Full wwPDB X-ray Structure Validation Report (i)

Mar 6, 2026 – 03:46 PM UTC

PDB ID	:	2O1S / pdb_00002o1s
Title	:	1-deoxy-D-xylulose 5-phosphate synthase (DXS) from Escherichia coli
Authors	:	Xiang, S.; Usunow, G.; Lange, G.; Busch, M.; Tong, L.
Deposited on	:	2006-11-29
Resolution	:	2.40 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

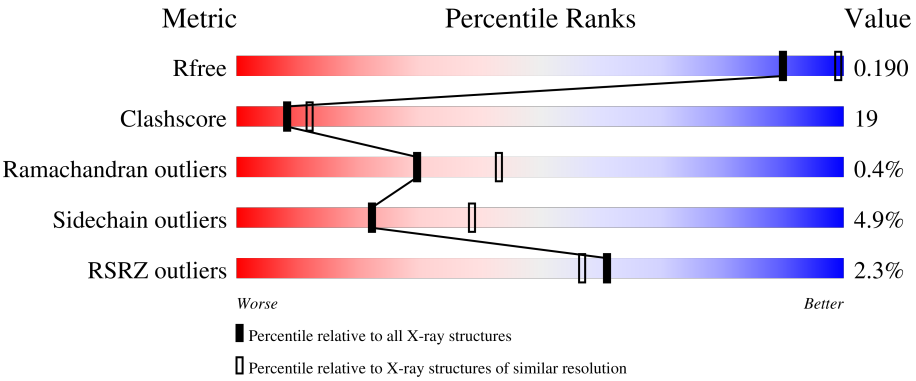
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	621	61% 22% · 14%
1	B	621	3% 50% 27% · 21%
1	C	621	% 60% 24% · 14%
1	D	621	3% 48% 27% · 22%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 16515 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 1-deoxy-D-xylulose-5-phosphate synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	536	Total	C	N	O	S	Se	0	0	0
			4122	2627	708	764	5	18			
1	B	493	Total	C	N	O	S	Se	0	0	0
			3800	2432	643	702	5	18			
1	C	536	Total	C	N	O	S	Se	0	0	0
			4123	2628	708	764	5	18			
1	D	487	Total	C	N	O	S	Se	0	0	0
			3734	2384	631	696	5	18			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP P77488
A	159	MSE	MET	modified residue	UNP P77488
A	164	MSE	MET	modified residue	UNP P77488
A	174	MSE	MET	modified residue	UNP P77488
A	183	MSE	MET	modified residue	UNP P77488
A	236	MSE	MET	modified residue	UNP P77488
A	269	MSE	MET	modified residue	UNP P77488
A	281	MSE	MET	modified residue	UNP P77488
A	340	MSE	MET	modified residue	UNP P77488
A	346	MSE	MET	modified residue	UNP P77488
A	352	MSE	MET	modified residue	UNP P77488
A	446	MSE	MET	modified residue	UNP P77488
A	449	MSE	MET	modified residue	UNP P77488
A	460	MSE	MET	modified residue	UNP P77488
A	515	MSE	MET	modified residue	UNP P77488
A	532	MSE	MET	modified residue	UNP P77488
A	546	MSE	MET	modified residue	UNP P77488
A	562	MSE	MET	modified residue	UNP P77488
A	574	MSE	MET	modified residue	UNP P77488
A	600	MSE	MET	modified residue	UNP P77488
A	611	MSE	MET	modified residue	UNP P77488

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Chain	Residue	Modelled	Actual	Comment	Reference
A	621	LEU	-	cloning artifact	UNP P77488
B	1	MSE	MET	modified residue	UNP P77488
B	159	MSE	MET	modified residue	UNP P77488
B	164	MSE	MET	modified residue	UNP P77488
B	174	MSE	MET	modified residue	UNP P77488
B	183	MSE	MET	modified residue	UNP P77488
B	236	MSE	MET	modified residue	UNP P77488
B	269	MSE	MET	modified residue	UNP P77488
B	281	MSE	MET	modified residue	UNP P77488
B	340	MSE	MET	modified residue	UNP P77488
B	346	MSE	MET	modified residue	UNP P77488
B	352	MSE	MET	modified residue	UNP P77488
B	446	MSE	MET	modified residue	UNP P77488
B	449	MSE	MET	modified residue	UNP P77488
B	460	MSE	MET	modified residue	UNP P77488
B	515	MSE	MET	modified residue	UNP P77488
B	532	MSE	MET	modified residue	UNP P77488
B	546	MSE	MET	modified residue	UNP P77488
B	562	MSE	MET	modified residue	UNP P77488
B	574	MSE	MET	modified residue	UNP P77488
B	600	MSE	MET	modified residue	UNP P77488
B	611	MSE	MET	modified residue	UNP P77488
B	621	LEU	-	cloning artifact	UNP P77488
C	1	MSE	MET	modified residue	UNP P77488
C	159	MSE	MET	modified residue	UNP P77488
C	164	MSE	MET	modified residue	UNP P77488
C	174	MSE	MET	modified residue	UNP P77488
C	183	MSE	MET	modified residue	UNP P77488
C	236	MSE	MET	modified residue	UNP P77488
C	269	MSE	MET	modified residue	UNP P77488
C	281	MSE	MET	modified residue	UNP P77488
C	340	MSE	MET	modified residue	UNP P77488
C	346	MSE	MET	modified residue	UNP P77488
C	352	MSE	MET	modified residue	UNP P77488
C	446	MSE	MET	modified residue	UNP P77488
C	449	MSE	MET	modified residue	UNP P77488
C	460	MSE	MET	modified residue	UNP P77488
C	515	MSE	MET	modified residue	UNP P77488
C	532	MSE	MET	modified residue	UNP P77488
C	546	MSE	MET	modified residue	UNP P77488
C	562	MSE	MET	modified residue	UNP P77488
C	574	MSE	MET	modified residue	UNP P77488

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Chain	Residue	Modelled	Actual	Comment	Reference
C	600	MSE	MET	modified residue	UNP P77488
C	611	MSE	MET	modified residue	UNP P77488
C	621	LEU	-	cloning artifact	UNP P77488
D	1	MSE	MET	modified residue	UNP P77488
D	159	MSE	MET	modified residue	UNP P77488
D	164	MSE	MET	modified residue	UNP P77488
D	174	MSE	MET	modified residue	UNP P77488
D	183	MSE	MET	modified residue	UNP P77488
D	236	MSE	MET	modified residue	UNP P77488
D	269	MSE	MET	modified residue	UNP P77488
D	281	MSE	MET	modified residue	UNP P77488
D	340	MSE	MET	modified residue	UNP P77488
D	346	MSE	MET	modified residue	UNP P77488
D	352	MSE	MET	modified residue	UNP P77488
D	446	MSE	MET	modified residue	UNP P77488
D	449	MSE	MET	modified residue	UNP P77488
D	460	MSE	MET	modified residue	UNP P77488
D	515	MSE	MET	modified residue	UNP P77488
D	532	MSE	MET	modified residue	UNP P77488
D	546	MSE	MET	modified residue	UNP P77488
D	562	MSE	MET	modified residue	UNP P77488
D	574	MSE	MET	modified residue	UNP P77488
D	600	MSE	MET	modified residue	UNP P77488
D	611	MSE	MET	modified residue	UNP P77488
D	621	LEU	-	cloning artifact	UNP P77488

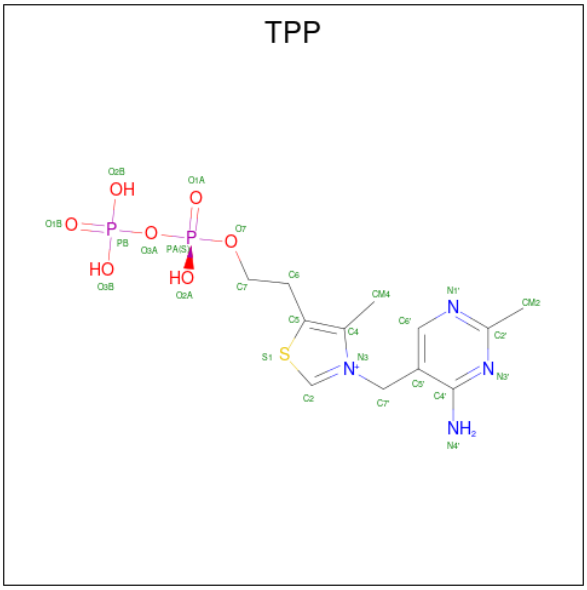
- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0

- Molecule 3 is POTASSIUM ION (CCD ID: K) (formula: K).

