



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:15 AM GMT

PDB ID : 3OAB  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

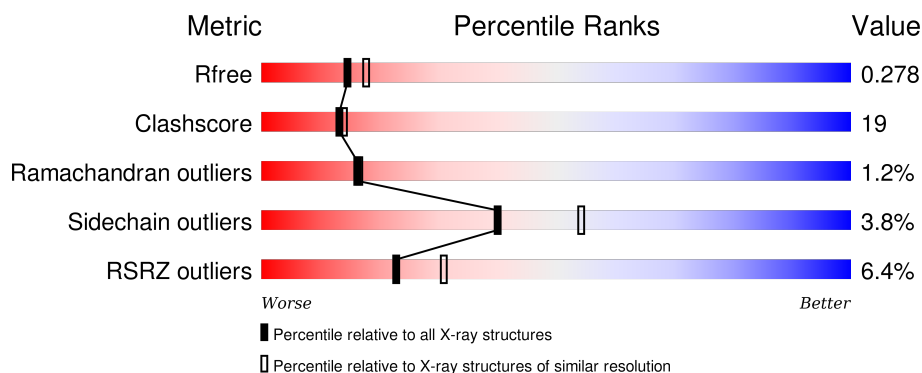
# 1 Overall quality at a glance

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))
$R_{free}$	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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>3%</div> <div>64%</div> <div>28%</div> <div>5%</div> </div>
1	D	295	<div> <div>6%</div> <div>64%</div> <div>34%</div> <div>•</div> </div>
2	B	264	<div> <div>10%</div> <div>66%</div> <div>24%</div> <div>• • 6%</div> </div>
2	C	264	<div> <div>6%</div> <div>65%</div> <div>25%</div> <div>• 8%</div> </div>

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
5	MG	D	901	-	-	-	X

## 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:

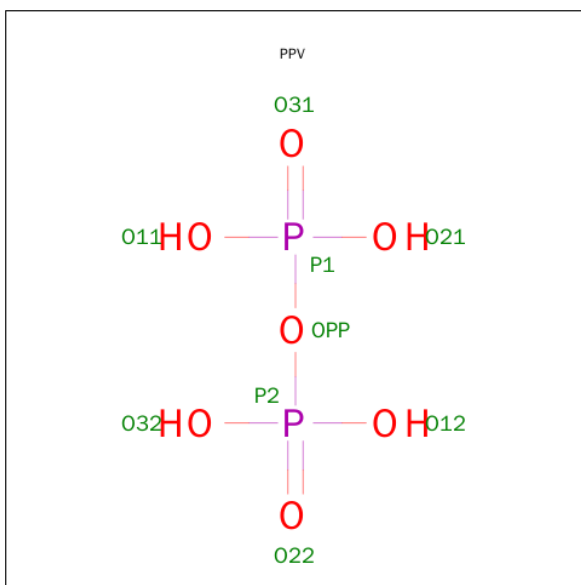
Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	EXPRESSION TAG	UNP Q9SBR4
B	?	-	LEU	DELETION	UNP Q9SBR4
B	?	-	THR	DELETION	UNP Q9SBR4
B	?	-	ASP	DELETION	UNP Q9SBR4
B	?	-	GLY	DELETION	UNP Q9SBR4
B	?	-	SER	DELETION	UNP Q9SBR4
B	?	-	ARG	DELETION	UNP Q9SBR4
B	?	-	PRO	DELETION	UNP Q9SBR4
B	?	-	VAL	DELETION	UNP Q9SBR4
B	?	-	SER	DELETION	UNP Q9SBR4

