



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:02 PM UTC

PDB ID : 3OAB / pdb_00003oab
Title : Mint deletion mutant of heterotetrameric geranyl pyrophosphate synthase in complex with ligands
Authors : Hsieh, F.-L.; Chang, T.-H.; Ko, T.-P.; Wang, A.H.-J.
Deposited on : 2010-08-05
Resolution : 2.30 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

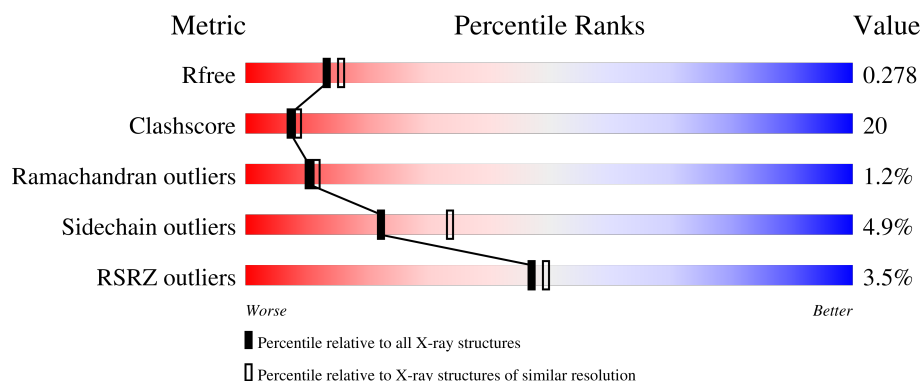
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	295	0% 61% 27% 6% 5%
1	D	295	2% 57% 39% .
2	B	264	9% 59% 28% 6% 6%
2	C	264	2% 61% 28% . 8%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8759 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 Geranyl diphosphate synthase large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	279	Total	C	N	O	S	0	0	0
			2120	1338	372	392	18			
1	D	295	Total	C	N	O	S	0	0	0
			2232	1406	391	417	18			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP Q9SBR3
D	1	MET	-	expression tag	UNP Q9SBR3

- Molecule 2 is a protein called Geranyl diphosphate synthase small subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	249	Total	C	N	O	S	0	0	0
			1881	1189	325	353	14			
2	C	242	Total	C	N	O	S	0	0	0
			1831	1160	315	342	14			

There are 38 discrepancies between the modelled and reference sequences:

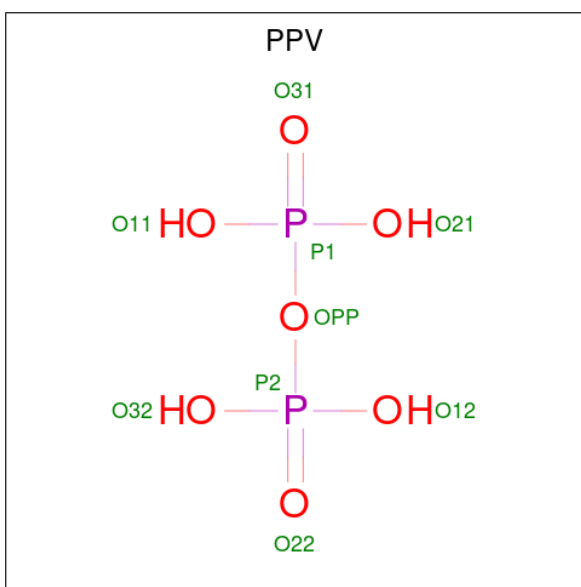
Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	expression tag	UNP Q9SBR4
B	?	-	LEU	deletion	UNP Q9SBR4
B	?	-	THR	deletion	UNP Q9SBR4
B	?	-	ASP	deletion	UNP Q9SBR4
B	?	-	GLY	deletion	UNP Q9SBR4
B	?	-	SER	deletion	UNP Q9SBR4
B	?	-	ARG	deletion	UNP Q9SBR4
B	?	-	PRO	deletion	UNP Q9SBR4
B	?	-	VAL	deletion	UNP Q9SBR4
B	?	-	SER	deletion	UNP Q9SBR4

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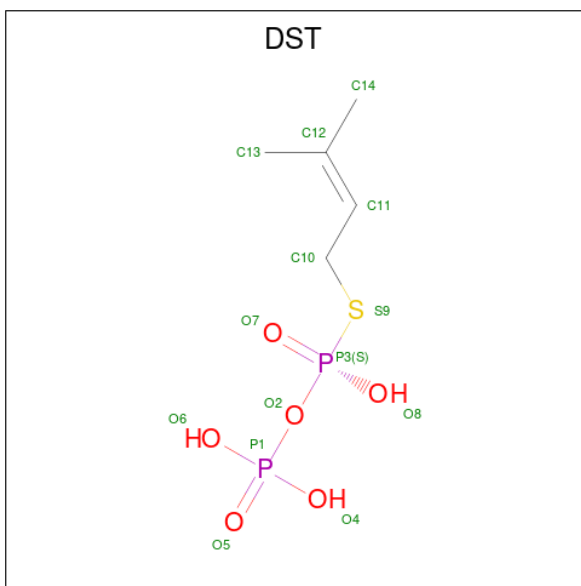
Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	LYS	deletion	UNP Q9SBR4
B	267	HIS	-	expression tag	UNP Q9SBR4
B	268	HIS	-	expression tag	UNP Q9SBR4
B	269	HIS	-	expression tag	UNP Q9SBR4
B	270	HIS	-	expression tag	UNP Q9SBR4
B	271	HIS	-	expression tag	UNP Q9SBR4
B	272	HIS	-	expression tag	UNP Q9SBR4
B	273	HIS	-	expression tag	UNP Q9SBR4
B	274	HIS	-	expression tag	UNP Q9SBR4
C	1	MET	-	expression tag	UNP Q9SBR4
C	?	-	LEU	deletion	UNP Q9SBR4
C	?	-	THR	deletion	UNP Q9SBR4
C	?	-	ASP	deletion	UNP Q9SBR4
C	?	-	GLY	deletion	UNP Q9SBR4
C	?	-	SER	deletion	UNP Q9SBR4
C	?	-	ARG	deletion	UNP Q9SBR4
C	?	-	PRO	deletion	UNP Q9SBR4
C	?	-	VAL	deletion	UNP Q9SBR4
C	?	-	SER	deletion	UNP Q9SBR4
C	?	-	LYS	deletion	UNP Q9SBR4
C	267	HIS	-	expression tag	UNP Q9SBR4
C	268	HIS	-	expression tag	UNP Q9SBR4
C	269	HIS	-	expression tag	UNP Q9SBR4
C	270	HIS	-	expression tag	UNP Q9SBR4
C	271	HIS	-	expression tag	UNP Q9SBR4
C	272	HIS	-	expression tag	UNP Q9SBR4
C	273	HIS	-	expression tag	UNP Q9SBR4
C	274	HIS	-	expression tag	UNP Q9SBR4

- Molecule 3 is PYROPHOSPHATE (CCD ID: PPV) (formula: $\text{H}_4\text{O}_7\text{P}_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			9	7	2		

- Molecule 4 is DIMETHYLALLYL S-THIOLODIPHOSPHATE (CCD ID: DST) (formula: $C_5H_{12}O_6P_2S$).

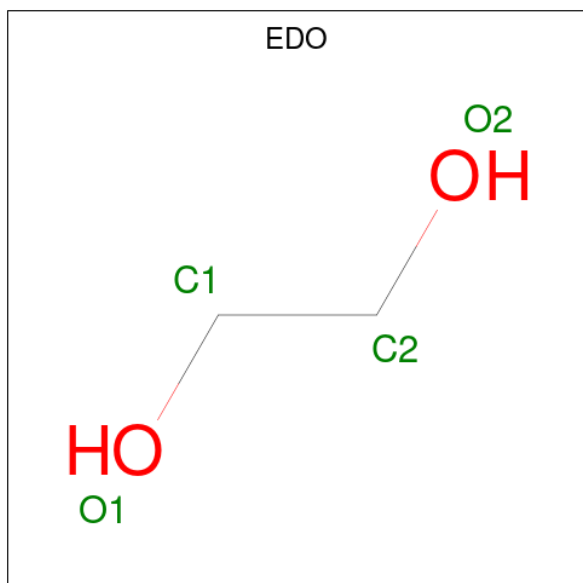


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	P	S	0
			14	5	6	2	1	0
4	D	1	Total	C	O	P	S	0
			14	5	6	2	1	0