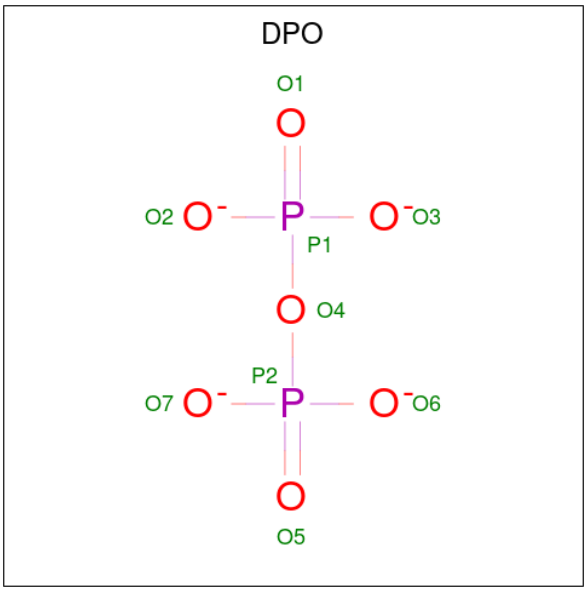
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total K 1 1	0	0
3	B	1	Total K 1 1	0	0
3	C	1	Total K 1 1	0	0
3	D	1	Total K 1 1	0	0

- Molecule 4 is THIAMINE DIPHOSPHATE (CCD ID: TPP) (formula: $C_{12}H_{19}N_4O_7P_2S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O P S 26 12 4 7 2 1	0	0
4	C	1	Total C N O P S 26 12 4 7 2 1	0	0

- Molecule 5 is DIPHOSPHATE (CCD ID: DPO) (formula: O_7P_2).



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

- Molecule 6 is water.

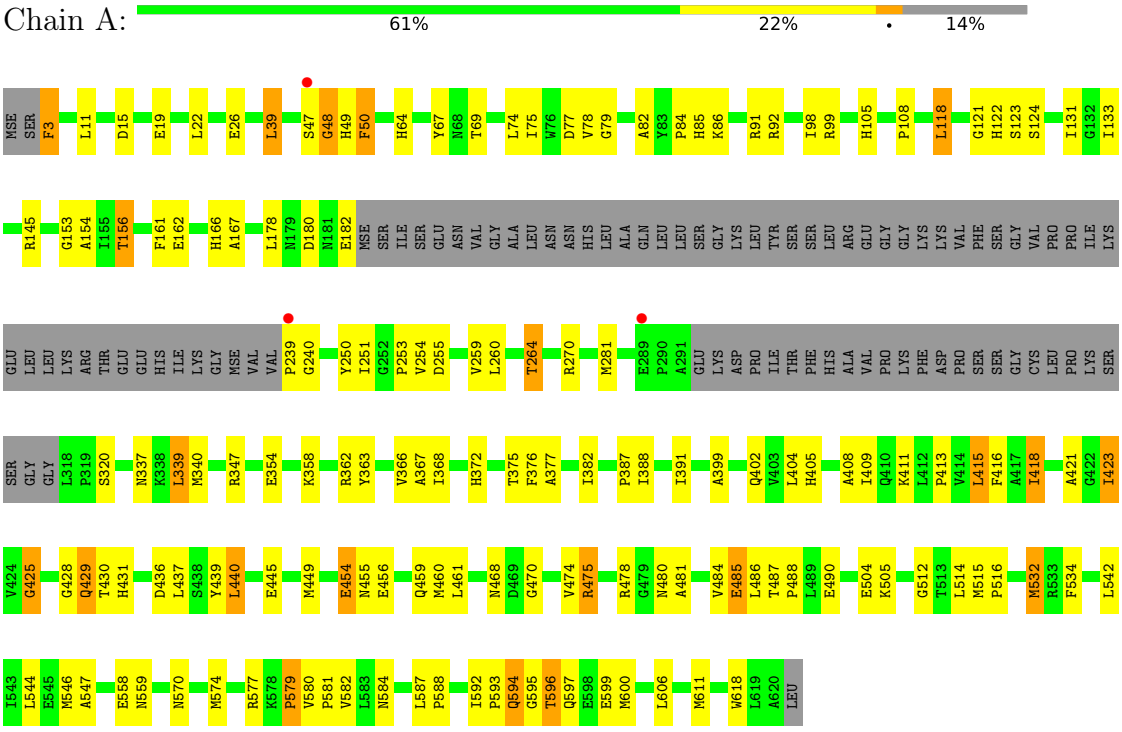
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	210	Total O 210 210	0	0
6	B	134	Total O 134 134	0	0
6	C	186	Total O 186 186	0	0
6	D	128	Total O 128 128	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

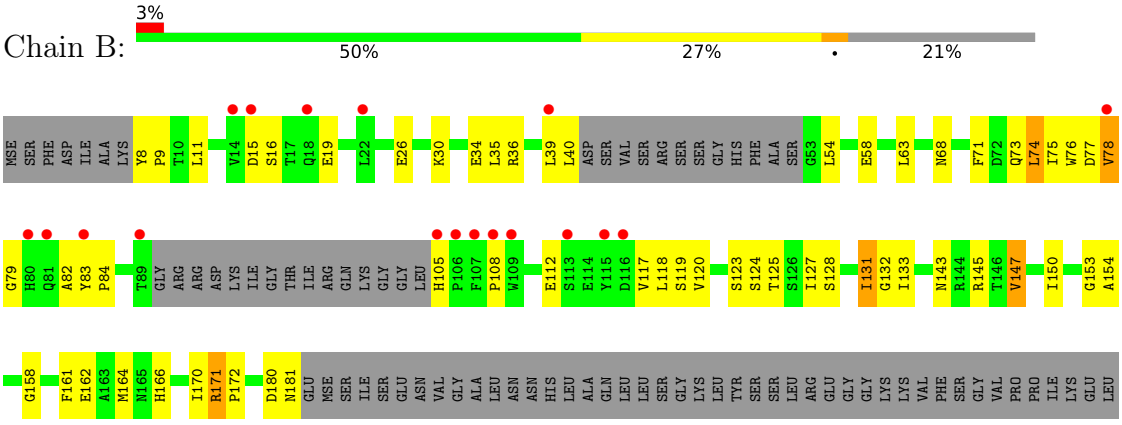
• Molecule 1: 1-deoxy-D-xylulose-5-phosphate synthase

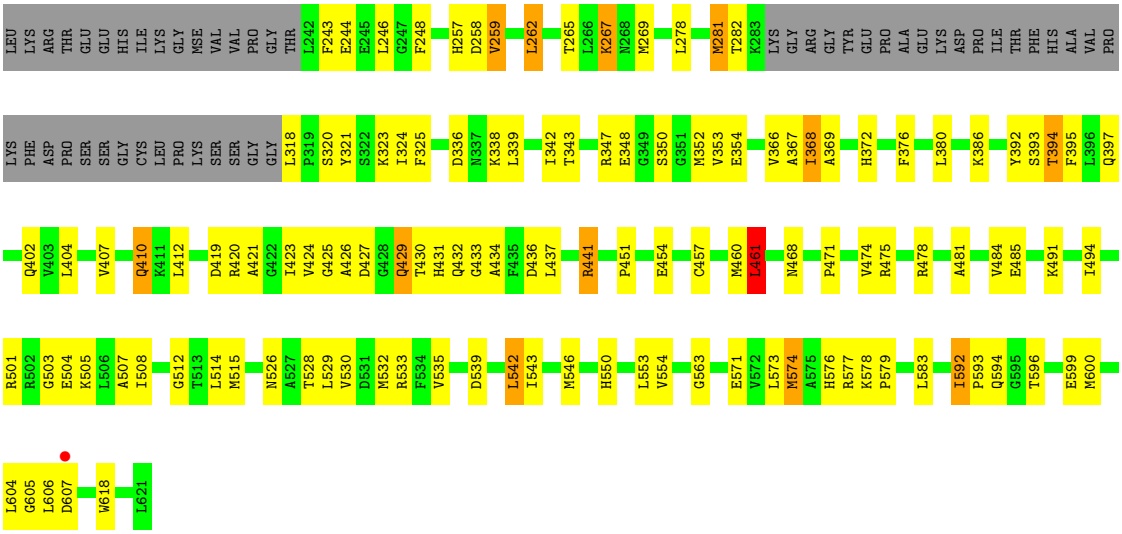
Chain A:



