



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:26 AM GMT

PDB ID : 3AQ0
Title : Ligand-bound form of Arabidopsis medium/long-chain length prenyl pyrophosphate synthase (surface polar residue mutant)
Authors : Hsieh, F.-L.; Chang, T.-H.; Ko, T.-P.; Wang, A.H.-J.
Deposited on : 2010-10-24
Resolution : 2.65 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/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 : 1.7 (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

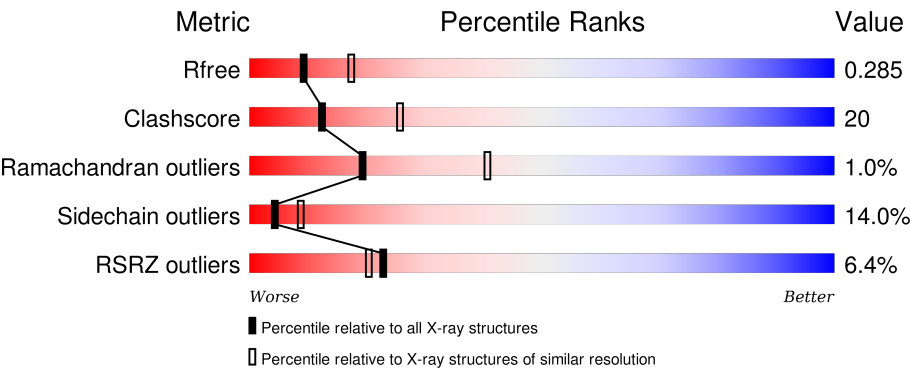
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	91344	3152 (2.70-2.62)
Clashscore	102246	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)
RSRZ outliers	91569	3161 (2.70-2.62)

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. 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	348	<div><div>5%</div><div><div></div><div>65%</div><div>25%</div><div>• 6%</div></div></div>
1	B	348	<div><div>6%</div><div><div></div><div>58%</div><div>25%</div><div>7%</div><div>10%</div></div></div>
1	C	348	<div><div>7%</div><div><div></div><div>64%</div><div>24%</div><div>5%</div><div>6%</div></div></div>
1	D	348	<div><div>5%</div><div><div></div><div>62%</div><div>20%</div><div>7%</div><div>• 10%</div></div></div>
1	E	348	<div><div>8%</div><div><div></div><div>66%</div><div>23%</div><div>5%</div><div>7%</div></div></div>

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Mol	Chain	Length	Quality of chain
1	F	348	
1	G	348	
1	H	348	

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
6	PEG	B	1002	-	-	-	X
6	PEG	D	1002	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 20426 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	326	Total	C	N	O	S	0	0	0
			2488	1563	434	479	12			
1	B	313	Total	C	N	O	S	0	0	0
			2394	1507	414	461	12			
1	C	327	Total	C	N	O	S	0	0	0
			2496	1567	434	483	12			
1	D	312	Total	C	N	O	S	0	0	0
			2388	1506	410	460	12			
1	E	325	Total	C	N	O	S	0	0	0
			2478	1556	432	478	12			
1	F	310	Total	C	N	O	S	0	0	0
			2368	1492	408	456	12			
1	G	314	Total	C	N	O	S	0	0	0
			2400	1514	415	459	12			
1	H	324	Total	C	N	O	S	0	0	0
			2471	1552	431	476	12			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	EXPRESSION TAG	UNP Q9FT89
A	178	ALA	GLU	ENGINEERED MUTATION	UNP Q9FT89
A	179	ALA	GLN	ENGINEERED MUTATION	UNP Q9FT89
A	281	ALA	GLU	ENGINEERED MUTATION	UNP Q9FT89
A	282	ALA	LYS	ENGINEERED MUTATION	UNP Q9FT89
B	1	GLY	-	EXPRESSION TAG	UNP Q9FT89
B	178	ALA	GLU	ENGINEERED MUTATION	UNP Q9FT89
B	179	ALA	GLN	ENGINEERED MUTATION	UNP Q9FT89
B	281	ALA	GLU	ENGINEERED MUTATION	UNP Q9FT89
B	282	ALA	LYS	ENGINEERED MUTATION	UNP Q9FT89
C	1	GLY	-	EXPRESSION TAG	UNP Q9FT89
C	178	ALA	GLU	ENGINEERED MUTATION	UNP Q9FT89
C	179	ALA	GLN	ENGINEERED MUTATION	UNP Q9FT89

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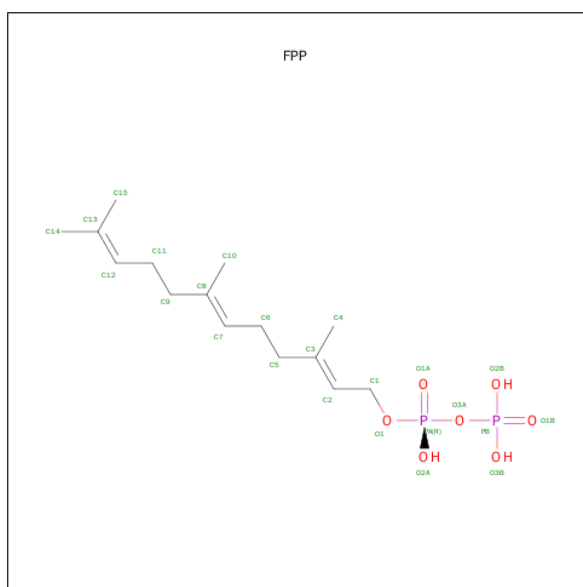
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Chain	Residue	Modelled	Actual	Comment	Reference
C	281	ALA	GLU	ENGINEERED MUTATION	UNP Q9FT89
C	282	ALA	LYS	ENGINEERED MUTATION	UNP Q9FT89
D	1	GLY	-	EXPRESSION TAG	UNP Q9FT89
D	178	ALA	GLU	ENGINEERED MUTATION	UNP Q9FT89
D	179	ALA	GLN	ENGINEERED MUTATION	UNP Q9FT89
D	281	ALA	GLU	ENGINEERED MUTATION	UNP Q9FT89
D	282	ALA	LYS	ENGINEERED MUTATION	UNP Q9FT89
E	1	GLY	-	EXPRESSION TAG	UNP Q9FT89
E	178	ALA	GLU	ENGINEERED MUTATION	UNP Q9FT89
E	179	ALA	GLN	ENGINEERED MUTATION	UNP Q9FT89
E	281	ALA	GLU	ENGINEERED MUTATION	UNP Q9FT89
E	282	ALA	LYS	ENGINEERED MUTATION	UNP Q9FT89
F	1	GLY	-	EXPRESSION TAG	UNP Q9FT89
F	178	ALA	GLU	ENGINEERED MUTATION	UNP Q9FT89
F	179	ALA	GLN	ENGINEERED MUTATION	UNP Q9FT89
F	281	ALA	GLU	ENGINEERED MUTATION	UNP Q9FT89
F	282	ALA	LYS	ENGINEERED MUTATION	UNP Q9FT89
G	1	GLY	-	EXPRESSION TAG	UNP Q9FT89
G	178	ALA	GLU	ENGINEERED MUTATION	UNP Q9FT89
G	179	ALA	GLN	ENGINEERED MUTATION	UNP Q9FT89
G	281	ALA	GLU	ENGINEERED MUTATION	UNP Q9FT89
G	282	ALA	LYS	ENGINEERED MUTATION	UNP Q9FT89
H	1	GLY	-	EXPRESSION TAG	UNP Q9FT89
H	178	ALA	GLU	ENGINEERED MUTATION	UNP Q9FT89
H	179	ALA	GLN	ENGINEERED MUTATION	UNP Q9FT89
H	281	ALA	GLU	ENGINEERED MUTATION	UNP Q9FT89
H	282	ALA	LYS	ENGINEERED MUTATION	UNP Q9FT89

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

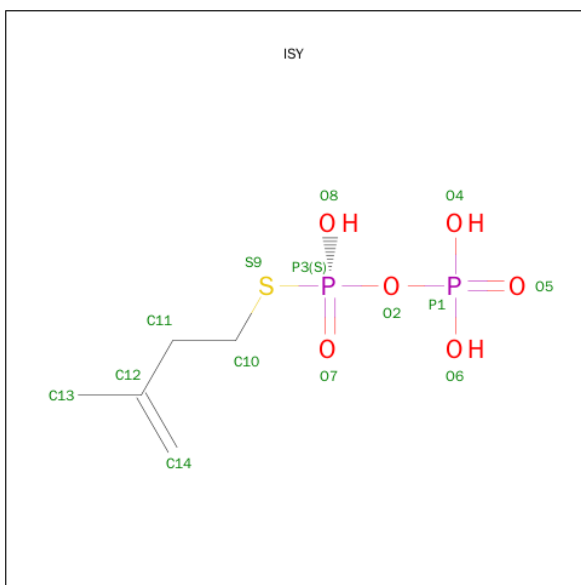
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	H	2	Total Mg 2 2	0	0
2	A	2	Total Mg 2 2	0	0
2	C	2	Total Mg 2 2	0	0
2	E	2	Total Mg 2 2	0	0

- Molecule 3 is FARNESYL DIPHOSPHATE (three-letter code: FPP) (formula: C₁₅H₂₈O₇P₂).



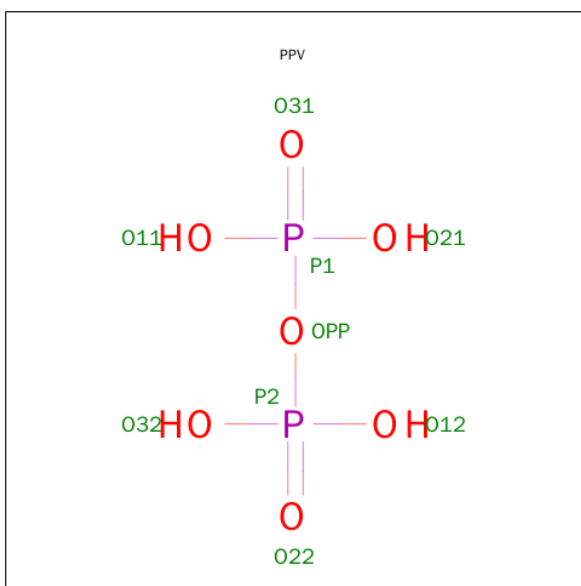
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			24	15	7	2		
3	B	1	Total	C	O	P	0	0
			24	15	7	2		
3	C	1	Total	C	O	P	0	0
			24	15	7	2		
3	E	1	Total	C	O	P	0	0
			24	15	7	2		
3	G	1	Total	C	O	P	0	0
			24	15	7	2		
3	H	1	Total	C	O	P	0	0
			24	15	7	2		

- Molecule 4 is 3-METHYLBUT-3-ENYLSULFANYL(PHOSPHONOOXY)PHOSPHINIC ACID (three-letter code: ISY) (formula: C₅H₁₂O₆P₂S).



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

- Molecule 5 is PYROPHOSPHATE (three-letter code: PPV) (formula: $\text{H}_4\text{O}_7\text{P}_2$).



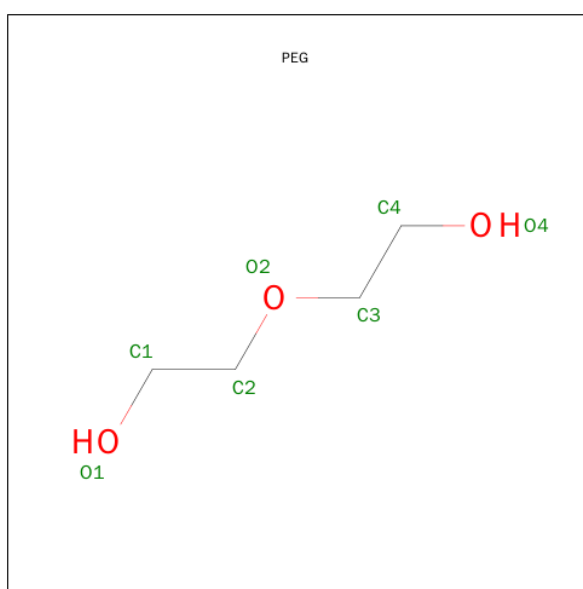
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	P	0	0
			9	7	2		
5	C	1	Total	O	P	0	0
			9	7	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	O	P	0	0
			9	7	2		
5	E	1	Total	O	P	0	0
			9	7	2		
5	F	1	Total	O	P	0	0
			9	7	2		
5	G	1	Total	O	P	0	0
			9	7	2		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			7	4	3		
6	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	83	Total	O	0	0
			83	83		
7	B	98	Total	O	0	0
			98	98		
7	C	116	Total	O	0	0
			116	116		

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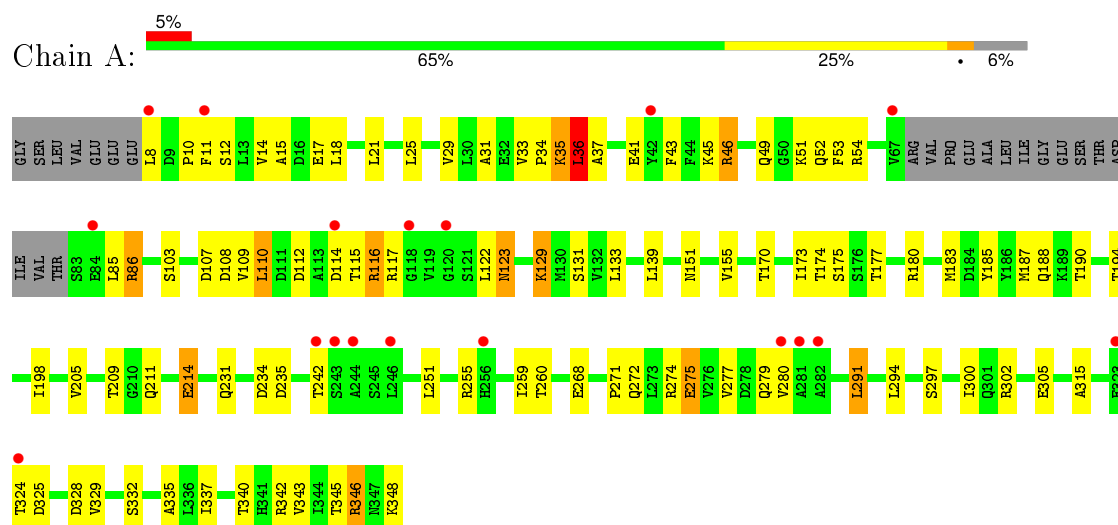
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	100	Total 100	O 100	0	0
7	E	67	Total 67	O 67	0	0
7	F	78	Total 78	O 78	0	0
7	G	77	Total 77	O 77	0	0
7	H	76	Total 76	O 76	0	0

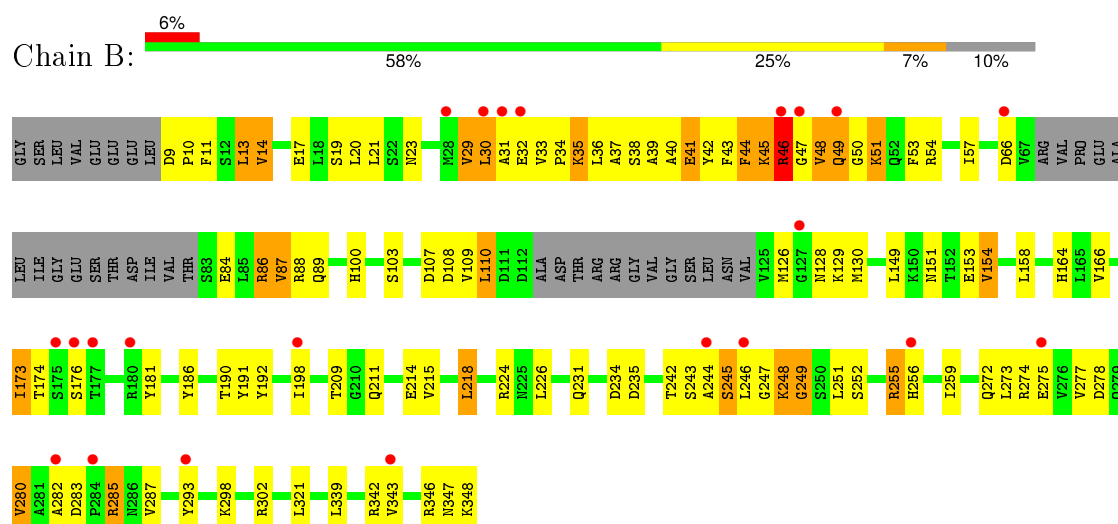
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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