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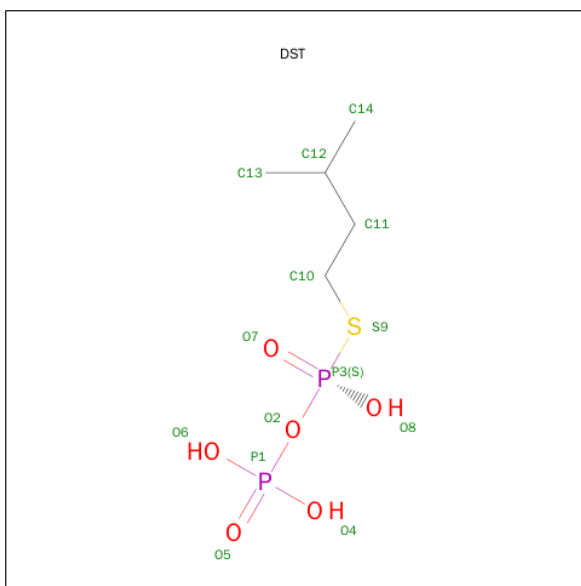
Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	LYS	DELETION	UNP Q9SBR4
B	267	HIS	-	EXPRESSION TAG	UNP Q9SBR4
B	268	HIS	-	EXPRESSION TAG	UNP Q9SBR4
B	269	HIS	-	EXPRESSION TAG	UNP Q9SBR4
B	270	HIS	-	EXPRESSION TAG	UNP Q9SBR4
B	271	HIS	-	EXPRESSION TAG	UNP Q9SBR4
B	272	HIS	-	EXPRESSION TAG	UNP Q9SBR4
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 (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	0	0
			9	7	2		

- Molecule 4 is DIMETHYLALLYL S-THIOLODIPHOSPHATE (three-letter code: DST) (formula:  $C_5H_{14}O_6P_2S$ ).

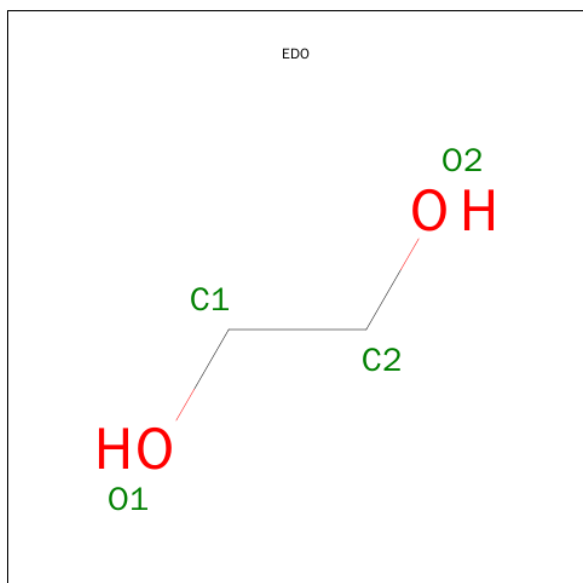


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	O	P	S	0	0
			14	5	6	2	1		
4	D	1	Total	C	O	P	S	0	0
			14	5	6	2	1		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

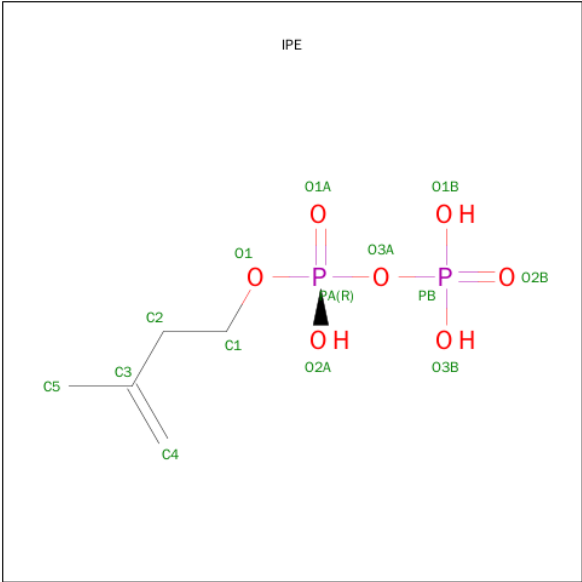
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Mg	0	0
			2	2		
5	D	2	Total	Mg	0	0
			2	2		

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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 (three-letter code: IPE) (formula: C<sub>5</sub>H<sub>12</sub>O<sub>7</sub>P<sub>2</sub>).



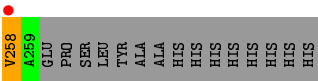
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	D	1	Total	C	O	P	0	0
			14	5	7	2		

- Molecule 8 is water.

