



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 6, 2020 – 11:46 pm BST

PDB ID : 3KRF
Title : Mint heterotetrameric geranyl pyrophosphate synthase in complex with magnesium, IPP, and DMASPP (I)
Authors : Chang, T.-H.; Hsieh, F.-L.; Ko, T.-P.; Wang, A.H.-J.
Deposited on : 2009-11-18
Resolution : 2.20 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

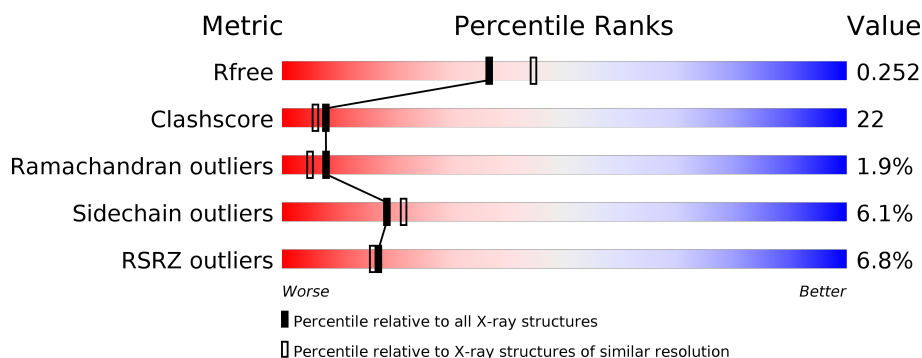
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 on 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	<div> <div>2%</div> <div> <div></div> <div>65%</div> <div>26%</div> <div>5%</div> </div> </div>
1	D	295	<div> <div>6%</div> <div> <div></div> <div>68%</div> <div>27%</div> <div></div> </div> </div>
2	B	274	<div> <div>9%</div> <div> <div></div> <div>57%</div> <div>31%</div> <div>5%</div> <div>5%</div> </div> </div>
2	C	274	<div> <div>9%</div> <div> <div></div> <div>62%</div> <div>27%</div> <div></div> <div>5%</div> </div> </div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 9075 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	259	Total	C	N	O	S	0	0	0
			1954	1233	339	368	14			
2	C	259	Total	C	N	O	S	0	0	0
			1954	1233	339	368	14			

There are 18 discrepancies between the modelled and reference sequences:

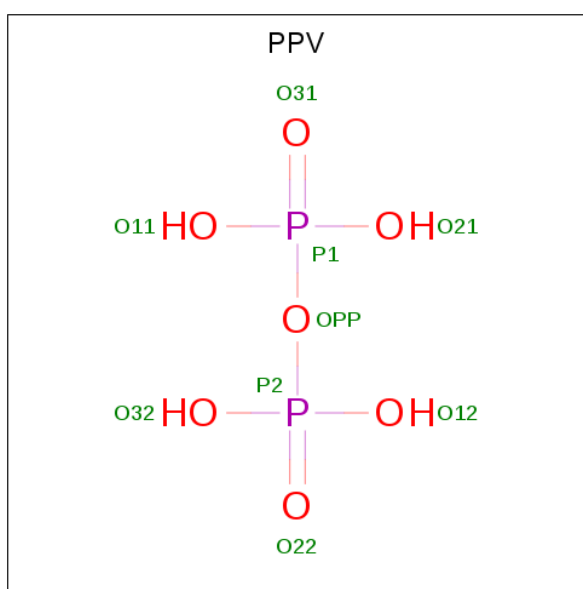
Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	EXPRESSION TAG	UNP Q9SBR4
B	267	HIS	-	EXPRESSION TAG	UNP Q9SBR4
B	268	HIS	-	EXPRESSION TAG	UNP Q9SBR4
B	269	HIS	-	EXPRESSION TAG	UNP Q9SBR4
B	270	HIS	-	EXPRESSION TAG	UNP Q9SBR4
B	271	HIS	-	EXPRESSION TAG	UNP Q9SBR4
B	272	HIS	-	EXPRESSION TAG	UNP Q9SBR4
B	273	HIS	-	EXPRESSION TAG	UNP Q9SBR4
B	274	HIS	-	EXPRESSION TAG	UNP Q9SBR4
C	1	MET	-	EXPRESSION TAG	UNP Q9SBR4

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Chain	Residue	Modelled	Actual	Comment	Reference
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 (three-letter code: PPV) (formula: $\text{H}_4\text{O}_7\text{P}_2$).



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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

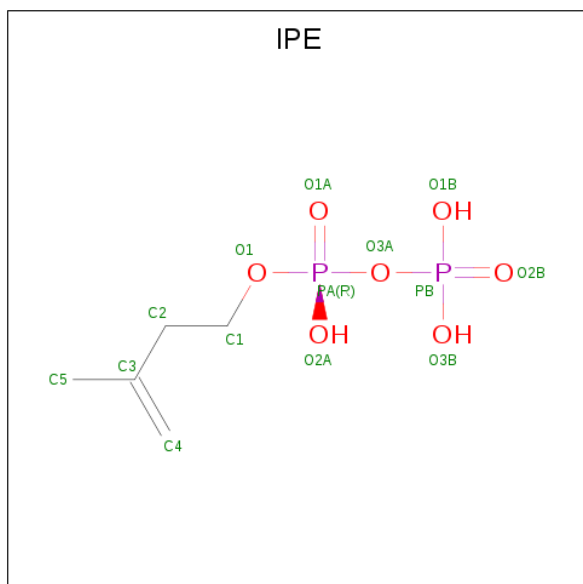
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Mg 2 2	0	0
4	D	2	Total Mg 2 2	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $\text{C}_2\text{H}_6\text{O}_2$).



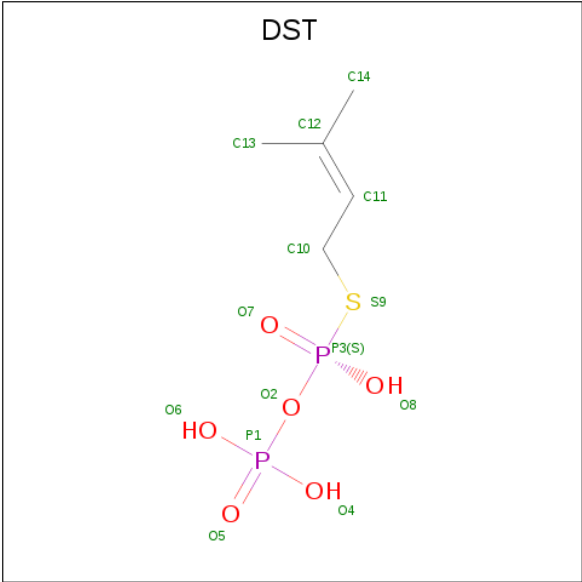
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is 3-METHYLBUT-3-ENYL TRIHYDROGEN DIPHOSPHATE (three-letter code: IPE) (formula: $C_5H_{12}O_7P_2$).



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

- Molecule 7 is DIMETHYLALLYL S-THIOLODIPHOSPHATE (three-letter code: DST) (formula: $C_5H_{12}O_6P_2S$).