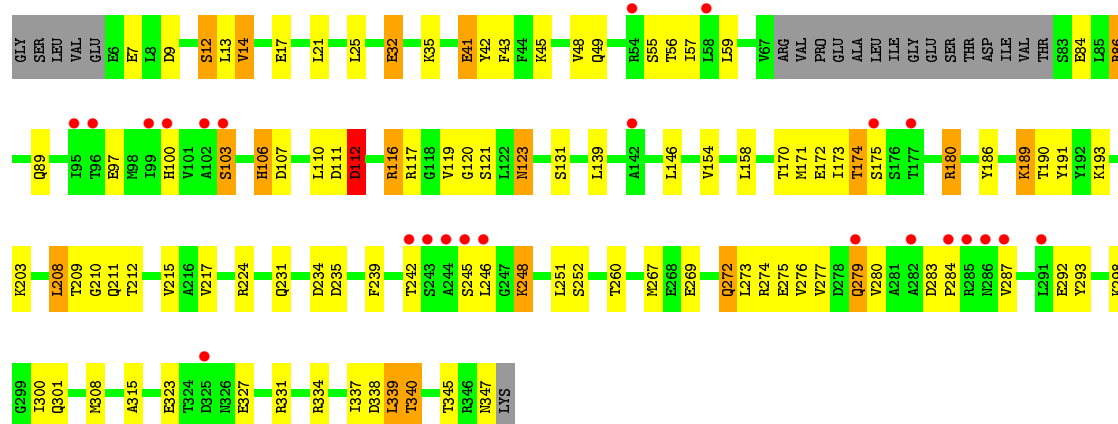


• Molecule 1: Geranyl diphosphate synthase

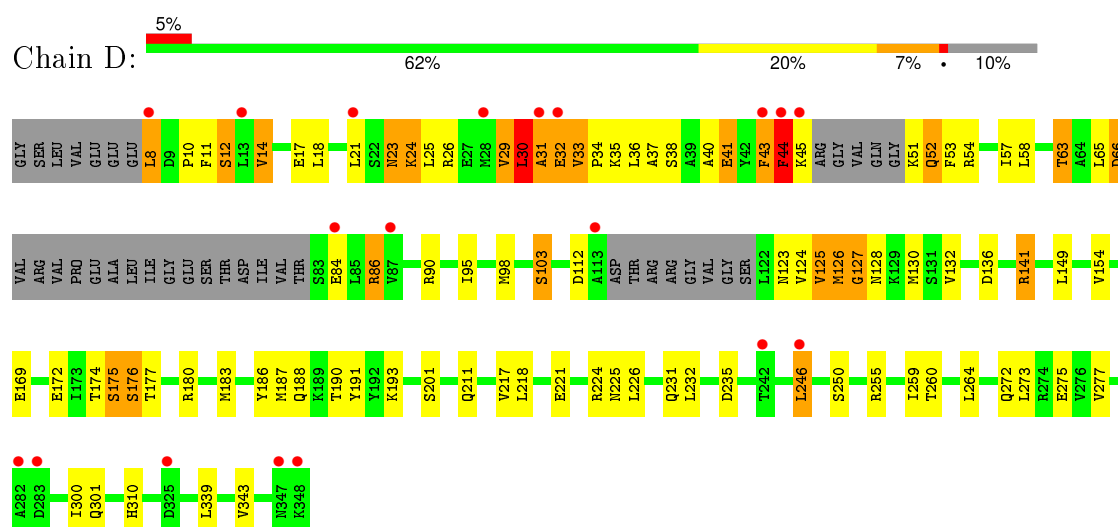


• Molecule 1: Geranyl diphosphate synthase

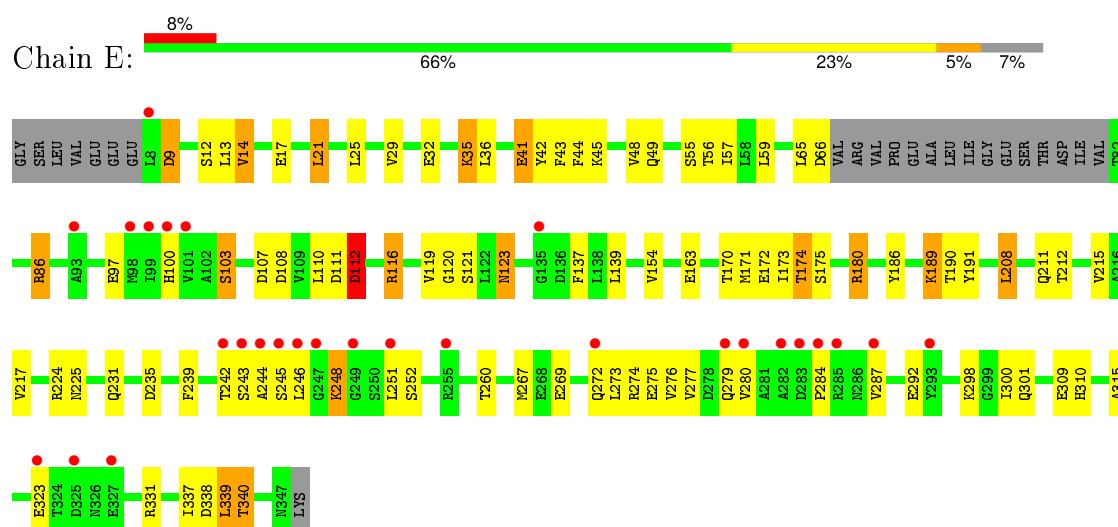




• Molecule 1: Geranyl diphosphate synthase

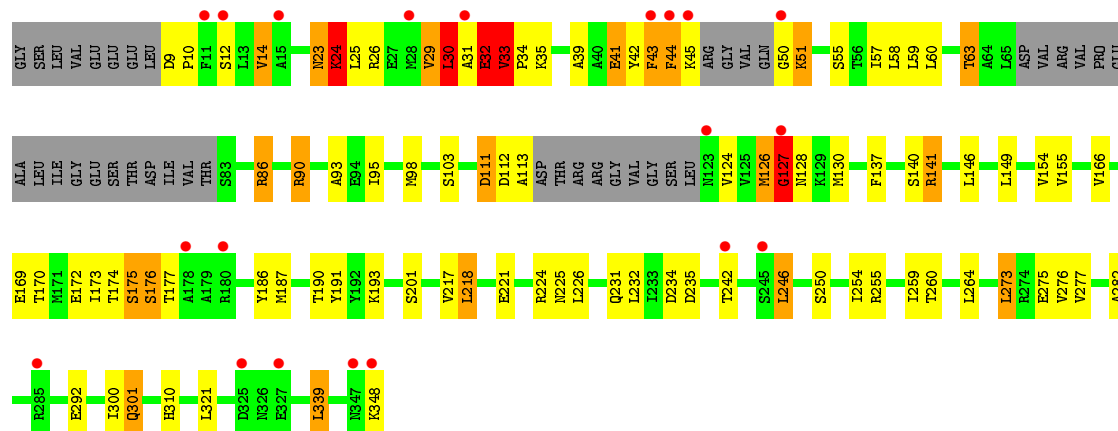


• Molecule 1: Geranyl diphosphate synthase

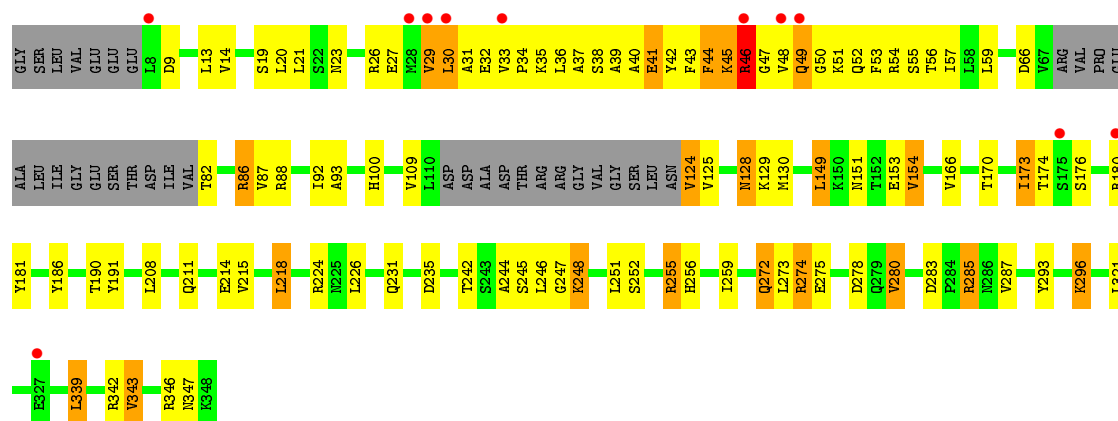


• Molecule 1: Geranyl diphosphate synthase

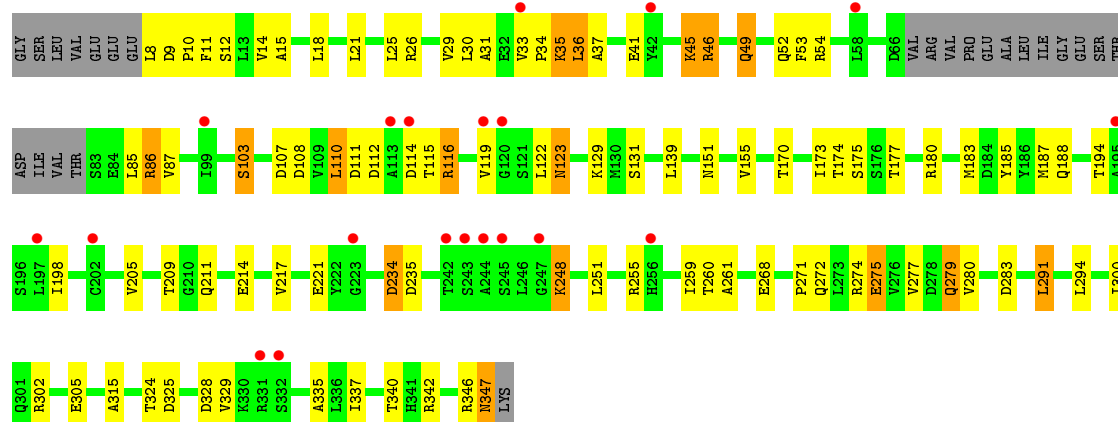




• Molecule 1: Geranyl diphosphate synthase



• Molecule 1: Geranyl diphosphate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	115.96Å 115.96Å 385.87Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.65 29.83 – 2.65	Depositor EDS
% Data completeness (in resolution range)	98.6 (30.00-2.65) 98.7 (29.83-2.65)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 2.64Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.222 , 0.274 0.250 , 0.285	Depositor DCC
R_{free} test set	4167 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	69.0	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 61.6	EDS
Estimated twinning fraction	0.944 for H, K, L 0.056 for -H-K, K, -L 0.047 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.944 for H, K, L 0.056 for -H-K, K, -L	Depositor
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 83457 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	20426	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.45% 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, 0.375 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, PEG, ISY, FPP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.45	0/2516	0.64	2/3399 (0.1%)
1	B	0.61	0/2421	0.70	1/3269 (0.0%)
1	C	0.56	1/2524 (0.0%)	0.68	2/3412 (0.1%)
1	D	0.53	0/2414	0.67	0/3260
1	E	0.47	1/2506 (0.0%)	0.66	1/3388 (0.0%)
1	F	0.49	0/2394	0.67	3/3232 (0.1%)
1	G	0.61	0/2427	0.71	1/3278 (0.0%)
1	H	0.42	0/2499	0.62	0/3378
All	All	0.52	2/19701 (0.0%)	0.67	10/26616 (0.0%)

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	B	0	1
1	D	0	2
1	F	0	1
1	G	0	1
All	All	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	217	VAL	CB-CG1	-6.83	1.38	1.52
1	E	217	VAL	CB-CG2	-6.45	1.39	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	36	LEU	CA-CB-CG	6.40	130.03	115.30
1	G	149	LEU	CA-CB-CG	6.23	129.63	115.30
1	E	217	VAL	CG1-CB-CG2	-6.13	101.09	110.90
1	F	32	GLU	CB-CA-C	-6.09	98.22	110.40
1	F	127	GLY	N-CA-C	5.83	127.67	113.10
1	C	112	ASP	CB-CG-OD2	5.68	123.41	118.30
1	C	217	VAL	CG1-CB-CG2	-5.21	102.57	110.90
1	B	158	LEU	CA-CB-CG	-5.08	103.61	115.30
1	A	36	LEU	CB-CG-CD1	5.08	119.63	111.00
1	F	31	ALA	C-N-CA	5.06	134.35	121.70

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	35	LYS	Peptide
1	D	31	ALA	Peptide
1	D	32	GLU	Peptide
1	F	32	GLU	Peptide
1	G	35	LYS	Peptide

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	2488	0	2546	67	2
1	B	2394	0	2446	161	0
1	C	2496	0	2545	91	0
1	D	2388	0	2442	131	0
1	E	2478	0	2531	81	0
1	F	2368	0	2419	115	0
1	G	2400	0	2465	169	0
1	H	2471	0	2524	74	2
2	A	2	0	0	0	0
2	C	2	0	0	0	0
2	E	2	0	0	0	0
2	H	2	0	0	0	0
3	A	24	0	25	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	24	0	25	6	0
3	C	24	0	25	7	0
3	E	24	0	25	2	0
3	G	24	0	25	4	0
3	H	24	0	25	2	0
4	A	14	0	9	3	0
4	H	14	0	9	2	0
5	B	9	0	0	3	0
5	C	9	0	0	0	0
5	D	9	0	0	0	0
5	E	9	0	0	0	0
5	F	9	0	0	0	0
5	G	9	0	0	0	0
6	B	7	0	10	1	0
6	D	7	0	10	0	0
7	A	83	0	0	5	0
7	B	98	0	0	8	0
7	C	116	0	0	5	0
7	D	100	0	0	6	0
7	E	67	0	0	0	0
7	F	78	0	0	3	0
7	G	77	0	0	5	0
7	H	76	0	0	3	0
All	All	20426	0	20106	781	2