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

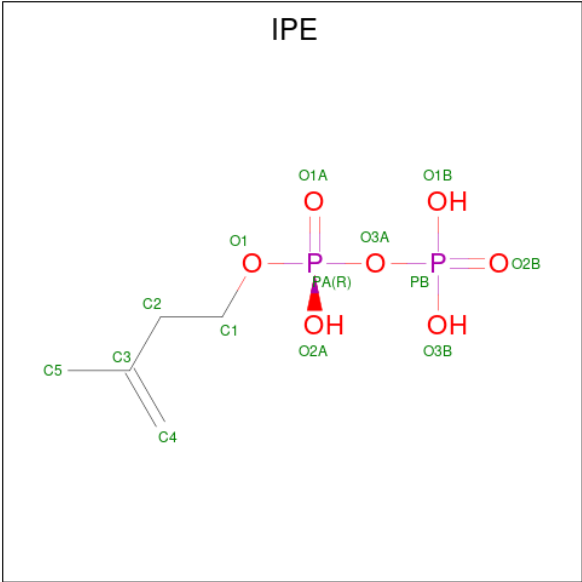
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Mg	0	0
			2	2		
5	D	2	Total	Mg	0	0
			2	2		

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

- Molecule 7 is 3-METHYLBUT-3-ENYL TRIHYDROGEN DIPHOSPHATE (CCD ID: IPE) (formula: C₅H₁₂O₇P₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	D	1	Total	C	O	P	0	0
			14	5	7	2		

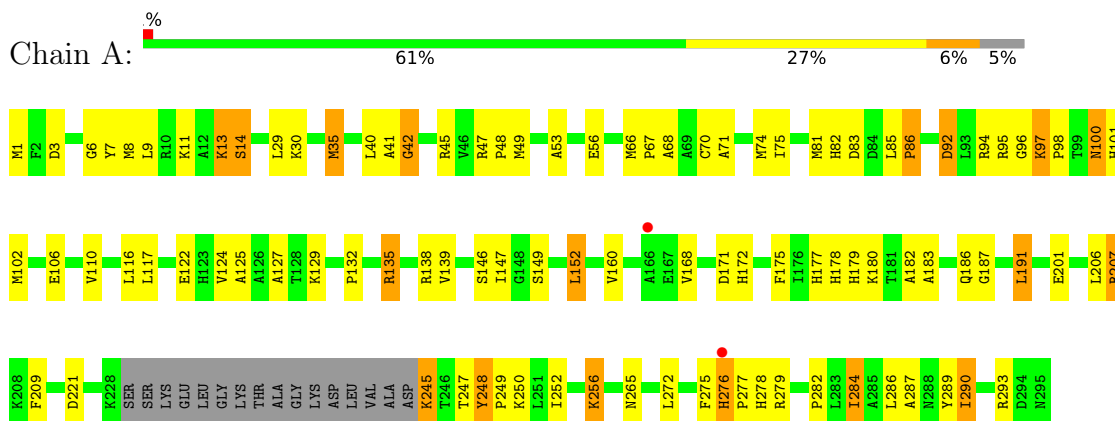
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	195	Total	O	0	0
			195	195		
8	B	148	Total	O	0	0
			148	148		
8	C	119	Total	O	0	0
			119	119		
8	D	174	Total	O	0	0
			174	174		

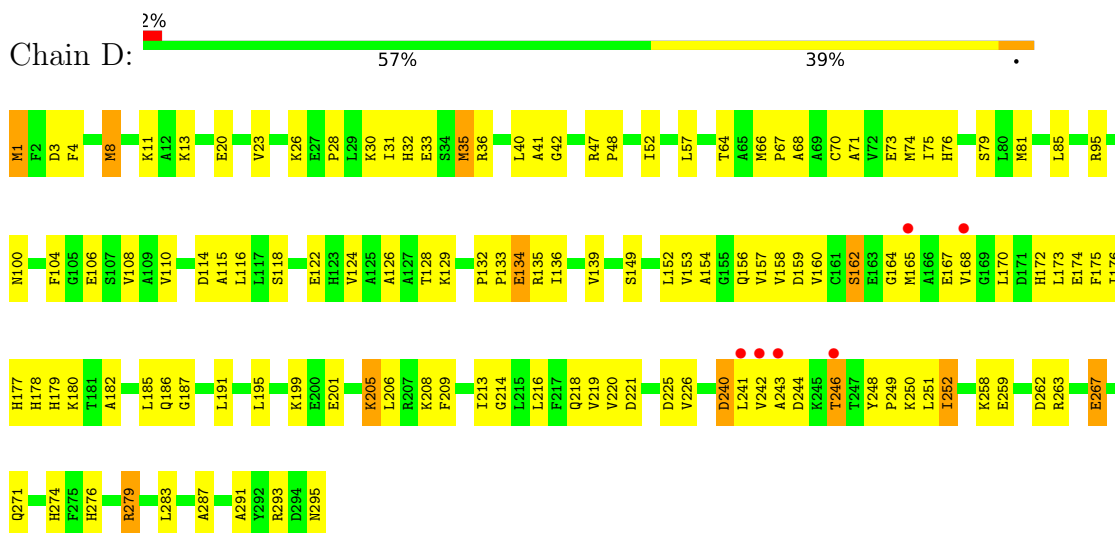
3 Residue-property plots

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.

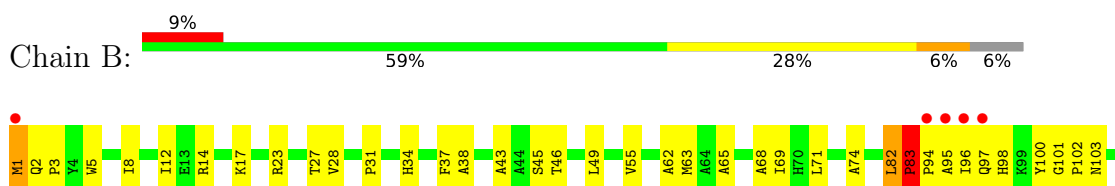
• Molecule 1: Geranyl diphosphate synthase large subunit

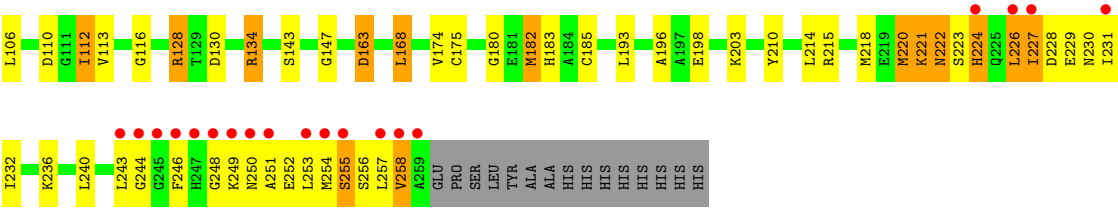


• Molecule 1: Geranyl diphosphate synthase large subunit

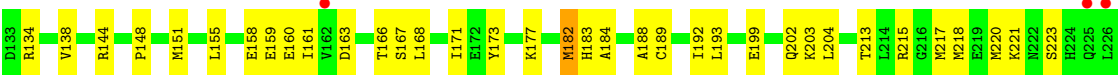
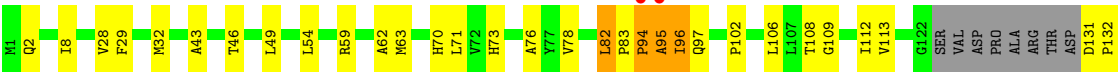


• Molecule 2: Geranyl diphosphate synthase small subunit





● Molecule 2: Geranyl diphosphate synthase small subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	51.27Å 109.26Å 182.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.96 – 2.30 24.96 – 2.30	Depositor EDS
% Data completeness (in resolution range)	92.1 (24.96-2.30) 92.1 (24.96-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.80 (at 2.28Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.208 , 0.277 0.210 , 0.278	Depositor DCC
R_{free} test set	2152 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	28.7	Xtriage
Anisotropy	0.859	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 43.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8759	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.99% 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: DST, PPV, IPE, MG, EDO

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	1.24	5/2155 (0.2%)	1.22	8/2903 (0.3%)
1	D	1.14	10/2268 (0.4%)	1.14	6/3055 (0.2%)
2	B	1.14	6/1919 (0.3%)	1.18	14/2595 (0.5%)
2	C	1.01	2/1867 (0.1%)	1.25	11/2521 (0.4%)
All	All	1.14	23/8209 (0.3%)	1.19	39/11074 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
2	B	0	1
All	All	0	3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	75	ILE	CA-CB	-6.91	1.45	1.54
1	D	287	ALA	CA-CB	-6.41	1.43	1.53
1	A	35	MET	SD-CE	6.37	1.95	1.79
2	B	1	MET	SD-CE	6.34	1.95	1.79
2	C	63	MET	SD-CE	6.19	1.95	1.79
1	A	53	ALA	CA-CB	-6.06	1.44	1.53
1	A	1	MET	SD-CE	6.05	1.94	1.79
2	B	74	ALA	CA-CB	-5.98	1.44	1.53
1	D	8	MET	SD-CE	5.97	1.94	1.79
1	D	8	MET	CG-SD	5.80	1.95	1.80
2	B	113	VAL	CA-CB	-5.78	1.51	1.54
1	A	152	LEU	CA-C	5.73	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	116	GLY	CA-C	5.57	1.58	1.52
2	C	78	VAL	CA-CB	-5.50	1.48	1.54
1	D	276	HIS	CA-C	5.46	1.58	1.53
1	D	1	MET	SD-CE	5.45	1.93	1.79
2	B	182	MET	SD-CE	5.43	1.93	1.79
1	D	114	ASP	C-O	-5.42	1.17	1.24
1	D	136	ILE	CA-CB	-5.33	1.48	1.54
1	D	118	SER	N-CA	-5.24	1.40	1.46
1	D	35	MET	CG-SD	5.14	1.93	1.80
2	B	68	ALA	CA-CB	5.06	1.61	1.53
1	A	290	ILE	CA-CB	-5.03	1.48	1.54