• Molecule 1: 1-deoxy-D-xylulose-5-phosphate synthase

Chain B:

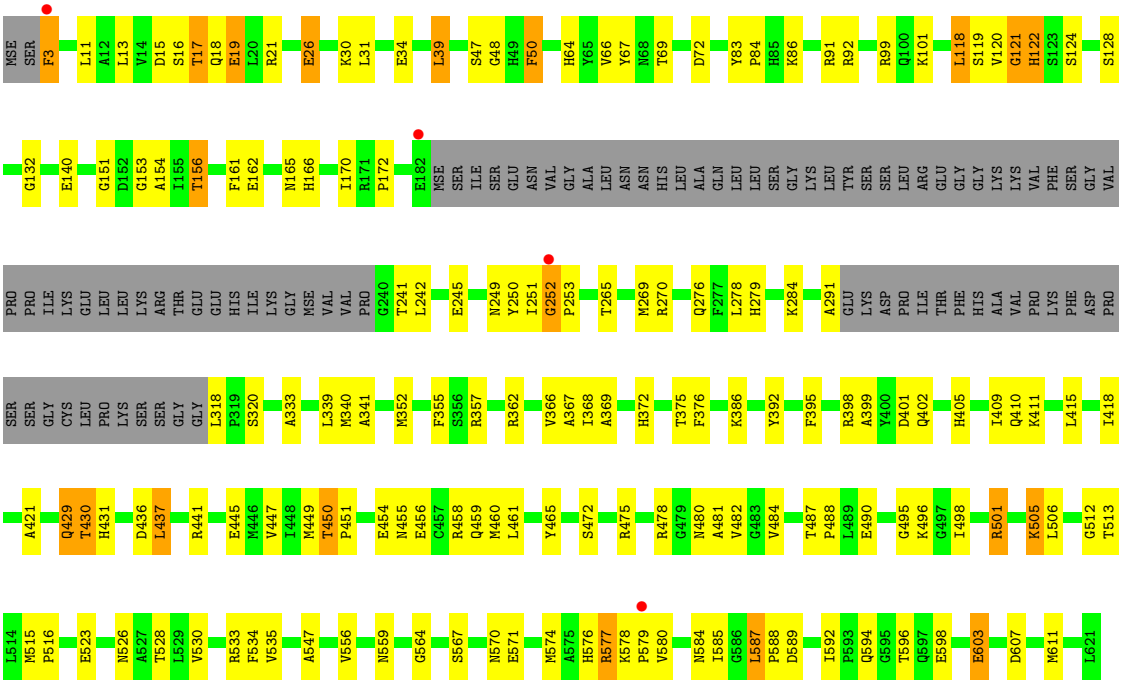




• Molecule 1: 1-deoxy-D-xylulose-5-phosphate synthase

Chain C:

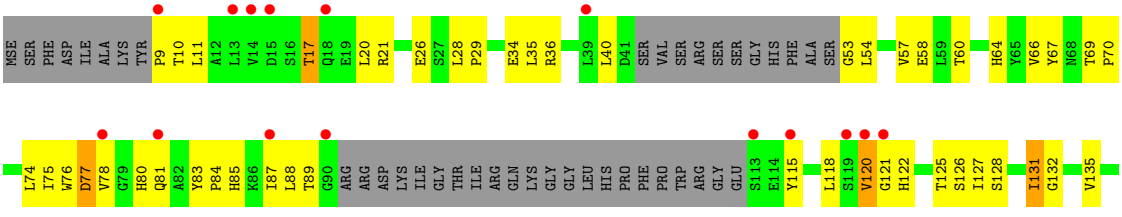


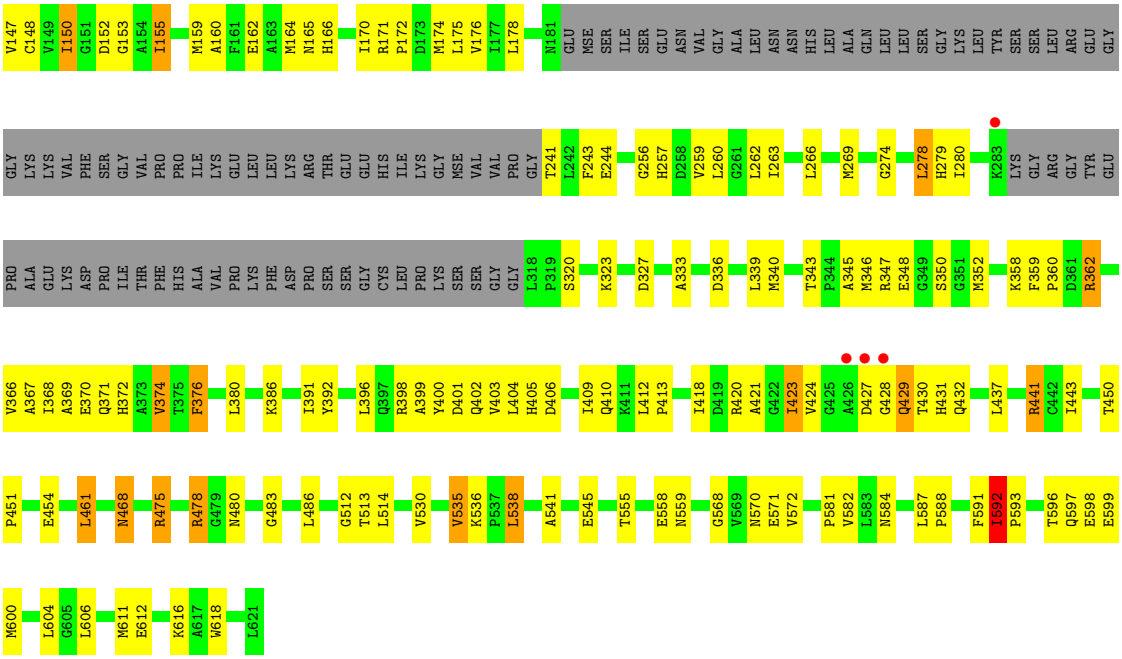


• Molecule 1: 1-deoxy-D-xylulose-5-phosphate synthase

Chain D:






V147 C148 V149 I150 G151 D152 G153 A154 I155 M159 A160 F161 E162 A163 M164 N165 H166 I170 R171 P172 D173 M174 L175 V176 I177 L178 N181
GLU MSE SER ILE SER GLU ASN VAL GLY ALA LEU ASN ASN HIS LEU ALA GLN LEU LEU SER GLY LYS LEU TYR SER SER LEU ARG GLU GLY
GLY LYS LYS VAL PHE SER GLY VAL PRO PRO ILE LYS GLU LEU LEU LYS ARG THR GLU GLU HIS ILE LYS GLY MSE VAL VAL PRO GLY
T241 L242 F243 E244 G256 H257 D258 V259 L260 G261 L262 I263 L266 M269 G274 L278 H279 I280 K283
LYS GLY ARG GLY TYR GLU
PRO ALA GLU LYS ASP PRO ILE THR PHE HIS ALA VAL PRO LYS PHE ASP PRO SER SER GLY CYS LEU PRO LYS SER SER GLY GLY L318 P319 S320 K323 D327 A333 D336 L339 M340 T343 P344 A345 M346 R347 E348 G349 S350 G351 M352 K358 F359 P360 D361 R362
V366 A367 I368 A369 E370 Q371 H372 A373 V374 T375 F376 L380 K386 I391 Y392 L396 Q397 R398 A399 Y400 D401 Q402 V403 L404 H405 D406 I409 Q410 K411 L412 P413 I418 D419 R420 A421 G422 I423 V424 G425 A426 D427 G428 Q429 T430 H431 Q432 L437 R441 C442 I443 T450
P451 E454 L461 M468 R475 R478 G479 N480 G483 L486 G512 T513 L514 V530 V535 K536 P537 L538 A541 E545 T555 E558 N559 G568 V569 N570 E571 V572 P581 V582 L583 N584 L587 P588 F591 I592 P593 T596 Q597 E598 E599
M600 L604 G605 L606 M611 E612 K616 A617 W618 L621

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	86.79Å 171.15Å 94.80Å 90.00° 107.25° 90.00°	Depositor
Resolution (Å)	30.00 – 2.40 30.00 – 2.41	Depositor EDS
% Data completeness (in resolution range)	89.0 (30.00-2.40) 89.6 (30.00-2.41)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	7.30 (at 2.42Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.191 , 0.234 0.192 , 0.190	Depositor DCC
R_{free} test set	4603 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	15.5	Xtriage
Anisotropy	0.312	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 40.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	16515	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, DPO, K, TPP

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	0.39	0/4191	0.91	12/5644 (0.2%)
1	B	0.39	0/3861	0.93	11/5203 (0.2%)
1	C	0.39	0/4191	0.94	15/5644 (0.3%)
1	D	0.37	0/3788	0.93	16/5101 (0.3%)
All	All	0.39	0/16031	0.93	54/21592 (0.3%)

There are no bond length outliers.

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	376	PHE	N-CA-C	-7.51	103.17	111.36
1	C	15	ASP	N-CA-C	-7.43	104.36	113.50
1	C	122	HIS	N-CA-C	-7.03	101.25	110.53
1	C	513	THR	N-CA-C	7.01	121.54	113.19
1	B	606	LEU	N-CA-C	-6.89	105.66	112.97
1	D	450	THR	CA-C-N	6.77	127.18	119.93
1	D	450	THR	C-N-CA	6.77	127.18	119.93
1	D	592	ILE	CA-C-N	6.66	126.61	120.21
1	D	592	ILE	C-N-CA	6.66	126.61	120.21
1	D	120	VAL	N-CA-C	6.44	118.06	107.24
1	A	478	ARG	N-CA-C	-6.43	99.54	109.76
1	B	376	PHE	N-CA-C	-6.17	104.64	111.36
1	A	512	GLY	N-CA-C	6.15	120.55	111.76
1	D	461	LEU	N-CA-C	-6.14	104.67	111.36
1	B	461	LEU	N-CA-C	-6.04	104.61	111.07
1	C	587	LEU	CA-C-N	5.92	125.89	120.21
1	C	587	LEU	C-N-CA	5.92	125.89	120.21
1	A	122	HIS	N-CA-C	-5.92	101.72	110.48
1	A	425	GLY	N-CA-C	5.85	118.64	111.45
1	B	468	ASN	N-CA-C	5.83	120.09	112.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	514	LEU	N-CA-C	-5.79	105.87	113.17
1	D	468	ASN	N-CA-C	5.78	120.03	112.92
1	D	513	THR	N-CA-C	5.69	121.22	113.37
1	C	50	PHE	N-CA-C	-5.65	105.27	111.82
1	D	478	ARG	N-CA-C	-5.64	102.13	110.48
1	B	592	ILE	N-CA-C	5.62	113.47	108.63
1	A	461	LEU	N-CA-C	-5.62	105.06	111.07
1	A	468	ASN	N-CA-C	5.60	120.10	112.88
1	C	512	GLY	N-CA-C	5.59	120.18	112.52
1	B	426	ALA	N-CA-C	5.50	118.79	111.75
1	A	532	MSE	N-CA-C	5.48	118.01	111.71
1	C	461	LEU	N-CA-C	-5.41	105.46	111.36
1	C	418	ILE	N-CA-C	5.37	115.05	106.88
1	C	450	THR	CA-C-N	5.37	125.30	119.76
1	C	450	THR	C-N-CA	5.37	125.30	119.76
1	C	535	VAL	N-CA-C	-5.36	104.79	112.35
1	A	15	ASP	N-CA-C	-5.35	107.41	114.31
1	B	425	GLY	N-CA-C	5.31	117.98	111.45
1	B	592	ILE	CA-C-N	5.27	125.56	119.92
1	B	592	ILE	C-N-CA	5.27	125.56	119.92
1	D	512	GLY	N-CA-C	5.25	119.27	111.76
1	D	274	GLY	CA-C-N	5.25	126.40	119.84
1	D	274	GLY	C-N-CA	5.25	126.40	119.84
1	C	528	THR	N-CA-C	-5.21	103.15	110.50
1	B	434	ALA	N-CA-C	5.21	119.79	113.38
1	B	512	GLY	N-CA-C	5.20	119.20	111.76
1	A	454	GLU	N-CA-C	5.19	117.68	111.71
1	D	376	PHE	N-CA-C	-5.17	105.72	111.36
1	D	535	VAL	N-CA-C	-5.15	105.49	113.16
1	D	441	ARG	N-CA-C	5.10	116.84	111.28
1	A	50	PHE	N-CA-C	-5.09	105.86	111.71
1	A	428	GLY	N-CA-C	5.04	123.06	112.17
1	A	418	ILE	N-CA-C	5.04	114.86	107.15
1	C	124	SER	N-CA-C	5.00	119.33	113.23