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 (781) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:VAL:HG13	1:B:49:GLN:CA	1.34	1.55
1:G:46:ARG:HD2	1:G:49:GLN:CA	1.43	1.49
1:C:274:ARG:NH2	1:F:30:LEU:HD11	1.15	1.39
1:B:48:VAL:HG22	1:B:50:GLY:N	1.40	1.34
1:G:46:ARG:CD	1:G:49:GLN:HA	1.60	1.31
1:D:30:LEU:HD11	1:E:274:ARG:NH2	1.48	1.28
1:B:48:VAL:CG1	1:B:49:GLN:HA	1.71	1.20
1:C:274:ARG:NH2	1:F:30:LEU:CD1	2.06	1.18
1:B:46:ARG:HE	1:B:48:VAL:HG12	1.01	1.13
1:B:256:HIS:CE1	7:B:551:HOH:O	2.02	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:VAL:CG1	1:B:49:GLN:CA	2.29	1.09
1:D:44:PHE:CE2	1:G:26:ARG:HD2	1.87	1.08
1:B:48:VAL:HG22	1:B:49:GLN:C	1.72	1.08
1:G:86:ARG:HG3	1:G:86:ARG:HH11	1.17	1.07
1:C:274:ARG:HH21	1:F:30:LEU:CD1	1.65	1.06
1:B:46:ARG:NH2	1:B:48:VAL:HG11	1.70	1.05
1:B:46:ARG:NE	1:B:48:VAL:HG12	1.71	1.05
1:G:49:GLN:HE21	1:G:49:GLN:C	1.60	1.05
1:B:46:ARG:HE	1:B:48:VAL:CG1	1.69	1.03
1:C:193:LYS:HE3	3:C:1002:FPP:H11	1.34	1.03
1:A:175:SER:HB3	1:A:185:TYR:OH	1.57	1.03
1:G:46:ARG:CG	1:G:47:GLY:H	1.71	1.02
1:G:255:ARG:HH11	1:G:255:ARG:HG3	1.23	1.02
1:G:255:ARG:HH11	1:G:255:ARG:CG	1.71	1.02
1:B:255:ARG:HG3	1:B:255:ARG:HH11	1.21	1.01
7:A:583:HOH:O	1:C:308:MET:HE1	1.58	1.01
1:C:211:GLN:HG2	1:C:215:VAL:HG11	1.40	1.01
1:D:26:ARG:O	1:D:30:LEU:HB2	1.61	1.01
1:B:48:VAL:CG2	1:B:49:GLN:C	2.28	1.00
1:B:46:ARG:HH21	1:B:48:VAL:CG1	1.72	0.99
1:F:26:ARG:O	1:F:30:LEU:HB2	1.62	0.99
1:B:88:ARG:NH2	1:B:149:LEU:O	1.96	0.99
1:G:46:ARG:HD2	1:G:49:GLN:HA	1.00	0.98
1:D:127:GLY:HA2	1:D:130:MET:HB2	1.42	0.98
1:C:193:LYS:HE3	3:C:1002:FPP:C1	1.92	0.98
1:B:48:VAL:HG13	1:B:49:GLN:C	1.83	0.97
1:B:255:ARG:CG	1:B:255:ARG:HH11	1.78	0.97
1:B:86:ARG:HH11	1:B:86:ARG:HG3	1.23	0.97
1:D:141:ARG:HH11	1:D:141:ARG:HG3	1.28	0.97
1:G:86:ARG:CG	1:G:86:ARG:HH11	1.78	0.96
1:B:48:VAL:HG22	1:B:50:GLY:CA	1.95	0.96
1:D:30:LEU:HD11	1:E:274:ARG:HH22	1.23	0.96
1:G:46:ARG:CD	1:G:47:GLY:H	1.78	0.95
1:B:48:VAL:CG2	1:B:50:GLY:N	2.30	0.95
1:A:342:ARG:O	1:A:346:ARG:HG3	1.67	0.94
1:B:48:VAL:CG1	1:B:49:GLN:C	2.36	0.94
1:C:106:HIS:HD2	1:D:136:ASP:OD2	1.49	0.93
1:D:44:PHE:CZ	1:G:29:VAL:HG11	2.03	0.93
1:H:175:SER:HB3	1:H:185:TYR:OH	1.69	0.93
1:G:46:ARG:HD2	1:G:49:GLN:CB	1.98	0.93
1:G:43:PHE:O	1:G:46:ARG:HB3	1.68	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:THR:O	1:A:174:THR:HG22	1.70	0.92
1:G:46:ARG:CG	1:G:47:GLY:N	2.30	0.92
1:A:35:LYS:HD2	1:B:174:THR:HG21	1.49	0.92
1:H:175:SER:OG	1:H:180:ARG:HG3	1.70	0.91
1:G:46:ARG:HG3	1:G:47:GLY:N	1.82	0.91
1:G:46:ARG:HD3	1:G:47:GLY:H	1.34	0.91
1:E:315:ALA:HB2	1:E:340:THR:HG21	1.52	0.91
1:B:46:ARG:NH2	1:B:48:VAL:CG1	2.30	0.91
1:D:30:LEU:CD1	1:E:274:ARG:NH2	2.33	0.91
1:E:65:LEU:O	1:E:66:ASP:HB3	1.71	0.91
1:B:46:ARG:NE	1:B:48:VAL:CG1	2.30	0.91
1:C:86:ARG:HH11	1:C:86:ARG:CG	1.84	0.91
1:B:46:ARG:HH21	1:B:48:VAL:HG11	1.26	0.90
1:D:14:VAL:HG21	1:G:59:LEU:HB2	1.53	0.90
1:G:88:ARG:NH2	1:G:149:LEU:O	2.05	0.90
1:C:274:ARG:HH22	1:F:30:LEU:HD11	1.17	0.90
1:C:315:ALA:HB2	1:C:340:THR:HG21	1.52	0.90
1:F:141:ARG:HH11	1:F:141:ARG:HG3	1.36	0.89
1:A:175:SER:OG	1:A:180:ARG:HG3	1.72	0.88
1:G:46:ARG:CD	1:G:49:GLN:CA	2.30	0.88
1:F:186:TYR:OH	1:F:235:ASP:OD2	1.90	0.87
1:E:86:ARG:CG	1:E:86:ARG:HH11	1.87	0.87
1:D:41:GLU:HG2	1:H:173:ILE:HG23	1.55	0.86
1:B:48:VAL:CG2	1:B:50:GLY:CA	2.51	0.86
1:B:86:ARG:HH11	1:B:86:ARG:CG	1.88	0.86
1:D:126:MET:C	1:D:128:ASN:H	1.76	0.86
1:G:46:ARG:HD2	1:G:49:GLN:N	1.90	0.85
1:H:170:THR:O	1:H:174:THR:HG22	1.75	0.85
1:C:106:HIS:CD2	1:D:136:ASP:OD2	2.29	0.85
1:G:40:ALA:O	1:G:44:PHE:CE1	2.29	0.85
1:A:173:ILE:HG23	1:F:41:GLU:HG2	1.58	0.85
1:G:49:GLN:NE2	1:G:49:GLN:C	2.30	0.85
1:G:273:LEU:HD12	1:G:293:TYR:CB	2.08	0.84
1:B:255:ARG:HG3	1:B:255:ARG:NH1	1.90	0.84
1:D:186:TYR:OH	1:D:235:ASP:OD2	1.94	0.84
1:H:86:ARG:CG	1:H:86:ARG:HH11	1.90	0.83
1:D:30:LEU:HD21	1:E:274:ARG:HH21	1.41	0.83
1:B:48:VAL:CG2	1:B:50:GLY:HA2	2.08	0.83
1:D:25:LEU:HD21	1:G:49:GLN:OE1	1.78	0.82
1:C:32:GLU:HG2	7:C:377:HOH:O	1.78	0.82
1:B:43:PHE:O	1:B:46:ARG:HG3	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:255:ARG:HG3	1:G:255:ARG:NH1	1.90	0.81
1:B:43:PHE:O	1:B:46:ARG:CG	2.29	0.80
1:G:174:THR:HG21	1:H:35:LYS:HD2	1.61	0.80
1:C:193:LYS:CE	3:C:1002:FPP:H11	2.09	0.80
1:B:186:TYR:OH	1:B:235:ASP:OD2	2.00	0.80
1:B:342:ARG:HD3	3:B:1001:FPP:H42	1.61	0.80
1:B:46:ARG:CZ	1:B:48:VAL:CG1	2.60	0.80
1:G:45:LYS:NZ	7:G:361:HOH:O	2.10	0.80
1:G:186:TYR:OH	1:G:235:ASP:OD2	1.99	0.80
1:G:44:PHE:H	1:G:44:PHE:HD1	1.30	0.80
1:B:48:VAL:CG1	1:B:49:GLN:O	2.30	0.79
1:D:17:GLU:CD	1:G:86:ARG:HH12	1.85	0.79
1:B:244:ALA:HB3	7:B:545:HOH:O	1.80	0.79
1:B:48:VAL:HG13	1:B:49:GLN:HA	0.80	0.79
1:G:48:VAL:CG2	1:G:48:VAL:O	2.30	0.79
7:A:583:HOH:O	1:C:308:MET:CE	2.22	0.79
1:B:44:PHE:N	1:B:44:PHE:HD1	1.80	0.79
1:D:30:LEU:HD11	1:E:274:ARG:HH21	1.42	0.79
1:D:124:VAL:HG23	7:D:477:HOH:O	1.82	0.78
1:G:49:GLN:NE2	1:G:50:GLY:N	2.30	0.78
1:A:86:ARG:CG	1:A:86:ARG:HH11	1.97	0.78
1:D:14:VAL:HG23	1:G:59:LEU:HD13	1.65	0.78
1:A:271:PRO:O	1:A:274:ARG:HG3	1.84	0.78
1:G:53:PHE:HB3	3:G:1001:FPP:H92	1.65	0.77
1:D:17:GLU:OE1	1:G:86:ARG:NH1	2.17	0.77
1:D:127:GLY:HA2	1:D:130:MET:CB	2.14	0.77
1:A:35:LYS:HD2	1:B:174:THR:CG2	2.14	0.77
1:G:46:ARG:NE	1:G:49:GLN:HA	1.98	0.77
1:G:40:ALA:O	1:G:44:PHE:CD1	2.36	0.77
1:B:44:PHE:H	1:B:44:PHE:HD1	1.33	0.77
1:B:48:VAL:HG21	1:B:50:GLY:HA2	1.66	0.77
1:G:86:ARG:NH1	1:G:86:ARG:HG3	1.93	0.76
1:B:47:GLY:O	1:B:48:VAL:HB	1.85	0.76
1:B:40:ALA:O	1:B:44:PHE:CD1	2.39	0.76
1:E:275:GLU:O	1:E:279:GLN:NE2	2.18	0.75
1:D:44:PHE:CD2	1:G:26:ARG:HD2	2.20	0.75
1:G:273:LEU:HD12	1:G:293:TYR:CG	2.20	0.75
1:B:256:HIS:HE1	7:B:551:HOH:O	1.53	0.75
1:D:44:PHE:CE2	1:G:29:VAL:HG11	2.20	0.74
1:E:211:GLN:HG3	1:E:215:VAL:HG11	1.69	0.74
1:C:123:ASN:H	1:C:123:ASN:HD22	1.34	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:VAL:HG11	1:B:49:GLN:O	1.88	0.74
1:G:46:ARG:CD	1:G:49:GLN:HB2	2.17	0.74
1:G:128:ASN:C	1:G:128:ASN:HD22	1.91	0.74
1:G:211:GLN:HE21	1:G:215:VAL:HG11	1.53	0.74
1:G:273:LEU:HD12	1:G:293:TYR:HB3	1.70	0.74
1:G:46:ARG:CD	1:G:49:GLN:CB	2.63	0.73
1:C:275:GLU:O	1:C:279:GLN:NE2	2.22	0.73
1:F:175:SER:O	1:F:177:THR:N	2.21	0.73
1:B:243:SER:HB3	7:B:543:HOH:O	1.87	0.73
1:E:14:VAL:HG11	1:E:56:THR:HG23	1.69	0.73
1:D:126:MET:C	1:D:128:ASN:N	2.39	0.73
1:A:86:ARG:HH11	1:A:86:ARG:HG2	1.54	0.73
1:C:274:ARG:HH21	1:F:30:LEU:HD11	0.92	0.73
1:G:174:THR:CG2	1:H:35:LYS:HD2	2.18	0.72
1:H:9:ASP:HB2	1:H:10:PRO:HD2	1.70	0.72
1:B:49:GLN:HG2	1:B:50:GLY:N	2.02	0.72
1:B:86:ARG:HG3	1:B:86:ARG:NH1	1.99	0.72
1:G:44:PHE:N	1:G:44:PHE:CD1	2.56	0.72
1:H:342:ARG:O	1:H:346:ARG:HG3	1.90	0.72
1:D:14:VAL:HG23	1:G:59:LEU:CD1	2.20	0.72
1:F:175:SER:O	1:F:176:SER:C	2.26	0.71
1:H:11:PHE:HE1	1:H:53:PHE:CE1	2.09	0.71
1:B:273:LEU:HD23	1:B:277:VAL:HG23	1.72	0.71
1:A:11:PHE:HE1	1:A:53:PHE:HE1	1.37	0.71
1:H:337:ILE:O	1:H:340:THR:HB	1.91	0.71
1:G:44:PHE:N	1:G:44:PHE:HD1	1.88	0.71
1:A:277:VAL:O	1:A:280:VAL:HG12	1.90	0.71
1:A:11:PHE:HE1	1:A:53:PHE:CE1	2.08	0.71
1:B:49:GLN:CG	1:B:50:GLY:N	2.53	0.71
1:D:30:LEU:CD2	1:E:274:ARG:HH21	2.04	0.71
1:E:86:ARG:HG3	1:E:86:ARG:HH11	1.56	0.71
1:B:46:ARG:CZ	1:B:48:VAL:HG12	2.20	0.70
1:B:44:PHE:CD1	1:B:44:PHE:N	2.53	0.70
1:G:242:THR:H	1:G:245:SER:HB3	1.55	0.70
1:G:36:LEU:O	1:G:39:ALA:N	2.24	0.70
1:H:11:PHE:HE1	1:H:53:PHE:HE1	1.38	0.70
1:B:48:VAL:HG13	1:B:49:GLN:N	2.06	0.70
1:B:255:ARG:HB2	1:B:256:HIS:HD2	1.56	0.70
1:H:277:VAL:O	1:H:280:VAL:HG12	1.92	0.69
1:G:49:GLN:HE21	1:G:50:GLY:N	1.88	0.69
1:C:86:ARG:HH11	1:C:86:ARG:HG2	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:86:ARG:HH11	1:C:86:ARG:HG3	1.57	0.69
1:F:255:ARG:HG2	1:F:255:ARG:HH11	1.57	0.69
1:H:31:ALA:O	1:H:37:ALA:HB2	1.92	0.69
1:D:14:VAL:HG21	1:G:59:LEU:CB	2.21	0.69
1:A:107:ASP:O	1:A:110:LEU:O	2.10	0.69
1:B:36:LEU:O	1:B:39:ALA:N	2.25	0.69
1:G:46:ARG:HG2	1:G:49:GLN:HB2	1.75	0.69
1:C:284:PRO:O	1:C:287:VAL:HG12	1.93	0.68
1:H:10:PRO:HB3	1:H:335:ALA:HB1	1.74	0.68
1:H:116:ARG:NH2	3:H:1002:FPP:O2B	2.26	0.68
1:D:44:PHE:N	1:D:44:PHE:CD2	2.58	0.68
1:B:17:GLU:HG2	1:F:90:ARG:HH11	1.58	0.68
1:G:273:LEU:CD1	1:G:293:TYR:HB3	2.23	0.68
1:B:21:LEU:HD11	1:F:93:ALA:HB3	1.74	0.68
1:D:125:VAL:HG12	1:D:126:MET:H	1.59	0.68
1:B:273:LEU:HD12	1:B:293:TYR:HB3	1.76	0.68
1:A:209:THR:OG1	1:A:211:GLN:HG2	1.94	0.68
1:A:173:ILE:HG23	1:F:41:GLU:CG	2.24	0.68
1:D:23:ASN:O	1:D:26:ARG:N	2.26	0.68
1:H:86:ARG:HH11	1:H:86:ARG:HG2	1.59	0.68
1:D:41:GLU:O	1:D:44:PHE:O	2.12	0.67
1:D:255:ARG:HH11	1:D:255:ARG:HG2	1.59	0.67
1:A:337:ILE:O	1:A:340:THR:HB	1.93	0.67
1:C:7:GLU:OE1	1:C:334:ARG:NE	2.20	0.67
1:D:14:VAL:CG2	1:G:59:LEU:CD1	2.73	0.67
1:B:211:GLN:HE21	1:B:215:VAL:HG11	1.58	0.67
1:H:248:LYS:HB2	7:H:521:HOH:O	1.94	0.67
1:E:284:PRO:O	1:E:287:VAL:HG12	1.95	0.67
1:D:40:ALA:HB1	1:G:29:VAL:HG22	1.77	0.67
1:B:108:ASP:O	1:B:110:LEU:HD22	1.94	0.67
1:D:14:VAL:O	1:D:14:VAL:CG2	2.43	0.67
1:B:10:PRO:HB3	1:F:60:LEU:HD11	1.77	0.67
1:A:51:LYS:O	7:A:638:HOH:O	2.13	0.67
1:A:110:LEU:C	1:A:112:ASP:H	1.98	0.66
1:B:248:LYS:HE3	7:B:546:HOH:O	1.93	0.66
1:E:337:ILE:O	1:E:340:THR:HB	1.95	0.66
1:H:209:THR:OG1	1:H:211:GLN:HG2	1.94	0.66
1:A:31:ALA:O	1:A:37:ALA:HB2	1.94	0.66
1:D:57:ILE:HD11	1:D:226:LEU:CD2	2.26	0.66
1:C:211:GLN:HG2	1:C:215:VAL:CG1	2.20	0.66
1:D:30:LEU:O	1:D:32:GLU:N	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:203:LYS:NZ	7:C:382:HOH:O	2.28	0.66
1:B:48:VAL:CG2	1:B:49:GLN:O	2.44	0.66
1:G:273:LEU:CD1	1:G:293:TYR:CB	2.74	0.66
1:F:23:ASN:O	1:F:26:ARG:N	2.24	0.65
1:D:18:LEU:HD22	1:G:52:GLN:HB3	1.77	0.65
1:D:190:THR:HG23	1:D:231:GLN:HG2	1.79	0.65
1:D:141:ARG:HH11	1:D:141:ARG:CG	2.04	0.65
1:D:10:PRO:HG2	1:G:339:LEU:HD13	1.77	0.65
1:H:271:PRO:O	1:H:274:ARG:HG3	1.96	0.65
1:B:31:ALA:O	1:B:32:GLU:HG2	1.97	0.64
1:F:14:VAL:O	1:F:14:VAL:CG2	2.44	0.64
1:E:86:ARG:HG2	1:E:86:ARG:HH11	1.62	0.64
1:A:129:LYS:HG3	1:B:109:VAL:O	1.98	0.64
1:E:35:LYS:HD2	1:F:174:THR:OG1	1.97	0.64
1:D:103:SER:HB3	7:D:576:HOH:O	1.98	0.64
1:D:141:ARG:NH1	1:D:141:ARG:HG3	2.07	0.64
1:G:255:ARG:HH11	1:G:255:ARG:HG2	1.61	0.64
1:F:126:MET:SD	1:F:126:MET:O	2.56	0.64
1:D:38:SER:HA	1:H:173:ILE:HG22	1.79	0.64
1:A:10:PRO:HB3	1:A:335:ALA:HB1	1.79	0.64
1:E:180:ARG:HD3	1:E:180:ARG:O	1.97	0.64
1:B:13:LEU:HD12	1:F:60:LEU:CD2	2.28	0.63
1:C:274:ARG:O	1:C:277:VAL:HG12	1.98	0.63
1:E:277:VAL:O	1:E:280:VAL:HG12	1.99	0.63
1:E:116:ARG:NH2	3:E:1002:FPP:O2B	2.32	0.63
1:D:174:THR:HG22	7:D:565:HOH:O	1.99	0.63
1:A:175:SER:CB	1:A:185:TYR:OH	2.41	0.62
1:D:14:VAL:CG2	1:G:59:LEU:HD12	2.28	0.62
1:G:46:ARG:HD2	1:G:49:GLN:HB2	1.77	0.62
1:C:274:ARG:HH22	1:F:30:LEU:CD1	1.94	0.62
1:C:277:VAL:O	1:C:280:VAL:HG12	1.99	0.62
1:A:175:SER:HG	1:A:180:ARG:HG3	1.63	0.62
1:G:128:ASN:C	1:G:128:ASN:ND2	2.53	0.62
1:E:171:MET:HA	1:E:174:THR:HG22	1.81	0.62
1:G:36:LEU:HG	1:G:37:ALA:N	2.15	0.62
1:B:242:THR:H	1:B:245:SER:HB3	1.65	0.62
1:D:14:VAL:HG23	1:D:14:VAL:O	2.00	0.62
1:B:54:ARG:NH2	5:B:1000:PPV:O31	2.31	0.62
1:C:180:ARG:O	1:C:180:ARG:HD3	2.00	0.62
1:H:107:ASP:O	1:H:110:LEU:O	2.16	0.62
1:D:43:PHE:HA	1:D:45:LYS:N	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:VAL:CB	1:B:49:GLN:C	2.67	0.62
1:H:86:ARG:HH11	1:H:86:ARG:HG3	1.64	0.62
1:C:14:VAL:HG11	1:C:56:THR:HG23	1.82	0.61
1:G:124:VAL:CB	1:G:125:VAL:HA	2.30	0.61
