



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:59 AM UTC

PDB ID : 3G4F / pdb_00003g4f
Title : Crystal Structure of (+)- α -Cadinene Synthase from *Gossypium arboreum* in complex with 2-fluorofarnesyl diphosphate
Authors : Gennadios, H.A.; Di Costanzo, L.; Christianson, D.W.
Deposited on : 2009-02-03
Resolution : 2.65 Å (reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

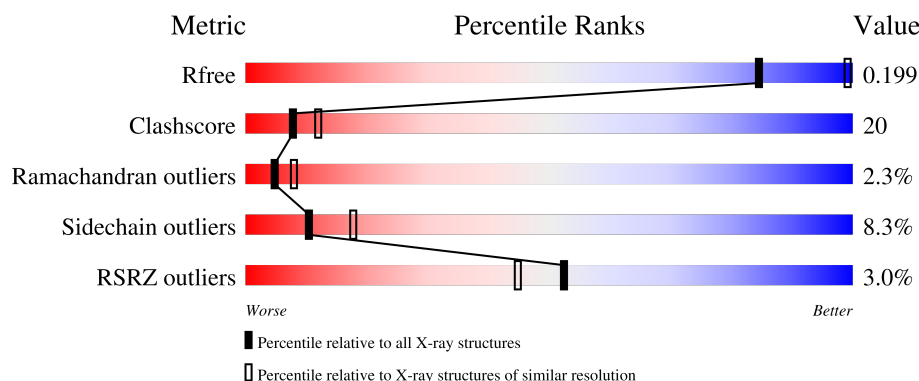
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	554	% 61% 27% 5% 7%
1	B	554	4% 53% 34% 5% 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	FPF	B	802	-	-	X	-

2 Entry composition [i](#)

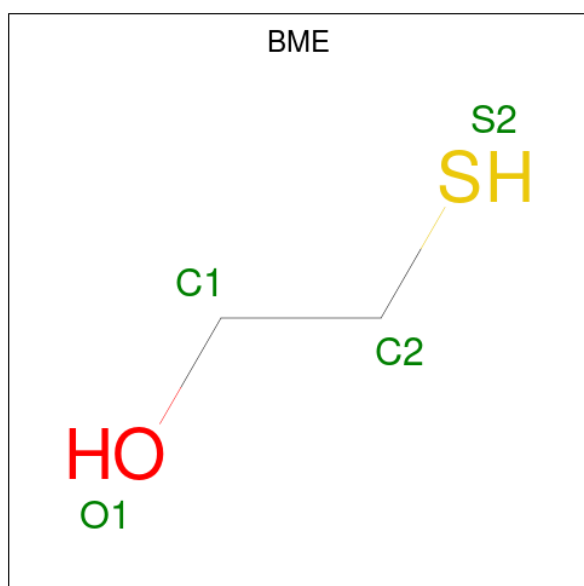
There are 5 unique types of molecules in this entry. The entry contains 8658 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (+)-delta-cadinene synthase isozyme XC1.

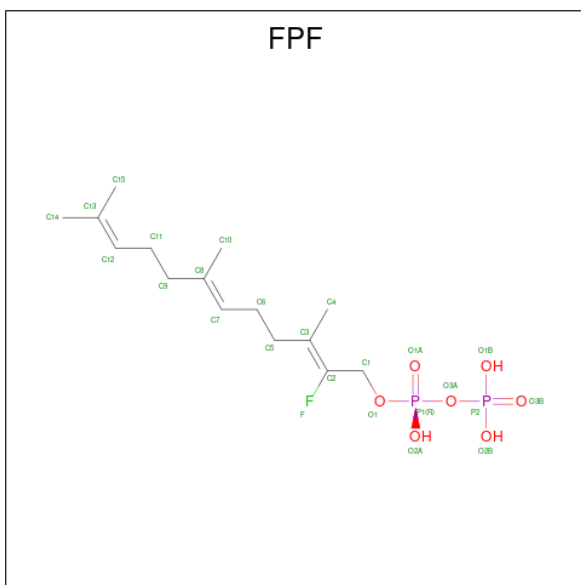
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	515	Total	C	N	O	S	18	0	0
			4209	2688	701	798	22			
1	B	515	Total	C	N	O	S	18	0	0
			4209	2688	701	798	22			

- Molecule 2 is BETA-MERCAPTOETHANOL (CCD ID: BME) (formula: C₂H₆OS).



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

- Molecule 3 is (2Z,6E)-2-fluoro-3,7,11-trimethyldodeca-2,6,10-trien-1-yl trihydrogen diphosphate (CCD ID: FPF) (formula: C₁₅H₂₇FO₇P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 25	C 15	F 1	O 7	P 2	0	0
3	B	1	Total 25	C 15	F 1	O 7	P 2	0	0

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	3	Total Mg 3 3	0	0
4	B	3	Total Mg 3 3	0	0

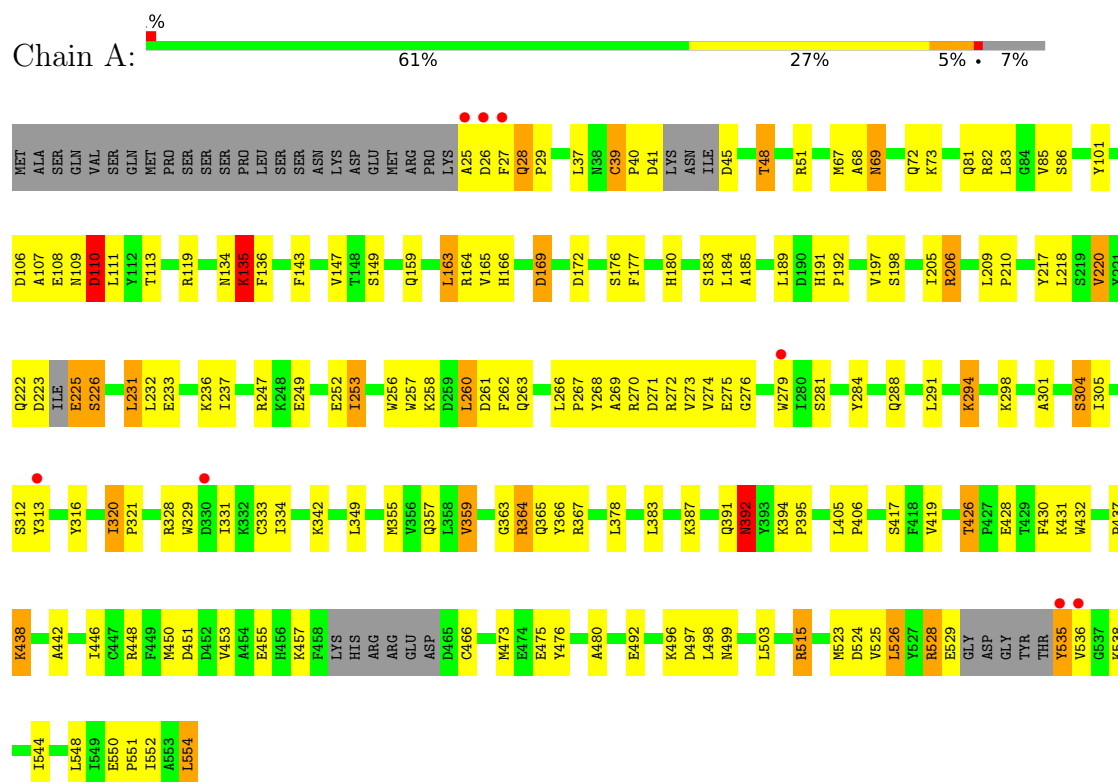
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	119	Total O 119 119	0	0
5	B	57	Total O 57 57	0	0