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	4122	0	4133	136	0
1	B	3800	0	3813	176	0
1	C	4123	0	4136	154	0
1	D	3734	0	3757	180	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	26	0	16	2	0
4	C	26	0	16	3	0
5	B	9	0	0	0	0
5	D	9	0	0	0	0
6	A	210	0	0	7	0
6	B	134	0	0	6	0
6	C	186	0	0	4	0
6	D	128	0	0	4	0
All	All	16515	0	15871	610	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 (610) 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:350:SER:HB2	1:B:352:MSE:HE2	1.34	1.10
1:B:503:GLY:H	1:B:528:THR:HG22	1.19	1.08
1:D:423:ILE:HD11	1:D:597:GLN:HA	1.39	1.04
1:A:581:PRO:HA	1:B:574:MSE:HE1	1.42	1.02
1:A:596:THR:HG22	1:A:599:GLU:H	1.19	1.01
1:B:420:ARG:HD3	1:B:478:ARG:HB2	1.45	0.99
1:A:570:ASN:HD21	1:A:584:ASN:HD21	1.08	0.99
1:C:429:GLN:H	1:C:429:GLN:HE21	1.03	0.98
1:B:265:THR:HG22	1:B:269:MSE:HE2	1.46	0.98
1:D:350:SER:HB2	1:D:352:MSE:HE2	1.45	0.97
1:C:269:MSE:HE1	1:C:278:LEU:HD22	1.48	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:570:ASN:HD21	1:C:584:ASN:HD21	1.16	0.94
1:A:429:GLN:H	1:A:429:GLN:NE2	1.66	0.93
1:B:437:LEU:HG	1:B:475:ARG:HH11	1.32	0.93
1:C:265:THR:HG22	1:C:269:MSE:HE2	1.51	0.93
1:C:402:GLN:HE21	1:D:159:MSE:HE1	1.33	0.92
1:A:156:THR:HG21	1:A:367:ALA:HB1	1.52	0.92
1:C:118:LEU:HD12	1:C:120:VAL:HG13	1.52	0.91
1:C:249:ASN:HD22	1:C:276:GLN:HE22	1.07	0.90
1:A:429:GLN:H	1:A:429:GLN:HE21	0.91	0.90
1:C:429:GLN:H	1:C:429:GLN:NE2	1.71	0.88
1:A:429:GLN:HE21	1:A:429:GLN:N	1.71	0.88
1:A:459:GLN:HE22	1:A:490:GLU:H	1.22	0.88
1:C:429:GLN:HE21	1:C:429:GLN:N	1.73	0.87
1:B:503:GLY:N	1:B:528:THR:HG22	1.89	0.86
1:D:420:ARG:HD3	1:D:478:ARG:HB2	1.58	0.86
1:D:570:ASN:HD21	1:D:584:ASN:HD21	1.23	0.85
1:B:574:MSE:HE3	1:B:574:MSE:HA	1.59	0.84
1:B:503:GLY:H	1:B:528:THR:CG2	1.90	0.84
1:C:17:THR:HG21	1:C:69:THR:HG23	1.59	0.84
1:D:404:LEU:HD13	1:D:443:ILE:HG12	1.62	0.82
1:B:574:MSE:HA	1:B:574:MSE:CE	2.10	0.82
1:C:64:HIS:ND1	1:C:69:THR:HG21	1.96	0.81
1:C:402:GLN:NE2	1:D:159:MSE:HE1	1.96	0.80
1:C:121:GLY:HA3	1:C:430:THR:OG1	1.81	0.80
1:D:596:THR:HB	1:D:599:GLU:HG3	1.64	0.80
1:B:63:LEU:HD13	1:B:74:LEU:HD21	1.64	0.79
1:B:437:LEU:HG	1:B:475:ARG:NH1	1.98	0.79
1:B:75:ILE:HD11	1:B:133:ILE:HD12	1.65	0.78
1:B:164:MSE:HE1	1:B:243:PHE:HD1	1.49	0.78
1:C:118:LEU:HD11	6:C:3003:HOH:O	1.82	0.77
1:B:269:MSE:HE1	1:B:278:LEU:HD22	1.64	0.77
1:D:36:ARG:HG3	1:D:54:LEU:HD22	1.64	0.77
1:D:343:THR:HB	1:D:352:MSE:HE1	1.66	0.77
1:C:437:LEU:HD13	1:C:475:ARG:HD3	1.65	0.76
1:C:437:LEU:CD1	1:C:475:ARG:HD3	2.14	0.76
1:B:508:ILE:HG12	1:B:554:VAL:CG1	2.16	0.75
1:B:421:ALA:HB1	1:B:475:ARG:HH21	1.49	0.75
1:C:556:VAL:HG13	1:C:611:MSE:HE1	1.68	0.75
1:C:118:LEU:HD12	1:C:120:VAL:CG1	2.17	0.74
1:C:26:GLU:CD	1:C:26:GLU:H	1.97	0.73
1:C:156:THR:HG21	1:C:368:ILE:H	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:372:HIS:HE1	1:D:166:HIS:ND1	1.87	0.72
1:C:459:GLN:HE22	1:C:490:GLU:H	1.37	0.72
1:A:581:PRO:HA	1:B:574:MSE:CE	2.20	0.71
1:B:338:LYS:HB3	1:B:386:LYS:HG2	1.72	0.71
1:A:156:THR:HG21	1:A:367:ALA:CB	2.19	0.71
1:B:120:VAL:O	1:B:430:THR:HG21	1.90	0.71
1:A:166:HIS:ND1	1:B:372:HIS:HE1	1.87	0.71
1:B:437:LEU:CG	1:B:475:ARG:HH11	2.02	0.71
1:C:585:ILE:HG21	1:C:611:MSE:HE2	1.73	0.71
1:B:596:THR:HG22	1:B:599:GLU:HB2	1.73	0.71
1:B:596:THR:HG23	1:B:599:GLU:H	1.55	0.70
1:C:156:THR:HG21	1:C:367:ALA:HB1	1.74	0.70
1:A:459:GLN:NE2	1:A:490:GLU:H	1.90	0.69
1:C:366:VAL:HG12	1:C:369:ALA:HB3	1.75	0.69
1:A:456:GLU:O	1:A:460:MSE:HG3	1.92	0.69
1:C:269:MSE:CE	1:C:278:LEU:HD22	2.21	0.69
1:D:420:ARG:CD	1:D:478:ARG:HB2	2.22	0.68
1:D:26:GLU:CD	1:D:26:GLU:H	2.00	0.68
1:C:556:VAL:CG1	1:C:611:MSE:HE1	2.23	0.68
1:D:40:LEU:HD21	1:D:54:LEU:HD11	1.74	0.68
1:D:343:THR:CB	1:D:352:MSE:HE1	2.23	0.68
1:C:17:THR:HG23	1:C:21:ARG:NH1	2.09	0.68
1:B:508:ILE:HG12	1:B:554:VAL:HG11	1.74	0.67
1:C:596:THR:HG22	1:C:598:GLU:H	1.60	0.67
1:D:423:ILE:HD13	1:D:600:MSE:HB2	1.77	0.67
1:D:347:ARG:HA	1:D:352:MSE:HE3	1.77	0.67
1:C:410:GLN:HE22	1:D:118:LEU:HD12	1.60	0.67
1:B:420:ARG:CD	1:B:478:ARG:HB2	2.23	0.67
1:B:368:ILE:N	1:B:368:ILE:HD12	2.10	0.66
1:C:30:LYS:HE3	1:C:34:GLU:OE2	1.95	0.66
1:B:258:ASP:O	1:B:262:LEU:HD22	1.96	0.66
1:A:436:ASP:O	1:A:440:LEU:HB2	1.96	0.65
1:A:337:ASN:HA	1:A:362:ARG:NH2	2.12	0.65
1:A:423:ILE:HD11	1:A:597:GLN:HA	1.77	0.65
1:C:118:LEU:HD22	1:D:410:GLN:HE22	1.60	0.65
1:C:437:LEU:HB2	1:C:559:ASN:CG	2.22	0.65
1:B:267:LYS:HB2	1:B:267:LYS:NZ	2.12	0.65