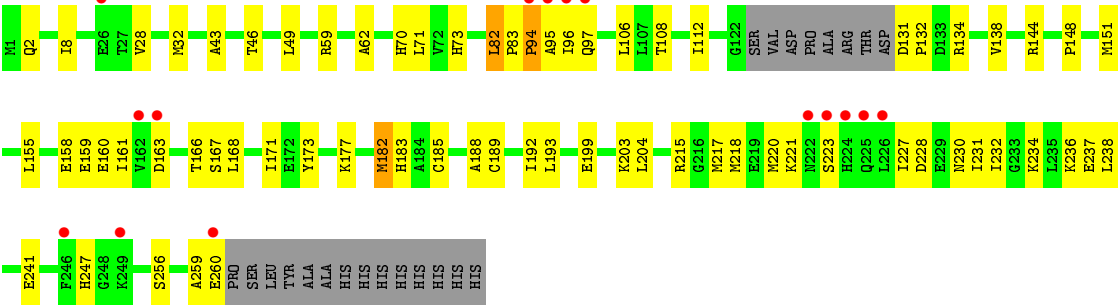
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	195	Total	O	0	0
			195	195		
8	B	148	Total	O	0	0
			148	148		
8	C	119	Total	O	0	0
			119	119		
8	D	174	Total	O	0	0
			174	174		







● 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, $\alpha$ , $\beta$ , $\gamma$	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) 91.9 (24.96-2.30)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.80 (at 2.28Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.208 , 0.277 0.210 , 0.278	Depositor DCC
$R_{free}$ test set	2143 reflections (4.99%)	DCC
Wilson B-factor (Å <sup>2</sup> )	28.7	Xtriage
Anisotropy	0.859	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 49.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 43011 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8759	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	1.00	2/2155 (0.1%)	0.90	1/2903 (0.0%)
1	D	0.90	1/2268 (0.0%)	0.83	0/3055
2	B	0.90	2/1919 (0.1%)	0.84	1/2595 (0.0%)
2	C	0.81	0/1867	0.87	4/2521 (0.2%)
All	All	0.91	5/8209 (0.1%)	0.86	6/11074 (0.1%)

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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	200	GLU	CG-CD	7.89	1.63	1.51
1	A	119	PHE	CE2-CZ	5.70	1.48	1.37
2	B	200	GLU	CB-CG	5.52	1.62	1.52
1	D	8	MET	CG-SD	5.42	1.95	1.81
1	A	189	VAL	CB-CG2	-5.27	1.41	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	82	LEU	C-N-CD	-11.23	95.90	120.60
2	C	82	LEU	C-N-CA	8.37	157.17	122.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	207	ARG	NE-CZ-NH1	-7.29	116.66	120.30
2	C	82	LEU	N-CA-C	-6.76	92.74	111.00
2	C	94	PRO	N-CA-C	-5.73	97.20	112.10
2	B	110	ASP	CB-CG-OD1	-5.14	113.67	118.30

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	66	0
1	D	2232	0	2264	98	0
2	B	1881	0	1871	86	0
2	C	1831	0	1822	65	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
8	B	148	0	0	7	0
8	C	119	0	0	5	0
8	D	174	0	0	7	0
All	All	8759	0	8138	308	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 19.