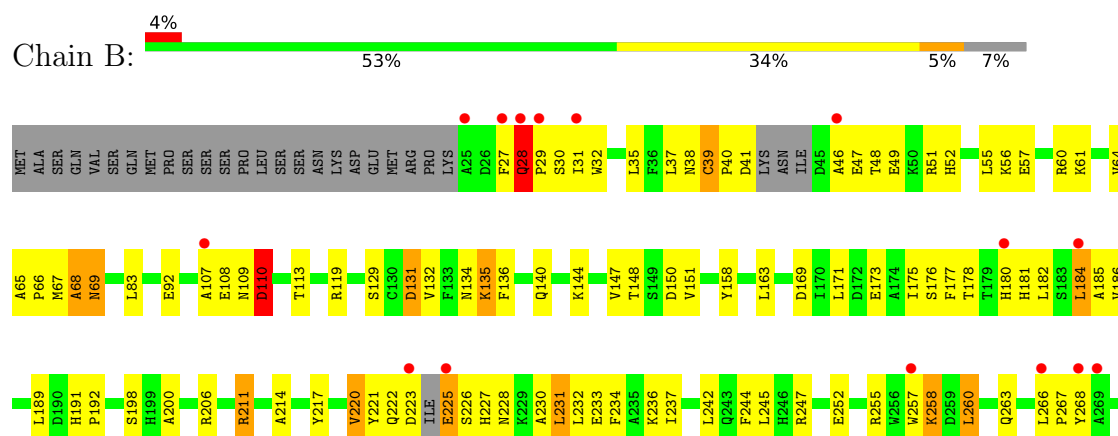
3 Residue-property plots [i](#)

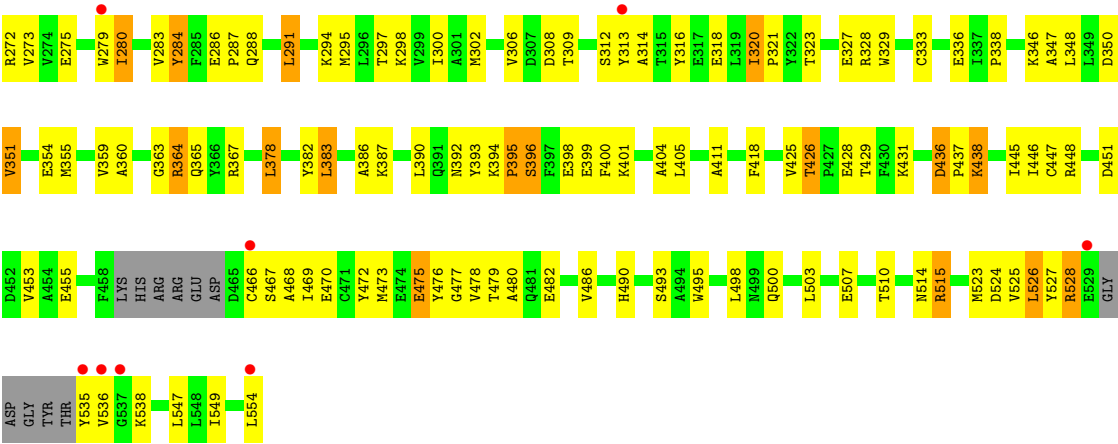
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: (+)-delta-cadinene synthase isozyme XC1



- Molecule 1: (+)-delta-cadinene synthase isozyme XC1





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α , β , γ	158.19Å 158.19Å 158.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.70 – 2.65 47.70 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.70-2.65) 99.9 (47.70-2.75)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.84 (at 2.73Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.201 , 0.256 0.203 , 0.199	Depositor DCC
R_{free} test set	1745 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	57.2	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.027 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8658	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.42% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, FPF, BME

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	0.71	0/4304	0.96	5/5821 (0.1%)
1	B	0.58	2/4304 (0.0%)	0.91	6/5821 (0.1%)
All	All	0.65	2/8608 (0.0%)	0.93	11/11642 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	221	TYR	C-N	8.16	1.45	1.34
1	B	227	HIS	CB-CG	5.21	1.57	1.50

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	549	ILE	N-CA-C	7.30	117.28	110.42
1	B	436	ASP	CA-C-N	7.11	127.53	119.92
1	B	436	ASP	C-N-CA	7.11	127.53	119.92
1	A	147	VAL	N-CA-C	5.67	116.40	110.62
1	B	493	SER	N-CA-C	-5.51	105.28	112.23
1	A	85	VAL	CB-CA-C	-5.35	105.12	111.65
1	A	39	CYS	CA-C-N	5.35	125.29	119.78
1	A	39	CYS	C-N-CA	5.35	125.29	119.78
1	B	411	ALA	N-CA-C	-5.30	105.58	111.36
1	A	281	SER	N-CA-C	-5.04	106.39	112.54
1	B	351	VAL	CB-CA-C	-5.04	105.44	111.88

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	4209	0	4091	147	0
1	B	4209	0	4091	184	0
2	A	8	0	12	3	0
3	A	25	0	24	1	0
3	B	25	0	24	10	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
5	A	119	0	0	7	0
5	B	57	0	0	5	0
All	All	8658	0	8242	332	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 20.