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	82	LEU	CA-C-N	12.57	157.17	127.00
2	C	82	LEU	C-N-CA	12.57	157.17	127.00
2	C	82	LEU	N-CA-C	-11.40	92.74	109.50
2	C	82	LEU	C-N-CD	-11.23	95.90	120.60
2	C	94	PRO	N-CA-C	-10.46	97.20	112.26
2	C	95	ALA	N-CA-C	-8.13	101.78	112.34
2	B	198	GLU	N-CA-C	6.82	119.58	111.33
1	A	276	HIS	CA-C-N	6.33	127.75	119.84
1	A	276	HIS	C-N-CA	6.33	127.75	119.84
1	A	284	ILE	N-CA-C	-6.06	104.44	110.62
2	B	226	LEU	N-CA-C	-6.03	103.66	113.19
2	B	180	GLY	N-CA-C	5.95	119.87	112.73
2	B	147	GLY	CA-C-N	5.92	125.59	119.56
2	B	147	GLY	C-N-CA	5.92	125.59	119.56
2	C	109	GLY	N-CA-C	-5.86	105.70	112.50
1	A	125	ALA	N-CA-C	5.55	117.41	111.36
1	A	191	LEU	N-CA-C	-5.54	104.87	111.69
2	B	82	LEU	CA-C-N	5.54	140.28	127.00
2	B	82	LEU	C-N-CA	5.54	140.28	127.00
1	D	76	HIS	N-CA-C	-5.50	105.18	111.07
2	B	23	ARG	CA-C-N	-5.49	114.72	120.38
2	B	23	ARG	C-N-CA	-5.49	114.72	120.38
2	C	184	ALA	N-CA-C	-5.42	105.37	111.28
1	D	240	ASP	N-CA-C	-5.39	106.75	113.38
1	D	291	ALA	N-CA-C	5.33	118.25	111.69
1	D	126	ALA	N-CA-C	5.32	119.77	113.28
1	D	85	LEU	CA-C-N	5.32	125.64	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	85	LEU	C-N-CA	5.32	125.64	119.47
2	C	213	THR	N-CA-C	-5.23	105.58	111.28
2	B	38	ALA	N-CA-C	-5.22	107.08	113.50
2	B	112	ILE	N-CA-C	5.15	115.92	110.72
1	A	92	ASP	N-CA-C	-5.15	107.13	113.41
2	B	83	PRO	CA-C-N	5.13	126.25	119.84
2	B	83	PRO	C-N-CA	5.13	126.25	119.84
2	C	29	PHE	N-CA-C	5.09	119.12	113.01
1	A	275	PHE	N-CA-C	-5.07	101.85	109.85
1	A	100	ASN	N-CA-C	5.03	116.45	111.07
2	B	103	ASN	N-CA-C	5.03	116.76	111.28
2	C	113	VAL	CA-C-O	5.02	122.05	118.69

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	248	TYR	Sidechain
1	A	289	TYR	Sidechain
2	B	210	TYR	Sidechain