1:B:57:ILE:HD11	1:B:226:LEU:HD23	1.82	0.61
1:A:315:ALA:HB2	1:A:340:THR:HG21	1.81	0.61
1:A:275:GLU:N	1:A:275:GLU:OE2	2.33	0.61
1:G:46:ARG:CG	1:G:49:GLN:HB2	2.30	0.61
1:C:274:ARG:HH21	1:F:30:LEU:CG	2.13	0.61
1:C:116:ARG:NH2	3:C:1002:FPP:O2B	2.34	0.61
1:C:110:LEU:O	1:C:111:ASP:HB2	1.99	0.61
1:H:110:LEU:C	1:H:112:ASP:H	2.03	0.61
1:B:41:GLU:HG2	1:E:173:ILE:HG23	1.82	0.61
1:B:17:GLU:HB2	1:F:59:LEU:HD13	1.81	0.61
1:B:283:ASP:OD1	1:B:285:ARG:HG3	1.99	0.61
1:G:46:ARG:HE	1:G:49:GLN:HG2	1.65	0.61
1:B:251:LEU:O	1:B:255:ARG:HG2	2.01	0.61
1:H:86:ARG:CG	1:H:86:ARG:NH1	2.60	0.60
1:E:154:VAL:HG21	1:E:208:LEU:HD13	1.82	0.60
1:H:275:GLU:N	1:H:275:GLU:OE2	2.34	0.60
1:C:42:TYR:O	1:C:45:LYS:HG3	2.00	0.60
1:D:125:VAL:CG1	1:D:126:MET:N	2.63	0.60
1:D:57:ILE:HD11	1:D:226:LEU:HD21	1.83	0.60
1:B:255:ARG:CG	1:B:255:ARG:NH1	2.48	0.60
1:D:33:VAL:H	1:D:34:PRO:HD2	1.66	0.60
1:G:48:VAL:HG22	1:G:48:VAL:O	2.01	0.60
1:D:17:GLU:CD	1:G:86:ARG:NH1	2.53	0.60
1:B:256:HIS:NE2	1:F:113:ALA:HB1	2.15	0.60
1:H:175:SER:HB3	1:H:185:TYR:CZ	2.36	0.60
1:B:242:THR:HB	1:B:245:SER:HB3	1.82	0.60
1:G:255:ARG:CG	1:G:255:ARG:NH1	2.42	0.60
1:A:175:SER:HB3	1:A:185:TYR:CZ	2.36	0.60
1:H:54:ARG:NH1	4:H:1003:ISY:S9	2.74	0.60
1:F:41:GLU:O	1:F:44:PHE:O	2.20	0.60
1:G:57:ILE:HD11	1:G:226:LEU:HD23	1.84	0.60
1:D:175:SER:O	1:D:177:THR:N	2.35	0.60
1:E:274:ARG:O	1:E:277:VAL:HG12	2.02	0.60
1:D:44:PHE:HZ	1:G:29:VAL:HG11	1.64	0.60
1:D:17:GLU:OE2	1:G:86:ARG:NH1	2.35	0.60
1:E:137:PHE:HB2	1:F:166:VAL:HG11	1.82	0.60
1:G:46:ARG:HD3	1:G:47:GLY:N	2.12	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:123:ASN:HD22	1:E:123:ASN:H	1.50	0.60
1:C:100:HIS:O	1:C:103:SER:HB2	2.02	0.60
1:G:166:VAL:HG12	1:H:36:LEU:HD11	1.82	0.60
1:F:126:MET:SD	1:F:126:MET:N	2.75	0.59
1:F:43:PHE:H	1:F:45:LYS:C	2.05	0.59
1:G:242:THR:N	1:G:245:SER:HB3	2.16	0.59
1:G:48:VAL:HG23	1:G:48:VAL:O	2.01	0.59
1:C:86:ARG:NH1	1:C:86:ARG:CG	2.56	0.59
1:C:171:MET:HA	1:C:174:THR:HG22	1.85	0.59
1:E:100:HIS:O	1:E:103:SER:HB2	2.01	0.59
1:F:169:GLU:HA	1:F:169:GLU:OE1	2.03	0.59
1:F:275:GLU:OE1	1:F:275:GLU:HA	2.02	0.59
1:D:30:LEU:CD1	1:E:274:ARG:HH22	2.04	0.59
1:G:49:GLN:NE2	1:G:50:GLY:CA	2.65	0.59
1:G:47:GLY:O	1:G:48:VAL:C	2.38	0.59
1:D:18:LEU:O	1:G:52:GLN:NE2	2.36	0.59
1:F:141:ARG:NH1	1:F:141:ARG:HG3	2.12	0.59
1:C:337:ILE:O	1:C:340:THR:HB	2.03	0.59
1:G:242:THR:HB	1:G:245:SER:HB3	1.85	0.59
1:B:14:VAL:HG11	1:F:59:LEU:HB3	1.83	0.59
1:A:108:ASP:OD1	1:A:116:ARG:NH1	2.34	0.59
1:D:44:PHE:CD2	1:G:26:ARG:CD	2.86	0.58
1:A:123:ASN:H	1:A:123:ASN:HD22	1.51	0.58
1:H:175:SER:CB	1:H:185:TYR:OH	2.47	0.58
1:C:111:ASP:O	1:C:112:ASP:C	2.41	0.58
1:B:273:LEU:HD23	1:B:277:VAL:CG2	2.32	0.58
1:E:248:LYS:NZ	1:E:248:LYS:HB2	2.18	0.58
1:D:30:LEU:CD1	1:E:274:ARG:HH21	2.06	0.58
1:B:273:LEU:HD12	1:B:293:TYR:CB	2.33	0.58
1:B:10:PRO:HG2	1:F:339:LEU:HD13	1.86	0.58
1:F:126:MET:HB2	1:F:130:MET:HB2	1.85	0.58
1:C:173:ILE:HG23	1:G:41:GLU:HG2	1.85	0.58
1:G:181:TYR:OH	1:G:278:ASP:OD1	2.22	0.58
1:B:40:ALA:O	1:B:44:PHE:CE1	2.57	0.58
1:B:17:GLU:CG	1:F:90:ARG:HH11	2.17	0.58
1:G:29:VAL:CG1	1:G:30:LEU:N	2.67	0.58
1:D:169:GLU:HA	1:D:169:GLU:OE1	2.03	0.57
1:G:23:ASN:HD21	1:H:279:GLN:CD	2.08	0.57
1:C:248:LYS:NZ	1:C:248:LYS:HB2	2.19	0.57
1:D:141:ARG:NH1	1:D:141:ARG:CG	2.66	0.57
1:B:57:ILE:CD1	1:B:226:LEU:HD23	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:242:THR:HG22	1:C:248:LYS:HD3	1.84	0.57
1:B:234:ASP:OD2	1:B:346:ARG:NH2	2.36	0.57
1:B:242:THR:N	1:B:245:SER:HB3	2.20	0.57
1:E:42:TYR:O	1:E:45:LYS:HG3	2.04	0.57
1:F:33:VAL:H	1:F:34:PRO:HD2	1.70	0.57
1:G:242:THR:HG22	1:G:244:ALA:N	2.18	0.57
1:C:107:ASP:O	1:C:110:LEU:O	2.22	0.57
1:D:58:LEU:HD21	1:D:201:SER:HB3	1.86	0.57
1:F:44:PHE:O	1:F:45:LYS:HB2	2.04	0.57
1:H:123:ASN:HD22	1:H:123:ASN:H	1.53	0.57
1:E:36:LEU:HB2	1:F:170:THR:HG21	1.86	0.57
1:B:246:LEU:N	1:B:247:GLY:HA2	2.20	0.57
1:D:63:THR:HG23	1:D:86:ARG:NH2	2.20	0.57
1:D:57:ILE:CD1	1:D:226:LEU:HD23	2.35	0.56
1:B:46:ARG:HH21	1:B:48:VAL:HG12	1.63	0.56
1:B:48:VAL:HG21	1:B:49:GLN:O	2.06	0.56
1:B:46:ARG:NH2	1:B:48:VAL:HG12	2.13	0.56
1:C:17:GLU:OE2	1:C:86:ARG:NH1	2.36	0.56
1:E:55:SER:OG	1:E:97:GLU:OE1	2.23	0.56
1:E:119:VAL:CG1	1:E:120:GLY:N	2.68	0.56
1:A:52:GLN:OE1	7:A:438:HOH:O	2.18	0.56
1:A:133:LEU:HB3	1:B:166:VAL:HG13	1.87	0.56
1:A:54:ARG:NH2	4:A:1003:ISY:H11	2.20	0.56
1:C:327:GLU:HG3	7:C:589:HOH:O	2.05	0.56
1:G:57:ILE:CD1	1:G:226:LEU:HD23	2.34	0.56
1:G:40:ALA:O	1:G:44:PHE:HE1	1.88	0.56
1:E:309:GLU:HG2	1:H:187:MET:HG3	1.87	0.56
1:B:130:MET:HE3	1:F:39:ALA:HB2	1.88	0.56
1:H:175:SER:HG	1:H:180:ARG:HG3	1.71	0.56
1:C:154:VAL:HG21	1:C:208:LEU:HD13	1.87	0.56
1:A:194:THR:O	1:A:198:ILE:HD12	2.06	0.56
1:D:125:VAL:HG12	1:D:126:MET:N	2.21	0.56
1:D:18:LEU:HD23	1:G:55:SER:HB3	1.88	0.56
1:B:342:ARG:HD3	3:B:1001:FPP:C4	2.35	0.56
1:H:315:ALA:HB2	1:H:340:THR:HG21	1.87	0.56
1:H:108:ASP:OD1	1:H:116:ARG:NH1	2.39	0.56
1:G:181:TYR:CE1	1:G:259:ILE:HD13	2.41	0.56
1:F:57:ILE:HD11	1:F:226:LEU:CD2	2.36	0.56
1:B:218:LEU:HD23	1:B:321:LEU:HD23	1.87	0.56
1:B:245:SER:C	1:B:247:GLY:HA2	2.26	0.56
1:B:17:GLU:OE1	1:F:86:ARG:NH1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:37:ALA:CB	1:H:174:THR:O	2.53	0.55
1:H:122:LEU:HD23	1:H:131:SER:HA	1.88	0.55
1:A:242:THR:HA	1:A:348:LYS:HG2	1.88	0.55
1:B:36:LEU:HG	1:B:37:ALA:N	2.21	0.55
1:G:46:ARG:HB2	1:G:46:ARG:NH1	2.22	0.55
1:B:242:THR:HG22	1:B:244:ALA:N	2.21	0.55
1:G:29:VAL:HG13	1:G:30:LEU:N	2.22	0.55
1:G:255:ARG:HB2	1:G:256:HIS:HD2	1.71	0.55
1:F:141:ARG:HH11	1:F:141:ARG:CG	2.14	0.55
1:D:187:MET:HE3	1:D:232:LEU:HD21	1.88	0.55
1:G:170:THR:OG1	1:H:36:LEU:HD12	2.07	0.55
1:D:187:MET:CE	1:D:232:LEU:HD21	2.37	0.55
1:E:119:VAL:HG12	1:E:120:GLY:N	2.22	0.55
1:D:21:LEU:HD11	1:G:93:ALA:HB3	1.89	0.55
1:B:181:TYR:OH	1:B:278:ASP:OD1	2.20	0.55
1:F:95:ILE:HA	1:F:98:MET:HE2	1.89	0.55
1:D:63:THR:HG23	1:D:86:ARG:HH21	1.71	0.54
1:C:41:GLU:O	1:C:43:PHE:O	2.25	0.54
6:B:1002:PEG:H42	1:F:137:PHE:HB2	1.89	0.54
1:D:246:LEU:HD11	1:D:300:ILE:HG13	1.90	0.54
1:E:17:GLU:OE2	1:E:86:ARG:NH1	2.37	0.54
1:B:46:ARG:CZ	1:B:48:VAL:HG11	2.31	0.54
1:G:46:ARG:HB2	1:G:46:ARG:CZ	2.38	0.54
1:D:127:GLY:CA	1:D:130:MET:HB2	2.27	0.54
1:C:170:THR:O	1:C:174:THR:HB	2.07	0.54
1:C:86:ARG:HG3	1:C:86:ARG:NH1	2.20	0.54
1:H:33:VAL:CG1	1:H:34:PRO:HD2	2.37	0.54
1:H:29:VAL:HG12	1:H:29:VAL:O	2.08	0.54
1:H:324:THR:HG21	1:H:329:VAL:HG11	1.89	0.54
1:E:86:ARG:NH1	1:E:86:ARG:HG3	2.21	0.54
1:B:89:GLN:NE2	1:B:209:THR:OG1	2.39	0.54
1:F:246:LEU:HD11	1:F:300:ILE:HG13	1.90	0.54
1:F:23:ASN:C	1:F:23:ASN:OD1	2.46	0.54
1:G:343:VAL:HG23	3:G:1001:FPP:H102	1.88	0.54
1:F:63:THR:HG23	1:F:86:ARG:HH21	1.73	0.54
1:A:294:LEU:HD21	1:A:300:ILE:HD11	1.90	0.54
1:E:111:ASP:O	1:E:112:ASP:C	2.46	0.54
1:C:146:LEU:HD21	1:C:158:LEU:HD13	1.90	0.53
1:F:30:LEU:O	1:F:32:GLU:C	2.47	0.53
1:B:242:THR:HG22	1:B:244:ALA:H	1.72	0.53
1:B:29:VAL:CG1	1:B:30:LEU:N	2.71	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:LEU:C	1:A:112:ASP:N	2.62	0.53
1:D:41:GLU:CG	1:H:173:ILE:HG23	2.33	0.53
1:B:17:GLU:HB3	1:F:90:ARG:HD3	1.90	0.53
1:H:103:SER:HB2	3:H:1002:FPP:H61	1.90	0.53
1:D:8:LEU:O	1:D:12:SER:OG	2.25	0.53
1:H:294:LEU:HD21	1:H:300:ILE:HD11	1.91	0.53
1:F:14:VAL:O	1:F:14:VAL:HG23	2.09	0.53
1:F:126:MET:HA	1:F:128:ASN:N	2.23	0.53
1:A:18:LEU:HD21	1:A:52:GLN:HB2	1.91	0.53
1:F:57:ILE:CD1	1:F:226:LEU:HD23	2.39	0.53
1:E:41:GLU:O	1:E:43:PHE:O	2.25	0.53
1:C:123:ASN:N	1:C:123:ASN:HD22	2.05	0.52
1:H:54:ARG:NH2	4:H:1003:ISY:H11	2.24	0.52
1:A:33:VAL:CG1	1:A:34:PRO:HD2	2.40	0.52
1:H:194:THR:O	1:H:198:ILE:HD12	2.08	0.52
1:G:181:TYR:HE1	1:G:259:ILE:HD13	1.74	0.52
1:C:9:ASP:HB3	1:C:12:SER:OG	2.09	0.52
1:C:14:VAL:HG21	1:C:59:LEU:HB2	1.92	0.52
1:G:272:GLN:HG2	7:G:532:HOH:O	2.09	0.52
1:D:90:ARG:HG2	1:G:21:LEU:HD21	1.90	0.52
1:G:46:ARG:HE	1:G:49:GLN:CG	2.22	0.52
1:A:35:LYS:CD	1:B:174:THR:HG21	2.32	0.52
1:G:124:VAL:HB	1:G:125:VAL:HA	1.91	0.52
1:D:126:MET:O	1:D:128:ASN:N	2.42	0.52
1:B:21:LEU:CD1	1:F:93:ALA:HB3	2.40	0.52
1:C:119:VAL:CG1	1:C:120:GLY:N	2.73	0.52
1:G:31:ALA:O	1:G:32:GLU:HG2	2.09	0.52
1:F:33:VAL:H	1:F:34:PRO:CD	2.23	0.52
1:E:267:MET:HE2	1:E:277:VAL:HG11	1.92	0.51
1:F:190:THR:HG23	1:F:231:GLN:HG2	1.92	0.51
1:D:44:PHE:HE1	7:H:504:HOH:O	1.93	0.51
1:G:49:GLN:NE2	1:G:50:GLY:HA3	2.25	0.51
1:G:151:ASN:HB3	1:G:154:VAL:HG13	1.92	0.51
1:B:31:ALA:C	1:B:32:GLU:HG2	2.31	0.51
1:F:63:THR:HG23	1:F:86:ARG:NH2	2.26	0.51
1:F:50:GLY:HA2	7:F:398:HOH:O	2.09	0.51
1:A:151:ASN:O	1:A:155:VAL:HG23	2.11	0.51
1:B:130:MET:CE	1:F:39:ALA:HB2	2.41	0.51
1:G:251:LEU:O	1:G:255:ARG:HG2	2.10	0.51
1:A:36:LEU:HD21	1:B:166:VAL:HG12	1.92	0.51
1:A:122:LEU:HD23	1:A:131:SER:HA	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:242:THR:HG22	1:G:244:ALA:H	1.75	0.51
1:A:29:VAL:HG12	1:A:29:VAL:O	2.11	0.51
1:H:261:ALA:HB3	7:H:392:HOH:O	2.11	0.50
1:B:107:ASP:HB3	7:B:385:HOH:O	2.09	0.50
1:F:41:GLU:HG3	1:F:42:TYR:N	2.25	0.50
1:G:211:GLN:NE2	1:G:215:VAL:HG11	2.25	0.50
1:D:259:ILE:HG22	1:D:264:LEU:HG	1.92	0.50
1:B:34:PRO:C	1:B:36:LEU:H	2.15	0.50
1:D:37:ALA:HB3	1:H:174:THR:O	2.11	0.50
1:A:86:ARG:CG	1:A:86:ARG:NH1	2.65	0.50
1:F:58:LEU:HD21	1:F:201:SER:HB3	1.93	0.50
1:E:191:TYR:CE1	1:E:224:ARG:HG3	2.47	0.50
1:D:23:ASN:O	1:D:25:LEU:N	2.45	0.50
1:E:116:ARG:HH22	3:E:1002:FPP:PB	2.34	0.50
1:D:259:ILE:HD11	1:D:277:VAL:CG1	2.41	0.50
1:A:324:THR:HG21	1:A:329:VAL:HG11	1.94	0.50
1:B:45:LYS:O	1:B:46:ARG:O	2.30	0.50
1:D:57:ILE:HD11	1:D:226:LEU:HD23	1.93	0.50
1:D:191:TYR:CE1	1:D:224:ARG:HG3	2.47	0.50
1:H:234:ASP:OD1	1:H:346:ARG:NH2	2.38	0.49
1:H:259:ILE:HG12	1:H:277:VAL:HG11	1.94	0.49
1:D:275:GLU:OE1	1:D:275:GLU:HA	2.11	0.49
1:C:274:ARG:HH21	1:F:30:LEU:CD2	2.24	0.49
1:G:36:LEU:O	1:G:39:ALA:HB3	2.12	0.49
1:B:51:LYS:HD2	5:B:1000:PPV:O22	2.12	0.49
1:B:57:ILE:HD11	1:B:226:LEU:CD2	2.42	0.49
1:E:110:LEU:O	1:E:111:ASP:HB2	2.12	0.49
1:G:45:LYS:O	1:G:46:ARG:O	2.30	0.49
1:A:345:THR:O	1:A:346:ARG:C	2.50	0.49
1:E:43:PHE:O	1:E:44:PHE:HB2	2.12	0.49
1:F:221:GLU:OE1	1:F:224:ARG:NH1	2.45	0.49
1:G:30:LEU:N	1:G:33:VAL:HG23	2.28	0.49
1:F:57:ILE:HD11	1:F:226:LEU:HD21	1.94	0.49
1:E:191:TYR:HE1	1:E:224:ARG:HG3	1.75	0.49
1:B:38:SER:O	1:B:42:TYR:CD2	2.65	0.49
1:F:23:ASN:OD1	1:F:24:LYS:N	2.45	0.49
1:D:11:PHE:CD1	1:G:56:THR:HG21	2.48	0.49
1:C:190:THR:HG23	1:C:231:GLN:HG2	1.94	0.49
1:C:267:MET:HE2	1:C:277:VAL:HG11	1.95	0.49
1:B:29:VAL:HG13	1:B:30:LEU:N	2.28	0.49
1:D:8:LEU:HB2	1:G:342:ARG:NH2	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:239:PHE:HA	1:C:251:LEU:HD23	1.95	0.49
1:B:181:TYR:CE1	1:B:259:ILE:HD13	2.48	0.49
1:D:30:LEU:HD21	1:E:274:ARG:NH2	2.19	0.49
1:E:14:VAL:HG21	1:E:59:LEU:HB2	1.95	0.49
1:H:151:ASN:O	1:H:155:VAL:HG23	2.13	0.49
1:E:186:TYR:OH	1:E:235:ASP:OD1	2.22	0.49
1:E:86:ARG:CG	1:E:86:ARG:NH1	2.58	0.48
1:E:239:PHE:HA	1:E:251:LEU:HD23	1.95	0.48
1:D:36:LEU:HD13	1:G:130:MET:HE3	1.95	0.48
1:D:53:PHE:HZ	1:D:343:VAL:CG2	2.26	0.48
1:F:42:TYR:O	1:F:43:PHE:CD1	2.66	0.48
1:D:172:GLU:OE1	1:D:172:GLU:HA	2.13	0.48
1:D:25:LEU:O	1:D:29:VAL:HB	2.14	0.48
1:F:29:VAL:O	1:F:30:LEU:O	2.31	0.48
1:H:205:VAL:O	1:H:209:THR:HG23	2.14	0.48
1:D:21:LEU:HD11	1:G:93:ALA:CB	2.43	0.48
1:C:210:GLY:HA3	7:C:419:HOH:O	2.13	0.48
1:G:191:TYR:CE1	1:G:224:ARG:HG3	2.49	0.48