All (332) 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:438:LYS:N	1:A:438:LYS:HE3	1.63	1.12
1:B:291:LEU:HD22	1:B:295:MET:HE2	1.34	1.09
1:A:320:ILE:HG13	1:A:321:PRO:HD3	1.28	1.08
1:A:438:LYS:HE3	1:A:438:LYS:H	0.88	1.02
1:A:438:LYS:H	1:A:438:LYS:CE	1.75	1.00
1:B:538:LYS:H	1:B:538:LYS:HD2	1.29	0.98
1:A:28:GLN:NE2	1:A:263:GLN:HA	1.78	0.97
1:A:28:GLN:HB3	1:A:29:PRO:CA	1.97	0.94
1:A:27:PHE:HB3	1:A:267:PRO:HA	1.49	0.92
1:A:28:GLN:HB3	1:A:29:PRO:HA	1.50	0.92
1:B:211:ARG:HG2	1:B:211:ARG:HH11	1.35	0.91
1:A:536:VAL:O	3:A:801:FPF:H12	1.70	0.91
1:B:320:ILE:HG13	1:B:321:PRO:HD3	1.53	0.90
1:A:320:ILE:HG13	1:A:321:PRO:CD	2.04	0.86
1:A:392:ASN:HB2	1:B:140:GLN:HG3	1.58	0.84
1:B:211:ARG:HH11	1:B:211:ARG:CG	1.91	0.84
1:B:186:VAL:HA	1:B:189:LEU:HD12	1.63	0.80
1:A:108:GLU:HB2	1:A:135:LYS:NZ	1.96	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:475:GLU:HG3	1:B:476:TYR:CD2	2.18	0.78
1:B:180:HIS:CE1	1:B:184:LEU:HD11	2.18	0.77
1:A:119:ARG:HG3	1:A:163:LEU:HD13	1.66	0.77
1:A:69:ASN:C	1:A:69:ASN:HD22	1.93	0.75
1:A:252:GLU:OE1	1:A:294:LYS:HE3	1.86	0.75
1:B:28:GLN:HB3	1:B:29:PRO:HA	1.69	0.75
1:A:28:GLN:CB	1:A:29:PRO:HA	2.17	0.74
1:B:347:ALA:O	1:B:351:VAL:HG23	1.87	0.74
1:A:39:CYS:HG	2:A:1274:BME:HS2	1.35	0.74
1:B:242:LEU:HD21	1:B:287:PRO:HG3	1.70	0.73
1:A:367:ARG:HG2	1:A:430:PHE:CE2	2.24	0.72
1:B:186:VAL:O	1:B:189:LEU:HB2	1.90	0.72
1:B:490:HIS:CE1	5:B:604:HOH:O	2.43	0.71
1:A:108:GLU:HB2	1:A:135:LYS:HZ1	1.55	0.71
1:B:27:PHE:HB3	1:B:267:PRO:HA	1.72	0.70
1:B:478:VAL:HB	1:B:482:GLU:OE1	1.92	0.70
1:B:28:GLN:NE2	1:B:263:GLN:HA	2.06	0.69
1:B:328:ARG:NH2	1:B:333:CYS:SG	2.65	0.69
1:B:525:VAL:HG12	1:B:526:LEU:HD13	1.73	0.69
1:A:328:ARG:NH2	1:A:333:CYS:SG	2.65	0.69
1:B:318:GLU:O	1:B:321:PRO:HD2	1.92	0.69
1:B:222:GLN:HE22	1:B:236:LYS:HZ1	1.41	0.68
1:A:276:GLY:HA2	1:A:279:TRP:CE3	2.28	0.68
1:B:467:SER:HB3	1:B:470:GLU:HG3	1.75	0.68
1:B:60:ARG:O	1:B:64:VAL:HG23	1.94	0.67
1:A:106:ASP:O	1:A:108:GLU:HA	1.95	0.67
1:A:206:ARG:HG3	1:A:206:ARG:O	1.90	0.67
1:B:320:ILE:HG13	1:B:321:PRO:CD	2.24	0.67
1:B:404:ALA:HB3	5:B:579:HOH:O	1.94	0.67
3:B:802:FPP:H4	3:B:802:FPP:H7	1.76	0.66
1:B:448:ARG:HD3	5:B:610:HOH:O	1.96	0.66
1:B:28:GLN:HB3	1:B:29:PRO:CA	2.27	0.65
1:B:312:SER:C	1:B:314:ALA:H	2.04	0.65
1:A:222:GLN:HE22	1:A:236:LYS:HZ1	1.45	0.65
1:A:473:MET:HE3	1:A:480:ALA:N	2.12	0.65
1:B:472:TYR:CE2	1:B:486:VAL:HG21	2.31	0.65
1:A:359:VAL:HG13	1:A:364:ARG:HB2	1.77	0.64
1:A:40:PRO:O	1:A:41:ASP:HB2	1.97	0.64
1:B:525:VAL:HG12	1:B:526:LEU:CD1	2.28	0.64
1:A:83:LEU:HD12	1:A:231:LEU:HD13	1.80	0.63
1:B:500:GLN:NE2	1:B:503:LEU:HD12	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:TYR:HA	1:A:220:VAL:HG13	1.81	0.63
1:B:182:LEU:O	1:B:186:VAL:HG23	2.00	0.62
1:B:225:GLU:O	1:B:226:SER:HB3	1.98	0.62
1:A:276:GLY:HA2	1:A:279:TRP:HE3	1.63	0.62
1:B:272:ARG:NH2	1:B:535:TYR:N	2.47	0.62
1:A:261:ASP:C	1:A:263:GLN:H	2.08	0.61
1:B:108:GLU:HB2	1:B:135:LYS:HZ1	1.65	0.61
1:A:191:HIS:CG	1:A:192:PRO:HA	2.36	0.61
1:B:28:GLN:CB	1:B:29:PRO:HA	2.30	0.61
1:B:359:VAL:CG1	1:B:364:ARG:HB2	2.29	0.61
1:A:312:SER:OG	1:A:313:TYR:N	2.26	0.61
1:B:284:TYR:HB3	1:B:515:ARG:NH2	2.16	0.60
1:A:222:GLN:HE22	1:A:236:LYS:NZ	2.00	0.60
1:B:527:TYR:HE2	3:B:802:FPF:H4B	1.67	0.60
1:B:109:ASN:HB3	1:B:113:THR:HB	1.83	0.60
1:A:222:GLN:NE2	1:A:236:LYS:NZ	2.50	0.60
1:A:270:ARG:NH1	5:A:642:HOH:O	2.34	0.60
1:B:527:TYR:CE2	3:B:802:FPF:H4B	2.36	0.59
1:A:109:ASN:HB3	1:A:113:THR:HB	1.83	0.59
1:A:328:ARG:CZ	1:A:333:CYS:SG	2.91	0.58
1:B:359:VAL:HG13	1:B:364:ARG:HB2	1.85	0.58
1:A:83:LEU:HD22	1:A:218:LEU:HD23	1.86	0.58
1:B:40:PRO:HB2	1:B:244:PHE:HE1	1.68	0.58
1:B:180:HIS:O	1:B:184:LEU:HG	2.04	0.58
1:B:52:HIS:HB2	1:B:237:ILE:HG21	1.86	0.58
1:B:298:LYS:HZ3	1:B:354:GLU:CD	2.11	0.58
1:B:328:ARG:HH22	1:B:336:GLU:HG3	1.67	0.58
1:A:107:ALA:HA	1:A:108:GLU:CB	2.31	0.57
1:A:109:ASN:HB3	1:A:113:THR:CG2	2.34	0.57
1:B:211:ARG:HG2	1:B:211:ARG:NH1	2.05	0.57
1:A:525:VAL:HG12	1:A:526:LEU:HD13	1.87	0.57
1:B:316:TYR:CE1	1:B:387:LYS:HB2	2.39	0.57
1:A:535:TYR:HB2	1:A:536:VAL:HA	1.87	0.57
1:B:228:ASN:C	1:B:228:ASN:OD1	2.46	0.56
1:A:119:ARG:HG3	1:A:163:LEU:CD1	2.35	0.56
1:B:535:TYR:CE1	3:B:802:FPF:H15A	2.39	0.56
1:A:83:LEU:CD1	1:A:231:LEU:HD13	2.35	0.56
1:A:108:GLU:HB2	1:A:135:LYS:HZ2	1.70	0.56
1:B:393:TYR:CE2	1:B:395:PRO:HA	2.41	0.56
1:B:40:PRO:HB2	1:B:244:PHE:CE1	2.40	0.56
1:B:401:LYS:C	5:B:579:HOH:O	2.48	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:GLU:HB2	1:B:135:LYS:NZ	2.21	0.55
1:B:438:LYS:H	1:B:438:LYS:HZ2	1.54	0.55
1:A:107:ALA:HA	1:A:108:GLU:HB3	1.89	0.55
1:A:180:HIS:CE1	1:A:184:LEU:HD11	2.42	0.55
1:A:364:ARG:HD2	1:A:367:ARG:CZ	2.37	0.55
1:B:48:THR:O	1:B:51:ARG:HB3	2.06	0.55
1:B:418:PHE:HB3	1:B:425:VAL:HG21	1.89	0.55
1:B:447:CYS:HA	1:B:523:MET:HG3	1.87	0.55
1:B:46:ALA:HA	1:B:49:GLU:HB2	1.89	0.55
1:A:82:ARG:HD2	5:A:670:HOH:O	2.07	0.55