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	2120	0	2146	72	0
1	D	2232	0	2264	104	0
2	B	1881	0	1871	91	0
2	C	1831	0	1822	71	0
3	A	9	0	0	0	0
4	A	14	0	10	1	0
4	D	14	0	10	5	0
5	A	2	0	0	0	0
5	D	2	0	0	0	0
6	C	4	0	6	0	0
7	D	14	0	9	2	0
8	A	195	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	148	0	0	7	0
8	C	119	0	0	5	0
8	D	174	0	0	8	0
All	All	8759	0	8138	331	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 (331) 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:139:VAL:HG13	1:A:191:LEU:HD22	1.33	1.04
1:D:279:ARG:HH11	1:D:279:ARG:HB3	1.22	0.99
1:D:4:PHE:HB2	1:D:8:MET:HE3	1.46	0.97
1:A:94:ARG:O	1:A:95:ARG:HG2	1.63	0.97
1:D:139:VAL:HG13	1:D:191:LEU:HD22	1.52	0.91
1:A:102:MET:HE2	1:A:102:MET:HA	1.50	0.91
2:B:249:LYS:HD3	2:B:253:LEU:HB2	1.51	0.90
1:D:205:LYS:HD2	1:D:274:HIS:HB2	1.52	0.89
2:B:218:MET:HE1	2:B:232:ILE:HD11	1.52	0.88
1:D:158:VAL:O	1:D:162:SER:HB3	1.75	0.87
2:B:82:LEU:HA	2:B:83:PRO:O	1.74	0.86
2:B:249:LYS:HE2	2:B:253:LEU:HD13	1.57	0.86
1:D:279:ARG:HH11	1:D:279:ARG:CB	1.89	0.84
2:B:128:ARG:HH11	2:B:128:ARG:CG	1.92	0.82
1:D:4:PHE:HB2	1:D:8:MET:CE	2.10	0.82
1:D:225:ASP:OD2	1:D:240:ASP:HB2	1.80	0.81
2:B:215:ARG:HD3	2:B:257:LEU:HD21	1.63	0.80
1:D:128:THR:O	1:D:129:LYS:HD3	1.81	0.80
1:A:101:HIS:CD2	1:A:102:MET:HE3	2.17	0.80
7:D:801:IPE:H53	4:D:802:DST:H133	1.64	0.80
2:C:236:LYS:HE3	8:C:442:HOH:O	1.83	0.79
2:C:108:THR:O	2:C:112:ILE:HG12	1.83	0.78
1:A:171:ASP:OD2	8:A:298:HOH:O	2.00	0.78
2:B:128:ARG:HH11	2:B:128:ARG:HG2	1.46	0.78
1:D:1:MET:HA	1:D:1:MET:HE2	1.64	0.78
2:C:97:GLN:HA	2:C:97:GLN:OE1	1.85	0.77
2:C:96:ILE:HG22	2:C:97:GLN:H	1.49	0.77
2:B:215:ARG:NH1	2:B:257:LEU:HD11	2.01	0.76
1:A:149:SER:HB2	8:A:470:HOH:O	1.86	0.75
2:B:249:LYS:O	2:B:253:LEU:N	2.19	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:173:LEU:HD22	1:D:251:LEU:HD12	1.68	0.75
1:D:168:VAL:HG23	1:D:251:LEU:HD11	1.69	0.75
1:D:168:VAL:HG21	1:D:246:THR:HG23	1.66	0.75
1:D:30:LYS:HE3	1:D:108:VAL:HG21	1.70	0.73
2:B:96:ILE:HG22	2:B:97:GLN:H	1.54	0.72
2:B:65:ALA:O	2:B:69:ILE:HG13	1.91	0.70
2:B:8:ILE:HG23	2:B:49:LEU:HD12	1.72	0.70
1:D:106:GLU:O	1:D:110:VAL:HG23	1.92	0.70
1:A:127:ALA:O	1:A:129:LYS:HD2	1.92	0.70
2:C:218:MET:HE1	2:C:232:ILE:HD13	1.74	0.70
2:C:237:GLU:O	2:C:241:GLU:HG3	1.91	0.70
2:B:232:ILE:O	2:B:236:LYS:HG2	1.93	0.69
2:B:71:LEU:HD22	2:B:112:ILE:HG23	1.75	0.68
2:B:253:LEU:HD12	2:B:256:SER:OG	1.94	0.68
2:C:188:ALA:O	2:C:192:ILE:HG13	1.94	0.68
1:A:187:GLY:O	1:A:191:LEU:HG	1.93	0.68
1:D:279:ARG:HH11	1:D:279:ARG:CG	2.07	0.68
1:A:30:LYS:HD3	8:A:412:HOH:O	1.93	0.67
1:D:134:GLU:H	1:D:134:GLU:CD	2.02	0.67
1:D:201:GLU:OE2	8:D:303:HOH:O	2.12	0.67
2:B:82:LEU:HD12	2:B:82:LEU:O	1.95	0.67
2:B:246:PHE:C	2:B:251:ALA:HB1	2.20	0.67
2:B:221:LYS:HG2	2:B:227:ILE:CG2	2.24	0.67
2:B:130:ASP:O	2:B:134:ARG:HG3	1.95	0.67
2:C:28:VAL:HG22	1:D:157:VAL:CG2	2.25	0.66
1:A:138:ARG:HD2	8:A:420:HOH:O	1.96	0.65
2:C:97:GLN:NE2	8:C:335:HOH:O	2.29	0.65
2:C:217:MET:HE2	2:C:231:ILE:HG21	1.79	0.65
1:D:64:THR:OG1	8:D:306:HOH:O	2.14	0.65
1:A:13:LYS:HD3	1:A:13:LYS:C	2.22	0.64
2:B:94:PRO:HA	8:B:555:HOH:O	1.97	0.64
2:B:230:ASN:HB3	8:B:318:HOH:O	1.97	0.64
2:C:260:GLU:OE2	2:C:260:GLU:HA	1.98	0.64
2:B:249:LYS:CD	2:B:253:LEU:HB2	2.27	0.64
2:C:218:MET:HE1	2:C:232:ILE:CD1	2.28	0.64
2:C:28:VAL:HG22	1:D:157:VAL:HG21	1.80	0.63
2:C:94:PRO:C	2:C:96:ILE:N	2.52	0.63
2:B:2:GLN:HE21	2:B:2:GLN:HA	1.62	0.63
1:D:205:LYS:HD2	1:D:274:HIS:CB	2.26	0.63
1:A:290:ILE:HG23	1:A:293:ARG:HH22	1.64	0.62
2:C:234:LYS:O	2:C:238:LEU:HG	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:230:ASN:O	2:C:234:LYS:HG3	2.00	0.62
2:B:249:LYS:HE2	2:B:253:LEU:HD22	1.83	0.61
1:D:81:MET:HE3	1:D:100:ASN:ND2	2.15	0.61
2:B:168:LEU:HD12	2:B:231:ILE:HG13	1.82	0.61
1:D:173:LEU:CD2	1:D:251:LEU:HD12	2.31	0.60
2:B:221:LYS:HG2	2:B:227:ILE:HG21	1.83	0.60
1:D:226:VAL:HG12	1:D:226:VAL:O	2.00	0.60
1:D:226:VAL:HG22	1:D:241:LEU:HD23	1.84	0.60
2:B:5:TRP:HE1	2:B:253:LEU:HD11	1.67	0.59
2:B:97:GLN:HA	8:B:556:HOH:O	2.01	0.59
2:C:138:VAL:HG13	2:C:189:CYS:SG	2.42	0.59
2:C:71:LEU:HD22	2:C:112:ILE:HG23	1.85	0.59
2:C:151:MET:O	2:C:155:LEU:HG	2.02	0.59
2:B:182:MET:HE3	2:B:185:CYS:HB3	1.84	0.58
1:A:207:ARG:NH1	8:A:362:HOH:O	2.37	0.58
2:C:97:GLN:OE1	2:C:97:GLN:CA	2.51	0.58
2:B:229:GLU:OE1	2:B:229:GLU:HA	2.04	0.58
2:B:1:MET:O	2:B:5:TRP:HD1	1.86	0.58
2:C:259:ALA:O	2:C:260:GLU:CB	2.51	0.58
1:A:247:THR:HB	1:A:249:PRO:HD2	1.85	0.58
2:C:8:ILE:CG2	2:C:49:LEU:HD12	2.34	0.58
2:B:246:PHE:O	2:B:251:ALA:HB1	2.04	0.58
1:D:279:ARG:HB3	1:D:279:ARG:NH1	2.05	0.57
1:A:102:MET:HA	1:A:102:MET:CE	2.32	0.57
1:D:71:ALA:HB2	1:D:124:VAL:HG23	1.86	0.57
1:A:83:ASP:CG	4:A:804:DST:H102	2.30	0.57
2:B:69:ILE:HG23	2:B:182:MET:HE2	1.87	0.57
1:D:168:VAL:HG23	1:D:251:LEU:HD21	1.86	0.56
2:B:249:LYS:CE	2:B:253:LEU:HD13	2.32	0.56
2:C:134:ARG:O	2:C:138:VAL:HG23	2.06	0.56
1:A:290:ILE:HG23	1:A:293:ARG:NH2	2.21	0.56
2:B:94:PRO:HB3	8:B:297:HOH:O	2.05	0.56
1:D:57:LEU:HD22	1:D:283:LEU:HD12	1.88	0.56
1:A:94:ARG:O	1:A:95:ARG:CG	2.47	0.56
1:D:187:GLY:O	1:D:191:LEU:HG	2.05	0.55
2:C:62:ALA:HA	2:C:193:LEU:HD13	1.88	0.55
1:D:48:PRO:HG3	1:D:73:GLU:HB2	1.89	0.55
7:D:801:IPE:C5	4:D:802:DST:H133	2.35	0.55
2:C:228:ASP:OD2	2:C:230:ASN:HB2	2.06	0.55
2:B:227:ILE:HG13	2:B:227:ILE:O	2.07	0.55
1:A:245:LYS:HB3	1:A:250:LYS:NZ	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:54:LEU:HD22	2:C:254:MET:HE3	1.89	0.55
2:C:227:ILE:O	2:C:227:ILE:HG12	2.06	0.55
1:A:252:ILE:HD12	1:A:256:LYS:HB3	1.88	0.55
2:B:14:ARG:HB2	2:B:14:ARG:NH1	2.22	0.55
2:C:218:MET:O	2:C:221:LYS:HB3	2.07	0.54
1:D:180:LYS:O	4:D:802:DST:H131	2.06	0.54
1:A:68:ALA:HA	1:A:124:VAL:HG22	1.89	0.54
2:B:228:ASP:OD2	2:B:230:ASN:HB2	2.07	0.54
1:D:206:LEU:O	1:D:209:PHE:HB3	2.06	0.54
2:B:248:GLY:N	2:B:251:ALA:HB3	2.22	0.54
1:D:293:ARG:HD2	1:D:295:ASN:O	2.08	0.54
2:C:83:PRO:CB	2:C:94:PRO:CD	2.84	0.54
2:B:128:ARG:CG	2:B:128:ARG:NH1	2.62	0.54
2:B:221:LYS:HG2	2:B:227:ILE:HG22	1.89	0.53
2:B:43:ALA:HB3	2:B:183:HIS:HE1	1.73	0.53
1:D:176:ILE:HG22	1:D:177:HIS:N	2.22	0.53
2:B:218:MET:HA	2:B:221:LYS:HG3	1.91	0.53
1:D:156:GLN:HE22	4:D:802:DST:H112	1.72	0.53
2:B:98:HIS:HB2	8:B:288:HOH:O	2.07	0.53
2:C:228:ASP:HB2	2:C:230:ASN:OD1	2.09	0.53
1:D:279:ARG:CG	1:D:279:ARG:NH1	2.67	0.53
2:C:259:ALA:O	2:C:260:GLU:HB2	2.08	0.53
2:B:228:ASP:HB3	2:B:231:ILE:HG12	1.91	0.52
2:C:83:PRO:HB2	2:C:94:PRO:CD	2.39	0.52
1:D:70:CYS:HB3	1:D:74:MET:HE3	1.91	0.52
1:D:162:SER:O	1:D:162:SER:OG	2.27	0.52
1:D:68:ALA:HA	1:D:124:VAL:HG22	1.91	0.52
1:D:128:THR:C	1:D:129:LYS:HD3	2.34	0.52
2:B:175:CYS:SG	2:B:220:MET:HG3	2.49	0.52
2:B:249:LYS:HD3	2:B:249:LYS:C	2.34	0.52
2:C:8:ILE:HG23	2:C:49:LEU:HD12	1.90	0.52
2:B:218:MET:CE	2:B:232:ILE:HD11	2.31	0.52
2:B:1:MET:O	2:B:5:TRP:CD1	2.62	0.52
1:A:85:LEU:HD12	2:B:106:LEU:HD21	1.91	0.52
1:A:40:LEU:C	1:A:42:GLY:H	2.18	0.51
2:B:43:ALA:HB3	2:B:183:HIS:CE1	2.45	0.51
1:A:35:MET:HG2	1:A:116:LEU:HG	1.90	0.51
2:B:31:PRO:HG3	2:B:100:TYR:CE1	2.45	0.51
2:B:214:LEU:CD2	2:B:258:VAL:HG12	2.40	0.51
2:C:166:THR:HG22	2:C:171:ILE:HG13	1.93	0.51
2:B:55:VAL:HG11	2:B:196:ALA:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:70:HIS:O	2:C:73:HIS:HB3	2.09	0.51
1:A:180:LYS:NZ	8:A:587:HOH:O	2.42	0.51
1:D:178:HIS:O	1:D:182:ALA:HB3	2.11	0.50
2:C:158:GLU:C	2:C:160:GLU:H	2.19	0.50
1:A:56:GLU:O	1:A:279:ARG:HD3	2.11	0.50
1:D:162:SER:HB2	1:D:172:HIS:NE2	2.27	0.50
1:D:226:VAL:HG22	1:D:241:LEU:CD2	2.41	0.50
1:D:52:ILE:HD11	1:D:66:MET:CE	2.42	0.50
1:D:178:HIS:C	1:D:178:HIS:ND1	2.69	0.50