All (308) 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: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
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
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:CG	2:B:128:ARG:HH11	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
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:HG2	2:B:128:ARG:HH11	1.46	0.78
2:C:97:GLN:OE1	2:C:97:GLN:HA	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
2:B:249:LYS:O	2:B:253:LEU:N	2.19	0.75
1:A:149:SER:HB2	8:A:470:HOH:O	1.86	0.75
1:D:173:LEU:HD22	1:D:251:LEU:HD12	1.68	0.75
1:D:168:VAL:HG21	1:D:246:THR:HG23	1.66	0.75
1:D:168:VAL:HG23	1:D:251:LEU:HD11	1.69	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: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: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
2:B:71:LEU:HD22	2:B:112:ILE:HG23	1.75	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:LYS:HD3	8:A:412:HOH:O	1.93	0.67
1:D:201:GLU:OE2	8:D:303:HOH:O	2.12	0.67
2:B:82:LEU:O	2:B:82:LEU:HD12	1.95	0.67
1:D:4:PHE:HB2	1:D:8:MET:HE3	1.75	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
1:D:64:THR:OG1	8:D:306:HOH:O	2.14	0.65
2:C:260:GLU:HA	2:C:260:GLU:OE2	1.98	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:B:249:LYS:CD	2:B:253:LEU:HB2	2.27	0.64
1:D:4:PHE:HB2	1:D:8:MET:HE1	1.78	0.64
2:C:28:VAL:HG22	1:D:157:VAL:HG21	1.80	0.63
2:B:2:GLN:HA	2:B:2:GLN:HE21	1.62	0.63
1:D:205:LYS:HD2	1:D:274:HIS:CB	2.26	0.63
1:D:134:GLU:CD	1:D:134:GLU:H	2.02	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
2:C:230:ASN:O	2:C:234:LYS:HG3	2.00	0.62
2:B:246:PHE:C	2:B:251:ALA:HB1	2.20	0.61
2:B:249:LYS:HE2	2:B:253:LEU:HD22	1.83	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:218:MET:CE	2:B:232:ILE:HD11	2.31	0.60
2:B:221:LYS:HG2	2:B:227:ILE:HG21	1.83	0.60
1:A:102:MET:HA	1:A:102:MET:CE	2.32	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
1:A:13:LYS:HD3	1:A:13:LYS:C	2.22	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:94:PRO:C	2:C:96:ILE:N	2.52	0.59
2:C:151:MET:O	2:C:155:LEU:HG	2.02	0.59
2:C:97:GLN:CA	2:C:97:GLN:OE1	2.51	0.58
1:A:207:ARG:NH1	8:A:362:HOH:O	2.37	0.58
2:B:218:MET:HE1	2:B:221:LYS:HE3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:71:ALA:HB2	1:D:124:VAL:HG23	1.86	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
2:B:94:PRO:HB3	8:B:297:HOH:O	2.05	0.56
1:A:290:ILE:HG23	1:A:293:ARG:NH2	2.21	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
7:D:801:IPE:C5	4:D:802:DST:H133	2.35	0.55
1:D:48:PRO:HG3	1:D:73:GLU:HB2	1.89	0.55
2:C:62:ALA:HA	2:C:193:LEU:HD13	1.88	0.55
2:C:182:MET:HE3	2:C:182:MET:HA	1.87	0.55
2:C:228:ASP:OD2	2:C:230:ASN:HB2	2.06	0.55
2:B:227:ILE:O	2:B:227:ILE:HG13	2.07	0.55
1:A:245:LYS:HB3	1:A:250:LYS:NZ	2.22	0.55
2:C:227:ILE:O	2:C:227:ILE:HG12	2.06	0.55
2:B:14:ARG:NH1	2:B:14:ARG:HB2	2.22	0.55
1:A:252:ILE:HD12	1:A:256:LYS:HB3	1.88	0.55
1:D:180:LYS:O	4:D:802:DST:H131	2.06	0.54
2:C:218:MET:O	2:C:221:LYS:HB3	2.07	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:NH1	2:B:128:ARG:CG	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
1:D:156:GLN:HE22	4:D:802:DST:H112	1.72	0.53
2:B:218:MET:HA	2:B:221:LYS:HG3	1.91	0.53
2:B:98:HIS:HB2	8:B:288:HOH:O	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:279:ARG:NH1	1:D:279:ARG:CG	2.67	0.53