1:H:86:ARG:NH1	1:H:86:ARG:HG3	2.27	0.48
1:C:173:ILE:HD13	1:G:42:TYR:OH	2.13	0.48
1:B:191:TYR:CE1	1:B:224:ARG:HG3	2.49	0.48
1:A:109:VAL:O	1:B:129:LYS:HE2	2.13	0.48
1:C:119:VAL:HG12	1:C:120:GLY:N	2.29	0.48
1:F:259:ILE:HD11	1:F:277:VAL:CG1	2.43	0.48
1:C:235:ASP:OD1	1:C:260:THR:HB	2.13	0.48
1:D:23:ASN:C	1:D:23:ASN:OD1	2.52	0.47
1:B:173:ILE:HG23	1:B:174:THR:HG23	1.96	0.47
1:H:251:LEU:CD1	1:H:291:LEU:HD21	2.43	0.47
1:D:95:ILE:HA	1:D:98:MET:HE2	1.96	0.47
1:D:66:ASP:H	1:D:211:GLN:HE21	1.61	0.47
1:D:30:LEU:CG	1:E:274:ARG:HH21	2.27	0.47
1:F:25:LEU:O	1:F:29:VAL:HB	2.14	0.47
1:D:128:ASN:O	1:D:132:VAL:HG23	2.14	0.47
1:G:53:PHE:CD1	1:G:53:PHE:N	2.81	0.47
1:E:107:ASP:O	1:E:110:LEU:O	2.33	0.47
1:D:180:ARG:HD2	7:D:378:HOH:O	2.14	0.47
1:G:51:LYS:HB3	1:G:53:PHE:CE1	2.50	0.47
1:B:211:GLN:NE2	1:B:215:VAL:HG11	2.27	0.47
1:D:259:ILE:HD11	1:D:277:VAL:HG11	1.95	0.47
1:D:221:GLU:OE1	1:D:224:ARG:NH1	2.47	0.47
1:C:274:ARG:HH21	1:F:30:LEU:HD21	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:44:PHE:CD2	1:F:44:PHE:N	2.82	0.47
1:G:49:GLN:HE21	1:G:50:GLY:CA	2.27	0.47
1:G:128:ASN:HD22	1:G:129:LYS:N	2.12	0.47
1:E:14:VAL:CG1	1:E:56:THR:HG23	2.41	0.47
1:C:193:LYS:HE3	3:C:1002:FPP:C2	2.41	0.47
1:H:110:LEU:C	1:H:112:ASP:N	2.67	0.47
1:B:84:GLU:O	1:B:87:VAL:HG12	2.15	0.47
1:F:187:MET:HE3	1:F:232:LEU:HD21	1.97	0.47
1:G:273:LEU:HD12	1:G:293:TYR:CD1	2.49	0.47
1:F:126:MET:HA	1:F:127:GLY:C	2.35	0.47
1:E:170:THR:O	1:E:174:THR:HB	2.15	0.47
1:C:191:TYR:HE1	1:C:224:ARG:HG3	1.80	0.47
1:D:44:PHE:N	1:D:44:PHE:HD2	2.13	0.47
1:F:44:PHE:O	1:F:45:LYS:CB	2.64	0.46
1:F:186:TYR:HD2	1:F:187:MET:HE2	1.79	0.46
1:H:33:VAL:HG12	1:H:34:PRO:HD2	1.97	0.46
1:F:9:ASP:HB3	1:F:10:PRO:HD3	1.97	0.46
1:B:173:ILE:C	1:B:173:ILE:HD13	2.36	0.46
1:C:172:GLU:HG3	1:C:189:LYS:HD2	1.97	0.46
1:C:42:TYR:OH	1:C:119:VAL:HG12	2.15	0.46
1:G:57:ILE:HD11	1:G:226:LEU:CD2	2.44	0.46
1:E:65:LEU:O	1:E:66:ASP:CB	2.46	0.46
1:D:11:PHE:CE2	3:G:1001:FPP:H41	2.51	0.46
1:E:121:SER:OG	1:E:123:ASN:ND2	2.48	0.46
1:A:54:ARG:NH1	4:A:1003:ISY:S9	2.83	0.46
1:G:82:THR:HA	1:G:86:ARG:HB2	1.97	0.46
1:G:173:ILE:HD13	1:G:173:ILE:C	2.35	0.46
1:B:46:ARG:NE	1:B:49:GLN:HA	2.31	0.46
1:H:9:ASP:CB	1:H:10:PRO:HD2	2.39	0.46
1:H:11:PHE:CE1	1:H:53:PHE:HE1	2.27	0.46
1:H:324:THR:HG21	1:H:329:VAL:CG1	2.45	0.46
1:G:19:SER:O	1:G:23:ASN:HB2	2.15	0.46
1:A:268:GLU:OE2	1:A:302:ARG:NH2	2.42	0.46
1:A:251:LEU:CD1	1:A:291:LEU:HD21	2.46	0.46
1:A:251:LEU:HD13	1:A:291:LEU:HD21	1.98	0.46
1:B:256:HIS:ND1	7:B:551:HOH:O	2.24	0.46
1:G:124:VAL:HG12	1:G:125:VAL:HA	1.98	0.46
1:G:19:SER:OG	1:H:283:ASP:HB2	2.16	0.46
1:A:17:GLU:OE2	1:A:86:ARG:NH1	2.49	0.46
1:C:334:ARG:NH2	7:C:589:HOH:O	2.49	0.46
1:C:273:LEU:HD12	1:C:276:VAL:HB	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:146:LEU:HB3	1:F:155:VAL:HG22	1.97	0.46
1:A:110:LEU:O	1:A:112:ASP:N	2.49	0.45
1:B:13:LEU:HD12	1:F:60:LEU:HD23	1.97	0.45
1:B:173:ILE:HG23	1:B:174:THR:H	1.81	0.45
1:D:57:ILE:HD13	1:D:226:LEU:HD23	1.98	0.45
1:E:108:ASP:OD1	1:E:116:ARG:NH1	2.49	0.45
1:C:55:SER:O	1:C:59:LEU:HG	2.16	0.45
1:D:175:SER:O	1:D:176:SER:C	2.55	0.45
3:A:1002:FPP:H41	7:A:439:HOH:O	2.17	0.45
1:G:218:LEU:HD23	1:G:321:LEU:HD23	1.97	0.45
1:B:45:LYS:O	1:B:46:ARG:C	2.54	0.45
1:G:34:PRO:C	1:G:36:LEU:H	2.19	0.45
1:G:248:LYS:O	1:G:248:LYS:CD	2.65	0.45
1:A:11:PHE:CE1	1:A:53:PHE:CE1	2.98	0.45
1:D:186:TYR:HD2	1:D:187:MET:HE2	1.80	0.45
1:H:11:PHE:CE1	1:H:53:PHE:CE1	2.98	0.45
1:B:21:LEU:HD21	1:F:90:ARG:O	2.16	0.45
1:C:116:ARG:HH22	3:C:1002:FPP:PB	2.40	0.45
1:C:123:ASN:H	1:C:123:ASN:ND2	2.10	0.45
1:C:173:ILE:O	1:C:173:ILE:HG22	2.16	0.45
1:H:183:MET:O	1:H:187:MET:HB2	2.16	0.45
1:D:259:ILE:CD1	1:D:277:VAL:HG11	2.47	0.45
1:G:33:VAL:HB	1:G:34:PRO:HD3	1.98	0.45
1:G:274:ARG:HB2	1:G:274:ARG:HH11	1.82	0.45
1:G:30:LEU:H	1:G:33:VAL:HG23	1.82	0.45
1:A:175:SER:CB	1:A:185:TYR:CZ	2.99	0.45
1:F:57:ILE:HD13	1:F:226:LEU:HD23	1.99	0.45
1:D:37:ALA:HB1	1:H:174:THR:O	2.16	0.44
1:B:30:LEU:N	1:B:33:VAL:HG23	2.32	0.44
1:F:126:MET:CG	1:F:126:MET:O	2.65	0.44
1:C:248:LYS:HZ3	1:C:248:LYS:HB2	1.81	0.44
1:C:191:TYR:CE1	1:C:224:ARG:HG3	2.51	0.44
1:A:235:ASP:HB3	1:A:260:THR:HB	1.99	0.44
1:B:255:ARG:HB2	1:B:256:HIS:CD2	2.46	0.44
1:B:173:ILE:O	7:B:549:HOH:O	2.21	0.44
1:G:246:LEU:O	7:G:350:HOH:O	2.21	0.44
1:G:248:LYS:HE2	7:G:355:HOH:O	2.16	0.44
1:A:205:VAL:O	1:A:209:THR:HG23	2.17	0.44
1:F:124:VAL:N	7:F:697:HOH:O	2.32	0.44
1:C:121:SER:OG	1:C:123:ASN:ND2	2.49	0.44
1:B:17:GLU:HG2	1:F:90:ARG:NH1	2.29	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:191:TYR:CE1	1:F:224:ARG:HG3	2.53	0.44
1:E:190:THR:HG23	1:E:231:GLN:HG2	2.00	0.44
1:E:273:LEU:HD12	1:E:276:VAL:HB	2.00	0.44
1:D:18:LEU:HD11	1:G:56:THR:OG1	2.17	0.44
1:A:259:ILE:HG12	1:A:277:VAL:HG11	1.98	0.44
1:F:57:ILE:HD11	1:F:226:LEU:HD23	2.00	0.44
1:D:65:LEU:O	1:D:66:ASP:CB	2.64	0.44
1:F:218:LEU:HD23	1:F:321:LEU:HD23	1.99	0.44
1:C:84:GLU:HA	1:C:84:GLU:OE1	2.17	0.44
1:H:110:LEU:O	1:H:112:ASP:N	2.51	0.44
1:A:324:THR:HG21	1:A:329:VAL:CG1	2.48	0.44
1:F:259:ILE:HG22	1:F:264:LEU:HG	1.99	0.44
1:B:11:PHE:CE1	1:F:51:LYS:HE2	2.52	0.44
1:B:298:LYS:O	1:B:302:ARG:HG3	2.17	0.44
1:A:214:GLU:HG2	1:A:214:GLU:H	1.57	0.44
1:E:42:TYR:OH	1:E:119:VAL:HG12	2.18	0.44
1:E:339:LEU:HA	1:E:339:LEU:HD12	1.86	0.44
1:B:54:ARG:NH2	1:B:100:HIS:CE1	2.86	0.43
1:F:255:ARG:NH1	1:F:255:ARG:HG2	2.30	0.43
1:B:198:ILE:HG12	3:B:1001:FPP:H143	2.01	0.43
1:G:245:SER:C	1:G:247:GLY:HA2	2.39	0.43
1:B:17:GLU:CG	1:F:90:ARG:NH1	2.80	0.43
1:B:151:ASN:HB3	1:B:154:VAL:HG13	2.00	0.43
1:G:280:VAL:HG22	1:G:287:VAL:HG23	1.99	0.43
1:E:13:LEU:HD11	1:E:331:ARG:HD2	2.00	0.43
1:E:175:SER:OG	1:E:180:ARG:HG2	2.17	0.43
1:D:8:LEU:CB	1:G:342:ARG:NH2	2.82	0.43
1:H:235:ASP:HB3	1:H:260:THR:HB	2.00	0.43
1:G:31:ALA:C	1:G:32:GLU:HG2	2.39	0.43
1:D:180:ARG:HB3	7:D:574:HOH:O	2.17	0.43
1:H:175:SER:CB	1:H:185:TYR:CZ	3.00	0.43
1:F:141:ARG:CG	1:F:141:ARG:NH1	2.74	0.43
1:B:17:GLU:CB	1:F:90:ARG:HD3	2.47	0.43
1:E:242:THR:HG22	1:E:248:LYS:HD2	2.00	0.43
1:H:268:GLU:OE2	1:H:302:ARG:NH2	2.43	0.43
1:B:280:VAL:HG22	1:B:287:VAL:HG23	2.00	0.43
1:D:51:LYS:O	1:D:52:GLN:C	2.57	0.43
1:B:190:THR:HG23	1:B:231:GLN:HG2	2.00	0.43
1:G:49:GLN:HE22	1:G:50:GLY:HA3	1.84	0.43
1:B:173:ILE:HG23	1:B:174:THR:N	2.33	0.43
1:B:33:VAL:HB	1:B:34:PRO:HD3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:10:PRO:CG	1:G:339:LEU:HD13	2.47	0.43
1:E:248:LYS:HZ2	1:E:248:LYS:HB2	1.83	0.43
1:E:29:VAL:O	1:E:29:VAL:HG12	2.17	0.43
1:D:24:LYS:O	1:D:24:LYS:HG2	2.19	0.43
1:G:242:THR:HB	1:G:245:SER:CB	2.48	0.43
1:B:13:LEU:HD12	1:F:60:LEU:HD22	1.98	0.43
1:G:154:VAL:HG11	1:G:208:LEU:HD13	2.00	0.43
1:G:190:THR:HG23	1:G:231:GLN:HG2	2.00	0.43
1:F:29:VAL:C	1:F:30:LEU:O	2.57	0.43
1:G:173:ILE:HD13	1:G:173:ILE:O	2.19	0.43
1:C:89:GLN:NE2	1:C:209:THR:HG22	2.34	0.43
1:B:282:ALA:HB2	1:F:282:ALA:HB2	2.00	0.43
1:D:235:ASP:HB3	1:D:260:THR:HB	2.01	0.43
1:A:54:ARG:HH22	4:A:1003:ISY:H11	1.84	0.43
1:F:259:ILE:CD1	1:F:277:VAL:HG11	2.48	0.43
1:D:225:ASN:HB3	1:D:310:HIS:O	2.18	0.43
1:G:283:ASP:OD1	1:G:285:ARG:HG3	2.18	0.43
1:H:18:LEU:HD21	1:H:52:GLN:HB2	2.01	0.43
1:G:36:LEU:O	1:G:39:ALA:CB	2.67	0.43
1:D:23:ASN:C	1:D:25:LEU:N	2.71	0.42
1:F:235:ASP:HB3	1:F:260:THR:HB	2.01	0.42
1:G:41:GLU:HG3	1:G:42:TYR:N	2.22	0.42
1:C:239:PHE:HB3	1:C:246:LEU:CD1	2.49	0.42
1:E:225:ASN:HB3	1:E:310:HIS:O	2.19	0.42
1:D:23:ASN:OD1	1:D:24:LYS:N	2.52	0.42
1:B:35:LYS:HA	1:E:174:THR:OG1	2.19	0.42
1:F:57:ILE:CD1	1:F:226:LEU:CD2	2.98	0.42
1:E:235:ASP:OD1	1:E:260:THR:HB	2.20	0.42
1:F:29:VAL:CG1	1:F:30:LEU:N	2.83	0.42
1:B:17:GLU:HB2	1:F:59:LEU:CD1	2.49	0.42
1:D:191:TYR:HE1	1:D:224:ARG:HG3	1.82	0.42
1:H:251:LEU:HD13	1:H:291:LEU:HD21	2.00	0.42
1:H:217:VAL:O	1:H:221:GLU:HG2	2.19	0.42
1:C:283:ASP:OD1	1:C:284:PRO:HD2	2.20	0.42
1:F:273:LEU:HA	1:F:276:VAL:HG13	2.01	0.42
1:F:254:ILE:HD12	1:F:254:ILE:HA	1.88	0.42
1:G:40:ALA:C	1:G:44:PHE:HE1	2.22	0.42
1:E:21:LEU:HD22	1:E:59:LEU:HD11	2.02	0.42
1:F:14:VAL:O	1:F:14:VAL:HG22	2.20	0.42
1:D:33:VAL:H	1:D:34:PRO:CD	2.32	0.42
1:C:173:ILE:CD1	1:G:42:TYR:OH	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:239:PHE:HB3	1:E:246:LEU:CD1	2.50	0.42
1:B:46:ARG:CZ	1:B:46:ARG:HB3	2.48	0.42
1:F:23:ASN:O	1:F:26:ARG:HB2	2.20	0.42
1:G:173:ILE:HG23	1:G:174:THR:HG23	2.01	0.42
1:G:346:ARG:HB3	3:G:1001:FPP:H2	2.02	0.42
1:D:23:ASN:O	1:D:26:ARG:HB2	2.19	0.42
1:G:246:LEU:N	1:G:247:GLY:HA2	2.35	0.42
1:D:183:MET:HE2	1:D:264:LEU:HB2	2.02	0.42
1:D:29:VAL:CG1	1:D:30:LEU:N	2.83	0.42
1:B:57:ILE:HD11	3:B:1001:FPP:H91	2.01	0.42
1:A:123:ASN:H	1:A:123:ASN:ND2	2.17	0.42
1:F:23:ASN:O	1:F:25:LEU:N	2.53	0.42
1:B:248:LYS:O	1:B:249:GLY:C	2.58	0.42
1:E:180:ARG:HH22	1:E:189:LYS:CD	2.33	0.42
1:B:19:SER:O	1:B:23:ASN:HB2	2.20	0.42
1:G:46:ARG:NE	1:G:49:GLN:CB	2.83	0.41
1:B:86:ARG:NH1	1:B:86:ARG:CG	2.60	0.41
1:A:343:VAL:HA	1:A:346:ARG:HD2	2.01	0.41
1:E:112:ASP:OD1	1:E:112:ASP:N	2.53	0.41
1:F:259:ILE:HD11	1:F:277:VAL:HG11	2.02	0.41
1:A:183:MET:O	1:A:187:MET:HB2	2.20	0.41
1:H:29:VAL:CG1	1:H:29:VAL:O	2.67	0.41
1:C:193:LYS:NZ	3:C:1002:FPP:H11	2.35	0.41
1:D:141:ARG:HA	1:D:141:ARG:HD2	1.80	0.41
1:B:54:ARG:NH1	5:B:1000:PPV:O31	2.50	0.41
1:E:172:GLU:OE1	1:E:189:LYS:HE2	2.20	0.41
1:E:9:ASP:C	1:E:9:ASP:OD1	2.58	0.41
1:G:34:PRO:HA	1:G:36:LEU:HD23	2.02	0.41
1:B:14:VAL:CG1	1:F:59:LEU:HB3	2.49	0.41
1:E:42:TYR:OH	1:E:119:VAL:CG1	2.68	0.41
1:D:183:MET:CE	1:D:264:LEU:HB2	2.50	0.41
1:G:180:ARG:HD3	7:G:533:HOH:O	2.20	0.41
1:C:106:HIS:CD2	1:D:136:ASP:CG	2.92	0.41
1:F:301:GLN:HB3	7:F:364:HOH:O	2.20	0.41
1:C:272:GLN:NE2	1:C:293:TYR:OH	2.53	0.41
1:B:53:PHE:HB3	3:B:1001:FPP:H92	2.02	0.41
1:C:175:SER:OG	1:C:180:ARG:HG2	2.21	0.41
1:C:42:TYR:OH	1:C:119:VAL:CG1	2.67	0.41
1:F:33:VAL:N	1:F:34:PRO:CD	2.84	0.41
1:E:163:GLU:HA	1:F:140:SER:HB2	2.02	0.41
1:C:339:LEU:HA	1:C:339:LEU:HD12	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:PHE:CE1	1:A:53:PHE:HE1	2.27	0.41
1:C:180:ARG:HH22	1:C:189:LYS:HD3	1.85	0.41
1:H:45:LYS:O	1:H:49:GLN:HG3	2.20	0.41
1:E:55:SER:O	1:E:59:LEU:HG	2.21	0.41
1:C:43:PHE:HB3	1:C:117:ARG:NH1	2.35	0.41
1:B:49:GLN:HG2	1:B:50:GLY:H	1.80	0.41
1:G:46:ARG:CD	1:G:47:GLY:N	2.62	0.41
1:G:46:ARG:NE	1:G:49:GLN:CA	2.74	0.41
1:D:18:LEU:CD2	1:G:55:SER:HB3	2.49	0.41
1:F:255:ARG:CG	1:F:255:ARG:HH11	2.27	0.41
1:D:57:ILE:CD1	1:D:226:LEU:CD2	2.92	0.41
1:A:43:PHE:HB3	1:A:117:ARG:NH1	2.36	0.41
1:B:36:LEU:O	1:B:39:ALA:HB3	2.21	0.41
1:G:92:ILE:HD12	1:G:208:LEU:HD22	2.03	0.41
1:G:54:ARG:NH2	1:G:100:HIS:CE1	2.89	0.41
1:E:243:SER:O	1:E:244:ALA:HB3	2.21	0.41
1:F:172:GLU:OE1	1:F:172:GLU:HA	2.20	0.41
1:G:296:LYS:HA	1:G:296:LYS:HD3	1.89	0.41
1:D:188:GLN:NE2	7:D:386:HOH:O	2.53	0.41
1:C:13:LEU:HD11	1:C:331:ARG:HD2	2.03	0.40
1:H:347:ASN:H	1:H:347:ASN:ND2	2.19	0.40
1:A:190:THR:HG23	1:A:231:GLN:HG2	2.03	0.40
1:F:42:TYR:C	1:F:43:PHE:CG	2.94	0.40
1:B:198:ILE:HG21	3:B:1001:FPP:H141	2.03	0.40
1:B:54:ARG:HG2	1:B:198:ILE:HD13	2.03	0.40
1:B:273:LEU:CD2	1:B:277:VAL:CG2	2.99	0.40
1:E:43:PHE:O	1:E:44:PHE:CB	2.70	0.40
1:G:109:VAL:HA	1:G:128:ASN:HB2	2.04	0.40
1:C:173:ILE:O	1:C:173:ILE:CG2	2.68	0.40
1:F:225:ASN:HB3	1:F:310:HIS:O	2.21	0.40
1:C:186:TYR:OH	1:C:235:ASP:OD1	2.32	0.40
1:B:164:HIS:O	1:B:192:TYR:HB3	2.21	0.40
1:F:111:ASP:OD1	1:F:111:ASP:N	2.55	0.40