2:B:1:MET:HG3	2:B:2:GLN:N	2.27	0.50
2:B:255:SER:O	2:B:258:VAL:HG23	2.12	0.50
1:A:45:ARG:O	1:A:48:PRO:HD2	2.12	0.50
1:D:156:GLN:O	1:D:160:VAL:HG13	2.12	0.50
2:C:2:GLN:HE22	2:C:256:SER:HB2	1.77	0.50
2:C:43:ALA:HB3	2:C:183:HIS:CE1	2.47	0.50
2:C:8:ILE:HG12	2:C:59:ARG:NH1	2.28	0.49
2:C:43:ALA:HB3	2:C:183:HIS:HE1	1.77	0.49
1:D:248:TYR:C	1:D:250:LYS:H	2.18	0.49
1:D:11:LYS:NZ	8:D:376:HOH:O	2.41	0.49
1:A:171:ASP:OD2	1:A:172:HIS:N	2.45	0.49
2:B:214:LEU:HD23	2:B:258:VAL:HG12	1.93	0.49
2:C:217:MET:CE	2:C:231:ILE:HG21	2.43	0.49
1:D:152:LEU:HA	1:D:179:HIS:O	2.12	0.49
1:D:226:VAL:O	1:D:226:VAL:CG1	2.60	0.49
1:A:94:ARG:C	1:A:95:ARG:HG2	2.37	0.49
2:B:221:LYS:CG	2:B:227:ILE:HG21	2.43	0.49
1:A:66:MET:HB3	1:A:67:PRO:HD3	1.94	0.49
1:D:170:LEU:O	1:D:174:GLU:HB2	2.13	0.49
1:A:29:LEU:HD11	2:C:173:TYR:CE2	2.47	0.49
2:B:5:TRP:HZ2	2:B:253:LEU:HG	1.77	0.49
2:C:94:PRO:O	2:C:95:ALA:C	2.52	0.49
1:D:219:VAL:HG22	1:D:248:TYR:CD2	2.47	0.49
1:A:221:ASP:OD1	1:A:293:ARG:NH1	2.33	0.49
1:A:13:LYS:HD2	8:A:382:HOH:O	2.12	0.48
2:C:28:VAL:HG22	1:D:157:VAL:HG23	1.94	0.48
2:B:34:HIS:HE1	8:B:391:HOH:O	1.96	0.48
2:C:71:LEU:HB3	2:C:112:ILE:HG22	1.94	0.48
2:B:249:LYS:HE2	2:B:253:LEU:CD1	2.36	0.48
2:B:220:MET:O	2:B:221:LYS:C	2.56	0.48
2:B:220:MET:HE2	2:B:220:MET:HA	1.96	0.48
2:C:158:GLU:C	2:C:160:GLU:N	2.72	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ARG:C	1:A:48:PRO:HD2	2.39	0.48
1:A:81:MET:HE3	1:A:100:ASN:ND2	2.29	0.48
1:A:47:ARG:HB2	1:A:48:PRO:HD3	1.95	0.48
1:A:92:ASP:O	1:A:98:PRO:HA	2.14	0.48
1:D:165:MET:HG2	8:D:406:HOH:O	2.13	0.48
2:C:221:LYS:HG3	2:C:227:ILE:CG2	2.44	0.47
1:D:23:VAL:O	1:D:36:ARG:HD2	2.14	0.47
2:B:163:ASP:O	2:B:224:HIS:HB3	2.14	0.47
2:B:14:ARG:HB2	2:B:14:ARG:HH11	1.79	0.47
1:A:122:GLU:HB2	2:B:143:SER:OG	2.14	0.47
2:B:254:MET:C	2:B:256:SER:H	2.23	0.47
1:D:52:ILE:HD11	1:D:66:MET:HE1	1.96	0.47
1:D:158:VAL:O	1:D:158:VAL:HG12	2.13	0.47
1:A:71:ALA:O	1:A:74:MET:HB2	2.14	0.46
1:A:7:TYR:CZ	1:A:11:LYS:HE2	2.50	0.46
2:C:247:HIS:CD2	8:C:483:HOH:O	2.69	0.46
1:D:153:VAL:O	1:D:157:VAL:HG22	2.16	0.46
1:D:267:GLU:O	1:D:271:GLN:HG2	2.16	0.46
1:D:248:TYR:HD1	1:D:252:ILE:HD11	1.80	0.46
1:A:168:VAL:HG13	1:A:172:HIS:HB3	1.96	0.46
2:B:94:PRO:O	2:B:95:ALA:C	2.58	0.46
2:B:240:LEU:N	2:B:240:LEU:HD23	2.30	0.46
2:B:248:GLY:O	2:B:252:GLU:HB2	2.16	0.46
2:C:199:GLU:O	2:C:203:LYS:HG2	2.15	0.46
1:D:66:MET:HB3	1:D:67:PRO:HD3	1.97	0.46
1:A:186:GLN:CD	1:A:207:ARG:HG2	2.41	0.45
2:B:2:GLN:HA	2:B:2:GLN:NE2	2.30	0.45
2:C:155:LEU:HD13	8:C:411:HOH:O	2.15	0.45
1:A:132:PRO:HG2	1:A:135:ARG:HB2	1.98	0.45
2:B:2:GLN:HB3	8:B:474:HOH:O	2.16	0.45
1:D:167:GLU:N	1:D:167:GLU:CD	2.74	0.45
2:B:221:LYS:O	2:B:222:ASN:C	2.60	0.45
2:C:94:PRO:C	2:C:96:ILE:H	2.24	0.45
1:A:209:PHE:CE1	1:A:272:LEU:HD11	2.52	0.45
1:D:135:ARG:CG	1:D:135:ARG:HH11	2.29	0.45
1:D:149:SER:O	1:D:154:ALA:HB2	2.17	0.45
2:B:253:LEU:O	2:B:256:SER:N	2.50	0.45
2:C:76:ALA:HB2	2:C:151:MET:HE3	1.99	0.45
2:C:82:LEU:HD11	2:C:106:LEU:HD13	1.99	0.45
1:D:175:PHE:CD1	1:D:175:PHE:C	2.94	0.45
1:D:20:GLU:HG2	1:D:40:LEU:HD13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:28:PRO:HG2	1:D:31:ILE:HB	1.98	0.44
1:A:82:HIS:ND1	2:B:110:ASP:OD2	2.47	0.44
2:B:12:ILE:HD13	2:B:45:SER:HB3	1.98	0.44
2:B:62:ALA:HA	2:B:193:LEU:HD13	1.99	0.44
1:D:259:GLU:O	1:D:262:ASP:HB2	2.16	0.44
2:C:144:ARG:HG2	1:D:122:GLU:CD	2.41	0.44
1:D:3:ASP:OD2	1:D:3:ASP:C	2.56	0.44
1:D:168:VAL:CG2	1:D:251:LEU:HD21	2.47	0.44
1:A:70:CYS:O	1:A:74:MET:HG3	2.18	0.44
1:A:248:TYR:N	1:A:249:PRO:CD	2.80	0.44
1:A:13:LYS:HD3	1:A:14:SER:N	2.32	0.44
1:D:157:VAL:HG23	1:D:158:VAL:N	2.33	0.44
1:A:265:ASN:OD1	1:A:287:ALA:HB1	2.18	0.44
1:A:276:HIS:HA	1:A:277:PRO:HD3	1.79	0.44
1:D:263:ARG:NH2	8:D:404:HOH:O	2.51	0.44
1:D:158:VAL:HG21	1:D:175:PHE:CE1	2.53	0.44
1:D:164:GLY:O	1:D:244:ASP:OD2	2.36	0.44
1:D:33:GLU:HG2	1:D:104:PHE:CE2	2.53	0.44
1:D:263:ARG:HB2	1:D:263:ARG:HH11	1.83	0.43
1:D:132:PRO:HD2	1:D:135:ARG:NE	2.33	0.43
1:A:71:ALA:HB2	1:A:124:VAL:HG23	1.98	0.43
2:B:168:LEU:HD23	2:B:226:LEU:HD23	2.00	0.43
1:A:40:LEU:C	1:A:42:GLY:N	2.77	0.43
1:A:206:LEU:HD23	1:A:206:LEU:HA	1.85	0.43
1:A:86:PRO:HD3	1:A:101:HIS:CD2	2.54	0.43
2:B:250:ASN:HA	2:B:253:LEU:HB3	2.01	0.43
2:C:148:PRO:HD3	1:D:115:ALA:HB1	2.00	0.43
1:A:8:MET:SD	1:A:49:MET:HG3	2.59	0.43
1:A:178:HIS:O	1:A:182:ALA:HB3	2.19	0.43
2:C:167:SER:O	2:C:171:ILE:HG13	2.19	0.43
2:C:218:MET:HE1	2:C:232:ILE:CG1	2.47	0.43
1:D:26:LYS:HG3	1:D:32:HIS:CE1	2.54	0.42
1:A:147:ILE:HD13	1:A:147:ILE:HG21	1.74	0.42
2:B:28:VAL:O	2:B:31:PRO:HD2	2.19	0.42
1:D:185:LEU:HD13	1:D:214:GLY:HA2	2.01	0.42
1:A:127:ALA:O	1:A:129:LYS:CD	2.66	0.42
2:B:253:LEU:O	2:B:254:MET:C	2.62	0.42
2:C:131:ASP:HB3	2:C:132:PRO:HD3	1.99	0.42
2:C:161:ILE:HG23	2:C:166:THR:HG21	2.00	0.42
2:C:182:MET:HA	2:C:182:MET:CE	2.49	0.42
2:C:32:MET:HG3	2:C:112:ILE:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:79:SER:OG	4:D:802:DST:H142	2.18	0.42
2:B:2:GLN:N	2:B:3:PRO:HD2	2.34	0.42
2:B:243:LEU:HD23	2:B:243:LEU:HA	1.90	0.42
1:D:178:HIS:HE1	8:D:344:HOH:O	2.02	0.42
1:D:248:TYR:HB2	1:D:249:PRO:HD3	2.02	0.42
1:A:146:SER:HB2	1:A:183:ALA:O	2.20	0.42
2:B:203:LYS:NZ	2:B:244:GLY:O	2.40	0.42
2:C:151:MET:HA	2:C:177:LYS:O	2.20	0.42
1:A:245:LYS:HB3	1:A:250:LYS:HZ1	1.85	0.42
2:B:253:LEU:C	2:B:255:SER:N	2.75	0.42
1:D:165:MET:CG	8:D:406:HOH:O	2.67	0.42
1:D:242:VAL:O	1:D:243:ALA:C	2.63	0.42
1:A:3:ASP:OD2	1:A:6:GLY:HA3	2.20	0.41
2:C:177:LYS:HA	2:C:177:LYS:HD2	1.77	0.41
1:A:175:PHE:O	1:A:179:HIS:HD2	2.02	0.41
1:A:286:LEU:O	1:A:290:ILE:HG13	2.20	0.41
2:C:8:ILE:HG22	2:C:46:THR:HG22	2.03	0.41
1:A:106:GLU:O	1:A:110:VAL:HG23	2.21	0.41
2:B:182:MET:HE3	2:B:182:MET:HA	2.02	0.41
1:D:139:VAL:HG21	1:D:195:LEU:HG	2.02	0.41
1:D:176:ILE:HG22	1:D:177:HIS:ND1	2.35	0.41
1:D:258:LYS:O	1:D:259:GLU:C	2.63	0.41
1:A:96:GLY:C	1:A:97:LYS:HD2	2.45	0.41
1:A:152:LEU:C	1:A:152:LEU:HD23	2.45	0.41
1:A:279:ARG:O	1:A:282:PRO:HD2	2.21	0.41
2:C:95:ALA:C	2:C:96:ILE:HG13	2.46	0.41
1:D:263:ARG:HB2	1:D:263:ARG:NH1	2.34	0.41
2:C:204:LEU:HD23	2:C:204:LEU:HA	1.85	0.41
1:D:213:ILE:HA	1:D:216:LEU:HB3	2.03	0.41
2:B:63:MET:HB2	2:B:63:MET:HE2	1.71	0.41
1:D:279:ARG:NH1	1:D:279:ARG:HG2	2.36	0.41
2:B:101:GLY:O	2:B:102:PRO:C	2.64	0.41
1:D:41:ALA:HB3	1:D:95:ARG:HD3	2.02	0.41
1:D:132:PRO:HB2	1:D:134:GLU:OE1	2.20	0.41
1:D:168:VAL:CG2	1:D:251:LEU:HD11	2.44	0.41
1:A:75:ILE:HD12	1:A:117:LEU:HD13	2.03	0.41
2:C:168:LEU:HD23	2:C:168:LEU:HA	1.93	0.41
1:D:35:MET:CE	1:D:116:LEU:HD23	2.51	0.41
1:D:159:ASP:OD2	1:D:159:ASP:C	2.64	0.41
1:D:216:LEU:O	1:D:220:VAL:HG23	2.20	0.41
1:D:71:ALA:HB2	1:D:124:VAL:CG2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:236:LYS:O	2:B:240:LEU:HG	2.21	0.40
2:C:131:ASP:HB3	2:C:132:PRO:CD	2.51	0.40
1:A:290:ILE:HA	1:A:293:ARG:HH21	1.85	0.40
2:B:17:LYS:HG2	2:B:37:PHE:CZ	2.55	0.40
1:D:47:ARG:HB2	8:D:318:HOH:O	2.21	0.40
2:B:163:ASP:OD1	2:B:163:ASP:N	2.54	0.40
1:D:218:GLN:O	1:D:221:ASP:N	2.54	0.40
1:A:94:ARG:HH21	1:A:94:ARG:HG3	1.86	0.40
1:A:177:HIS:HD2	1:A:248:TYR:OH	2.05	0.40
1:A:290:ILE:O	1:A:293:ARG:NH2	2.54	0.40
2:C:215:ARG:NH1	8:C:402:HOH:O	2.52	0.40
2:C:203:LYS:HA	2:C:203:LYS:HD2	1.86	0.40
2:C:218:MET:HE1	2:C:232:ILE:HG12	2.03	0.40
1:D:209:PHE:CE2	1:D:213:ILE:HD13	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	275/295 (93%)	262 (95%)	11 (4%)	2 (1%)	18	23
1	D	293/295 (99%)	275 (94%)	16 (6%)	2 (1%)	18	23
2	B	247/264 (94%)	229 (93%)	11 (4%)	7 (3%)	4	2
2	C	238/264 (90%)	227 (95%)	9 (4%)	2 (1%)	16	20
All	All	1053/1118 (94%)	993 (94%)	47 (4%)	13 (1%)	10	12