2:C:228:ASP:HB2	2:C:230:ASN:OD1	2.09	0.53
2:C:259:ALA:O	2:C:260:GLU:HB2	2.08	0.53
2:C:83:PRO:HB2	2:C:94:PRO:CD	2.39	0.52
2:B:228:ASP:HB3	2:B:231:ILE:HG12	1.91	0.52
1:D:68:ALA:HA	1:D:124:VAL:HG22	1.91	0.52
1:A:83:ASP:CG	4:A:804:DST:H102	2.30	0.52
2:B:175:CYS:SG	2:B:220:MET:HG3	2.49	0.52
2:C:8:ILE:HG23	2:C:49:LEU:HD12	1.90	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
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:C:166:THR:HG22	2:C:171:ILE:HG13	1.93	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:B:55:VAL:HG11	2:B:196:ALA:HB2	1.93	0.51
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
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:A:56:GLU:O	1:A:279:ARG:HD3	2.11	0.50
1:D:52:ILE:HD11	1:D:66:MET:CE	2.42	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:D:156:GLN:O	1:D:160:VAL:HG13	2.12	0.50
1:A:45:ARG:O	1:A:48:PRO:HD2	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: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:226:VAL:CG1	1:D:226:VAL:O	2.60	0.49
1:D:152:LEU:HA	1:D:179:HIS:O	2.12	0.49
2:B:221:LYS:CG	2:B:227:ILE:HG21	2.43	0.49
2:C:218:MET:HE2	2:C:232:ILE:HG12	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:5:TRP:HZ2	2:B:253:LEU:HG	1.77	0.49
1:D:219:VAL:HG22	1:D:248:TYR:CD2	2.47	0.49
1:A:29:LEU:HD11	2:C:173:TYR:CE2	2.47	0.49
1:A:221:ASP:OD1	1:A:293:ARG:NH1	2.33	0.49
2:C:28:VAL:HG22	1:D:157:VAL:HG23	1.94	0.48
1:A:13:LYS:HD2	8:A:382:HOH:O	2.12	0.48
2:C:71:LEU:HB3	2:C:112:ILE:HG22	1.94	0.48
2:B:218:MET:HE1	2:B:232:ILE:HD11	1.94	0.48
2:B:34:HIS:HE1	8:B:391:HOH:O	1.96	0.48
2:B:249:LYS:HE2	2:B:253:LEU:CD1	2.36	0.48
1:A:47:ARG:HB2	1:A:48:PRO:HD3	1.95	0.48
1:D:165:MET:HG2	8:D:406:HOH:O	2.13	0.48
1:A:92:ASP:O	1:A:98:PRO:HA	2.14	0.48
1:D:128:THR:C	1:D:129:LYS:HD3	2.34	0.47
2:C:221:LYS:HG3	2:C:227:ILE:CG2	2.44	0.47
2:B:249:LYS:HD3	2:B:249:LYS:C	2.34	0.47
1:D:23:VAL:O	1:D:36:ARG:HD2	2.14	0.47
2:B:253:LEU:HD12	2:B:256:SER:HG	1.78	0.47
2:B:163:ASP:O	2:B:224:HIS:HB3	2.14	0.47
2:B:14:ARG:HH11	2:B:14:ARG:HB2	1.79	0.47
1:A:122:GLU:HB2	2:B:143:SER:OG	2.14	0.47
1:D:158:VAL:HG12	1:D:158:VAL:O	2.13	0.47
1:A:40:LEU:C	1:A:42:GLY:H	2.18	0.47
1:A:71:ALA:O	1:A:74:MET:HB2	2.14	0.46
1:A:102:MET:HA	1:A:102:MET:HE2	1.96	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:C:158:GLU:C	2:C:160:GLU:H	2.19	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
1:D:66:MET:HB3	1:D:67:PRO:HD3	1.97	0.46
2:C:199:GLU:O	2:C:203:LYS:HG2	2.15	0.46
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:D:248:TYR:C	1:D:250:LYS:H	2.18	0.45
2:B:2:GLN:HB3	8:B:474:HOH:O	2.16	0.45
1:D:178:HIS:ND1	1:D:178:HIS:C	2.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:PRO:HG2	1:A:135:ARG:HB2	1.98	0.45
1:D:162:SER:O	1:D:162:SER:OG	2.27	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
1:A:209:PHE:CE1	1:A:272:LEU:HD11	2.52	0.45
2:B:253:LEU:O	2:B:256:SER:N	2.50	0.45
2:C:82:LEU:HD11	2:C:106:LEU:HD13	1.99	0.45
1:D:28:PRO:HG2	1:D:31:ILE:HB	1.98	0.44
1:D:20:GLU:HG2	1:D:40:LEU:HD13	1.99	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
1:A:82:HIS:ND1	2:B:110:ASP:OD2	2.47	0.44
1:D:168:VAL:CG2	1:D:251:LEU:HD21	2.47	0.44
2:C:94:PRO:O	2:C:95:ALA:C	2.52	0.44
1:A:248:TYR:N	1:A:249:PRO:CD	2.80	0.44
1:A:70:CYS:O	1:A:74:MET:HG3	2.18	0.44
1:D:1:MET:HA	1:D:1:MET:CE	2.48	0.44
1:D:157:VAL:HG23	1:D:158:VAL:N	2.33	0.44
1:A:13:LYS:HD3	1:A:14:SER:N	2.32	0.44