1:A:166:HIS:HE1	1:A:497:ASP:OD1	1.90	0.55
1:B:56:LYS:HB2	1:B:234:PHE:HE1	1.72	0.55
1:B:180:HIS:CE1	1:B:184:LEU:CD1	2.87	0.55
1:B:295:MET:SD	1:B:355:MET:HG2	2.46	0.55
1:A:438:LYS:N	1:A:438:LYS:CE	2.50	0.54
1:B:510:THR:HG22	1:B:514:ASN:ND2	2.22	0.54
1:A:28:GLN:HG3	1:A:271:ASP:HB2	1.89	0.54
1:B:223:ASP:O	1:B:225:GLU:N	2.41	0.54
1:A:159:GLN:NE2	1:A:205:ILE:HG13	2.23	0.54
1:B:222:GLN:HE22	1:B:236:LYS:NZ	2.05	0.54
1:B:185:ALA:O	1:B:189:LEU:HG	2.08	0.54
1:B:192:PRO:HG3	1:B:223:ASP:HB3	1.89	0.54
1:B:119:ARG:HG3	1:B:163:LEU:HD13	1.89	0.54
1:A:25:ALA:N	1:A:267:PRO:HB2	2.23	0.53
1:A:538:LYS:H	1:A:538:LYS:HD2	1.72	0.53
1:A:225:GLU:O	1:A:226:SER:CB	2.56	0.53
1:B:472:TYR:CD2	1:B:472:TYR:O	2.61	0.53
1:A:143:PHE:HD2	1:A:177:PHE:CD1	2.26	0.53
1:A:266:LEU:HD22	1:A:268:TYR:CE1	2.44	0.53
1:B:510:THR:HG22	1:B:514:ASN:HD21	1.74	0.53
1:A:535:TYR:CB	1:A:536:VAL:HA	2.38	0.53
1:B:134:ASN:C	1:B:136:PHE:H	2.16	0.53
1:B:475:GLU:CG	1:B:476:TYR:CD2	2.91	0.53
1:A:110:ASP:OD2	1:A:110:ASP:N	2.30	0.53
1:B:222:GLN:NE2	1:B:236:LYS:NZ	2.57	0.53
1:B:255:ARG:HH12	1:B:258:LYS:NZ	2.07	0.52
1:B:257:TRP:CD2	1:B:273:VAL:HG21	2.44	0.52
1:B:438:LYS:H	1:B:438:LYS:CE	2.22	0.52
1:B:400:PHE:HZ	1:B:468:ALA:HB2	1.72	0.52
1:A:331:ILE:O	1:A:334:ILE:HG22	2.09	0.52
1:B:151:VAL:HG11	1:B:189:LEU:HD21	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:GLU:OE2	2:A:1273:BME:H21	2.08	0.52
1:B:398:GLU:HA	1:B:401:LYS:CB	2.40	0.52
1:B:247:ARG:HG3	1:B:247:ARG:HH11	1.75	0.51
1:B:225:GLU:O	1:B:226:SER:CB	2.57	0.51
1:A:83:LEU:CD2	1:A:218:LEU:HD23	2.41	0.51
1:A:222:GLN:NE2	1:A:236:LYS:HZ3	2.09	0.51
1:B:312:SER:C	1:B:314:ALA:N	2.69	0.51
1:B:405:LEU:CD2	1:B:445:ILE:HD13	2.41	0.51
1:A:27:PHE:CB	1:A:267:PRO:HA	2.31	0.51
1:A:391:GLN:O	1:A:392:ASN:C	2.53	0.51
1:B:131:ASP:C	1:B:131:ASP:OD1	2.53	0.51
1:B:40:PRO:HG3	1:B:247:ARG:HB3	1.92	0.50
1:B:346:LYS:HE3	1:B:350:ASP:OD2	2.10	0.50
1:A:426:THR:HG23	1:A:428:GLU:H	1.75	0.50
1:A:269:ALA:HB1	1:A:305:ILE:HD12	1.93	0.50
1:A:366:TYR:CD1	1:A:366:TYR:C	2.89	0.50
1:B:27:PHE:HB2	1:B:28:GLN:NE2	2.26	0.50
1:B:395:PRO:O	1:B:396:SER:C	2.53	0.50
1:B:479:THR:O	1:B:480:ALA:C	2.55	0.50
1:A:535:TYR:HB2	1:A:536:VAL:CA	2.41	0.50
1:B:524:ASP:O	1:B:528:ARG:HD2	2.11	0.50
1:B:38:ASN:O	1:B:39:CYS:C	2.54	0.49
1:B:191:HIS:CG	1:B:192:PRO:HA	2.47	0.49
1:A:442:ALA:O	1:A:446:ILE:HG13	2.11	0.49
1:A:27:PHE:HA	1:A:267:PRO:O	2.13	0.49
1:B:398:GLU:HA	1:B:401:LYS:HB2	1.94	0.49
1:A:261:ASP:C	1:A:263:GLN:N	2.70	0.49
1:A:288:GLN:HG2	5:A:601:HOH:O	2.12	0.49
1:A:432:TRP:O	1:A:437:PRO:HG3	2.12	0.49
1:A:475:GLU:HG3	1:A:476:TYR:CD2	2.48	0.49
1:B:323:THR:HG21	1:B:383:LEU:HD12	1.95	0.49
1:B:171:LEU:C	1:B:173:GLU:N	2.71	0.49
1:B:400:PHE:C	1:B:400:PHE:CD2	2.90	0.49
1:A:274:VAL:HG12	1:A:544:ILE:HD13	1.95	0.49
1:B:158:TYR:HE1	1:B:200:ALA:O	1.96	0.49
1:A:39:CYS:SG	2:A:1274:BME:S2	2.96	0.48
1:B:280:ILE:HD13	1:B:280:ILE:N	2.27	0.48
1:A:27:PHE:HB2	1:A:28:GLN:HE21	1.79	0.48
1:B:400:PHE:CZ	1:B:468:ALA:HB2	2.48	0.48
1:B:30:SER:C	1:B:32:TRP:H	2.19	0.48
1:A:69:ASN:C	1:A:69:ASN:ND2	2.63	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:LYS:HA	1:B:234:PHE:CE1	2.49	0.48
1:B:27:PHE:HB2	1:B:28:GLN:HE21	1.78	0.48
1:B:247:ARG:HG3	1:B:247:ARG:NH1	2.29	0.48
1:B:232:LEU:HD12	1:B:232:LEU:O	2.13	0.48
1:A:334:ILE:O	1:A:342:LYS:HE2	2.14	0.47
1:B:302:MET:O	1:B:306:VAL:HG23	2.14	0.47
1:B:436:ASP:N	1:B:437:PRO:HD3	2.29	0.47
1:A:450:MET:HB2	1:A:523:MET:HE2	1.96	0.47
1:A:316:TYR:CE1	1:A:387:LYS:HB2	2.49	0.47
1:B:275:GLU:OE2	1:B:536:VAL:HG11	2.14	0.47
1:B:312:SER:O	1:B:314:ALA:N	2.46	0.47
1:B:394:LYS:HD3	1:B:395:PRO:HD3	1.97	0.47
1:A:363:GLY:HA2	1:A:365:GLN:OE1	2.15	0.47
1:B:426:THR:HG23	1:B:428:GLU:H	1.79	0.47
1:A:69:ASN:ND2	1:A:72:GLN:H	2.13	0.47
1:A:109:ASN:HB3	1:A:113:THR:CB	2.44	0.47
1:A:279:TRP:CD1	1:A:526:LEU:HD23	2.49	0.47
1:B:109:ASN:HB3	1:B:113:THR:CG2	2.45	0.47
1:B:175:ILE:HG23	1:B:176:SER:H	1.80	0.47
1:B:245:LEU:O	1:B:245:LEU:HD12	2.15	0.47
1:B:308:ASP:O	1:B:309:THR:C	2.58	0.46
1:B:297:THR:O	1:B:300:ILE:HG22	2.15	0.46
3:B:802:FPF:H15A	3:B:802:FPF:H9A	1.97	0.46
1:B:175:ILE:HG23	1:B:176:SER:N	2.30	0.46
1:B:473:MET:O	1:B:477:GLY:HA2	2.14	0.46
1:B:67:MET:O	1:B:68:ALA:C	2.58	0.46
1:B:144:LYS:O	1:B:147:VAL:HB	2.16	0.46
1:A:27:PHE:HB2	1:A:28:GLN:NE2	2.30	0.46
1:B:363:GLY:HA2	1:B:365:GLN:OE1	2.16	0.46
1:B:476:TYR:O	1:B:478:VAL:HG13	2.16	0.46
1:A:101:TYR:HE2	5:A:645:HOH:O	1.98	0.46
1:B:455:GLU:OE1	3:B:802:FPF:F	2.24	0.46
1:B:55:LEU:HD11	1:B:233:GLU:OE1	2.16	0.46
1:B:448:ARG:CD	5:B:610:HOH:O	2.59	0.46
1:A:252:GLU:OE1	1:A:294:LYS:CE	2.60	0.45
1:A:301:ALA:O	1:A:304:SER:HB2	2.16	0.45
1:A:67:MET:HE2	1:A:72:GLN:HB3	1.98	0.45
1:A:81:GLN:HA	1:A:86:SER:HB3	1.98	0.45
1:B:396:SER:OG	1:B:399:GLU:HB2	2.15	0.45
1:B:252:GLU:HB2	1:B:294:LYS:HE3	1.98	0.45
1:B:438:LYS:HZ3	1:B:507:GLU:CD	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:GLU:O	1:A:226:SER:HB3	2.16	0.45