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

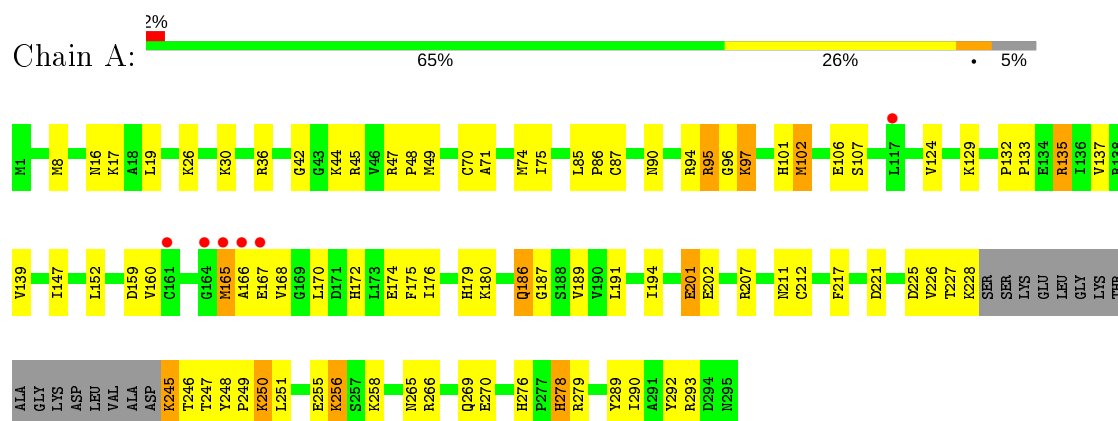
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	204	Total	O	0	0
			204	204		
8	B	172	Total	O	0	0
			172	172		
8	C	172	Total	O	0	0
			172	172		
8	D	213	Total	O	0	0
			213	213		

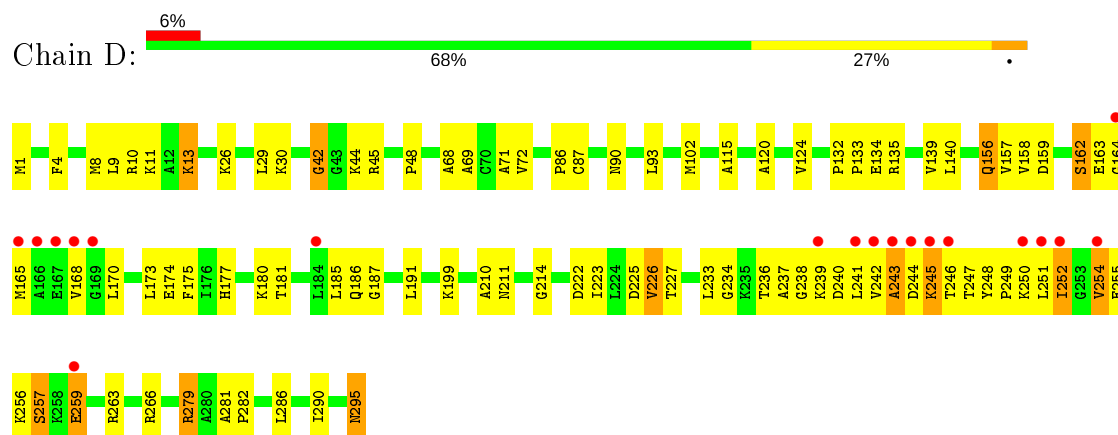
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

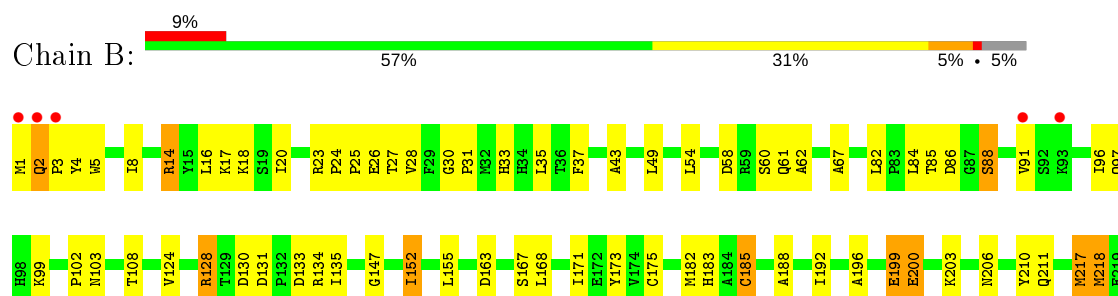
• Molecule 1: Geranyl diphosphate synthase large subunit

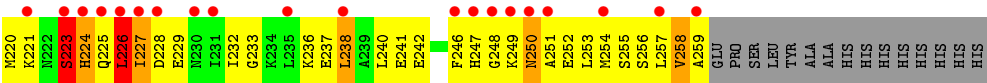


• Molecule 1: Geranyl diphosphate synthase large subunit

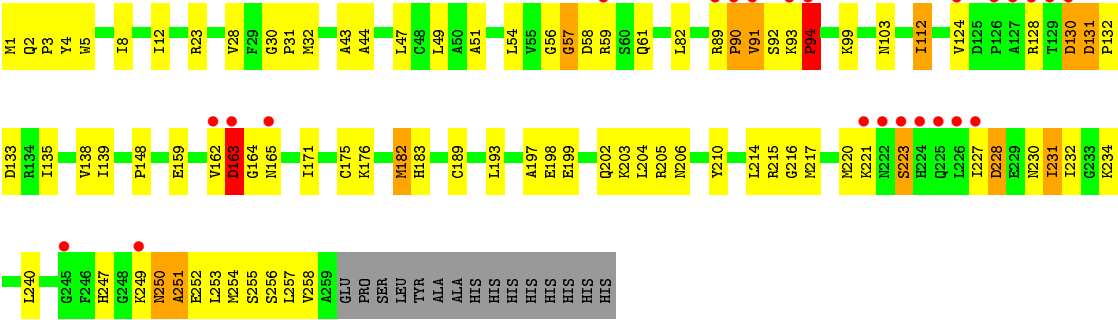


• Molecule 2: Geranyl diphosphate synthase small subunit





● 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	53.85Å 108.84Å 182.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.20 29.69 – 2.20	Depositor EDS
% Data completeness (in resolution range)	91.5 (30.00-2.20) 91.4 (29.69-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.12 (at 2.20Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.192 , 0.252 0.193 , 0.252	Depositor DCC
R_{free} test set	2541 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	32.1	Xtriage
Anisotropy	0.929	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 54.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9075	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.75% 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: PPV, MG, EDO, DST, IPE

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	1.01	3/2155 (0.1%)	0.93	2/2903 (0.1%)
1	D	0.91	1/2268 (0.0%)	0.92	1/3055 (0.0%)
2	B	0.90	3/1993 (0.2%)	0.92	3/2695 (0.1%)
2	C	0.83	0/1993	0.89	4/2695 (0.1%)
All	All	0.91	7/8409 (0.1%)	0.91	10/11348 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	185	CYS	CB-SG	-5.95	1.72	1.81
1	A	102	MET	CG-SD	5.73	1.96	1.81
1	A	212	CYS	CB-SG	5.54	1.91	1.82
2	B	200	GLU	CG-CD	5.30	1.59	1.51
1	D	259	GLU	CG-CD	5.18	1.59	1.51
1	A	255	GLU	CG-CD	5.11	1.59	1.51
2	B	199	GLU	CG-CD	5.00	1.59	1.51

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	226	LEU	N-CA-C	-7.21	91.55	111.00
2	B	86	ASP	N-CA-C	6.22	127.81	111.00
1	A	102	MET	CG-SD-CE	5.89	109.63	100.20
2	C	82	LEU	CA-CB-CG	5.85	128.76	115.30
2	C	23	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	A	36	ARG	NE-CZ-NH2	-5.74	117.43	120.30
2	C	23	ARG	NE-CZ-NH2	-5.56	117.52	120.30
2	C	163	ASP	N-CA-C	5.51	125.88	111.00
1	D	42	GLY	N-CA-C	5.17	126.01	113.10
2	B	238	LEU	CA-CB-CG	5.16	127.16	115.30

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	2120	0	2146	65	0
1	D	2232	0	2264	94	0
2	B	1954	0	1948	120	1
2	C	1954	0	1948	96	0
3	A	18	0	0	0	0
4	A	2	0	0	0	0
4	D	2	0	0	0	0
5	C	4	0	6	1	0
6	D	14	0	9	2	0
7	D	14	0	10	2	0
8	A	204	0	0	6	0
8	B	172	0	0	12	0
8	C	172	0	0	7	1
8	D	213	0	0	6	3
All	All	9075	0	8331	362	3

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 22.