2:B:218:MET:HE3	2:B:232:ILE:HD11	2.00	0.44
1:D:263:ARG:NH2	8:D:404:HOH:O	2.51	0.44
1:A:276:HIS:HA	1:A:277:PRO:HD3	1.79	0.44
1:A:265:ASN:OD1	1:A:287:ALA:HB1	2.18	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:1:MET:HE2	1:D:1:MET:HA	2.00	0.43
1:D:263:ARG:HH11	1:D:263:ARG:HB2	1.83	0.43
1:D:132:PRO:HD2	1:D:135:ARG:NE	2.33	0.43
2:B:220:MET:O	2:B:221:LYS:C	2.56	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:101:HIS:CD2	1:A:102:MET:HE2	2.53	0.43
1:A:45:ARG:C	1:A:48:PRO:HD2	2.39	0.43
1:A:206:LEU:HD23	1:A:206:LEU:HA	1.85	0.43
2:B:250:ASN:HA	2:B:253:LEU:HB3	2.01	0.43
1:A:86:PRO:HD3	1:A:101:HIS:CD2	2.54	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
2:C:167:SER:O	2:C:171:ILE:HG13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:HIS:O	1:A:182:ALA:HB3	2.19	0.43
2:C:158:GLU:C	2:C:160:GLU:N	2.72	0.42
1:D:26:LYS:HG3	1:D:32:HIS:CE1	2.54	0.42
2:B:28:VAL:O	2:B:31:PRO:HD2	2.19	0.42
1:A:147:ILE:HG21	1:A:147:ILE:HD13	1.74	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
1:D:3:ASP:C	1:D:3:ASP:OD2	2.56	0.42
2:C:182:MET:HA	2:C:182:MET:CE	2.49	0.42
2:C:161:ILE:HG23	2:C:166:THR:HG21	2.00	0.42
2:C:131:ASP:HB3	2:C:132:PRO:HD3	1.99	0.42
1:D:79:SER:OG	4:D:802:DST:H142	2.18	0.42
2:C:32:MET:HG3	2:C:112:ILE:HD11	2.01	0.42
2:B:254:MET:C	2:B:256:SER:H	2.23	0.42
2:B:2:GLN:N	2:B:3:PRO:HD2	2.34	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
2:B:243:LEU:HA	2:B:243:LEU:HD23	1.90	0.42
2:C:151:MET:HA	2:C:177:LYS:O	2.20	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
1:D:165:MET:CG	8:D:406:HOH:O	2.67	0.42
2:C:177:LYS:HA	2:C:177:LYS:HD2	1.77	0.41
1:A:3:ASP:OD2	1:A:6:GLY:HA3	2.20	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:175:PHE:O	1:A:179:HIS:HD2	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:A:106:GLU:O	1:A:110:VAL:HG23	2.21	0.41
1:A:279:ARG:O	1:A:282:PRO:HD2	2.21	0.41
1:D:263:ARG:HB2	1:D:263:ARG:NH1	2.34	0.41
1:D:213:ILE:HA	1:D:216:LEU:HB3	2.03	0.41
2:C:204:LEU:HA	2:C:204:LEU:HD23	1.85	0.41
1:D:279:ARG:HG2	1:D:279:ARG:NH1	2.36	0.41
2:B:94:PRO:O	2:B:95:ALA:C	2.58	0.41
1:D:168:VAL:CG2	1:D:251:LEU:HD11	2.44	0.41
1:D:132:PRO:HB2	1:D:134:GLU:OE1	2.20	0.41
1:D:41:ALA:HB3	1:D:95:ARG:HD3	2.02	0.41
1:A:186:GLN:CD	1:A:207:ARG:HG2	2.41	0.41
1:D:216:LEU:O	1:D:220:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:168:LEU:HD23	2:C:168:LEU:HA	1.93	0.41
1:A:75:ILE:HD12	1:A:117:LEU:HD13	2.03	0.41
1:D:35:MET:CE	1:D:116:LEU:HD23	2.51	0.41
1:D:71:ALA:HB2	1:D:124:VAL:CG2	2.50	0.41
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:167:GLU:CD	1:D:167:GLU:N	2.74	0.40
1:D:47:ARG:HB2	8:D:318:HOH:O	2.21	0.40
2:C:144:ARG:HG2	1:D:122:GLU:CD	2.41	0.40
2:C:94:PRO:C	2:C:96:ILE:H	2.24	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:HG3	1:A:94:ARG:HH21	1.86	0.40
2:B:221:LYS:O	2:B:222:ASN:C	2.60	0.40
1:A:290:ILE:O	1:A:293:ARG:NH2	2.54	0.40
1:A:177:HIS:HD2	1:A:248:TYR:OH	2.05	0.40
2:C:215:ARG:NH1	8:C:402:HOH:O	2.52	0.40
1:D:209:PHE:CE2	1:D:213:ILE:HD13	2.56	0.40
2:C:203:LYS:HD2	2:C:203:LYS:HA	1.86	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%)	26	31
1	D	293/295 (99%)	275 (94%)	16 (6%)	2 (1%)	26	31
2	B	247/264 (94%)	229 (93%)	11 (4%)	7 (3%)	6	4
2	C	238/264 (90%)	227 (95%)	9 (4%)	2 (1%)	24	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1053/1118 (94%)	993 (94%)	47 (4%)	13 (1%)	16	16