1:D:17:THR:HG23	1:D:21:ARG:NH1	2.12	0.65
1:C:291:ALA:C	1:C:478:ARG:HH12	2.06	0.64
1:D:429:GLN:NE2	1:D:429:GLN:H	1.95	0.64
1:B:421:ALA:HB1	1:B:475:ARG:NH2	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:386:LYS:HD3	1:C:465:TYR:CZ	2.33	0.63
1:A:570:ASN:HD21	1:A:584:ASN:ND2	1.90	0.63
1:B:164:MSE:HE1	1:B:243:PHE:CD1	2.33	0.63
1:D:17:THR:HG23	1:D:21:ARG:HH12	1.64	0.63
1:D:35:LEU:CD1	1:D:87:ILE:HD13	2.29	0.63
1:B:343:THR:HB	1:B:352:MSE:HE1	1.81	0.63
1:C:441:ARG:HH12	1:C:567:SER:HB3	1.64	0.63
1:C:454:GLU:CD	1:C:481:ALA:HB1	2.24	0.63
1:C:454:GLU:OE2	1:C:481:ALA:HB1	1.99	0.63
1:D:126:SER:OG	1:D:148:CYS:HB3	1.99	0.63
1:D:486:LEU:N	1:D:486:LEU:HD12	2.13	0.62
1:D:592:ILE:HG21	1:D:604:LEU:HD11	1.80	0.62
1:A:105:HIS:HA	1:A:594:GLN:HE22	1.63	0.62
1:A:153:GLY:O	1:A:156:THR:HB	1.98	0.62
1:B:421:ALA:HB1	1:B:475:ARG:HE	1.65	0.62
1:A:484:VAL:HG12	1:A:485:GLU:N	2.14	0.62
1:B:343:THR:CB	1:B:352:MSE:HE1	2.29	0.62
1:A:596:THR:CG2	1:A:599:GLU:H	2.06	0.62
1:C:482:VAL:CG2	1:C:484:VAL:HG13	2.30	0.62
1:A:595:GLY:HA3	1:A:600:MSE:CE	2.30	0.62
1:B:127:ILE:O	1:B:131:ILE:HG23	2.00	0.62
1:D:35:LEU:HD11	1:D:87:ILE:HG21	1.82	0.62
1:C:402:GLN:NE2	1:D:159:MSE:CE	2.63	0.61
1:C:153:GLY:O	1:C:156:THR:HB	2.00	0.61
1:D:150:ILE:HD12	1:D:150:ILE:O	2.01	0.61
1:A:411:LYS:HE2	1:A:445:GLU:CD	2.26	0.61
1:C:16:SER:HB3	1:C:19:GLU:OE1	2.01	0.61
1:C:436:ASP:OD1	1:C:475:ARG:HD2	2.01	0.61
1:B:26:GLU:CD	1:B:26:GLU:H	2.09	0.60
1:C:430:THR:OG1	1:C:431:HIS:HD2	1.84	0.60
1:C:607:ASP:O	1:C:611:MSE:HG3	2.01	0.60
1:B:429:GLN:H	1:B:429:GLN:NE2	1.98	0.60
1:D:150:ILE:HD12	1:D:178:LEU:HA	1.83	0.60
1:A:596:THR:HG22	1:A:599:GLU:N	2.04	0.60
1:B:74:LEU:HD22	1:B:147:VAL:HG13	1.83	0.60
1:B:170:ILE:HG13	1:B:172:PRO:HD3	1.83	0.60
1:D:405:HIS:HA	1:D:409:ILE:HD12	1.83	0.60
1:A:437:LEU:HB2	1:A:559:ASN:CG	2.27	0.60
1:B:105:HIS:HB2	1:B:112:GLU:OE1	2.02	0.60
1:A:595:GLY:HA3	1:A:600:MSE:HE3	1.84	0.60
1:B:79:GLY:HA3	1:B:108:PRO:HD2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:17:THR:HG22	1:C:18:GLN:NE2	2.16	0.60
1:C:505:LYS:HG3	1:C:506:LEU:HD13	1.84	0.60
1:C:570:ASN:HD21	1:C:584:ASN:ND2	1.95	0.60
1:A:459:GLN:HE22	1:A:490:GLU:N	1.94	0.59
1:C:170:ILE:HG13	1:C:172:PRO:HD3	1.84	0.59
1:D:429:GLN:HG3	1:D:592:ILE:O	2.02	0.59
1:B:454:GLU:OE1	1:B:481:ALA:HB1	2.02	0.59
1:A:423:ILE:HD12	1:A:425:GLY:H	1.67	0.59
1:D:423:ILE:O	1:D:423:ILE:HG13	2.02	0.59
1:B:504:GLU:HG2	1:B:526:ASN:ND2	2.18	0.58
1:D:36:ARG:HH21	1:D:57:VAL:HB	1.68	0.58
1:C:456:GLU:O	1:C:460:MSE:HG3	2.04	0.58
1:D:121:GLY:HA3	1:D:430:THR:CB	2.33	0.58
1:B:105:HIS:HA	1:B:594:GLN:NE2	2.19	0.58
1:B:494:ILE:HD12	1:B:494:ILE:N	2.19	0.58
1:A:339:LEU:O	1:A:340:MSE:HE2	2.04	0.58
1:B:494:ILE:HD12	1:B:494:ILE:H	1.69	0.58
1:B:484:VAL:HG12	1:B:485:GLU:N	2.19	0.58
1:C:122:HIS:H	1:D:405:HIS:CE1	2.21	0.58
1:D:339:LEU:HD23	1:D:339:LEU:C	2.28	0.58
1:D:596:THR:HB	1:D:599:GLU:CG	2.34	0.58
1:A:423:ILE:HD12	1:A:425:GLY:N	2.19	0.57
1:B:131:ILE:HD11	1:B:166:HIS:ND1	2.19	0.57
1:C:166:HIS:ND1	1:D:372:HIS:HE1	2.02	0.57
1:B:368:ILE:HD12	1:B:368:ILE:H	1.67	0.57
1:C:269:MSE:HE1	1:C:278:LEU:HB2	1.86	0.57
1:A:405:HIS:HE1	1:B:430:THR:HB	1.68	0.57
1:C:402:GLN:HE21	1:D:159:MSE:CE	2.14	0.57
1:B:58:GLU:HG3	1:B:259:VAL:HG22	1.86	0.57
1:C:333:ALA:O	1:C:362:ARG:NH2	2.38	0.57
1:D:84:PRO:HG2	6:D:4010:HOH:O	2.03	0.57
1:D:345:ALA:HB2	1:D:367:ALA:HA	1.86	0.57
1:A:64:HIS:HE1	1:A:85:HIS:ND1	2.03	0.56
1:C:17:THR:HG23	1:C:21:ARG:HH12	1.69	0.56
1:D:256:GLY:HA3	1:D:280:ILE:HG23	1.86	0.56
1:A:250:TYR:C	1:A:251:ILE:HD12	2.30	0.56
1:A:547:ALA:HB1	1:A:580:VAL:HG21	1.86	0.56
1:A:39:LEU:HD22	1:A:50:PHE:HB2	1.87	0.56
1:A:366:VAL:O	1:A:367:ALA:HB3	2.06	0.56
1:A:606:LEU:C	1:A:611:MSE:HE3	2.31	0.56
1:C:441:ARG:NH2	1:C:571:GLU:OE1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:HIS:HE1	1:B:166:HIS:ND1	2.03	0.56
1:B:437:LEU:HD21	1:B:475:ARG:HD2	1.88	0.56
1:D:84:PRO:HA	1:D:87:ILE:HG22	1.88	0.56
1:D:451:PRO:HD2	1:D:475:ARG:O	2.06	0.56
1:B:108:PRO:HG2	1:B:120:VAL:HG22	1.88	0.56
1:C:366:VAL:O	1:C:366:VAL:CG1	2.54	0.56
1:D:131:ILE:HG13	1:D:132:GLY:N	2.20	0.56
1:A:372:HIS:HD2	1:B:128:SER:OG	1.89	0.55
1:B:392:TYR:CE2	1:B:420:ARG:HG3	2.42	0.55
1:C:269:MSE:HE1	1:C:278:LEU:CD2	2.29	0.55
1:D:36:ARG:NH2	1:D:58:GLU:OE1	2.39	0.55
1:D:78:VAL:HB	1:D:80:HIS:ND1	2.21	0.55
1:A:75:ILE:HD11	1:A:133:ILE:HD12	1.88	0.55
1:C:495:GLY:O	1:C:496:LYS:HD2	2.06	0.55
4:A:3001:TPP:C2	4:A:3001:TPP:HN42	2.19	0.55