All (362) 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:D:102:MET:HG2	8:D:625:HOH:O	1.33	1.22
1:D:10:ARG:HD2	8:D:609:HOH:O	1.41	1.21
2:B:249:LYS:HD3	2:B:253:LEU:HB2	1.36	1.02
2:C:228:ASP:OD2	2:C:230:ASN:HB2	1.63	0.99
2:B:200:GLU:HG3	8:B:475:HOH:O	1.62	0.97
2:B:240:LEU:HD21	2:B:258:VAL:HG21	1.44	0.95
2:B:225:GLN:HA	2:B:227:ILE:HG23	1.47	0.95
2:B:250:ASN:HA	2:B:253:LEU:HB3	1.49	0.94
2:C:230:ASN:O	2:C:234:LYS:HG3	1.66	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:58:ASP:H	2:B:61:GLN:HE21	1.16	0.94
2:B:249:LYS:O	2:B:253:LEU:N	2.02	0.92
6:D:801:IPE:H53	7:D:802:DST:H133	1.50	0.92
1:D:135:ARG:HG3	1:D:135:ARG:HH11	1.34	0.90
2:B:249:LYS:HE2	2:B:253:LEU:HD13	1.54	0.87
1:D:4:PHE:HB2	1:D:8:MET:HE1	1.57	0.86
2:C:28:VAL:HG22	1:D:157:VAL:CG2	2.05	0.86
1:D:186:GLN:OE1	1:D:211:ASN:HB2	1.77	0.85
1:A:168:VAL:HG13	1:A:172:HIS:HB3	1.58	0.85
1:D:158:VAL:O	1:D:162:SER:HB3	1.76	0.84
2:B:1:MET:HG3	2:B:2:GLN:H	1.40	0.84
2:C:199:GLU:O	2:C:203:LYS:HG2	1.77	0.84
2:C:221:LYS:HG3	2:C:227:ILE:HG21	1.59	0.84
2:C:92:SER:HB3	2:C:94:PRO:HD2	1.62	0.82
2:C:124:VAL:HG22	2:C:135:ILE:HD12	1.63	0.80
2:C:214:LEU:HD11	2:C:232:ILE:HG23	1.64	0.80
2:C:43:ALA:O	2:C:47:LEU:HB2	1.82	0.80
1:D:223:ILE:HD11	1:D:257:SER:HB3	1.64	0.79
2:B:253:LEU:HD12	2:B:256:SER:OG	1.83	0.77
2:C:221:LYS:HE3	2:C:227:ILE:HD13	1.64	0.77
1:A:165:MET:HG2	1:A:165:MET:O	1.84	0.77
1:D:173:LEU:HD13	1:D:246:THR:HG22	1.66	0.77
1:D:223:ILE:O	1:D:227:THR:HG23	1.84	0.77
2:B:203:LYS:HD3	2:B:246:PHE:CE2	2.20	0.76
1:A:225:ASP:O	1:A:228:LYS:HD2	1.86	0.76
2:B:210:TYR:OH	8:B:327:HOH:O	2.03	0.76
2:B:2:GLN:HB2	2:B:3:PRO:HD3	1.68	0.75
2:B:1:MET:HG3	2:B:2:GLN:N	2.01	0.75
2:C:92:SER:C	2:C:94:PRO:HD2	2.07	0.74
2:B:221:LYS:HZ1	2:B:232:ILE:HG12	1.52	0.74
1:D:173:LEU:HD13	1:D:246:THR:O	1.87	0.73
1:A:276:HIS:HB2	1:A:279:ARG:HD2	1.69	0.73
2:C:28:VAL:HG22	1:D:157:VAL:HG23	1.72	0.72
2:B:124:VAL:HG22	2:B:135:ILE:HD12	1.70	0.72
2:C:61:GLN:HE21	2:C:128:ARG:HH21	1.38	0.72
1:D:170:LEU:HD23	1:D:251:LEU:HD13	1.70	0.72
2:C:28:VAL:HG22	1:D:157:VAL:HG21	1.69	0.72
2:B:26:GLU:HG3	8:B:443:HOH:O	1.90	0.71
1:A:101:HIS:CD2	1:A:102:MET:HE2	2.26	0.71
1:A:107:SER:HB2	2:B:88:SER:HB3	1.71	0.71
1:A:106:GLU:OE2	2:B:85:THR:HB	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:295:ASN:C	1:D:295:ASN:HD22	1.93	0.70
2:C:124:VAL:HG22	2:C:135:ILE:CD1	2.20	0.70
1:D:238:GLY:O	1:D:241:LEU:HB2	1.92	0.70
1:A:289:TYR:O	1:A:293:ARG:HG2	1.91	0.69
2:B:128:ARG:CG	2:B:128:ARG:HH11	2.06	0.69
1:D:173:LEU:HB2	1:D:246:THR:CG2	2.22	0.69
2:B:2:GLN:HB2	2:B:3:PRO:CD	2.24	0.68
1:D:4:PHE:HB2	1:D:8:MET:CE	2.23	0.68
1:D:236:THR:HG23	8:D:763:HOH:O	1.93	0.68
1:A:101:HIS:CD2	1:A:102:MET:CE	2.77	0.68
1:A:186:GLN:NE2	1:A:211:ASN:OD1	2.27	0.68
1:D:187:GLY:O	1:D:191:LEU:HG	1.93	0.68
2:B:60:SER:CB	8:B:628:HOH:O	2.41	0.68
1:D:233:LEU:HD12	1:D:237:ALA:HB2	1.76	0.68
2:B:128:ARG:HG2	2:B:128:ARG:HH11	1.57	0.67
1:D:279:ARG:HH11	1:D:279:ARG:CG	2.08	0.67
2:C:128:ARG:HH11	2:C:128:ARG:HA	1.60	0.67
2:B:221:LYS:HZ1	2:B:232:ILE:CG1	2.06	0.66
1:A:247:THR:OG1	1:A:250:LYS:HD2	1.95	0.66
1:A:94:ARG:O	1:A:95:ARG:HG2	1.95	0.66
2:B:58:ASP:H	2:B:61:GLN:NE2	1.90	0.66
1:A:187:GLY:O	1:A:191:LEU:HG	1.96	0.66
2:B:28:VAL:O	2:B:31:PRO:HD2	1.95	0.65
2:C:4:TYR:CZ	2:C:8:ILE:HD11	2.31	0.65
2:C:228:ASP:HB2	2:C:230:ASN:HD22	1.61	0.65
1:D:279:ARG:HH11	1:D:279:ARG:HB3	1.61	0.65
2:B:60:SER:HB3	8:B:628:HOH:O	1.95	0.65
1:D:173:LEU:HD22	1:D:251:LEU:HD12	1.80	0.64
1:A:95:ARG:O	1:A:95:ARG:HG3	1.97	0.64
2:C:32:MET:HG3	2:C:112:ILE:HD11	1.78	0.64
2:C:93:LYS:N	2:C:94:PRO:HD2	2.12	0.64
2:C:221:LYS:HG3	2:C:227:ILE:CG2	2.28	0.64
2:C:4:TYR:CE2	2:C:8:ILE:HD11	2.32	0.64
2:B:188:ALA:O	2:B:192:ILE:HG13	1.98	0.64
1:D:163:GLU:O	1:D:244:ASP:HB3	1.97	0.64
2:B:203:LYS:HD3	2:B:246:PHE:HE2	1.60	0.63
1:D:225:ASP:OD2	1:D:240:ASP:HB2	1.98	0.63
2:B:43:ALA:HB3	2:B:183:HIS:HE1	1.63	0.63
1:D:263:ARG:HG3	8:D:732:HOH:O	1.98	0.63
1:A:44:LYS:NZ	8:A:327:HOH:O	2.28	0.63
2:B:130:ASP:O	2:B:134:ARG:HG3	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:124:VAL:CG2	2:B:135:ILE:HD12	2.29	0.62
1:D:168:VAL:O	1:D:168:VAL:HG23	1.99	0.62
2:B:218:MET:CE	2:B:221:LYS:HZ2	2.13	0.62
2:B:25:PRO:HB2	2:B:27:THR:HG22	1.81	0.62
1:D:135:ARG:HG3	1:D:135:ARG:NH1	2.09	0.62
2:C:99:LYS:HE2	8:C:537:HOH:O	2.00	0.61
1:D:181:THR:OG1	6:D:801:IPE:H51	1.99	0.61
2:C:223:SER:HB3	8:C:760:HOH:O	1.99	0.61
2:C:215:ARG:HH11	2:C:215:ARG:HG2	1.66	0.61
2:C:56:GLY:O	2:C:57:GLY:O	2.19	0.61
1:D:173:LEU:HB2	1:D:246:THR:HG21	1.80	0.61
2:B:221:LYS:HZ1	2:B:232:ILE:CD1	2.13	0.61
1:A:180:LYS:HD2	8:A:296:HOH:O	2.00	0.60
1:A:226:VAL:HG12	1:A:227:THR:HG23	1.82	0.60
2:B:237:GLU:O	2:B:241:GLU:HG3	2.02	0.60
2:C:32:MET:CG	2:C:112:ILE:HD11	2.32	0.60
1:D:170:LEU:CD2	1:D:251:LEU:HD13	2.31	0.60
1:A:258:LYS:NZ	8:A:576:HOH:O	2.33	0.59
1:D:279:ARG:HH11	1:D:279:ARG:CB	2.14	0.59
2:B:23:ARG:HB2	2:B:24:PRO:HD2	1.84	0.59
1:D:252:ILE:HB	1:D:256:LYS:HB2	1.85	0.59
2:B:211:GLN:OE1	2:B:258:VAL:HG13	2.02	0.59
2:B:210:TYR:CE2	2:B:238:LEU:HD13	2.38	0.59
2:B:1:MET:HE3	8:B:580:HOH:O	2.02	0.58
2:B:253:LEU:O	2:B:256:SER:HB2	2.03	0.58
1:D:165:MET:HG2	1:D:168:VAL:HG12	1.85	0.58
1:A:101:HIS:HD2	1:A:102:MET:HE2	1.66	0.58
2:C:182:MET:HE3	2:C:182:MET:HA	1.85	0.58
2:C:132:PRO:HG3	1:D:134:GLU:HG3	1.85	0.58