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	83	PRO
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%)	213 (96%)	9 (4%)	37	50
1	D	234/234 (100%)	224 (96%)	10 (4%)	35	47
2	B	192/205 (94%)	183 (95%)	9 (5%)	32	43
2	C	186/205 (91%)	182 (98%)	4 (2%)	60	77
All	All	834/878 (95%)	802 (96%)	32 (4%)	40	54

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	13	LYS

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Mol	Chain	Res	Type
1	A	14	SER
1	A	86	PRO
1	A	97	LYS
1	A	135	ARG
1	A	207	ARG
1	A	245	LYS
1	A	278	HIS
2	B	2	GLN
2	B	27	THR
2	B	83	PRO
2	B	128	ARG
2	B	163	ASP
2	B	168	LEU
2	B	224	HIS
2	B	250	ASN
2	B	255	SER
2	C	159	GLU
2	C	182	MET
2	C	185	CYS
2	C	220	MET
1	D	13	LYS
1	D	133	PRO
1	D	162	SER
1	D	186	GLN
1	D	205	LYS
1	D	208	LYS
1	D	246	THR
1	D	267	GLU
1	D	279	ARG
1	D	295	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	177	HIS
1	A	179	HIS
1	A	271	GLN
1	A	276	HIS
2	B	2	GLN
2	B	98	HIS
2	B	156	HIS
2	B	183	HIS

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Mol	Chain	Res	Type
2	B	250	ASN
2	C	2	GLN
2	C	183	HIS
2	C	202	GLN
1	D	156	GLN
1	D	186	GLN
1	D	269	GLN
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
3	PPV	A	803	-	6,8,8	1.36	1 (16%)	11,13,13	1.87	1 (9%)
4	DST	A	804	5	8,13,13	1.09	1 (12%)	11,19,19	2.42	4 (36%)
6	EDO	C	805	-	3,3,3	0.60	0	2,2,2	0.32	0
7	IPE	D	801	-	10,13,13	2.28	1 (10%)	14,19,19	2.12	4 (28%)
4	DST	D	802	5	8,13,13	1.24	1 (12%)	11,19,19	2.45	5 (45%)



In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PPV	A	803	-	-	0/6/6/6	0/0/0/0
4	DST	A	804	5	-	0/9/13/13	0/0/0/0
6	EDO	C	805	-	-	0/1/1/1	0/0/0/0
7	IPE	D	801	-	-	0/13/13/13	0/0/0/0
4	DST	D	802	5	-	0/9/13/13	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	802	DST	C11-C12	-2.30	1.34	1.51
4	A	804	DST	P3-O8	-2.15	1.51	1.56
3	A	803	PPV	P1-O11	2.03	1.62	1.54
7	D	801	IPE	C4-C3	6.88	1.55	1.33

