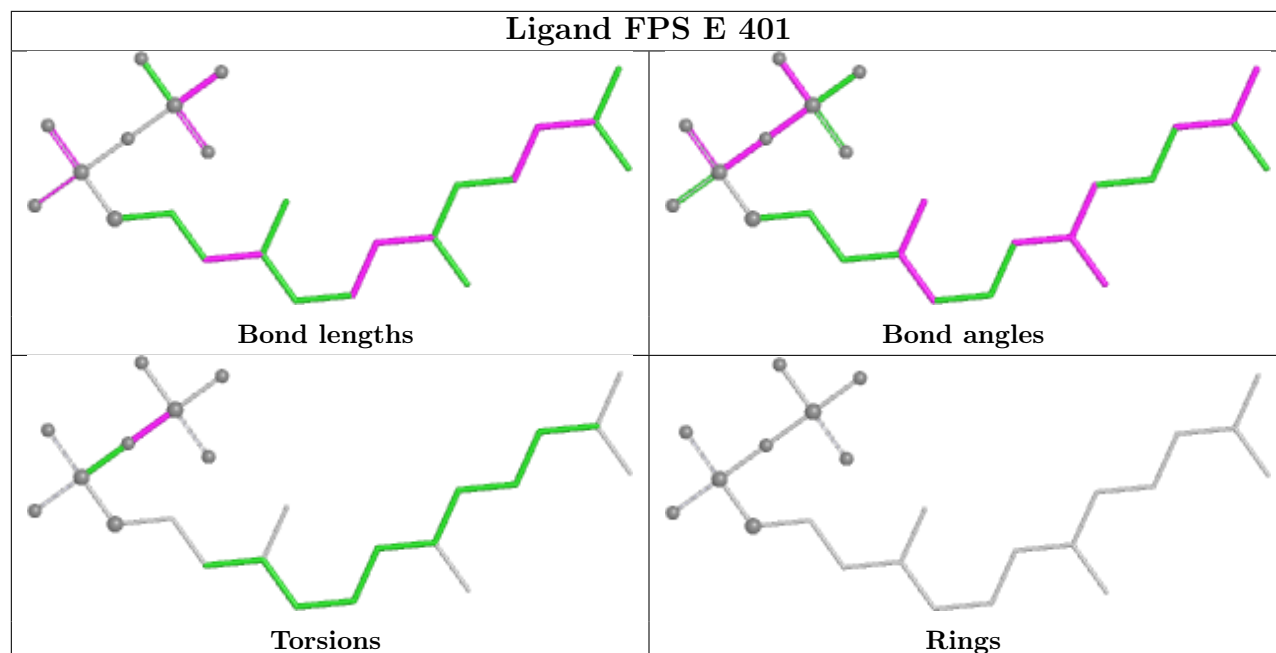
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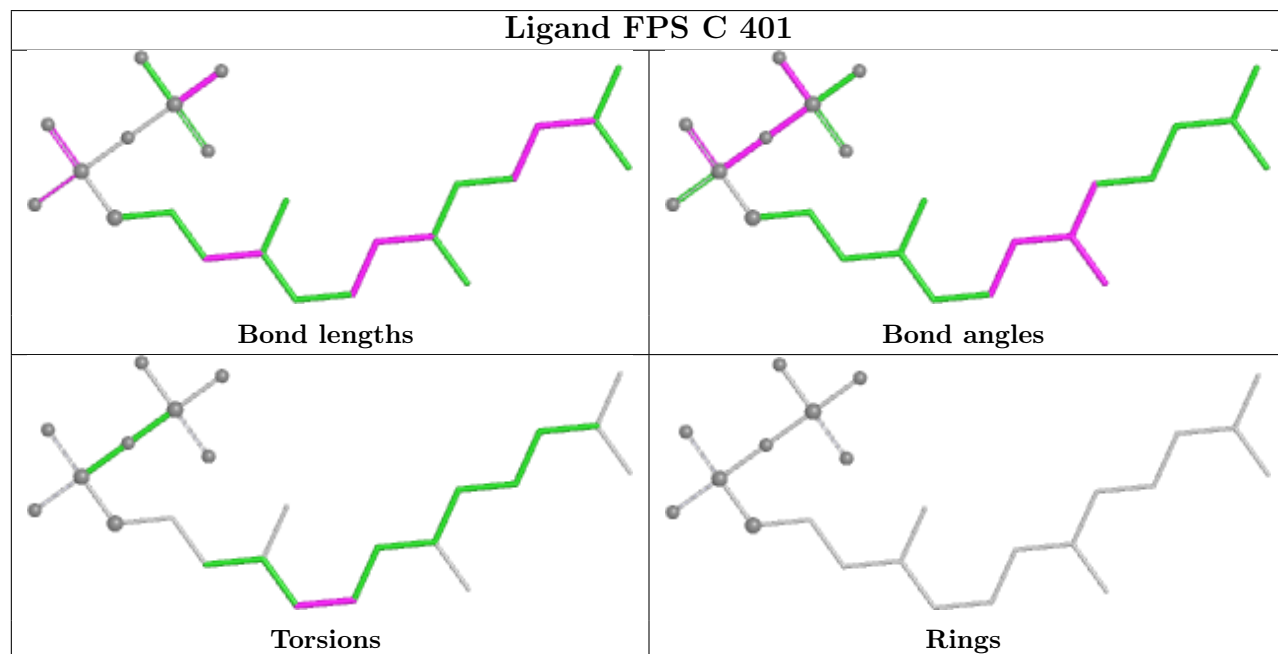
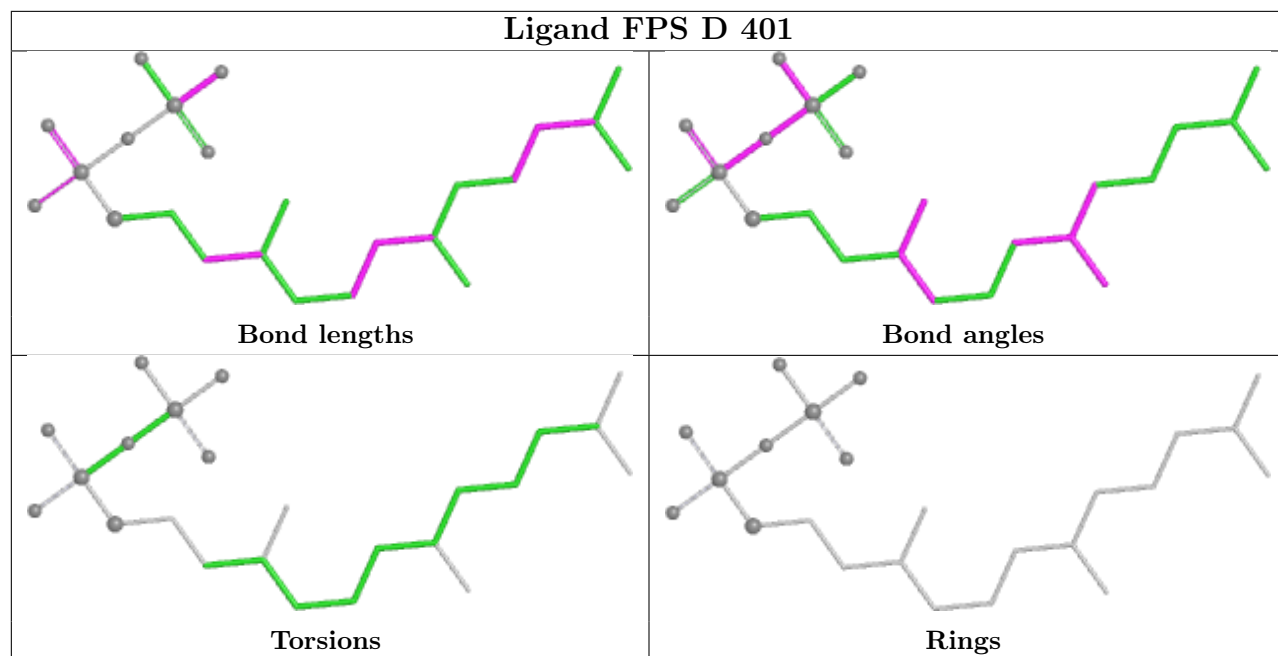
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	FPS	8	0
2	A	401	FPS	7	0
2	E	401	FPS	5	0
2	A	402	FPS	7	0
2	D	401	FPS	6	0
2	C	401	FPS	8	0
2	B	402	FPS	8	0