1:D:240:ASP:HA	1:D:245:LYS:HD2	1.85	0.58
2:B:131:ASP:O	2:B:135:ILE:HG13	2.02	0.58
2:C:221:LYS:CG	2:C:227:ILE:HG21	2.32	0.58
1:D:286:LEU:O	1:D:290:ILE:HG13	2.04	0.58
1:A:278:HIS:H	1:A:278:HIS:CD2	2.20	0.58
2:B:206:ASN:HD22	2:B:242:GLU:CD	2.06	0.58
1:D:132:PRO:HG2	1:D:135:ARG:HB2	1.84	0.58
2:B:248:GLY:O	2:B:252:GLU:HB2	2.03	0.58
2:B:43:ALA:HB3	2:B:183:HIS:CE1	2.39	0.57
2:C:227:ILE:HD11	2:C:232:ILE:HD11	1.86	0.57
1:A:217:PHE:O	1:A:221:ASP:HB2	2.04	0.57
2:B:221:LYS:NZ	2:B:232:ILE:HD11	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:165:MET:O	1:D:168:VAL:HG13	2.05	0.57
2:C:133:ASP:OD1	1:D:133:PRO:HG2	2.05	0.57
1:A:201:GLU:OE1	1:A:202:GLU:HG3	2.05	0.56
1:A:97:LYS:N	1:A:97:LYS:HD2	2.21	0.56
2:B:229:GLU:HA	2:B:232:ILE:HD12	1.86	0.56
2:C:182:MET:CE	2:C:182:MET:HA	2.35	0.56
1:A:139:VAL:HG23	1:A:194:ILE:HG21	1.86	0.56
2:B:20:ILE:O	2:B:33:HIS:HD2	1.90	0.55
2:B:249:LYS:CE	2:B:253:LEU:HD13	2.33	0.54
2:C:163:ASP:CG	2:C:164:GLY:N	2.60	0.54
2:B:221:LYS:HG2	2:B:227:ILE:CG2	2.37	0.54
2:C:54:LEU:HD11	2:C:251:ALA:HB2	1.90	0.54
2:B:221:LYS:NZ	2:B:232:ILE:CD1	2.70	0.54
1:A:47:ARG:HB2	1:A:48:PRO:HD3	1.90	0.54
2:B:196:ALA:HB1	2:B:200:GLU:HB2	1.90	0.54
1:D:68:ALA:HA	1:D:124:VAL:HG22	1.90	0.54
2:B:211:GLN:NE2	2:B:257:LEU:HB3	2.23	0.54
2:B:82:LEU:O	2:B:84:LEU:HG	2.07	0.54
2:C:228:ASP:HB2	2:C:230:ASN:ND2	2.22	0.54
2:B:128:ARG:O	2:B:131:ASP:HB2	2.08	0.53
2:C:228:ASP:CB	2:C:230:ASN:HD22	2.21	0.53
2:C:32:MET:HG3	2:C:112:ILE:CD1	2.38	0.53
2:C:202:GLN:HG2	8:C:499:HOH:O	2.07	0.53
2:C:92:SER:HB3	2:C:94:PRO:CD	2.34	0.53
1:D:222:ASP:HB3	1:D:249:PRO:HD2	1.90	0.53
2:C:44:ALA:HB2	2:C:183:HIS:CD2	2.42	0.53
2:C:162:VAL:HG12	2:C:165:ASN:HD22	1.73	0.53
1:D:295:ASN:C	1:D:295:ASN:ND2	2.62	0.53
2:C:250:ASN:C	2:C:252:GLU:H	2.13	0.53
1:A:96:GLY:C	1:A:97:LYS:HD2	2.29	0.52
1:D:181:THR:O	1:D:185:LEU:HD12	2.08	0.52
2:C:5:TRP:CH2	2:C:257:LEU:HD22	2.44	0.52
2:B:218:MET:HE3	2:B:221:LYS:HZ2	1.73	0.52
2:B:225:GLN:HA	2:B:227:ILE:CG2	2.32	0.52
2:C:221:LYS:CE	2:C:227:ILE:HD13	2.36	0.52
1:D:279:ARG:HH11	1:D:279:ARG:HG2	1.74	0.52
1:A:101:HIS:CD2	1:A:102:MET:HE3	2.44	0.52
1:A:129:LYS:HE2	8:A:336:HOH:O	2.10	0.52
2:C:8:ILE:CG2	2:C:49:LEU:HD12	2.40	0.52
1:A:71:ALA:O	1:A:74:MET:HB2	2.10	0.51
2:B:255:SER:HA	2:B:258:VAL:CG2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:173:LEU:CD1	1:D:246:THR:O	2.57	0.51
2:B:16:LEU:HD21	2:B:67:ALA:HB1	1.93	0.51
2:B:17:LYS:HG3	2:B:37:PHE:CZ	2.46	0.51
1:D:279:ARG:HG2	1:D:279:ARG:NH1	2.26	0.51
2:B:250:ASN:C	2:B:252:GLU:H	2.14	0.51
2:C:89:ARG:O	2:C:90:PRO:C	2.49	0.51
1:D:139:VAL:HG13	1:D:191:LEU:HD22	1.92	0.51
2:B:227:ILE:O	2:B:227:ILE:HG13	2.10	0.51
2:B:96:ILE:HG12	2:B:97:GLN:N	2.26	0.50
2:C:93:LYS:N	2:C:94:PRO:CD	2.73	0.50
2:B:163:ASP:O	2:B:224:HIS:HB3	2.11	0.50
2:B:220:MET:HE2	8:B:318:HOH:O	2.11	0.50
2:B:14:ARG:NH1	2:B:14:ARG:HB3	2.26	0.50
2:C:61:GLN:O	2:C:193:LEU:HD22	2.11	0.50
1:A:175:PHE:O	1:A:179:HIS:HD2	1.95	0.50
2:B:25:PRO:HB2	2:B:27:THR:CG2	2.42	0.50
1:A:95:ARG:HG3	1:A:97:LYS:HD3	1.94	0.50
2:B:54:LEU:HD13	2:B:250:ASN:HB3	1.92	0.50
1:A:133:PRO:O	1:A:137:VAL:HG23	2.12	0.49
2:B:128:ARG:NE	8:B:390:HOH:O	2.40	0.49
1:A:94:ARG:O	1:A:95:ARG:CG	2.58	0.49
2:B:5:TRP:HZ2	2:B:253:LEU:HG	1.78	0.49
1:A:132:PRO:HG2	1:A:135:ARG:HB2	1.95	0.49
2:B:221:LYS:HZ1	2:B:232:ILE:HD11	1.76	0.49
2:B:233:GLY:HA2	2:B:236:LYS:HG2	1.93	0.49
2:C:250:ASN:HA	2:C:253:LEU:HD12	1.93	0.49
2:C:240:LEU:HD21	2:C:258:VAL:HG23	1.93	0.49
2:B:227:ILE:HG22	8:B:291:HOH:O	2.13	0.49
2:B:206:ASN:HB3	2:B:242:GLU:HG3	1.94	0.49
1:D:279:ARG:NH1	1:D:279:ARG:CG	2.73	0.49
1:D:9:LEU:O	1:D:13:LYS:HD3	2.13	0.49
1:D:281:ALA:HB3	1:D:282:PRO:HD3	1.95	0.49
2:B:257:LEU:C	2:B:259:ALA:H	2.16	0.48
1:D:186:GLN:HA	1:D:210:ALA:HB1	1.94	0.48
1:D:26:LYS:HE2	1:D:26:LYS:HB3	1.62	0.48
1:D:86:PRO:HA	1:D:90:ASN:HB2	1.94	0.48
1:D:93:LEU:HG	1:D:234:GLY:O	2.13	0.48
2:B:249:LYS:O	2:B:252:GLU:C	2.51	0.48
2:C:176:LYS:NZ	8:C:346:HOH:O	2.36	0.48
1:D:134:GLU:H	1:D:134:GLU:CD	2.17	0.48
1:D:250:LYS:HG2	1:D:251:LEU:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:218:MET:CE	2:B:221:LYS:NZ	2.76	0.48
2:C:131:ASP:O	2:C:135:ILE:HG13	2.14	0.48
2:C:90:PRO:O	2:C:92:SER:N	2.47	0.48
1:D:71:ALA:HB2	1:D:124:VAL:HG23	1.94	0.48
2:C:202:GLN:NE2	2:C:205:ARG:HE	2.11	0.47
2:B:217:MET:O	2:B:221:LYS:HG3	2.14	0.47
2:C:90:PRO:HG3	2:C:159:GLU:O	2.14	0.47
2:B:35:LEU:HD12	2:B:108:THR:HG21	1.96	0.47
1:D:243:ALA:HB3	1:D:245:LYS:HG3	1.97	0.47
2:C:139:ILE:HD13	1:D:140:LEU:HD13	1.97	0.47
2:B:236:LYS:O	2:B:240:LEU:HG	2.15	0.47
1:A:245:LYS:NZ	1:A:245:LYS:HB2	2.30	0.47
2:C:61:GLN:NE2	2:C:128:ARG:HH21	2.09	0.46
2:B:218:MET:HE2	2:B:221:LYS:NZ	2.30	0.46
2:C:217:MET:CE	2:C:231:ILE:HG21	2.45	0.46
2:C:217:MET:HE3	2:C:231:ILE:HG21	1.96	0.46
2:C:89:ARG:O	2:C:91:VAL:N	2.48	0.46
2:C:138:VAL:HG13	2:C:189:CYS:SG	2.56	0.46
2:C:216:GLY:O	2:C:220:MET:HG2	2.16	0.46
1:D:247:THR:O	1:D:250:LYS:HB3	2.16	0.46
2:C:103:ASN:HB3	1:D:87:CYS:O	2.15	0.46
2:B:167:SER:HB2	8:B:292:HOH:O	2.14	0.46
2:B:255:SER:HA	2:B:258:VAL:HG22	1.97	0.46
2:C:93:LYS:O	2:C:94:PRO:C	2.54	0.46
1:A:256:LYS:HD2	8:A:574:HOH:O	2.13	0.46
2:B:14:ARG:CB	2:B:14:ARG:NH1	2.79	0.46
1:D:135:ARG:NH1	8:D:303:HOH:O	2.48	0.46
1:D:173:LEU:HB2	1:D:246:THR:HG22	1.95	0.46
2:B:221:LYS:HG2	2:B:227:ILE:HG22	1.98	0.46