All (2) 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)
1:A:15:ALA:O	1:H:46:ARG:NH1[1_665]	1.98	0.22
1:A:46:ARG:NH1	1:H:15:ALA:O[1_665]	2.19	0.01

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	322/348 (92%)	312 (97%)	9 (3%)	1 (0%)	46	72
1	B	307/348 (88%)	289 (94%)	15 (5%)	3 (1%)	19	41
1	C	323/348 (93%)	311 (96%)	11 (3%)	1 (0%)	46	72
1	D	304/348 (87%)	280 (92%)	14 (5%)	10 (3%)	5	9
1	E	321/348 (92%)	308 (96%)	12 (4%)	1 (0%)	46	72
1	F	302/348 (87%)	282 (93%)	14 (5%)	6 (2%)	9	21
1	G	308/348 (88%)	291 (94%)	16 (5%)	1 (0%)	46	72
1	H	320/348 (92%)	308 (96%)	11 (3%)	1 (0%)	46	72
All	All	2507/2784 (90%)	2381 (95%)	102 (4%)	24 (1%)	19	41

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	46	ARG
1	B	48	VAL
1	C	112	ASP
1	D	30	LEU
1	D	31	ALA
1	E	112	ASP
1	F	30	LEU
1	G	46	ARG
1	B	249	GLY
1	D	24	LYS
1	D	44	PHE
1	D	176	SER
1	F	24	LYS
1	F	112	ASP
1	F	176	SER
1	D	43	PHE
1	D	52	GLN