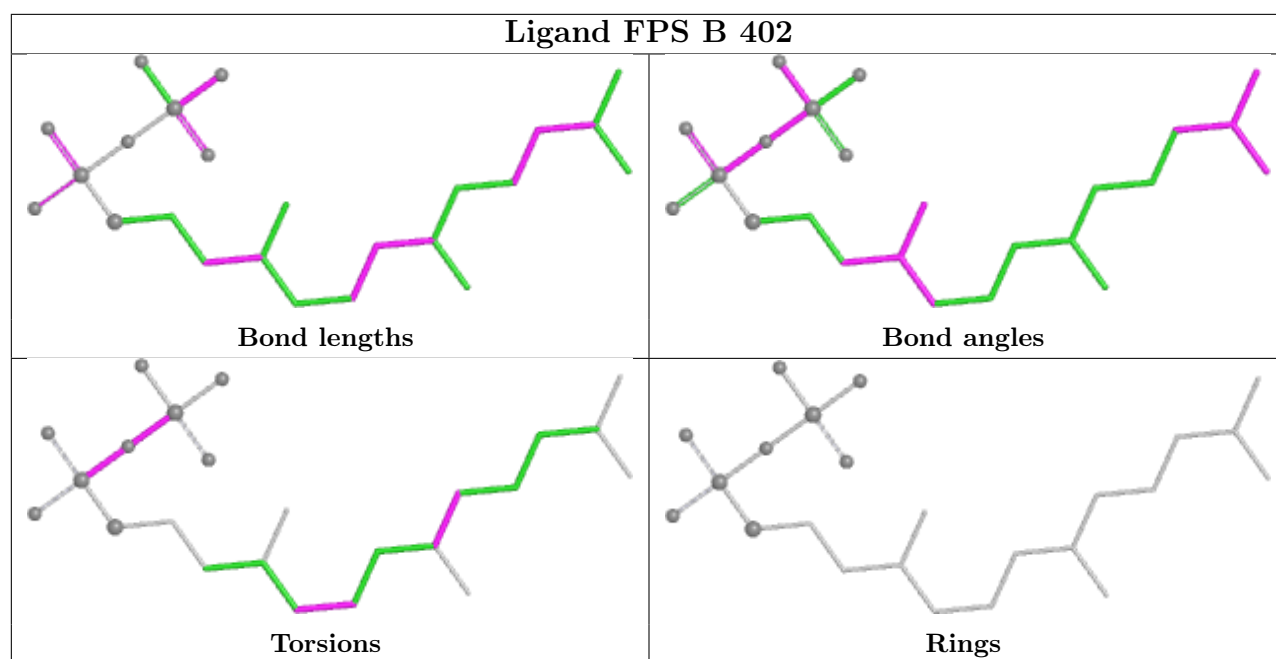
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	327/343 (95%)	-0.48	5 (1%) 72 77	19, 34, 60, 99	0
1	B	333/343 (97%)	-0.43	9 (2%) 56 63	22, 37, 65, 97	0
1	C	333/343 (97%)	-0.01	13 (3%) 43 49	23, 48, 102, 120	0
1	D	329/343 (95%)	0.04	10 (3%) 52 59	29, 56, 102, 126	0
1	E	329/343 (95%)	0.01	10 (3%) 52 59	24, 51, 103, 125	0
1	F	322/343 (93%)	0.38	11 (3%) 48 55	35, 77, 131, 151	0
All	All	1973/2058 (95%)	-0.09	58 (2%) 53 60	19, 48, 109, 151	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	324	LEU	4.5
1	C	322	VAL	4.2
1	E	321	ALA	4.2
1	E	322	VAL	3.8
1	D	322	VAL	3.8
1	E	324	LEU	3.8
1	C	321	ALA	3.7
1	E	316	ILE	3.6
1	F	314	VAL	3.4
1	C	323	THR	3.2
1	B	316	ILE	3.1
1	B	324	LEU	3.1
1	B	314	VAL	2.9
1	B	313	ALA	2.9
1	B	322	VAL	2.8
1	E	159	ASP	2.8
1	B	319	GLY	2.8
1	C	243	LEU	2.8
1	C	313	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	316	ILE	2.8
1	B	159	ASP	2.7
1	A	159	ASP	2.7
1	A	316	ILE	2.7
1	E	314	VAL	2.6
1	E	368	THR	2.6
1	D	88	ILE	2.5
1	F	325	MET	2.5
1	D	316	ILE	2.5
1	D	315	LYS	2.5
1	F	162	VAL	2.4
1	C	318	LYS	2.4
1	C	324	LEU	2.4
1	D	313	ALA	2.4
1	F	313	ALA	2.4
1	F	225	GLN	2.4
1	D	323	THR	2.4
1	A	313	ALA	2.3
1	B	321	ALA	2.3
1	D	314	VAL	2.3
1	C	310	PHE	2.3
1	A	314	VAL	2.3
1	E	325	MET	2.3
1	E	313	ALA	2.3
1	F	100	PHE	2.2
1	F	247	ALA	2.2
1	F	252	ILE	2.2
1	F	309	VAL	2.2
1	C	36	LEU	2.2
1	A	325	MET	2.2
1	C	314	VAL	2.2
1	C	312	GLY	2.2
1	F	242	LYS	2.1
1	D	327	ASP	2.1
1	C	368	THR	2.1
1	E	369	GLN	2.1
1	F	230	PHE	2.1
1	D	159	ASP	2.0
1	B	317	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