1:A:8:MET:SD	1:A:49:MET:HG3	2.56	0.46
2:C:162:VAL:CG1	2:C:165:ASN:HD22	2.29	0.46
8:C:719:HOH:O	1:D:87:CYS:HB3	2.16	0.46
2:B:171:ILE:HG22	2:B:217:MET:CE	2.46	0.45
1:A:71:ALA:HB2	1:A:124:VAL:HG23	1.98	0.45
2:B:30:GLY:N	2:B:31:PRO:CD	2.79	0.45
2:C:128:ARG:HH11	2:C:128:ARG:CA	2.29	0.45
2:C:250:ASN:OD1	2:C:250:ASN:N	2.49	0.45
1:A:165:MET:O	1:A:167:GLU:N	2.49	0.45
1:A:19:LEU:HD23	1:A:19:LEU:HA	1.81	0.45
1:A:186:GLN:OE1	1:A:207:ARG:CD	2.65	0.45
2:B:128:ARG:NH1	2:B:128:ARG:CG	2.71	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:168:LEU:HD11	2:B:226:LEU:HG	1.98	0.45
2:B:221:LYS:HG2	2:B:227:ILE:HB	1.98	0.45
2:B:250:ASN:O	2:B:254:MET:HG2	2.16	0.45
2:C:197:ALA:O	2:C:198:GLU:C	2.54	0.45
2:C:4:TYR:O	2:C:8:ILE:HG13	2.17	0.45
1:D:162:SER:OG	1:D:162:SER:O	2.32	0.45
1:D:168:VAL:HG21	1:D:250:LYS:HE2	1.99	0.45
2:B:155:LEU:HA	2:B:155:LEU:HD23	1.81	0.45
2:B:249:LYS:CD	2:B:253:LEU:HB2	2.26	0.45
2:C:128:ARG:HB2	2:C:131:ASP:CG	2.38	0.45
2:C:112:ILE:HD13	2:C:112:ILE:HA	1.74	0.45
2:C:202:GLN:NE2	8:C:499:HOH:O	2.33	0.45
1:A:245:LYS:HB2	1:A:245:LYS:HZ3	1.80	0.44
1:D:133:PRO:HD2	1:D:134:GLU:OE2	2.17	0.44
2:B:218:MET:HE2	2:B:221:LYS:HZ2	1.80	0.44
2:C:92:SER:CB	2:C:94:PRO:HD2	2.39	0.44
1:D:255:GLU:HA	1:D:255:GLU:OE2	2.18	0.44
1:A:176:ILE:CG2	1:A:180:LYS:HE3	2.48	0.44
2:C:5:TRP:CZ2	2:C:257:LEU:HB2	2.53	0.44
2:C:220:MET:O	2:C:223:SER:HB2	2.17	0.44
1:A:152:LEU:HA	1:A:179:HIS:O	2.18	0.44
1:A:160:VAL:HG22	8:A:370:HOH:O	2.18	0.44
2:B:14:ARG:CB	2:B:14:ARG:HH11	2.31	0.44
2:C:175:CYS:SG	2:C:220:MET:HG3	2.58	0.44
1:D:248:TYR:C	1:D:250:LYS:H	2.21	0.43
1:D:69:ALA:O	1:D:72:VAL:HG22	2.18	0.43
1:D:248:TYR:O	1:D:250:LYS:N	2.51	0.43
2:B:173:TYR:CE2	1:D:29:LEU:HD21	2.53	0.43
1:A:101:HIS:NE2	1:A:102:MET:HE3	2.34	0.43
2:C:8:ILE:HG22	2:C:49:LEU:HD12	2.01	0.43
2:C:227:ILE:O	2:C:227:ILE:HG23	2.19	0.43
1:D:44:LYS:HD3	1:D:295:ASN:HD22	1.82	0.43
2:C:253:LEU:O	2:C:256:SER:OG	2.21	0.43
1:A:16:ASN:OD1	1:A:45:ARG:NE	2.46	0.43
2:B:227:ILE:O	2:B:229:GLU:OE1	2.35	0.43
2:B:99:LYS:HG2	2:B:99:LYS:O	2.18	0.43
2:C:12:ILE:HD13	5:C:805:EDO:H22	1.99	0.43
1:D:239:LYS:HE3	8:D:624:HOH:O	2.19	0.43
1:D:252:ILE:O	1:D:256:LYS:HB2	2.19	0.43
2:C:90:PRO:O	2:C:91:VAL:C	2.56	0.43
1:D:164:GLY:O	1:D:244:ASP:OD2	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:171:ILE:HG22	2:B:217:MET:HE3	2.01	0.43
1:D:233:LEU:HD12	1:D:237:ALA:CB	2.47	0.43
1:A:290:ILE:O	1:A:293:ARG:HG3	2.18	0.42
1:A:30:LYS:HB3	1:A:30:LYS:HE2	1.83	0.42
2:B:147:GLY:O	2:B:152:ILE:HB	2.19	0.42
2:B:251:ALA:O	2:B:252:GLU:HG3	2.19	0.42
2:C:202:GLN:HE21	2:C:205:ARG:HE	1.66	0.42
2:C:215:ARG:HG2	2:C:215:ARG:NH1	2.31	0.42
1:D:180:LYS:O	7:D:802:DST:H131	2.19	0.42
1:A:170:LEU:O	1:A:174:GLU:HG3	2.20	0.42
2:B:229:GLU:HA	2:B:232:ILE:CD1	2.48	0.42
2:C:204:LEU:HA	2:C:204:LEU:HD23	1.82	0.42
2:C:2:GLN:OE1	2:C:256:SER:HB2	2.20	0.42
2:B:1:MET:HG3	2:B:2:GLN:HG2	2.01	0.42
2:C:130:ASP:CG	8:C:286:HOH:O	2.58	0.42
2:C:171:ILE:HG23	2:C:220:MET:HE3	2.00	0.42
2:C:89:ARG:O	2:C:89:ARG:HG3	2.20	0.42
1:D:175:PHE:C	1:D:175:PHE:CD1	2.93	0.42
1:A:165:MET:C	1:A:167:GLU:H	2.23	0.42
2:C:206:ASN:O	2:C:210:TYR:CD1	2.73	0.42
1:A:70:CYS:O	1:A:74:MET:HG3	2.20	0.42
1:A:87:CYS:O	2:B:103:ASN:HB3	2.20	0.42
2:C:30:GLY:N	2:C:31:PRO:CD	2.83	0.42
1:D:156:GLN:O	1:D:159:ASP:HB3	2.19	0.42
2:B:4:TYR:O	2:B:8:ILE:HG13	2.20	0.42
1:A:152:LEU:C	1:A:152:LEU:HD23	2.40	0.42
1:A:266:ARG:HG2	1:A:270:GLU:OE2	2.20	0.42
1:D:165:MET:HG2	1:D:168:VAL:CG1	2.50	0.42
2:B:220:MET:HB3	2:B:224:HIS:HE1	1.84	0.41
1:D:266:ARG:HH11	1:D:266:ARG:HG3	1.85	0.41
1:A:87:CYS:HB2	2:B:102:PRO:HB2	2.02	0.41
2:C:163:ASP:CG	2:C:164:GLY:H	2.23	0.41
1:D:9:LEU:HA	1:D:9:LEU:HD12	1.74	0.41
2:B:1:MET:O	2:B:5:TRP:CD1	2.73	0.41
2:B:221:LYS:HG2	8:B:291:HOH:O	2.20	0.41
2:B:249:LYS:HE2	2:B:253:LEU:HD22	2.02	0.41
1:D:71:ALA:HB1	1:D:120:ALA:HB1	2.03	0.41
2:B:24:PRO:HA	2:B:25:PRO:HA	1.88	0.41
1:A:265:ASN:O	1:A:269:GLN:HG3	2.21	0.41
2:C:148:PRO:HB3	1:D:115:ALA:HB1	2.02	0.41
1:A:85:LEU:HA	1:A:86:PRO:HD3	1.96	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:182:MET:HE1	2:B:185:CYS:SG	2.61	0.41
2:B:223:SER:HB3	2:B:224:HIS:H	1.61	0.41
2:B:211:GLN:HE22	2:B:257:LEU:HB3	1.86	0.41
1:A:107:SER:CB	2:B:88:SER:HB3	2.45	0.41
1:D:11:LYS:HD3	1:D:11:LYS:HA	1.92	0.41
1:D:185:LEU:HD13	1:D:214:GLY:HA2	2.03	0.41
1:D:45:ARG:HB3	1:D:48:PRO:HG2	2.03	0.41
1:A:170:LEU:HA	1:A:251:LEU:HD13	2.03	0.41
1:A:26:LYS:HE3	1:A:26:LYS:HB3	1.75	0.41
1:A:292:TYR:O	1:A:293:ARG:C	2.59	0.41
2:B:49:LEU:HD23	2:B:62:ALA:HB3	2.02	0.41
1:A:248:TYR:N	1:A:249:PRO:CD	2.85	0.40
2:C:2:GLN:HB3	2:C:3:PRO:HD2	2.03	0.40
1:D:248:TYR:C	1:D:250:LYS:N	2.75	0.40
2:B:175:CYS:SG	2:B:220:MET:HG3	2.62	0.40
2:B:18:LYS:O	2:B:18:LYS:HG2	2.21	0.40
2:B:199:GLU:HB3	8:B:487:HOH:O	2.21	0.40
2:B:247:HIS:C	2:B:251:ALA:HB3	2.41	0.40
1:D:86:PRO:HA	1:D:90:ASN:CB	2.52	0.40
1:A:75:ILE:HG21	1:A:147:ILE:HG21	2.03	0.40
1:D:226:VAL:HG11	1:D:254:VAL:CG2	2.52	0.40
1:D:259:GLU:OE1	1:D:263:ARG:NH1	2.52	0.40
1:A:17:LYS:HB2	1:A:17:LYS:HE3	1.84	0.40
2:C:51:ALA:N	2:C:254:MET:HE1	2.37	0.40
2:C:8:ILE:HD13	2:C:8:ILE:HG21	1.81	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:622:HOH:O	8:D:745:HOH:O[1_455]	2.00	0.20
2:B:60:SER:OG	8:D:339:HOH:O[3_555]	2.10	0.10
8:C:286:HOH:O	8:D:659:HOH:O[1_655]	2.17	0.03