1:A:526:LEU:HD12	1:A:526:LEU:HA	1.70	0.45
1:B:47:GLU:OE1	1:B:47:GLU:HA	2.17	0.45
1:A:223:ASP:O	1:A:225:GLU:N	2.50	0.45
1:A:446:ILE:O	1:A:450:MET:HG3	2.17	0.45
1:A:355:MET:HE3	1:A:419:VAL:HG11	2.00	0.44
1:A:417:SER:OG	1:A:515:ARG:HG2	2.16	0.44
1:B:364:ARG:HD2	1:B:367:ARG:CZ	2.48	0.44
1:B:178:THR:O	1:B:182:LEU:HG	2.17	0.44
1:B:316:TYR:O	1:B:320:ILE:HG23	2.17	0.44
1:A:550:GLU:HA	1:A:551:PRO:HD2	1.92	0.44
1:B:538:LYS:HD2	1:B:538:LYS:N	2.13	0.44
1:B:328:ARG:CZ	1:B:333:CYS:SG	3.06	0.44
1:B:110:ASP:OD2	1:B:110:ASP:N	2.47	0.44
1:B:228:ASN:OD1	1:B:230:ALA:N	2.51	0.44
1:A:111:LEU:HA	1:A:136:PHE:CZ	2.53	0.44
1:B:279:TRP:HE1	1:B:526:LEU:HD23	1.82	0.44
1:A:45:ASP:HB3	1:A:48:THR:HG23	1.99	0.43
1:A:453:VAL:CG1	1:A:457:LYS:HE3	2.48	0.43
1:A:260:LEU:HD12	1:A:260:LEU:HA	1.77	0.43
1:B:405:LEU:HD22	1:B:445:ILE:HD13	1.99	0.43
1:B:469:ILE:HD13	1:B:469:ILE:HA	1.88	0.43
1:A:426:THR:HG23	1:A:428:GLU:N	2.32	0.43
1:B:438:LYS:H	1:B:438:LYS:NZ	2.15	0.43
1:A:134:ASN:O	1:A:136:PHE:N	2.51	0.43
1:A:364:ARG:HD3	5:A:634:HOH:O	2.17	0.43
1:A:451:ASP:O	1:A:455:GLU:HG3	2.19	0.43
1:B:446:ILE:HD13	1:B:495:TRP:CE2	2.52	0.43
1:B:386:ALA:O	1:B:387:LYS:C	2.61	0.43
1:A:45:ASP:HB3	1:A:48:THR:CG2	2.48	0.43
1:B:236:LYS:HB3	1:B:554:LEU:CD2	2.49	0.43
1:B:69:ASN:HD22	1:B:69:ASN:H	1.66	0.43
1:B:426:THR:HG22	1:B:429:THR:H	1.84	0.43
1:A:73:LYS:HA	1:A:73:LYS:HD3	1.87	0.43
1:B:129:SER:O	1:B:132:VAL:HG22	2.18	0.43
1:B:242:LEU:HD23	1:B:242:LEU:HA	1.66	0.43
1:B:284:TYR:CD1	1:B:284:TYR:N	2.86	0.43
1:A:222:GLN:HA	1:A:232:LEU:HD22	2.01	0.43
1:A:169:ASP:HA	1:A:172:ASP:HB2	2.00	0.42
1:A:275:GLU:OE2	1:A:536:VAL:HG11	2.18	0.42
1:B:83:LEU:O	1:B:214:ALA:HB1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:ILE:O	1:B:283:VAL:HB	2.19	0.42
1:A:257:TRP:CG	1:A:273:VAL:HG21	2.55	0.42
1:B:535:TYR:HE1	3:B:802:FPF:H15A	1.84	0.42
1:B:107:ALA:HA	1:B:108:GLU:HA	1.76	0.42
1:B:316:TYR:HB2	1:B:390:LEU:HD12	2.01	0.42
1:A:197:VAL:O	1:A:198:SER:C	2.61	0.42
1:A:279:TRP:NE1	1:A:526:LEU:HD23	2.33	0.42
1:B:57:GLU:O	1:B:61:LYS:HG3	2.19	0.42
1:A:209:LEU:O	1:A:210:PRO:C	2.62	0.42
1:A:256:TRP:CE2	1:A:298:LYS:HD3	2.55	0.42
1:B:438:LYS:HE3	1:B:438:LYS:N	2.34	0.42
1:B:451:ASP:OD2	3:B:802:FPF:C2	2.67	0.42
1:A:163:LEU:HA	1:A:499:ASN:ND2	2.35	0.42
1:A:523:MET:HE3	1:A:523:MET:HB3	1.87	0.42
1:B:266:LEU:HD22	1:B:268:TYR:CE1	2.54	0.42
1:A:405:LEU:HB2	1:A:406:PRO:HD3	2.00	0.42
1:B:60:ARG:HG3	1:B:92:GLU:HG2	2.02	0.42
1:B:110:ASP:HB2	1:B:113:THR:H	1.83	0.42
1:B:279:TRP:NE1	1:B:526:LEU:HD23	2.35	0.42
1:A:233:GLU:O	1:A:237:ILE:HG13	2.19	0.42
1:A:272:ARG:NH2	1:A:535:TYR:N	2.67	0.42
1:A:529:GLU:CD	1:A:529:GLU:H	2.26	0.42
1:B:211:ARG:NH2	1:B:242:LEU:HD12	2.35	0.42
1:B:329:TRP:O	1:B:329:TRP:CD1	2.73	0.42
1:A:106:ASP:C	1:A:108:GLU:HA	2.44	0.42
1:A:143:PHE:HB2	1:A:177:PHE:CE1	2.55	0.42
1:A:448:ARG:O	1:A:448:ARG:HD3	2.20	0.41
1:A:51:ARG:HE	1:A:51:ARG:HA	1.84	0.41
1:A:185:ALA:O	1:A:189:LEU:HG	2.20	0.41
1:A:450:MET:HE2	1:A:450:MET:HB3	1.83	0.41
1:A:554:LEU:HD23	1:A:554:LEU:HA	1.80	0.41
1:B:55:LEU:O	1:B:56:LYS:C	2.63	0.41
1:B:217:TYR:HA	1:B:220:VAL:HG13	2.02	0.41
1:B:260:LEU:HD13	1:B:260:LEU:HA	1.81	0.41
1:A:288:GLN:CG	5:A:601:HOH:O	2.67	0.41
1:A:328:ARG:O	1:A:329:TRP:C	2.63	0.41
1:B:394:LYS:HA	1:B:395:PRO:HD3	1.76	0.41
1:A:68:ALA:HB3	1:A:72:GLN:NE2	2.36	0.41
1:A:231:LEU:HA	1:A:231:LEU:HD23	1.69	0.41
1:B:257:TRP:O	1:B:257:TRP:CD1	2.74	0.41
1:B:446:ILE:HD13	1:B:495:TRP:NE1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:THR:HG22	1:B:181:HIS:CE1	2.55	0.41
1:A:45:ASP:N	5:A:610:HOH:O	2.53	0.41
1:A:492:GLU:O	1:A:496:LYS:HG3	2.21	0.41
1:B:453:VAL:HG22	1:B:469:ILE:HD11	2.02	0.41
1:A:524:ASP:O	1:A:528:ARG:HG2	2.21	0.41
1:B:231:LEU:HA	1:B:231:LEU:HD23	1.77	0.41
1:B:535:TYR:HE1	3:B:802:FPP:C15	2.34	0.41
1:A:249:GLU:O	1:A:253:ILE:HD12	2.20	0.41
1:B:393:TYR:HE2	1:B:395:PRO:HA	1.83	0.41
1:B:398:GLU:HA	1:B:401:LYS:HB3	2.03	0.41
1:A:475:GLU:CG	1:A:476:TYR:CE2	3.04	0.41
1:B:323:THR:HG22	1:B:327:GLU:OE1	2.21	0.41
1:B:378:LEU:HD22	1:B:382:TYR:CZ	2.56	0.41
1:B:535:TYR:CB	1:B:536:VAL:HA	2.50	0.41
1:B:69:ASN:C	1:B:69:ASN:ND2	2.79	0.40
1:B:245:LEU:HD12	1:B:245:LEU:C	2.45	0.40
1:A:135:LYS:HE3	1:A:135:LYS:HB2	1.80	0.40
1:A:247:ARG:HD3	1:A:548:LEU:O	2.22	0.40
1:A:503:LEU:HD23	1:A:503:LEU:HA	1.80	0.40
1:A:28:GLN:HB3	1:A:29:PRO:CB	2.48	0.40
1:A:394:LYS:HA	1:A:395:PRO:HD3	1.94	0.40
1:B:436:ASP:H	1:B:437:PRO:HD3	1.86	0.40
1:B:455:GLU:HG2	3:B:802:FPP:H5	2.02	0.40
1:B:535:TYR:HB2	1:B:536:VAL:HA	2.03	0.40
1:A:257:TRP:CD2	1:A:273:VAL:HG21	2.57	0.40
1:B:65:ALA:HA	1:B:66:PRO:HD3	1.84	0.40
1:B:348:LEU:HD12	1:B:348:LEU:HA	1.78	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	505/554 (91%)	475 (94%)	22 (4%)	8 (2%)	7	12
1	B	505/554 (91%)	444 (88%)	46 (9%)	15 (3%)	3	5
All	All	1010/1108 (91%)	919 (91%)	68 (7%)	23 (2%)	5	8