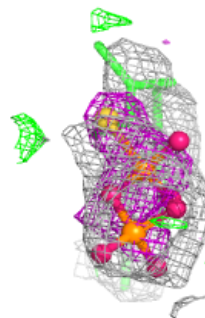
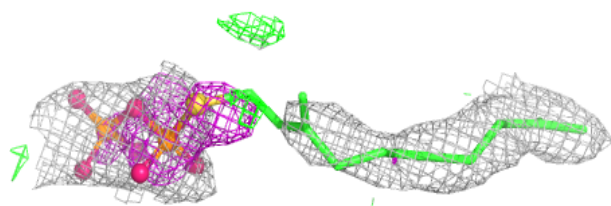
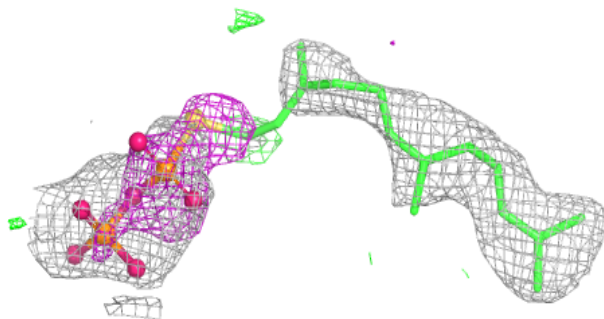
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FPS	C	401	24/24	0.77	0.17	44,81,105,105	0
2	FPS	A	402	24/24	0.78	0.18	77,106,126,126	0
2	FPS	B	402	24/24	0.79	0.16	44,77,98,98	0
2	FPS	E	402	24/24	0.81	0.16	56,90,119,119	0
2	FPS	D	401	24/24	0.87	0.16	72,96,118,118	0
2	FPS	B	401	24/24	0.87	0.14	33,83,107,107	0
2	FPS	E	401	24/24	0.88	0.14	52,90,109,109	0
2	FPS	A	401	24/24	0.88	0.14	48,78,107,107	0