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%)	265 (96%)	8 (3%)	2 (1%)	22	22
1	D	293/295 (99%)	266 (91%)	21 (7%)	6 (2%)	7	4
2	B	257/274 (94%)	238 (93%)	14 (5%)	5 (2%)	8	5
2	C	257/274 (94%)	233 (91%)	16 (6%)	8 (3%)	4	2
All	All	1082/1138 (95%)	1002 (93%)	59 (6%)	21 (2%)	8	5

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	223	SER
2	B	227	ILE
2	C	57	GLY
2	C	91	VAL
2	C	163	ASP
1	D	243	ALA
1	A	166	ALA
2	B	88	SER
2	B	258	VAL
2	C	249	LYS
2	C	90	PRO
2	C	94	PRO
2	C	251	ALA
2	B	226	LEU
2	C	223	SER
1	D	42	GLY
1	D	245	LYS
1	A	42	GLY
1	D	252	ILE
1	D	242	VAL
1	D	254	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	222/234 (95%)	208 (94%)	14 (6%)	18	20
1	D	234/234 (100%)	222 (95%)	12 (5%)	24	29
2	B	201/214 (94%)	189 (94%)	12 (6%)	19	22
2	C	201/214 (94%)	187 (93%)	14 (7%)	15	16
All	All	858/896 (96%)	806 (94%)	52 (6%)	18	21