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	135	LYS
1	A	466	CYS
1	B	360	ALA
1	B	475	GLU
1	B	28	GLN
1	B	68	ALA
1	B	177	PHE
1	B	466	CYS
1	A	226	SER
1	A	262	PHE
1	A	392	ASN
1	B	135	LYS
1	B	150	ASP
1	B	313	TYR
1	A	110	ASP
1	B	286	GLU
1	B	392	ASN
1	B	110	ASP
1	B	395	PRO
1	B	396	SER
1	B	338	PRO
1	A	165	VAL

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	456/492 (93%)	415 (91%)	41 (9%)	9	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	456/492 (93%)	421 (92%)	35 (8%)	12	20
All	All	912/984 (93%)	836 (92%)	76 (8%)	10	18

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

Mol	Chain	Res	Type
1	A	26	ASP
1	A	37	LEU
1	A	48	THR
1	A	69	ASN
1	A	110	ASP
1	A	135	LYS
1	A	149	SER
1	A	163	LEU
1	A	164	ARG
1	A	169	ASP
1	A	176	SER
1	A	183	SER
1	A	206	ARG
1	A	220	VAL
1	A	225	GLU
1	A	231	LEU
1	A	253	ILE
1	A	258	LYS
1	A	260	LEU
1	A	284	TYR
1	A	291	LEU
1	A	294	LYS
1	A	304	SER
1	A	320	ILE
1	A	349	LEU
1	A	357	GLN
1	A	359	VAL
1	A	364	ARG
1	A	378	LEU
1	A	383	LEU
1	A	392	ASN
1	A	426	THR
1	A	431	LYS
1	A	438	LYS
1	A	498	LEU
1	A	515	ARG