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	83	PRO

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Mol	Chain	Res	Type
2	B	163	ASP
2	B	227	ILE
2	C	223	SER
1	A	41	ALA
2	B	223	SER
2	C	163	ASP
2	B	221	LYS
2	B	222	ASN
1	D	42	GLY
1	D	252	ILE
2	B	258	VAL
1	A	42	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	222/234 (95%)	209 (94%)	13 (6%)	18	26
1	D	234/234 (100%)	223 (95%)	11 (5%)	23	35
2	B	192/205 (94%)	182 (95%)	10 (5%)	21	31
2	C	186/205 (91%)	179 (96%)	7 (4%)	29	44
All	All	834/878 (95%)	793 (95%)	41 (5%)	22	34

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	13	LYS
1	A	14	SER
1	A	86	PRO
1	A	97	LYS
1	A	135	ARG
1	A	160	VAL
1	A	201	GLU
1	A	207	ARG

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Mol	Chain	Res	Type
1	A	245	LYS
1	A	256	LYS
1	A	278	HIS
1	A	284	ILE
2	B	27	THR
2	B	46	THR
2	B	83	PRO
2	B	128	ARG
2	B	134	ARG
2	B	168	LEU
2	B	174	VAL
2	B	220	MET
2	B	224	HIS
2	B	255	SER
2	C	96	ILE
2	C	102	PRO
2	C	159	GLU
2	C	182	MET
2	C	202	GLN
2	C	220	MET
2	C	227	ILE
1	D	13	LYS
1	D	133	PRO
1	D	134	GLU
1	D	162	SER
1	D	186	GLN
1	D	199	LYS
1	D	205	LYS
1	D	208	LYS
1	D	246	THR
1	D	267	GLU
1	D	279	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	ASN
1	A	177	HIS
1	A	218	GLN
1	A	269	GLN
1	A	271	GLN
1	A	274	HIS

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Mol	Chain	Res	Type
1	A	276	HIS
2	B	2	GLN
2	B	98	HIS
2	B	156	HIS
2	B	183	HIS
2	B	247	HIS
2	B	250	ASN
2	C	2	GLN
2	C	73	HIS
2	C	81	HIS
2	C	98	HIS
2	C	183	HIS
2	C	202	GLN
1	D	76	HIS
1	D	100	ASN
1	D	156	GLN
1	D	186	GLN
1	D	269	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 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 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	$\# Z > 2$
6	EDO	C	805	-	3,3,3	0.59	0	2,2,2	0.28	0
4	DST	D	802	5	10,13,13	2.17	1 (10%)	12,19,19	2.60	4 (33%)
4	DST	A	804	5	10,13,13	2.17	3 (30%)	12,19,19	2.46	4 (33%)
7	IPE	D	801	-	12,13,13	4.47	3 (25%)	16,19,19	1.86	5 (31%)
3	PPV	A	803	-	6,8,8	1.42	0	12,13,13	0.95	0