1:B:429:GLN:NE2	1:B:593:PRO:HA	2.21	0.55
4:A:3001:TPP:HN42	4:A:3001:TPP:H2	1.72	0.55
1:B:507:ALA:HB3	1:B:553:LEU:HD23	1.88	0.55
1:A:156:THR:HG21	1:A:368:ILE:H	1.71	0.55
1:A:454:GLU:OE2	1:A:481:ALA:HB1	2.05	0.55
1:C:410:GLN:HE22	1:D:118:LEU:CD1	2.20	0.55
1:D:131:ILE:HG22	1:D:174:MSE:SE	2.56	0.55
1:D:155:ILE:HG13	1:D:178:LEU:HD13	1.89	0.55
1:D:127:ILE:O	1:D:131:ILE:HG23	2.07	0.54
1:D:428:GLY:O	1:D:432:GLN:HG2	2.07	0.54
1:D:118:LEU:HD21	1:D:125:THR:HG22	1.88	0.54
1:B:281:MSE:HE3	1:B:281:MSE:HA	1.89	0.54
1:B:437:LEU:HD22	1:B:535:VAL:HG21	1.89	0.54
1:B:451:PRO:HD2	1:B:475:ARG:O	2.07	0.54
1:C:128:SER:OG	1:D:372:HIS:HD2	1.91	0.54
1:C:454:GLU:O	1:C:458:ARG:HG3	2.07	0.54
1:B:596:THR:HG22	1:B:599:GLU:CD	2.32	0.54
4:C:3002:TPP:HN42	4:C:3002:TPP:C2	2.20	0.54
1:D:348:GLU:H	1:D:348:GLU:CD	2.16	0.54
1:A:577:ARG:HH11	1:A:577:ARG:HG2	1.72	0.54
1:D:9:PRO:HB2	1:D:34:GLU:OE1	2.06	0.54
1:A:145:ARG:HD2	6:A:3183:HOH:O	2.07	0.54
1:D:11:LEU:O	1:D:11:LEU:HD23	2.08	0.54
1:D:256:GLY:CA	1:D:280:ILE:HG23	2.38	0.54
1:B:441:ARG:NH2	1:B:571:GLU:CD	2.66	0.54
1:B:454:GLU:CD	1:B:481:ALA:HB1	2.32	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:501:ARG:NH2	1:C:526:ASN:HA	2.22	0.54
1:C:592:ILE:HD12	1:C:592:ILE:N	2.22	0.54
1:A:542:LEU:HD13	1:A:542:LEU:O	2.07	0.53
1:D:386:LYS:NZ	1:D:468:ASN:HD21	2.06	0.53
1:B:432:GLN:HE21	1:B:432:GLN:HA	1.73	0.53
1:D:89:THR:HG23	1:D:115:TYR:CD1	2.43	0.53
1:B:508:ILE:HA	1:B:554:VAL:HG13	1.90	0.53
1:D:241:THR:HG23	1:D:244:GLU:H	1.74	0.53
1:B:54:LEU:C	1:B:54:LEU:HD12	2.34	0.53
1:C:441:ARG:NH1	1:C:567:SER:HB3	2.24	0.53
1:D:58:GLU:HG2	1:D:257:HIS:O	2.08	0.53
1:D:159:MSE:HE3	1:D:398:ARG:CZ	2.39	0.53
1:A:47:SER:O	1:A:49:HIS:N	2.35	0.53
1:A:411:LYS:HD3	1:A:445:GLU:HG3	1.89	0.53
1:C:366:VAL:O	1:C:367:ALA:HB3	2.08	0.53
1:D:121:GLY:HA3	1:D:430:THR:HB	1.91	0.53
1:A:154:ALA:HA	1:A:368:ILE:HD12	1.90	0.53
1:B:410:GLN:HB2	1:B:412:LEU:HG	1.91	0.53
1:A:239:PRO:HG2	1:A:240:GLY:H	1.74	0.52
1:A:430:THR:OG1	1:A:431:HIS:HD2	1.91	0.52
1:B:347:ARG:HA	1:B:352:MSE:HE3	1.90	0.52
1:D:320:SER:HA	1:D:480:ASN:HA	1.91	0.52
1:D:427:ASP:HB3	1:D:431:HIS:HB2	1.91	0.52
1:A:454:GLU:CD	1:A:481:ALA:HB1	2.34	0.52
1:C:576:HIS:O	1:C:578:LYS:HG2	2.10	0.52
1:B:171:ARG:HD2	6:B:4009:HOH:O	2.08	0.52
1:C:366:VAL:HG12	1:C:366:VAL:O	2.09	0.52
1:C:447:VAL:HG22	1:C:472:SER:HA	1.91	0.52
1:D:66:VAL:HG21	1:D:266:LEU:HB3	1.90	0.52
1:D:437:LEU:HB2	1:D:559:ASN:CG	2.35	0.52
1:A:166:HIS:ND1	1:B:372:HIS:CE1	2.76	0.52
1:C:339:LEU:C	1:C:339:LEU:HD23	2.35	0.52
1:A:375:THR:HG21	1:B:125:THR:HG23	1.92	0.52
1:A:574:MSE:HE1	1:A:579:PRO:HA	1.92	0.52
1:A:347:ARG:HB2	1:A:363:TYR:OH	2.09	0.51
1:B:423:ILE:HG23	1:B:592:ILE:HD11	1.91	0.51
1:D:486:LEU:HD11	6:D:4126:HOH:O	2.11	0.51
1:C:411:LYS:HE2	1:C:445:GLU:OE1	2.10	0.51
1:B:366:VAL:O	1:B:367:ALA:HB3	2.10	0.51
1:B:592:ILE:O	1:B:592:ILE:HG13	2.10	0.51
1:B:324:ILE:HG13	1:B:325:PHE:N	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:17:THR:CG2	1:C:21:ARG:HH12	2.22	0.51
1:B:424:VAL:H	1:B:432:GLN:HE22	1.59	0.51
1:C:441:ARG:NH1	1:C:564:GLY:O	2.42	0.51
1:C:459:GLN:NE2	1:C:490:GLU:H	2.07	0.51
1:C:547:ALA:HB1	1:C:580:VAL:HG21	1.91	0.51
1:C:253:PRO:HA	1:C:279:HIS:O	2.09	0.51
1:C:375:THR:HG21	1:D:125:THR:HG23	1.93	0.51
1:C:577:ARG:HG2	1:D:618:TRP:CE2	2.45	0.51
1:D:66:VAL:HG23	1:D:67:TYR:CD2	2.46	0.51
1:D:20:LEU:C	1:D:20:LEU:HD23	2.36	0.51
1:C:455:ASN:O	1:C:459:GLN:HG2	2.11	0.51
1:A:606:LEU:O	1:A:611:MSE:HE3	2.11	0.50
1:B:150:ILE:CG1	1:B:154:ALA:HB3	2.41	0.50
1:C:487:THR:HB	1:C:488:PRO:HD2	1.93	0.50
1:D:77:ASP:OD2	1:D:150:ILE:HG22	2.12	0.50
1:D:421:ALA:HB1	1:D:475:ARG:CZ	2.41	0.50
1:A:154:ALA:C	1:A:156:THR:H	2.17	0.50
1:A:260:LEU:O	1:A:264:THR:HG22	2.11	0.50
1:A:253:PRO:HB2	1:A:281:MSE:HE2	1.93	0.50
1:D:241:THR:HG22	1:D:244:GLU:HB2	1.92	0.50
1:A:161:PHE:HB2	1:B:161:PHE:CD2	2.47	0.50
1:B:394:THR:HG21	1:B:431:HIS:HA	1.94	0.50
1:C:392:TYR:HB2	1:C:395:PHE:CD2	2.47	0.50
1:C:405:HIS:HA	1:C:409:ILE:HD12	1.94	0.50
1:C:459:GLN:HE22	1:C:490:GLU:N	2.07	0.50
1:D:570:ASN:HD21	1:D:584:ASN:ND2	2.03	0.50
1:A:436:ASP:OD2	1:A:475:ARG:HD2	2.12	0.50
1:B:539:ASP:O	1:B:543:ILE:HG13	2.11	0.50
1:A:339:LEU:HD21	1:A:388:ILE:HD12	1.94	0.50
1:A:596:THR:HG21	6:A:3048:HOH:O	2.11	0.50
1:B:421:ALA:HB1	1:B:475:ARG:NE	2.25	0.50
1:A:399:ALA:HA	1:A:402:GLN:NE2	2.26	0.49
1:A:596:THR:HG23	6:A:3185:HOH:O	2.12	0.49
1:C:251:ILE:O	1:C:252:GLY:O	2.30	0.49