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	ASN
1	A	95	ARG
1	A	97	LYS
1	A	135	ARG
1	A	159	ASP
1	A	165	MET
1	A	186	GLN
1	A	189	VAL
1	A	201	GLU
1	A	245	LYS
1	A	246	THR
1	A	250	LYS
1	A	256	LYS
1	A	278	HIS
2	B	2	GLN
2	B	14	ARG
2	B	91	VAL
2	B	128	ARG
2	B	133	ASP
2	B	152	ILE
2	B	217	MET
2	B	218	MET
2	B	223	SER
2	B	224	HIS
2	B	228	ASP
2	B	250	ASN
2	C	1	MET
2	C	58	ASP
2	C	59	ARG
2	C	94	PRO
2	C	112	ILE

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Mol	Chain	Res	Type
2	C	130	ASP
2	C	131	ASP
2	C	163	ASP
2	C	182	MET
2	C	228	ASP
2	C	231	ILE
2	C	247	HIS
2	C	250	ASN
2	C	255	SER
1	D	1	MET
1	D	13	LYS
1	D	30	LYS
1	D	156	GLN
1	D	162	SER
1	D	174	GLU
1	D	177	HIS
1	D	199	LYS
1	D	226	VAL
1	D	257	SER
1	D	279	ARG
1	D	295	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	ASN
1	A	177	HIS
1	A	179	HIS
1	A	186	GLN
1	A	211	ASN
1	A	278	HIS
2	B	2	GLN
2	B	33	HIS
2	B	61	GLN
2	B	81	HIS
2	B	156	HIS
2	B	183	HIS
2	B	202	GLN
2	B	224	HIS
2	B	225	GLN
2	B	250	ASN
2	C	33	HIS

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Mol	Chain	Res	Type
2	C	61	GLN
2	C	165	ASN
2	C	202	GLN
2	C	230	ASN
1	D	100	ASN
1	D	295	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 carbohydrates 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	IPE	D	801	-	11,13,13	3.55	3 (27%)	15,19,19	1.88	3 (20%)
3	PPV	A	804	4	6,8,8	1.55	2 (33%)	13,13,13	1.87	1 (7%)
3	PPV	A	803	-	6,8,8	1.35	0	13,13,13	2.02	1 (7%)
7	DST	D	802	4	9,13,13	1.26	1 (11%)	11,19,19	2.84	3 (27%)
5	EDO	C	805	-	3,3,3	0.95	0	2,2,2	0.43	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	IPE	D	801	-	-	4/13/13/13	-
3	PPV	A	804	4	-	0/6/6/6	-
3	PPV	A	803	-	-	0/6/6/6	-
7	DST	D	802	4	-	3/7/13/13	-
5	EDO	C	805	-	-	1/1/1/1	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	801	IPE	C2-C3	-8.69	1.35	1.51
6	D	801	IPE	C4-C3	7.50	1.54	1.33
7	D	802	DST	C11-C12	2.20	1.38	1.32
3	A	804	PPV	P2-O22	2.14	1.57	1.50
6	D	801	IPE	PA-O1A	2.05	1.58	1.50
3	A	804	PPV	P1-O11	2.02	1.62	1.54

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	803	PPV	P2-OPP-P1	-6.56	110.32	132.83
7	D	802	DST	O8-P3-O7	6.04	124.46	109.82
3	A	804	PPV	P2-OPP-P1	-5.81	112.90	132.83
7	D	802	DST	O4-P1-O2	5.68	123.67	104.64
6	D	801	IPE	O1B-PB-O3A	4.21	118.77	104.64
6	D	801	IPE	O1-C1-C2	-3.57	94.04	108.64
7	D	802	DST	O4-P1-O5	-3.29	97.80	110.68
6	D	801	IPE	O3B-PB-O3A	2.52	113.10	104.64

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	D	801	IPE	C1-O1-PA-O1A
7	D	802	DST	P3-O2-P1-O4
6	D	801	IPE	O1-C1-C2-C3
6	D	801	IPE	C1-O1-PA-O3A
5	C	805	EDO	O1-C1-C2-O2
6	D	801	IPE	PB-O3A-PA-O2A

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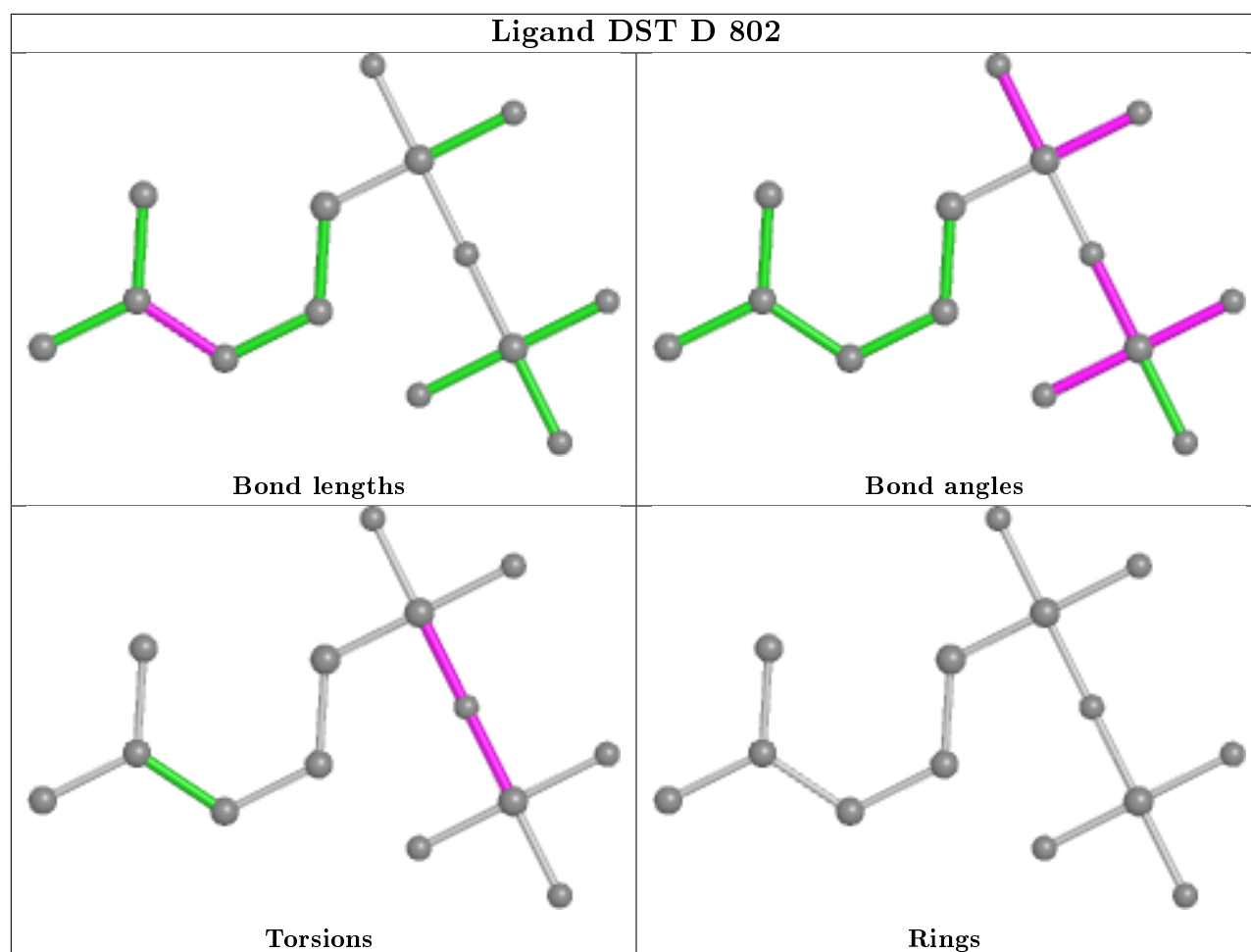
Mol	Chain	Res	Type	Atoms
7	D	802	DST	P3-O2-P1-O6
7	D	802	DST	P1-O2-P3-O8