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
6	EDO	C	805	-	-	1/1/1/1	-
4	DST	D	802	5	-	0/7/13/13	-
4	DST	A	804	5	-	0/7/13/13	-
7	IPE	D	801	-	-	3/13/13/13	-
3	PPV	A	803	-	-	1/6/6/6	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	801	IPE	C2-C3	-10.12	1.34	1.51
7	D	801	IPE	PA-O3A	-8.46	1.50	1.59
7	D	801	IPE	C4-C3	7.80	1.55	1.33
4	D	802	DST	P3-O7	6.24	1.60	1.46
4	A	804	DST	P3-O7	5.48	1.58	1.46
4	A	804	DST	P3-O8	-2.30	1.51	1.56
4	A	804	DST	C10-S9	-2.02	1.81	1.84

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	802	DST	O8-P3-O7	5.81	123.70	109.86
4	A	804	DST	O8-P3-O7	5.51	123.00	109.86
4	D	802	DST	O4-P1-O2	4.61	120.11	104.64
4	A	804	DST	O4-P1-O2	4.42	119.46	104.64
7	D	801	IPE	O1-C1-C2	-3.38	95.05	108.63
7	D	801	IPE	O3A-PA-O1A	-3.35	100.62	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	801	IPE	O1B-PB-O3A	3.18	115.31	104.64
4	D	802	DST	O6-P1-O2	3.02	114.77	104.64
4	A	804	DST	O6-P1-O4	-2.90	96.95	107.80
4	D	802	DST	O6-P1-O4	-2.54	98.29	107.80
7	D	801	IPE	O3B-PB-O3A	2.26	112.21	104.64
4	A	804	DST	O6-P1-O2	2.17	111.92	104.64
7	D	801	IPE	O3B-PB-O1B	-2.03	100.19	107.80

There are no chirality outliers.

All (5) torsion outliers are listed below:

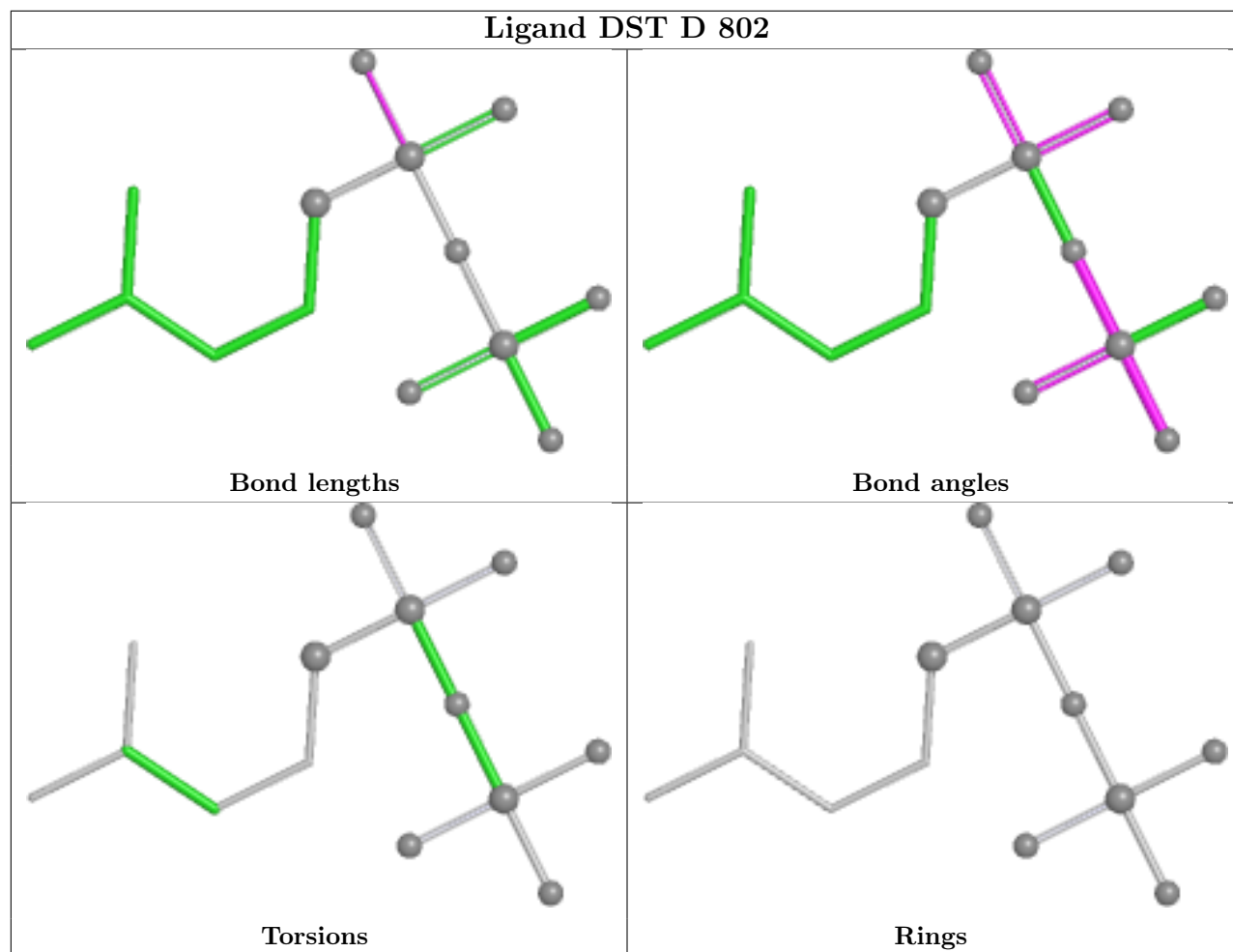
Mol	Chain	Res	Type	Atoms
3	A	803	PPV	P2-OPP-P1-O11
7	D	801	IPE	C1-O1-PA-O1A
7	D	801	IPE	C1-O1-PA-O3A
7	D	801	IPE	O1-C1-C2-C3
6	C	805	EDO	O1-C1-C2-O2

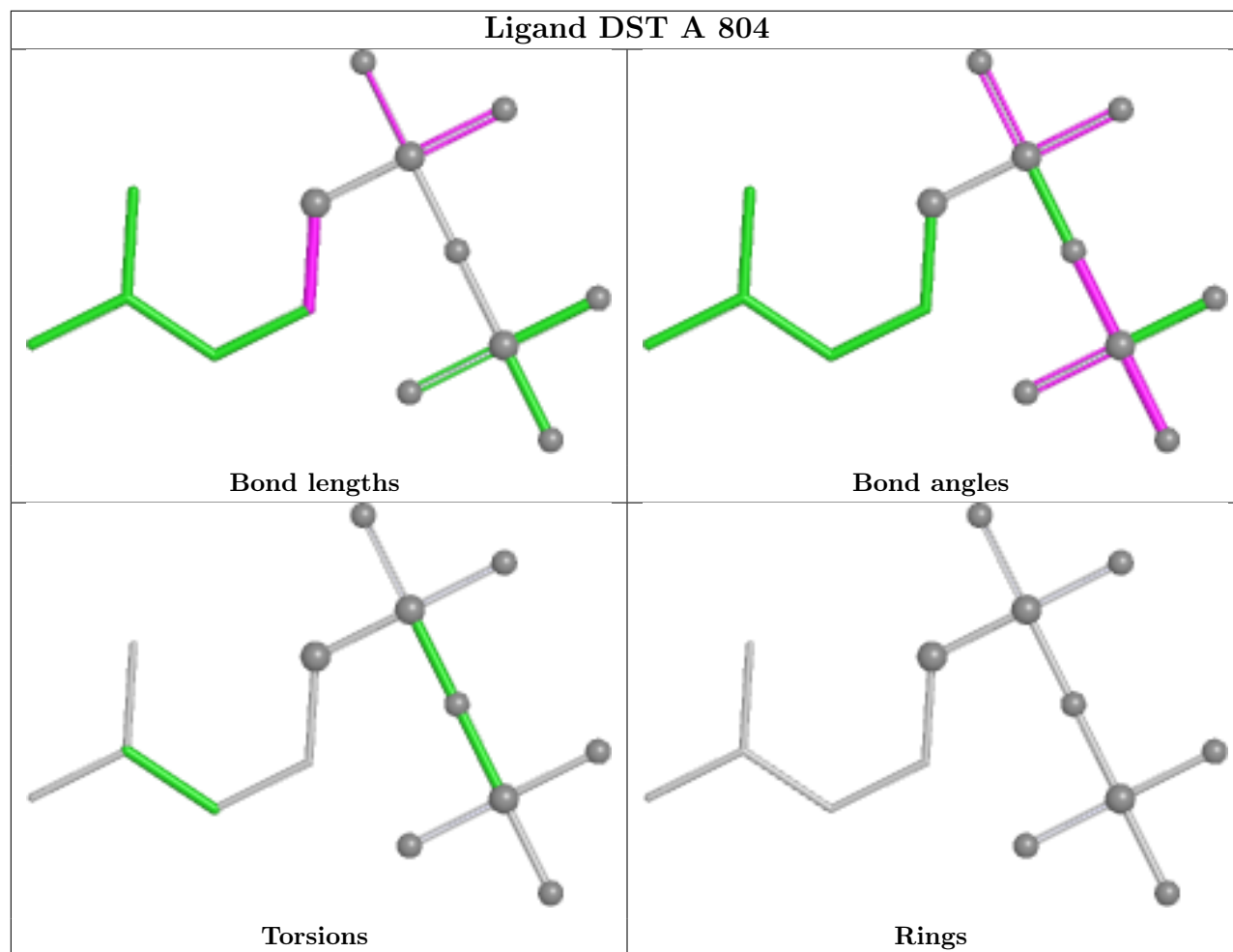
There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	802	DST	5	0
4	A	804	DST	1	0
7	D	801	IPE	2	0