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Mol	Chain	Res	Type
1	A	526	LEU
1	A	528	ARG
1	A	535	TYR
1	A	552	ILE
1	A	554	LEU
1	B	28	GLN
1	B	31	ILE
1	B	35	LEU
1	B	37	LEU
1	B	39	CYS
1	B	41	ASP
1	B	69	ASN
1	B	110	ASP
1	B	131	ASP
1	B	169	ASP
1	B	184	LEU
1	B	198	SER
1	B	206	ARG
1	B	211	ARG
1	B	220	VAL
1	B	225	GLU
1	B	231	LEU
1	B	258	LYS
1	B	260	LEU
1	B	280	ILE
1	B	284	TYR
1	B	288	GLN
1	B	291	LEU
1	B	320	ILE
1	B	364	ARG
1	B	378	LEU
1	B	383	LEU
1	B	426	THR
1	B	431	LYS
1	B	438	LYS
1	B	498	LEU
1	B	515	ARG
1	B	526	LEU
1	B	528	ARG
1	B	547	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	69	ASN
1	A	134	ASN
1	A	180	HIS
1	A	181	HIS
1	A	222	GLN
1	A	392	ASN
1	A	403	ASN
1	A	441	GLN
1	B	28	GLN
1	B	69	ASN
1	B	81	GLN
1	B	134	ASN
1	B	222	GLN
1	B	227	HIS
1	B	392	ASN
1	B	403	ASN
1	B	441	GLN
1	B	500	GLN

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](#)

Of 10 ligands modelled in this entry, 6 are monoatomic - leaving 4 for Mogul analysis.

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	BME	A	1273	-	3,3,3	0.32	0	2,2,2	0.90	0
2	BME	A	1274	-	3,3,3	0.37	0	2,2,2	1.41	0
3	FPF	A	801	4	22,24,24	2.92	7 (31%)	26,33,33	1.51	5 (19%)
3	FPF	B	802	4	22,24,24	2.87	6 (27%)	26,33,33	1.59	5 (19%)

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	BME	A	1273	-	-	0/1/1/1	-
2	BME	A	1274	-	-	0/1/1/1	-
3	FPF	A	801	4	-	8/22/28/28	-
3	FPF	B	802	4	-	5/22/28/28	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	801	FPF	P1-O3A	-9.00	1.49	1.59
3	B	802	FPF	P1-O3A	-8.79	1.50	1.59
3	B	802	FPF	P2-O3B	5.08	1.66	1.50
3	A	801	FPF	P2-O3B	5.06	1.66	1.50
3	B	802	FPF	C5-C3	4.27	1.56	1.51
3	A	801	FPF	C5-C3	4.10	1.56	1.51
3	B	802	FPF	C1-C2	3.49	1.54	1.48
3	A	801	FPF	C1-C2	3.28	1.54	1.48
3	A	801	FPF	P2-O1B	3.28	1.67	1.54
3	B	802	FPF	P2-O1B	3.11	1.66	1.54
3	A	801	FPF	O1-C1	-3.06	1.40	1.43
3	A	801	FPF	P2-O2B	2.97	1.65	1.54
3	B	802	FPF	P2-O2B	2.69	1.64	1.54

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	802	FPF	O1-C1-C2	-4.51	102.53	110.64
3	A	801	FPF	C10-C8-C9	3.06	120.55	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	801	FPF	O1-C1-C2	-2.78	105.65	110.64
3	B	802	FPF	C10-C8-C9	2.75	120.00	115.23
3	A	801	FPF	C4-C3-C5	2.62	120.97	115.33
3	B	802	FPF	O2A-P1-O3A	2.51	114.05	107.27
3	A	801	FPF	O2A-P1-O3A	2.46	113.92	107.27
3	B	802	FPF	C11-C12-C13	-2.03	120.89	127.64
3	B	802	FPF	O1B-P2-O3A	2.03	111.43	104.64
3	A	801	FPF	O1B-P2-O3A	2.02	111.42	104.64

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	802	FPF	C1-O1-P1-O1A
3	B	802	FPF	C1-O1-P1-O2A
3	B	802	FPF	C1-O1-P1-O3A
3	A	801	FPF	C12-C11-C9-C8
3	B	802	FPF	C12-C11-C9-C8
3	A	801	FPF	P1-O3A-P2-O3B
3	A	801	FPF	C1-O1-P1-O1A
3	A	801	FPF	C1-O1-P1-O2A
3	A	801	FPF	C1-O1-P1-O3A
3	B	802	FPF	C9-C11-C12-C13
3	A	801	FPF	C3-C5-C6-C7
3	A	801	FPF	P1-O3A-P2-O1B
3	A	801	FPF	P1-O3A-P2-O2B

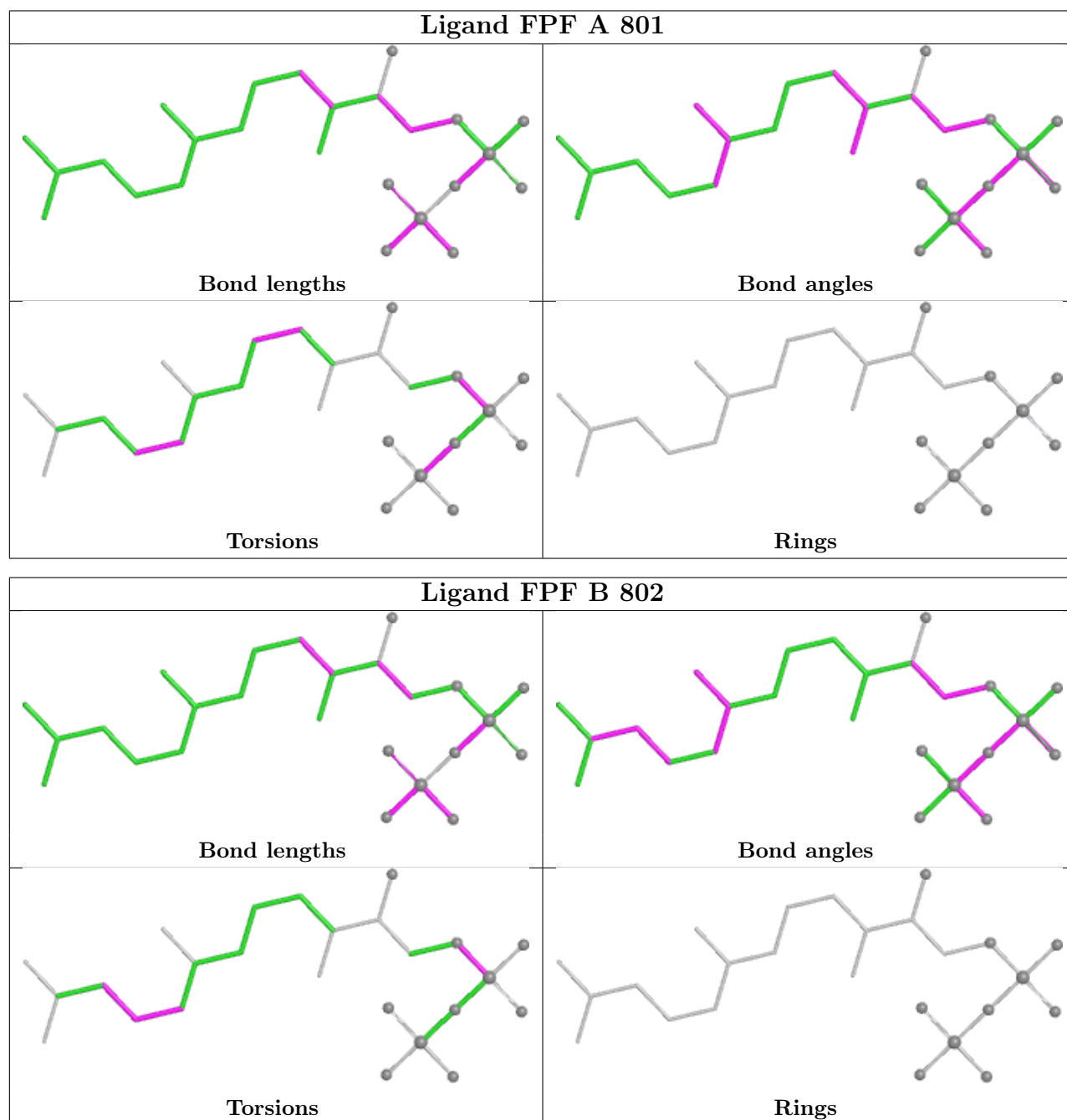
There are no ring outliers.