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	801	IPE	2	0
7	D	802	DST	2	0
5	C	805	EDO	1	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	279/295 (94%)	-0.29	6 (2%) 62 59	27, 39, 65, 98	0
1	D	295/295 (100%)	0.01	19 (6%) 19 18	26, 42, 96, 113	0
2	B	259/274 (94%)	0.22	25 (9%) 7 6	31, 46, 121, 132	0
2	C	259/274 (94%)	0.05	24 (9%) 8 7	29, 48, 97, 115	0
All	All	1092/1138 (95%)	-0.01	74 (6%) 17 16	26, 43, 100, 132	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	243	ALA	10.3
2	B	257	LEU	9.4
2	B	246	PHE	7.7
1	D	251	LEU	7.7
2	B	250	ASN	7.3
1	A	166	ALA	7.2
2	B	226	LEU	6.6
2	B	249	LYS	6.4
1	D	246	THR	6.3
1	D	166	ALA	5.9
2	C	127	ALA	5.8
2	C	126	PRO	5.8
2	C	222	ASN	5.4
2	B	224	HIS	5.3
2	B	248	GLY	5.1
2	C	226	LEU	5.1
2	B	221	LYS	5.0
1	D	242	VAL	4.9
1	D	165	MET	4.9
2	B	230	ASN	4.8
1	A	165	MET	4.8

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Mol	Chain	Res	Type	RSRZ
2	B	259	ALA	4.7
1	D	244	ASP	4.7
1	D	167	GLU	4.7
2	B	225	GLN	4.5
2	C	225	GLN	4.4
1	A	164	GLY	4.3
1	D	254	VAL	4.2
2	B	1	MET	4.2
2	C	128	ARG	4.1
2	B	91	VAL	4.0
2	C	224	HIS	4.0
2	B	93	LYS	3.9
2	B	251	ALA	3.8
1	D	168	VAL	3.5
2	C	163	ASP	3.3
2	B	254	MET	3.3
1	D	239	LYS	3.2
2	C	249	LYS	3.2
2	C	93	LYS	3.2
1	D	245	LYS	3.1
1	A	167	GLU	3.1
2	B	223	SER	3.0
2	B	3	PRO	3.0
2	C	227	ILE	2.9
2	C	90	PRO	2.9
1	D	250	LYS	2.8
2	C	94	PRO	2.8
2	B	2	GLN	2.7
1	D	164	GLY	2.7
2	B	247	HIS	2.6
2	C	165	ASN	2.6
2	B	231	ILE	2.6
2	C	91	VAL	2.5
2	C	223	SER	2.5
1	D	241	LEU	2.5
1	D	252	ILE	2.5
2	C	221	LYS	2.5
1	D	169	GLY	2.4
2	B	228	ASP	2.3
1	A	117	LEU	2.3
2	C	162	VAL	2.3
2	B	238	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	259	GLU	2.2
2	C	124	VAL	2.2
2	C	59	ARG	2.2
2	C	130	ASP	2.2
1	D	184	LEU	2.2
2	C	129	THR	2.2
2	B	227	ILE	2.1
2	C	89	ARG	2.1
2	B	235	LEU	2.1
1	A	161	CYS	2.1
2	C	245	GLY	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 carbohydrates in this entry.

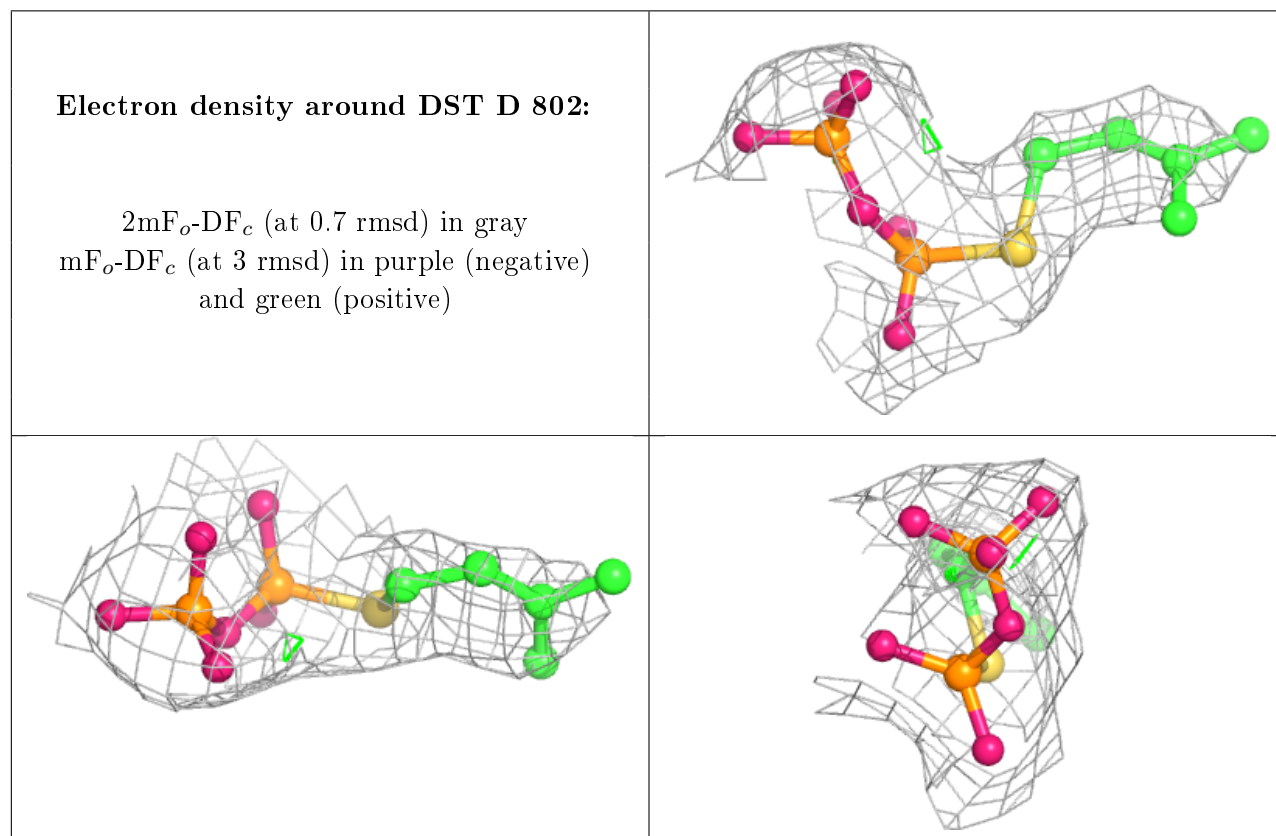
6.4 Ligands [i](#)

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	PPV	A	803	9/9	0.90	0.14	117,117,118,118	0
3	PPV	A	804	9/9	0.93	0.11	74,76,77,78	0
4	MG	A	903	1/1	0.94	0.06	52,52,52,52	0
4	MG	A	904	1/1	0.96	0.04	54,54,54,54	0
5	EDO	C	805	4/4	0.97	0.19	34,37,39,41	0
7	DST	D	802	14/14	0.97	0.21	54,61,66,66	0
6	IPE	D	801	14/14	0.98	0.18	42,45,47,50	0
4	MG	D	901	1/1	0.98	0.15	52,52,52,52	0
4	MG	D	902	1/1	0.98	0.14	53,53,53,53	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.