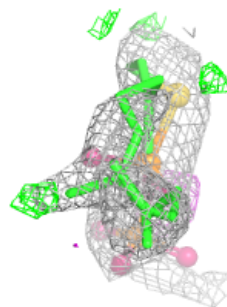
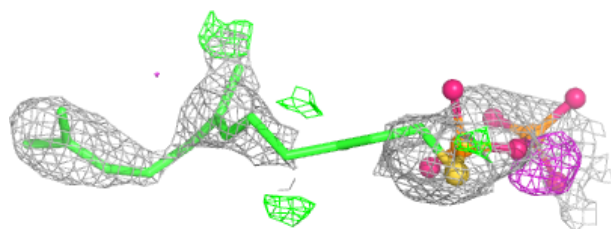
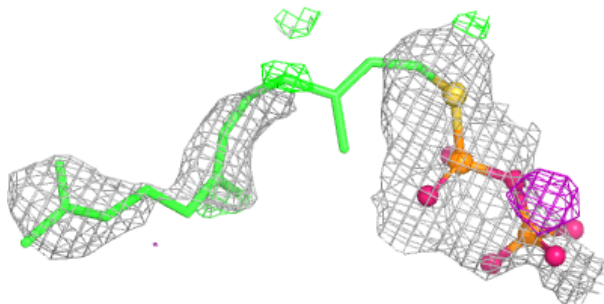
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FPS C 401:

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

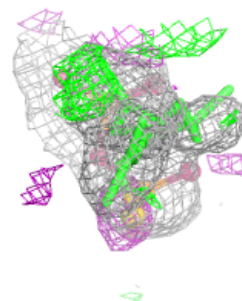
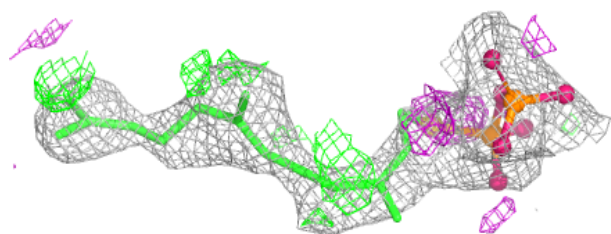
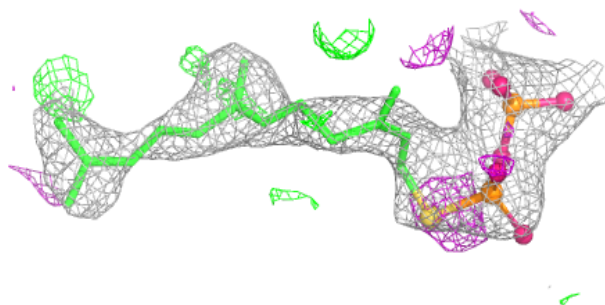
**Electron density around FPS A 402:**

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

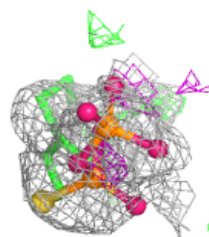
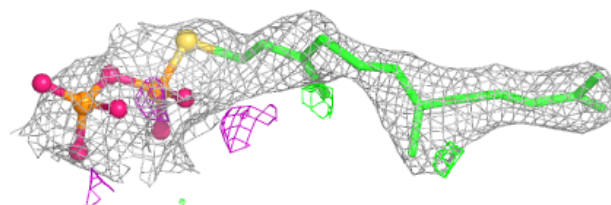
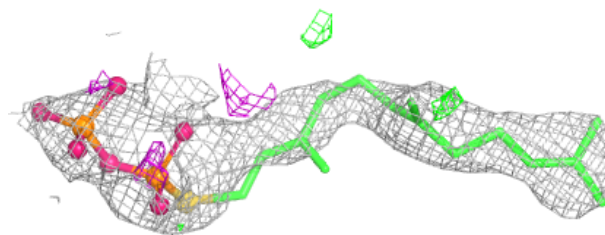


Electron density around FPS B 402:

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

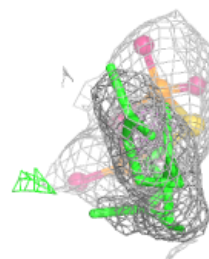
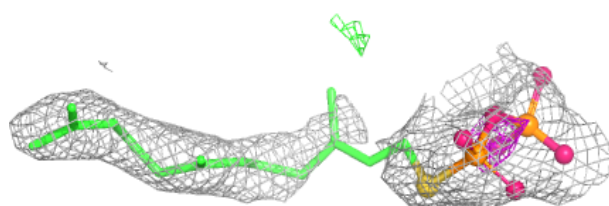
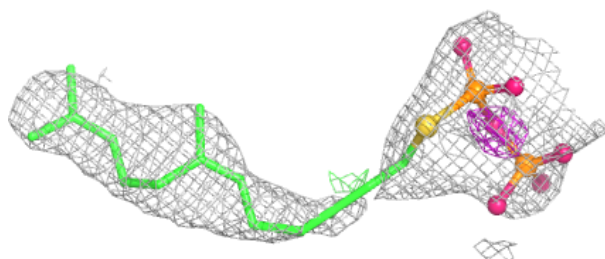
**Electron density around FPS E 402:**

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

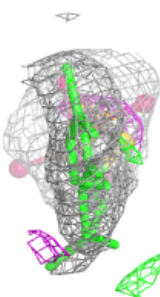
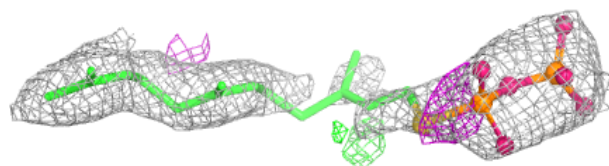
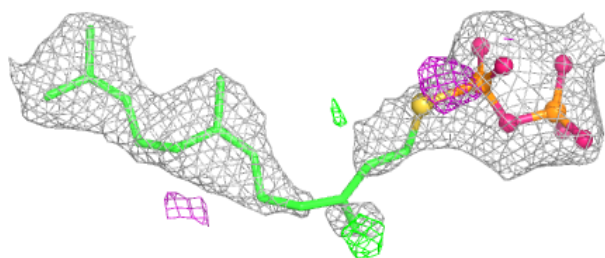


Electron density around FPS D 401:

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

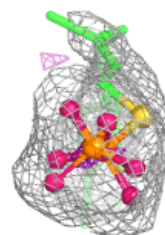
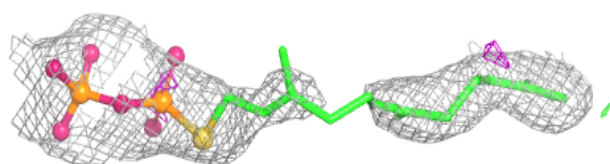
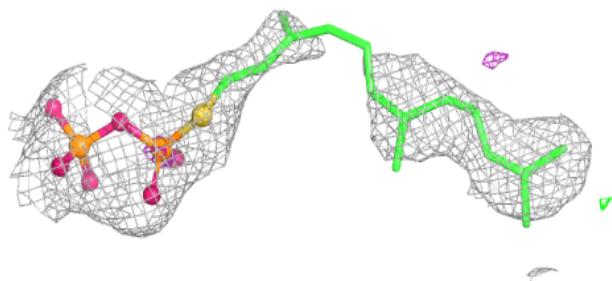
**Electron density around FPS B 401:**

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and green (positive)

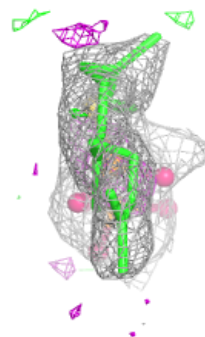
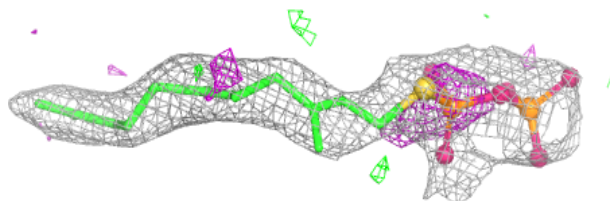


Electron density around FPS E 401:

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

**Electron density around FPS A 401:**

$2mF_o-DF_c$ (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.