4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1273	BME	1	0
2	A	1274	BME	2	0
3	A	801	FPF	1	0
3	B	802	FPF	10	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	514/554 (92%)	-0.22	8 (1%) 70 66	30, 51, 86, 115	2 (0%)
1	B	514/554 (92%)	0.30	23 (4%) 38 31	32, 76, 117, 159	2 (0%)
All	All	1028/1108 (92%)	0.04	31 (3%) 52 45	30, 63, 109, 159	4 (0%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	27	PHE	4.9
1	B	279	TRP	4.7
1	B	268	TYR	4.0
1	B	25	ALA	3.9
1	B	269	ALA	3.8
1	A	26	ASP	3.7
1	A	279	TRP	3.6
1	A	535	TYR	3.3
1	A	313	TYR	3.3
1	A	25	ALA	3.1
1	A	536	VAL	3.0
1	A	330	ASP	3.0
1	B	223	ASP	2.8
1	B	535	TYR	2.8
1	B	225	GLU	2.8
1	B	313	TYR	2.8
1	B	27	PHE	2.8
1	B	46	ALA	2.7
1	B	29	PRO	2.7
1	B	31	ILE	2.6
1	B	28	GLN	2.6
1	B	554	LEU	2.5
1	B	107	ALA	2.5
1	B	466	CYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	537	GLY	2.4
1	B	180	HIS	2.3
1	B	529	GLU	2.2
1	B	257	TRP	2.2
1	B	184	LEU	2.1
1	B	266	LEU	2.1
1	B	536	VAL	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](#)

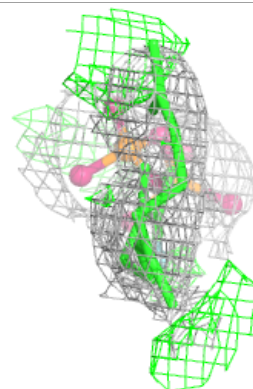
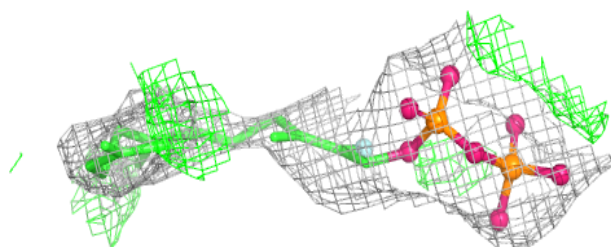
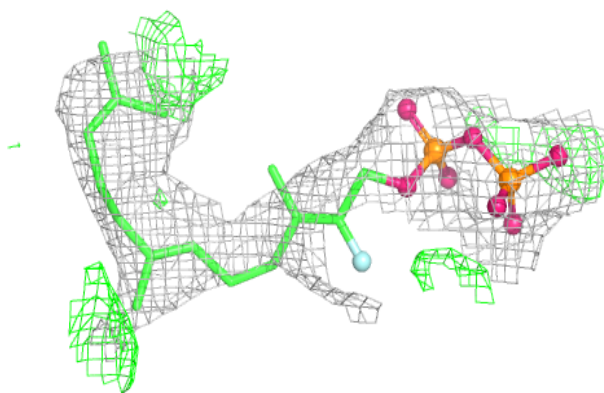
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	FPF	B	802	25/25	0.85	0.15	71,85,96,99	0
2	BME	A	1273	4/4	0.88	0.12	55,58,59,91	0
3	FPF	A	801	25/25	0.89	0.15	72,81,87,87	1
4	MG	A	606	1/1	0.90	0.11	68,68,68,68	0
4	MG	B	603	1/1	0.91	0.17	66,66,66,66	0
4	MG	A	605	1/1	0.94	0.21	49,49,49,49	0
4	MG	B	602	1/1	0.95	0.18	58,58,58,58	0
2	BME	A	1274	4/4	0.96	0.09	66,68,84,89	0
4	MG	A	604	1/1	0.97	0.13	46,46,46,46	0
4	MG	B	601	1/1	0.98	0.14	56,56,56,56	0

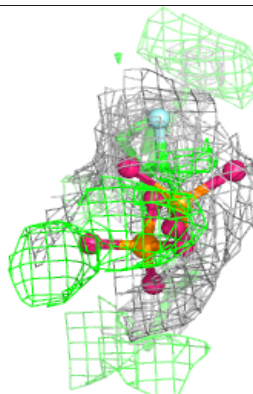
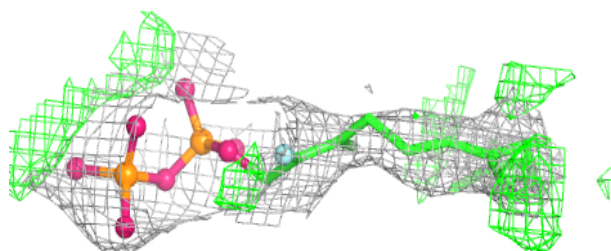
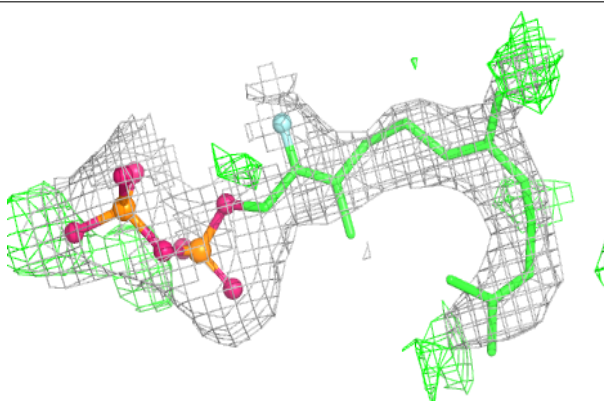
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FPF B 802:

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

**Electron density around FPF A 801:**

$2mF_o-DF_c$ (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.