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





5.7 Other polymers [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	279/295 (94%)	-0.29	2 (0%) 84 85	13, 29, 53, 81	0
1	D	295/295 (100%)	0.02	6 (2%) 65 66	21, 35, 80, 102	0
2	B	249/264 (94%)	0.15	24 (9%) 13 15	20, 32, 111, 128	0
2	C	242/264 (91%)	0.11	5 (2%) 63 65	22, 40, 75, 105	0
All	All	1065/1118 (95%)	-0.01	37 (3%) 47 49	13, 34, 81, 128	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	249	LYS	7.3
2	B	226	LEU	4.6
2	B	254	MET	4.4
2	B	250	ASN	4.4
1	D	243	ALA	4.2
2	C	94	PRO	4.0
2	B	257	LEU	3.9
2	B	248	GLY	3.8
2	C	162	VAL	3.4
2	B	246	PHE	3.4
2	B	258	VAL	3.3
2	B	251	ALA	3.3
2	B	259	ALA	3.2
1	D	241	LEU	3.2
1	A	166	ALA	3.1
2	B	97	GLN	3.1
2	C	226	LEU	3.1
2	B	1	MET	3.0
2	B	247	HIS	2.8
2	C	95	ALA	2.7
2	B	244	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	227	ILE	2.6
1	D	246	THR	2.5
2	B	245	GLY	2.5
2	B	94	PRO	2.3
1	A	276	HIS	2.3
2	B	96	ILE	2.3
1	D	165	MET	2.3
2	C	225	GLN	2.2
2	B	231	ILE	2.2
2	B	255	SER	2.2
2	B	253	LEU	2.1
2	B	95	ALA	2.1
1	D	242	VAL	2.1
2	B	224	HIS	2.1
1	D	168	VAL	2.1
2	B	243	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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
5	MG	D	901	1/1	0.80	0.15	58,58,58,58	0
3	PPV	A	803	9/9	0.87	0.09	88,89,90,91	0
4	DST	D	802	14/14	0.93	0.10	47,57,59,60	0
4	DST	A	804	14/14	0.93	0.09	46,50,53,56	0
6	EDO	C	805	4/4	0.93	0.07	25,28,30,32	0
5	MG	A	904	1/1	0.95	0.05	33,33,33,33	0
5	MG	D	902	1/1	0.96	0.05	54,54,54,54	0

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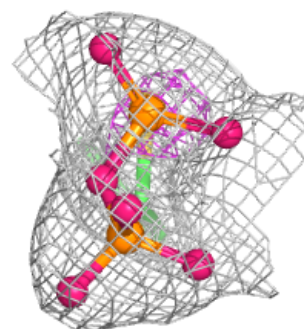
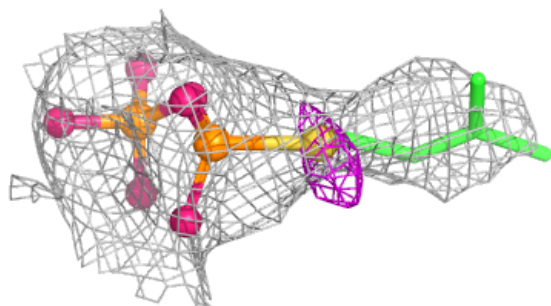
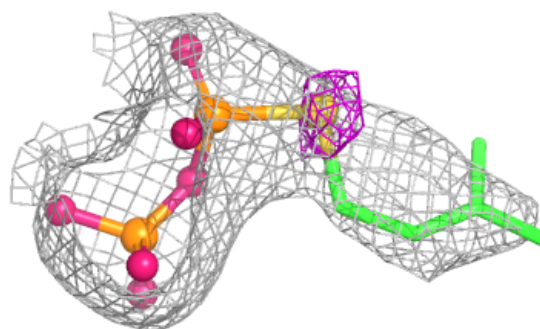
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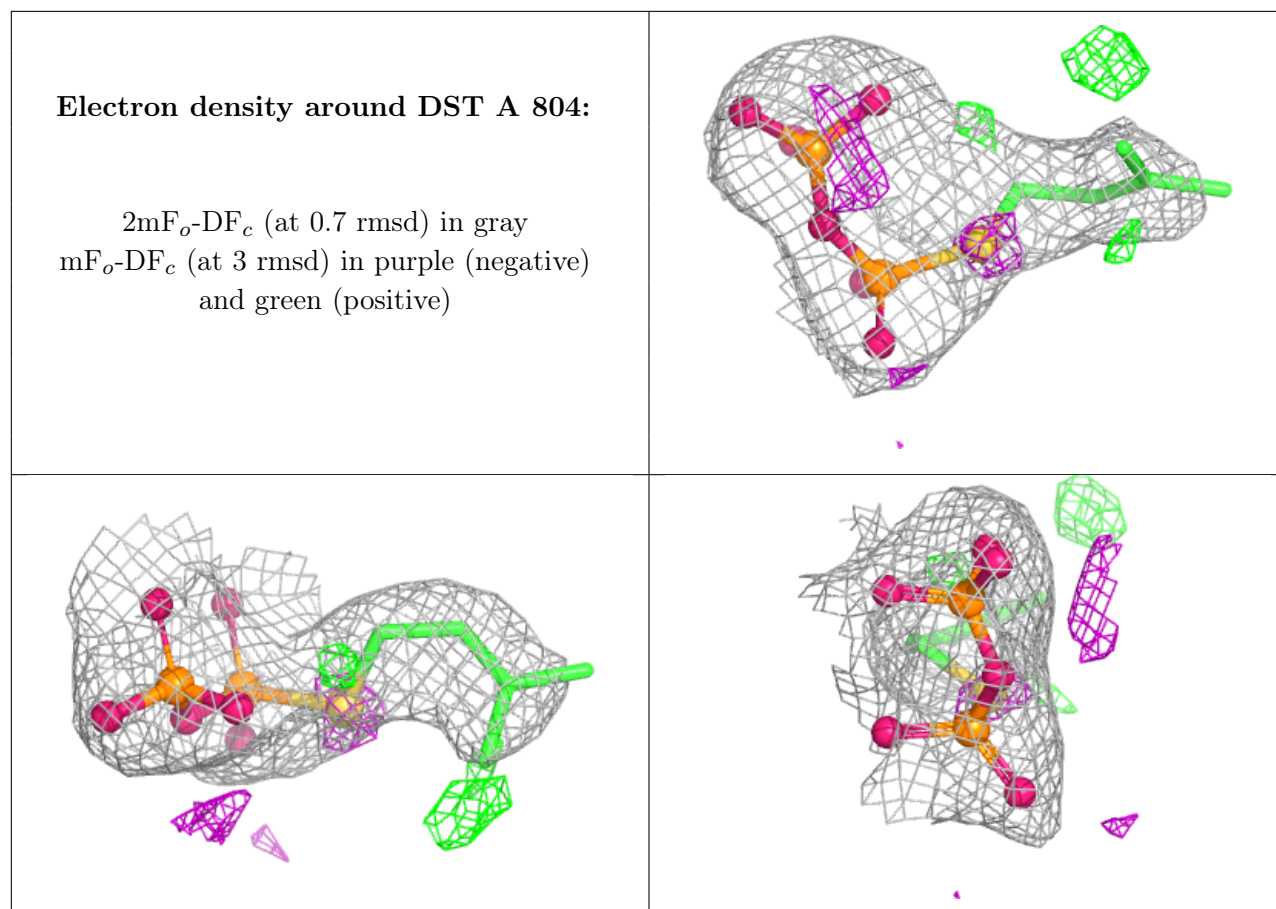
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	IPE	D	801	14/14	0.97	0.06	32,35,37,37	0
5	MG	A	903	1/1	0.99	0.02	32,32,32,32	0

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 DST D 802:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.