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Mol	Chain	Res	Type
1	D	123	ASN
1	A	346	ARG
1	H	111	ASP
1	D	33	VAL
1	F	33	VAL
1	D	127	GLY
1	F	127	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	266/285 (93%)	231 (87%)	35 (13%)	5	10
1	B	256/285 (90%)	218 (85%)	38 (15%)	4	8
1	C	267/285 (94%)	226 (85%)	41 (15%)	3	7
1	D	256/285 (90%)	225 (88%)	31 (12%)	6	12
1	E	265/285 (93%)	230 (87%)	35 (13%)	5	10
1	F	253/285 (89%)	217 (86%)	36 (14%)	4	8
1	G	257/285 (90%)	221 (86%)	36 (14%)	4	9
1	H	264/285 (93%)	225 (85%)	39 (15%)	4	8
All	All	2084/2280 (91%)	1793 (86%)	291 (14%)	4	9

All (291) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LEU
1	A	12	SER
1	A	14	VAL
1	A	21	LEU
1	A	25	LEU
1	A	35	LYS
1	A	36	LEU
1	A	41	GLU

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Mol	Chain	Res	Type
1	A	45	LYS
1	A	46	ARG
1	A	49	GLN
1	A	85	LEU
1	A	86	ARG
1	A	103	SER
1	A	110	LEU
1	A	114	ASP
1	A	115	THR
1	A	116	ARG
1	A	123	ASN
1	A	129	LYS
1	A	139	LEU
1	A	177	THR
1	A	188	GLN
1	A	214	GLU
1	A	234	ASP
1	A	255	ARG
1	A	272	GLN
1	A	275	GLU
1	A	279	GLN
1	A	291	LEU
1	A	297	SER
1	A	305	GLU
1	A	325	ASP
1	A	328	ASP
1	A	332	SER
1	B	9	ASP
1	B	13	LEU
1	B	14	VAL
1	B	20	LEU
1	B	29	VAL
1	B	30	LEU
1	B	41	GLU
1	B	44	PHE
1	B	45	LYS
1	B	46	ARG
1	B	49	GLN
1	B	51	LYS
1	B	66	ASP
1	B	86	ARG
1	B	87	VAL

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Mol	Chain	Res	Type
1	B	103	SER
1	B	110	LEU
1	B	126	MET
1	B	128	ASN
1	B	153	GLU
1	B	154	VAL
1	B	173	ILE
1	B	176	SER
1	B	214	GLU
1	B	218	LEU
1	B	245	SER
1	B	248	LYS
1	B	252	SER
1	B	255	ARG
1	B	272	GLN
1	B	274	ARG
1	B	275	GLU
1	B	280	VAL
1	B	285	ARG
1	B	339	LEU
1	B	343	VAL
1	B	347	ASN
1	B	348	LYS
1	C	12	SER
1	C	14	VAL
1	C	21	LEU
1	C	25	LEU
1	C	32	GLU
1	C	35	LYS
1	C	41	GLU
1	C	48	VAL
1	C	49	GLN
1	C	57	ILE
1	C	86	ARG
1	C	97	GLU
1	C	103	SER
1	C	106	HIS
1	C	112	ASP
1	C	116	ARG
1	C	123	ASN
1	C	131	SER
1	C	139	LEU

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Mol	Chain	Res	Type
1	C	174	THR
1	C	180	ARG
1	C	189	LYS
1	C	208	LEU
1	C	212	THR
1	C	234	ASP
1	C	245	SER
1	C	248	LYS
1	C	252	SER
1	C	269	GLU
1	C	272	GLN
1	C	279	GLN
1	C	292	GLU
1	C	298	LYS
1	C	300	ILE
1	C	301	GLN
1	C	323	GLU
1	C	338	ASP
1	C	339	LEU
1	C	340	THR
1	C	345	THR
1	C	347	ASN
1	D	8	LEU
1	D	12	SER
1	D	14	VAL
1	D	23	ASN
1	D	29	VAL
1	D	30	LEU
1	D	35	LYS
1	D	41	GLU
1	D	44	PHE
1	D	54	ARG
1	D	63	THR
1	D	66	ASP
1	D	84	GLU
1	D	86	ARG
1	D	103	SER
1	D	112	ASP
1	D	125	VAL
1	D	126	MET
1	D	141	ARG
1	D	149	LEU

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Mol	Chain	Res	Type
1	D	154	VAL
1	D	175	SER
1	D	193	LYS
1	D	217	VAL
1	D	218	LEU
1	D	246	LEU
1	D	250	SER
1	D	272	GLN
1	D	273	LEU
1	D	301	GLN
1	D	339	LEU
1	E	9	ASP
1	E	12	SER
1	E	14	VAL
1	E	21	LEU
1	E	25	LEU
1	E	32	GLU
1	E	35	LYS
1	E	41	GLU
1	E	48	VAL
1	E	49	GLN
1	E	57	ILE
1	E	86	ARG
1	E	103	SER
1	E	112	ASP
1	E	116	ARG
1	E	123	ASN
1	E	139	LEU
1	E	174	THR
1	E	180	ARG
1	E	189	LYS
1	E	208	LEU
1	E	212	THR
1	E	245	SER
1	E	248	LYS
1	E	252	SER
1	E	269	GLU
1	E	272	GLN
1	E	292	GLU
1	E	298	LYS
1	E	300	ILE
1	E	301	GLN

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Mol	Chain	Res	Type
1	E	323	GLU
1	E	338	ASP
1	E	339	LEU
1	E	340	THR
1	F	12	SER
1	F	14	VAL
1	F	23	ASN
1	F	24	LYS
1	F	29	VAL
1	F	30	LEU
1	F	33	VAL
1	F	35	LYS
1	F	41	GLU
1	F	43	PHE
1	F	44	PHE
1	F	51	LYS
1	F	55	SER
1	F	63	THR
1	F	86	ARG
1	F	90	ARG
1	F	103	SER
1	F	111	ASP
1	F	126	MET
1	F	141	ARG
1	F	149	LEU
1	F	154	VAL
1	F	173	ILE
1	F	175	SER
1	F	193	LYS
1	F	217	VAL
1	F	218	LEU
1	F	234	ASP
1	F	242	THR
1	F	246	LEU
1	F	250	SER
1	F	273	LEU
1	F	292	GLU
1	F	301	GLN
1	F	339	LEU
1	F	348	LYS
1	G	9	ASP
1	G	13	LEU

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Mol	Chain	Res	Type
1	G	14	VAL
1	G	20	LEU
1	G	27	GLU
1	G	29	VAL
1	G	30	LEU
1	G	38	SER
1	G	41	GLU
1	G	44	PHE
1	G	45	LYS
1	G	46	ARG
1	G	49	GLN
1	G	66	ASP
1	G	86	ARG
1	G	87	VAL
1	G	124	VAL
1	G	128	ASN
1	G	153	GLU
1	G	154	VAL
1	G	173	ILE
1	G	176	SER
1	G	214	GLU
1	G	218	LEU
1	G	248	LYS
1	G	252	SER
1	G	255	ARG
1	G	272	GLN
1	G	274	ARG
1	G	275	GLU
1	G	280	VAL
1	G	285	ARG
1	G	296	LYS
1	G	339	LEU
1	G	343	VAL
1	G	347	ASN
1	H	8	LEU
1	H	12	SER
1	H	14	VAL
1	H	21	LEU
1	H	25	LEU
1	H	26	ARG
1	H	30	LEU
1	H	35	LYS

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Mol	Chain	Res	Type
1	H	36	LEU
1	H	41	GLU
1	H	45	LYS
1	H	46	ARG
1	H	49	GLN
1	H	85	LEU
1	H	86	ARG
1	H	87	VAL
1	H	103	SER
1	H	110	LEU
1	H	114	ASP
1	H	115	THR
1	H	116	ARG
1	H	119	VAL
1	H	123	ASN
1	H	129	LYS
1	H	139	LEU
1	H	177	THR
1	H	188	GLN
1	H	214	GLU
1	H	234	ASP
1	H	248	LYS
1	H	255	ARG
1	H	272	GLN
1	H	275	GLU
1	H	279	GLN
1	H	291	LEU
1	H	305	GLU
1	H	325	ASP
1	H	328	ASP
1	H	347	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	ASN
1	A	211	GLN
1	A	312	ASN
1	B	211	GLN
1	B	256	HIS
1	B	279	GLN
1	B	347	ASN

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Mol	Chain	Res	Type
1	C	106	HIS
1	C	123	ASN
1	C	272	GLN
1	C	279	GLN
1	C	312	ASN
1	C	347	ASN
1	D	188	GLN
1	D	211	GLN
1	D	310	HIS
1	E	123	ASN
1	E	272	GLN
1	E	279	GLN
1	F	310	HIS
1	G	23	ASN
1	G	49	GLN
1	G	100	HIS
1	G	211	GLN
1	G	256	HIS
1	G	347	ASN
1	H	123	ASN
1	H	128	ASN
1	H	211	GLN
1	H	312	ASN
1	H	347	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 24 ligands modelled in this entry, 8 are monoatomic - leaving 16 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	FPP	A	1002	2	21,23,23	2.14	7 (33%)	27,31,31	1.31	4 (14%)
4	ISY	A	1003	-	7,13,13	2.93	4 (57%)	10,19,19	1.97	4 (40%)
5	PPV	B	1000	-	6,8,8	2.55	4 (66%)	11,13,13	1.53	2 (18%)
3	FPP	B	1001	-	21,23,23	2.17	9 (42%)	27,31,31	1.31	2 (7%)
6	PEG	B	1002	-	6,6,6	0.41	0	5,5,5	0.81	0
3	FPP	C	1002	2	21,23,23	2.19	9 (42%)	27,31,31	1.43	6 (22%)
5	PPV	C	1003	-	6,8,8	2.40	2 (33%)	11,13,13	1.30	1 (9%)
5	PPV	D	1000	-	6,8,8	2.61	4 (66%)	11,13,13	1.68	1 (9%)
6	PEG	D	1002	-	6,6,6	0.86	0	5,5,5	0.68	0
3	FPP	E	1002	2	21,23,23	2.16	8 (38%)	27,31,31	1.28	4 (14%)
5	PPV	E	1003	-	6,8,8	2.41	3 (50%)	11,13,13	1.52	2 (18%)
5	PPV	F	1000	-	6,8,8	2.52	4 (66%)	11,13,13	1.51	1 (9%)
5	PPV	G	1000	-	6,8,8	2.56	4 (66%)	11,13,13	1.63	2 (18%)
3	FPP	G	1001	-	21,23,23	2.16	8 (38%)	27,31,31	1.67	4 (14%)
3	FPP	H	1002	2	21,23,23	2.24	9 (42%)	27,31,31	1.39	2 (7%)
4	ISY	H	1003	-	7,13,13	2.97	3 (42%)	10,19,19	1.73	2 (20%)

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	FPP	A	1002	2	-	0/25/25/25	0/0/0/0
4	ISY	A	1003	-	-	0/9/13/13	0/0/0/0
5	PPV	B	1000	-	-	0/6/6/6	0/0/0/0
3	FPP	B	1001	-	-	0/25/25/25	0/0/0/0
6	PEG	B	1002	-	-	0/4/4/4	0/0/0/0
3	FPP	C	1002	2	-	0/25/25/25	0/0/0/0
5	PPV	C	1003	-	-	0/6/6/6	0/0/0/0
5	PPV	D	1000	-	-	0/6/6/6	0/0/0/0
6	PEG	D	1002	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FPP	E	1002	2	-	0/25/25/25	0/0/0/0
5	PPV	E	1003	-	-	0/6/6/6	0/0/0/0
5	PPV	F	1000	-	-	0/6/6/6	0/0/0/0
5	PPV	G	1000	-	-	0/6/6/6	0/0/0/0
3	FPP	G	1001	-	-	0/25/25/25	0/0/0/0
3	FPP	H	1002	2	-	0/25/25/25	0/0/0/0
4	ISY	H	1003	-	-	0/9/13/13	0/0/0/0