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	803	PPV	P2-OPP-P1	-5.70	113.56	132.67
7	D	801	IPE	O1-C1-C2	-2.83	95.05	108.63
4	A	804	DST	O6-P1-O4	-2.74	96.95	107.38
4	A	804	DST	P1-O2-P3	-2.67	123.72	132.67
4	D	802	DST	P1-O2-P3	-2.58	124.01	132.67
4	D	802	DST	O6-P1-O4	-2.39	98.29	107.38
7	D	801	IPE	PA-O3A-PB	-2.06	125.78	132.67
4	D	802	DST	O6-P1-O2	2.13	114.77	105.09
7	D	801	IPE	O1B-PB-O3A	2.25	115.31	105.09
4	A	804	DST	O4-P1-O2	3.17	119.46	105.09
4	D	802	DST	O4-P1-O2	3.31	120.11	105.09
4	A	804	DST	O8-P3-O7	5.19	123.00	110.05
7	D	801	IPE	O3A-PA-O1	5.39	117.24	102.94
4	D	802	DST	O8-P3-O7	5.47	123.70	110.05

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

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

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	279/295 (94%)	-0.07	10 (3%) 46 55	13, 29, 53, 81	0
1	D	295/295 (100%)	0.27	17 (5%) 26 35	21, 35, 80, 102	0
2	B	249/264 (94%)	0.48	26 (10%) 8 12	20, 33, 111, 128	0
2	C	242/264 (91%)	0.38	15 (6%) 24 32	22, 40, 75, 105	0
All	All	1065/1118 (95%)	0.25	68 (6%) 23 31	13, 34, 81, 128	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	248	GLY	9.5
2	C	225	GLN	7.2
2	B	249	LYS	7.1
2	B	1	MET	7.0
2	B	226	LEU	6.9
1	D	241	LEU	6.5
1	D	165	MET	6.4
2	B	227	ILE	6.2
2	B	250	ASN	6.2
1	D	243	ALA	6.1
2	C	94	PRO	5.9
2	C	222	ASN	5.8
2	B	251	ALA	5.8
2	C	96	ILE	5.8
2	C	95	ALA	5.7
1	A	166	ALA	5.7
2	B	225	GLN	5.6
2	C	163	ASP	5.4
2	B	96	ILE	5.3
2	B	97	GLN	5.0
1	D	168	VAL	4.9

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Mol	Chain	Res	Type	RSRZ
2	B	254	MET	4.8
2	B	94	PRO	4.8
1	D	166	ALA	4.8
1	D	242	VAL	4.7
1	D	167	GLU	4.6
1	D	164	GLY	4.6
2	B	246	PHE	4.5
2	B	95	ALA	4.3
1	D	244	ASP	4.2
1	D	251	LEU	4.0
2	C	162	VAL	3.9
2	B	253	LEU	3.5
1	A	167	GLU	3.4
2	C	97	GLN	3.4
2	C	226	LEU	3.3
1	D	1	MET	3.3
2	B	247	HIS	3.3
1	A	276	HIS	3.2
2	B	224	HIS	3.2
2	C	224	HIS	3.2
2	B	228	ASP	3.2
2	B	257	LEU	3.1
2	B	252	GLU	3.1
1	A	164	GLY	3.1
1	A	228	LYS	3.0
1	A	95	ARG	2.9
1	A	295	ASN	2.9
2	B	223	SER	2.9
1	A	245	LYS	2.9
2	B	2	GLN	2.8
2	B	163	ASP	2.7
1	D	170	LEU	2.7
1	A	165	MET	2.7
2	B	244	GLY	2.7
1	D	171	ASP	2.7
1	D	162	SER	2.7
2	B	258	VAL	2.6
1	A	163	GLU	2.5
2	C	260	GLU	2.4
1	D	256	LYS	2.4
2	C	223	SER	2.4
2	C	246	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	252	ILE	2.2
2	C	26	GLU	2.2
2	B	241	GLU	2.1
2	C	249	LYS	2.1
1	D	169	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	MG	D	901	1/1	0.80	0.45	8.46	58,58,58,58	0
6	EDO	C	805	4/4	0.95	0.17	1.23	25,28,30,32	0
3	PPV	A	803	9/9	0.91	0.12	-0.64	88,89,90,91	0
4	DST	A	804	14/14	0.97	0.10	-0.76	46,50,53,56	0
5	MG	D	902	1/1	0.88	0.09	-0.79	54,54,54,54	0
4	DST	D	802	14/14	0.96	0.12	-0.83	47,57,59,60	0
7	IPE	D	801	14/14	0.98	0.10	-0.85	32,35,37,37	0
5	MG	A	903	1/1	0.95	0.03	-	32,32,32,32	0
5	MG	A	904	1/1	0.94	0.04	-	33,33,33,33	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.