All (78) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1001	FPP	C11-C12	-4.08	1.39	1.50
3	E	1002	FPP	C6-C7	-4.00	1.39	1.50
3	G	1001	FPP	C11-C12	-3.97	1.39	1.50
3	A	1002	FPP	C11-C12	-3.97	1.39	1.50
3	C	1002	FPP	C11-C12	-3.94	1.39	1.50
3	H	1002	FPP	C11-C12	-3.94	1.39	1.50
3	H	1002	FPP	C6-C7	-3.92	1.39	1.50
3	E	1002	FPP	C11-C12	-3.91	1.39	1.50
3	B	1001	FPP	C6-C7	-3.79	1.39	1.50
3	G	1001	FPP	C6-C7	-3.76	1.40	1.50
3	A	1002	FPP	C6-C7	-3.68	1.40	1.50
3	C	1002	FPP	C6-C7	-3.55	1.40	1.50
4	A	1003	ISY	C10-C11	-3.29	1.40	1.51
4	H	1003	ISY	C10-C11	-3.25	1.41	1.51
4	A	1003	ISY	P3-O8	-3.04	1.48	1.56
3	G	1001	FPP	C1-C2	-2.97	1.39	1.49
4	H	1003	ISY	P3-O8	-2.86	1.49	1.56
3	E	1002	FPP	C1-C2	-2.82	1.39	1.49
3	H	1002	FPP	C1-C2	-2.78	1.39	1.49
3	A	1002	FPP	C1-C2	-2.62	1.40	1.49
3	C	1002	FPP	C1-C2	-2.58	1.40	1.49
3	B	1001	FPP	C1-C2	-2.50	1.40	1.49
5	F	1000	PPV	P2-O32	2.00	1.61	1.54
3	E	1002	FPP	PB-O3B	2.07	1.62	1.54
4	A	1003	ISY	P1-O6	2.08	1.62	1.54
3	H	1002	FPP	PB-O3B	2.10	1.62	1.54
3	B	1001	FPP	PB-O2B	2.12	1.62	1.54
5	E	1003	PPV	P2-O32	2.13	1.62	1.54
5	D	1000	PPV	P1-O21	2.14	1.62	1.54
5	F	1000	PPV	P1-O21	2.17	1.62	1.54
5	D	1000	PPV	P2-O32	2.18	1.62	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1001	FPP	PB-O3B	2.19	1.62	1.54
3	C	1002	FPP	C12-C13	2.21	1.39	1.32
3	G	1001	FPP	C12-C13	2.22	1.39	1.32
3	C	1002	FPP	C9-C8	2.23	1.56	1.51
5	G	1000	PPV	P2-O32	2.24	1.62	1.54
5	G	1000	PPV	P1-O21	2.25	1.62	1.54
3	B	1001	FPP	C12-C13	2.32	1.39	1.32
3	G	1001	FPP	PB-O3B	2.39	1.63	1.54
3	E	1002	FPP	C12-C13	2.55	1.40	1.32
5	B	1000	PPV	P2-O32	2.56	1.63	1.54
3	H	1002	FPP	PB-O2B	2.56	1.63	1.54
3	A	1002	FPP	C12-C13	2.58	1.40	1.32
3	C	1002	FPP	PB-O3B	2.58	1.64	1.54
3	H	1002	FPP	PA-O1A	2.63	1.60	1.51
3	A	1002	FPP	PA-O1A	2.81	1.61	1.51
3	C	1002	FPP	PA-O1A	2.82	1.61	1.51
5	B	1000	PPV	P2-O22	2.82	1.60	1.51
5	B	1000	PPV	P1-O21	2.87	1.65	1.54
3	E	1002	FPP	PA-O1A	2.89	1.61	1.51
3	H	1002	FPP	C12-C13	2.92	1.41	1.32
3	B	1001	FPP	PA-O1A	2.98	1.62	1.51
3	G	1001	FPP	C2-C3	2.99	1.38	1.33
5	E	1003	PPV	P2-O22	3.07	1.61	1.51
3	G	1001	FPP	C7-C8	3.15	1.39	1.33
3	E	1002	FPP	C7-C8	3.19	1.39	1.33
5	B	1000	PPV	P1-O31	3.27	1.61	1.51
5	E	1003	PPV	P1-O31	3.27	1.61	1.51
5	F	1000	PPV	P2-O22	3.28	1.61	1.51
3	H	1002	FPP	C7-C8	3.28	1.39	1.33
3	B	1001	FPP	C7-C8	3.31	1.39	1.33
5	G	1000	PPV	P1-O31	3.41	1.62	1.51
3	C	1002	FPP	C2-C3	3.46	1.39	1.33
5	G	1000	PPV	P2-O22	3.54	1.62	1.51
5	D	1000	PPV	P2-O22	3.55	1.62	1.51
5	F	1000	PPV	P1-O31	3.55	1.62	1.51
3	A	1002	FPP	C2-C3	3.59	1.40	1.33
5	D	1000	PPV	P1-O31	3.61	1.63	1.51
3	A	1002	FPP	C7-C8	3.62	1.40	1.33
5	C	1003	PPV	P2-O22	3.64	1.63	1.51
3	E	1002	FPP	C2-C3	3.67	1.40	1.33
3	B	1001	FPP	C2-C3	3.79	1.40	1.33
5	C	1003	PPV	P1-O31	3.82	1.63	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1002	FPP	C7-C8	3.82	1.40	1.33
3	H	1002	FPP	C2-C3	3.86	1.40	1.33
3	G	1001	FPP	PA-O1A	3.92	1.65	1.51
4	A	1003	ISY	C14-C12	5.60	1.51	1.33
4	H	1003	ISY	C14-C12	5.78	1.51	1.33

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	1001	FPP	PA-O3A-PB	-4.46	117.71	132.67
3	H	1002	FPP	PA-O3A-PB	-4.21	118.57	132.67
3	A	1002	FPP	PA-O3A-PB	-4.02	119.20	132.67
5	D	1000	PPV	P2-OPP-P1	-3.81	119.88	132.67
5	G	1000	PPV	P2-OPP-P1	-3.29	121.65	132.67
5	F	1000	PPV	P2-OPP-P1	-3.21	121.90	132.67
3	C	1002	FPP	PA-O3A-PB	-3.13	122.18	132.67
5	B	1000	PPV	P2-OPP-P1	-2.85	123.10	132.67
3	B	1001	FPP	PA-O3A-PB	-2.80	123.28	132.67
5	E	1003	PPV	P2-OPP-P1	-2.50	124.28	132.67
3	G	1001	FPP	C4-C3-C2	-2.49	118.61	123.50
3	C	1002	FPP	C4-C3-C2	-2.48	118.63	123.50
4	A	1003	ISY	P1-O2-P3	-2.40	124.63	132.67
3	A	1002	FPP	C4-C3-C2	-2.35	118.89	123.50
3	E	1002	FPP	PA-O3A-PB	-2.21	125.25	132.67
4	A	1003	ISY	C11-C10-S9	-2.16	109.45	113.13
5	G	1000	PPV	O21-P1-O31	-2.04	104.01	110.58
4	A	1003	ISY	O6-P1-O5	2.01	117.06	110.58
4	H	1003	ISY	O6-P1-O5	2.04	117.16	110.58
3	C	1002	FPP	O3B-PB-O2B	2.05	115.19	107.38
3	C	1002	FPP	C4-C3-C5	2.08	118.59	115.41
3	A	1002	FPP	C4-C3-C5	2.14	118.67	115.41
3	G	1001	FPP	O3A-PA-O1	2.15	108.64	102.94
3	E	1002	FPP	C4-C3-C5	2.20	118.77	115.41
3	E	1002	FPP	O2A-PA-O3A	2.22	115.15	105.09
3	A	1002	FPP	C10-C8-C9	2.26	118.86	115.41
5	C	1003	PPV	O32-P2-O12	2.30	116.14	107.38
5	E	1003	PPV	O12-P2-OPP	2.35	115.74	105.09
3	B	1001	FPP	O3A-PA-O1	2.36	109.19	102.94
3	C	1002	FPP	O2A-PA-O3A	2.45	116.19	105.09
5	B	1000	PPV	O12-P2-OPP	2.50	116.46	105.09
3	C	1002	FPP	C10-C8-C9	3.11	120.15	115.41
3	E	1002	FPP	C10-C8-C9	3.16	120.23	115.41

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	H	1002	FPP	C10-C8-C9	3.51	120.77	115.41
4	H	1003	ISY	O8-P3-O7	3.90	119.80	110.05
3	G	1001	FPP	C4-C3-C5	3.91	121.39	115.41
4	A	1003	ISY	O8-P3-O7	4.08	120.23	110.05

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1002	FPP	1	0
4	A	1003	ISY	3	0
5	B	1000	PPV	3	0
3	B	1001	FPP	6	0
6	B	1002	PEG	1	0
3	C	1002	FPP	7	0
3	E	1002	FPP	2	0
3	G	1001	FPP	4	0
3	H	1002	FPP	2	0
4	H	1003	ISY	2	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, 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	326/348 (93%)	0.40	18 (5%)	29 26	53, 82, 121, 153	0
1	B	313/348 (89%)	0.48	22 (7%)	19 17	49, 69, 125, 175	0
1	C	327/348 (93%)	0.34	24 (7%)	18 15	46, 69, 110, 141	0
1	D	312/348 (89%)	0.31	19 (6%)	25 22	49, 70, 109, 142	0
1	E	325/348 (93%)	0.40	28 (8%)	13 10	54, 79, 117, 144	0
1	F	310/348 (89%)	0.37	20 (6%)	22 20	52, 76, 108, 141	0
1	G	314/348 (90%)	0.32	11 (3%)	48 46	46, 66, 119, 166	0
1	H	324/348 (93%)	0.38	20 (6%)	24 22	57, 85, 121, 147	0
All	All	2551/2784 (91%)	0.38	162 (6%)	23 20	46, 75, 118, 175	0

All (162) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	244	ALA	9.9
1	A	244	ALA	8.4
1	H	243	SER	7.7
1	G	30	LEU	7.3
1	E	244	ALA	6.7
1	D	8	LEU	6.1
1	D	28	MET	5.4
1	D	43	PHE	5.4
1	E	245	SER	5.0
1	E	246	LEU	4.8
1	C	243	SER	4.5
1	E	8	LEU	4.5
1	F	31	ALA	4.5
1	B	30	LEU	4.4
1	E	247	GLY	4.3
1	C	244	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
1	G	48	VAL	4.3
1	A	243	SER	4.2
1	F	285	ARG	4.2
1	D	348	LYS	4.2
1	B	177	THR	4.2
1	F	348	LYS	4.2
1	H	331	ARG	4.1
1	E	272	GLN	3.9
1	G	33	VAL	3.9
1	C	287	VAL	3.9
1	A	282	ALA	3.8
1	B	31	ALA	3.8
1	F	245	SER	3.7
1	H	242	THR	3.7
1	D	113	ALA	3.7
1	C	245	SER	3.6
1	E	284	PRO	3.6
1	E	243	SER	3.5
1	E	279	GLN	3.5
1	F	325	ASP	3.5
1	C	96	THR	3.5
1	E	282	ALA	3.3
1	F	127	GLY	3.3
1	B	32	GLU	3.3
1	F	327	GLU	3.3
1	B	28	MET	3.3
1	F	180	ARG	3.2
1	B	175	SER	3.2
1	C	95	ILE	3.2
1	D	45	LYS	3.2
1	E	285	ARG	3.2
1	H	332	SER	3.2
1	D	347	ASN	3.2
1	F	178	ALA	3.2
1	B	46	ARG	3.1
1	A	67	VAL	3.1
1	H	202	CYS	3.1
1	F	242	THR	3.1
1	B	284	PRO	3.0
1	B	244	ALA	3.0
1	A	242	THR	3.0
1	A	323	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	279	GLN	3.0
1	G	175	SER	3.0
1	C	284	PRO	3.0
1	C	99	ILE	2.9
1	A	42	TYR	2.9
1	F	44	PHE	2.9
1	C	286	ASN	2.9
1	D	282	ALA	2.9
1	B	256	HIS	2.8
1	D	31	ALA	2.8
1	G	46	ARG	2.8
1	B	293	TYR	2.8
1	A	324	THR	2.8
1	G	8	LEU	2.7
1	G	29	VAL	2.7
1	A	114	ASP	2.7
1	F	45	LYS	2.7
1	D	44	PHE	2.7
1	C	246	LEU	2.7
1	E	135	GLY	2.7
1	E	255	ARG	2.7
1	C	325	ASP	2.7
1	F	28	MET	2.7
1	E	99	ILE	2.6
1	C	282	ALA	2.6
1	F	15	ALA	2.6
1	G	28	MET	2.6
1	A	281	ALA	2.6
1	C	58	LEU	2.6
1	C	175	SER	2.6
1	E	325	ASP	2.6
1	H	119	VAL	2.6
1	A	256	HIS	2.6
1	A	8	LEU	2.5
1	B	176	SER	2.5
1	D	283	ASP	2.5
1	C	285	ARG	2.5
1	E	93	ALA	2.5
1	H	120	GLY	2.5
1	H	247	GLY	2.5
1	H	114	ASP	2.5
1	E	280	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	249	GLY	2.4
1	E	293	TYR	2.4
1	B	275	GLU	2.4
1	E	251	LEU	2.4
1	E	98	MET	2.4
1	A	280	VAL	2.4
1	D	325	ASP	2.4
1	D	21	LEU	2.4
1	H	256	HIS	2.4
1	C	103	SER	2.3
1	A	246	LEU	2.3
1	A	84	GLU	2.3
1	E	100	HIS	2.3
1	E	327	GLU	2.3
1	B	49	GLN	2.3
1	H	245	SER	2.3
1	E	287	VAL	2.3
1	F	123	ASN	2.3
1	D	242	THR	2.3
1	B	66	ASP	2.3
1	D	84	GLU	2.3
1	C	142	ALA	2.3
1	A	120	GLY	2.3
1	H	99	ILE	2.3
1	C	102	ALA	2.2
1	A	118	GLY	2.2
1	C	177	THR	2.2
1	F	43	PHE	2.2
1	H	42	TYR	2.2
1	H	195	ALA	2.2
1	E	101	VAL	2.2
1	E	323	GLU	2.2
1	F	12	SER	2.2
1	H	113	ALA	2.2
1	B	343	VAL	2.2
1	G	327	GLU	2.2
1	H	197	LEU	2.1
1	G	180	ARG	2.1
1	G	49	GLN	2.1
1	B	47	GLY	2.1
1	B	127	GLY	2.1
1	C	100	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	54	ARG	2.1
1	D	32	GLU	2.1
1	D	13	LEU	2.1
1	B	282	ALA	2.1
1	F	50	GLY	2.1
1	C	291	LEU	2.1
1	C	242	THR	2.1
1	H	33	VAL	2.1
1	B	198	ILE	2.1
1	F	347	ASN	2.0
1	H	58	LEU	2.0
1	F	11	PHE	2.0
1	E	283	ASP	2.0
1	H	223	GLY	2.0
1	B	246	LEU	2.0
1	D	246	LEU	2.0
1	B	180	ARG	2.0
1	D	87	VAL	2.0
1	E	242	THR	2.0
1	A	11	PHE	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, 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	LLDF	B-factors(Å ²)	Q<0.9
6	PEG	D	1002	7/7	0.92	0.35	3.13	3,4,5,8	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	PEG	B	1002	7/7	0.90	0.42	1.98	22,23,24,27	0
5	PPV	F	1000	9/9	0.83	0.20	0.28	131,131,131,132	0
3	FPP	B	1001	24/24	0.92	0.23	-0.04	65,67,68,69	0
3	FPP	G	1001	24/24	0.94	0.21	-0.30	51,56,62,63	0
3	FPP	H	1002	24/24	0.94	0.17	-0.76	20,40,42,43	0
5	PPV	B	1000	9/9	0.90	0.14	-0.99	57,59,62,62	0
5	PPV	G	1000	9/9	0.93	0.12	-1.15	69,70,70,71	0
3	FPP	A	1002	24/24	0.94	0.16	-1.18	25,37,44,45	0
4	ISY	A	1003	14/14	0.94	0.15	-1.34	33,40,44,45	0
3	FPP	E	1002	24/24	0.96	0.13	-1.36	40,42,45,45	0
5	PPV	E	1003	9/9	0.97	0.11	-1.47	31,33,35,36	0
4	ISY	H	1003	14/14	0.96	0.14	-1.50	38,41,44,45	0
5	PPV	C	1003	9/9	0.94	0.13	-1.52	25,29,32,33	0
3	FPP	C	1002	24/24	0.97	0.13	-1.60	26,35,40,40	0
2	MG	A	1001	1/1	0.90	0.22	-	63,63,63,63	0
2	MG	E	1001	1/1	0.77	0.10	-	47,47,47,47	0
2	MG	A	1000	1/1	0.97	0.10	-	46,46,46,46	0
2	MG	H	1001	1/1	0.92	0.14	-	61,61,61,61	0
2	MG	C	1000	1/1	0.82	0.29	-	53,53,53,53	0
5	PPV	D	1000	9/9	0.84	0.22	-	109,109,110,110	0
2	MG	H	1000	1/1	0.96	0.14	-	42,42,42,42	0
2	MG	C	1001	1/1	0.87	0.12	-	36,36,36,36	0
2	MG	E	1000	1/1	0.88	0.17	-	62,62,62,62	0

6.5 Other polymers [i](#)

There are no such residues in this entry.