1:A:487:THR:HB	1:A:488:PRO:HD2	1.94	0.49
1:B:437:LEU:HD21	1:B:475:ARG:CD	2.41	0.49
1:D:20:LEU:HD12	1:D:88:LEU:HD22	1.94	0.49
1:C:430:THR:OG1	1:C:431:HIS:CD2	2.65	0.49
1:B:441:ARG:NH1	1:B:563:GLY:O	2.46	0.49
1:C:366:VAL:CG1	1:C:369:ALA:HB3	2.42	0.49
1:A:67:TYR:CE2	1:A:270:ARG:HD2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:PRO:HG2	6:A:3002:HOH:O	2.12	0.49
1:A:250:TYR:O	1:A:251:ILE:HD12	2.11	0.49
1:B:407:VAL:HG12	1:B:471:PRO:HB3	1.95	0.49
1:D:75:ILE:N	1:D:75:ILE:HD12	2.27	0.49
1:D:429:GLN:HB3	1:D:591:PHE:HB3	1.95	0.49
1:D:323:LYS:HE3	1:D:327:ASP:OD2	2.13	0.49
1:D:53:GLY:HA2	6:D:4037:HOH:O	2.13	0.48
1:A:423:ILE:HG23	1:A:558:GLU:OE1	2.13	0.48
1:B:505:LYS:O	1:B:550:HIS:HB3	2.12	0.48
1:C:67:TYR:CD1	1:C:270:ARG:HD2	2.48	0.48
1:D:77:ASP:HB2	1:D:150:ILE:HG22	1.95	0.48
1:D:159:MSE:HE3	1:D:398:ARG:NH1	2.28	0.48
1:C:118:LEU:CD2	1:D:410:GLN:HE22	2.26	0.48
1:B:542:LEU:O	1:B:546:MSE:HG2	2.13	0.48
1:C:437:LEU:HD11	1:C:475:ARG:HD3	1.95	0.48
1:B:77:ASP:O	1:B:78:VAL:HB	2.13	0.48
1:B:429:GLN:H	1:B:429:GLN:HE21	1.59	0.48
1:B:576:HIS:O	1:B:578:LYS:HD2	2.13	0.48
1:C:242:LEU:C	1:C:242:LEU:HD23	2.39	0.48
1:D:121:GLY:HA3	1:D:430:THR:OG1	2.14	0.48
1:D:441:ARG:HH22	1:D:571:GLU:CD	2.22	0.48
1:D:535:VAL:O	1:D:538:LEU:HD13	2.14	0.48
1:C:495:GLY:C	1:C:496:LYS:HD2	2.39	0.48
1:D:359:PHE:HB3	1:D:362:ARG:HG3	1.94	0.48
1:D:568:GLY:O	1:D:572:VAL:HG23	2.14	0.48
1:A:582:VAL:H	1:B:574:MSE:HE2	1.79	0.48
1:C:156:THR:HG21	1:C:368:ILE:N	2.27	0.48
1:D:159:MSE:CE	1:D:398:ARG:CZ	2.92	0.48
1:D:160:ALA:O	1:D:164:MSE:HG3	2.13	0.48
1:A:484:VAL:CG1	1:A:485:GLU:N	2.77	0.48
1:B:244:GLU:HA	1:B:248:PHE:O	2.14	0.48
1:D:83:TYR:N	1:D:84:PRO:HD2	2.29	0.48
1:D:259:VAL:HG13	1:D:260:LEU:N	2.29	0.48
1:D:366:VAL:O	1:D:367:ALA:HB3	2.13	0.48
1:A:437:LEU:H	1:A:559:ASN:ND2	2.12	0.47
1:B:143:ASN:ND2	1:B:145:ARG:HH12	2.12	0.47
1:A:39:LEU:CD2	1:A:50:PHE:HB2	2.44	0.47
1:B:475:ARG:O	1:B:475:ARG:HG3	2.14	0.47
1:B:494:ILE:H	1:B:494:ILE:CD1	2.26	0.47
1:C:249:ASN:HD22	1:C:276:GLN:NE2	1.91	0.47
1:D:89:THR:O	1:D:89:THR:HG22	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:TYR:N	1:B:84:PRO:HD2	2.29	0.47
1:D:423:ILE:HD11	1:D:597:GLN:CA	2.29	0.47
1:A:259:VAL:HG13	1:A:260:LEU:N	2.29	0.47
4:C:3002:TPP:HN42	4:C:3002:TPP:H2	1.80	0.47
1:A:546:MSE:HE2	1:A:546:MSE:HA	1.97	0.47
1:B:324:ILE:HD11	1:B:457:CYS:SG	2.54	0.47
1:B:339:LEU:HD23	1:B:339:LEU:C	2.39	0.47
1:C:118:LEU:HD13	1:C:119:SER:N	2.29	0.47
1:C:386:LYS:NZ	1:C:465:TYR:O	2.47	0.47
1:C:436:ASP:OD1	1:C:475:ARG:CD	2.62	0.47
1:D:64:HIS:HE1	1:D:85:HIS:ND1	2.13	0.47
1:D:164:MSE:HE1	1:D:243:PHE:HD1	1.78	0.47
1:D:358:LYS:C	1:D:360:PRO:HD3	2.40	0.47
1:B:350:SER:CB	1:B:352:MSE:HE2	2.26	0.47
1:A:118:LEU:HD23	1:B:410:GLN:OE1	2.15	0.47
1:B:158:GLY:O	1:B:162:GLU:HG3	2.15	0.47
1:C:399:ALA:HA	1:C:402:GLN:OE1	2.15	0.47
1:C:3:PHE:C	1:C:3:PHE:CD2	2.93	0.47
1:C:162:GLU:CD	1:D:369:ALA:HB1	2.40	0.47
1:C:250:TYR:CE1	1:C:252:GLY:HA2	2.50	0.47
1:C:589:ASP:OD2	1:D:536:LYS:NZ	2.48	0.47
1:D:17:THR:CG2	1:D:21:ARG:HH22	2.28	0.47
1:D:81:GLN:O	1:D:81:GLN:HG2	2.15	0.47
1:C:398:ARG:HA	1:D:401:ASP:HB2	1.97	0.46
1:D:262:LEU:O	1:D:266:LEU:HD13	2.15	0.46
1:A:182:GLU:OE2	1:A:182:GLU:HA	2.15	0.46
1:A:339:LEU:HD13	1:A:339:LEU:C	2.40	0.46
1:A:542:LEU:HD13	1:A:546:MSE:HG2	1.97	0.46
1:C:587:LEU:HA	1:C:588:PRO:HD3	1.76	0.46
1:B:16:SER:OG	1:B:19:GLU:HG3	2.16	0.46
1:C:161:PHE:CZ	1:D:165:ASN:ND2	2.83	0.46
1:D:405:HIS:HD2	1:D:406:ASP:OD1	1.97	0.46
1:A:98:ILE:O	1:A:99:ARG:HB2	2.16	0.46
1:B:441:ARG:NH2	1:B:571:GLU:OE2	2.44	0.46
1:C:13:LEU:O	1:C:19:GLU:HG2	2.16	0.46
1:D:423:ILE:CD1	1:D:600:MSE:HB2	2.42	0.46
1:A:3:PHE:CE1	1:A:92:ARG:HD2	2.51	0.46
1:A:180:ASP:O	1:A:281:MSE:HA	2.15	0.46
1:A:579:PRO:HB2	1:B:579:PRO:O	2.16	0.46
1:B:267:LYS:HB2	1:B:267:LYS:HZ2	1.79	0.46
1:D:64:HIS:HD2	1:D:69:THR:OG1	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:437:LEU:HD12	1:D:559:ASN:HB2	1.96	0.46
1:A:162:GLU:CD	1:B:369:ALA:HB1	2.40	0.46
1:B:74:LEU:HD12	1:B:76:TRP:NE1	2.31	0.46
1:B:265:THR:HG22	1:B:269:MSE:CE	2.33	0.46
1:B:596:THR:CG2	1:B:599:GLU:HB2	2.43	0.46
1:C:341:ALA:HB1	1:C:352:MSE:HE3	1.98	0.46
1:C:161:PHE:HZ	1:D:165:ASN:HD21	1.61	0.46
1:C:498:ILE:HG13	1:C:498:ILE:O	2.15	0.46
1:D:164:MSE:HE1	1:D:243:PHE:CD1	2.51	0.46
1:D:374:VAL:HG11	1:D:399:ALA:HB1	1.97	0.46
1:A:421:ALA:HB1	1:A:475:ARG:CZ	2.46	0.46
1:C:372:HIS:CE1	1:D:166:HIS:ND1	2.77	0.46
1:B:181:ASN:HA	1:B:282:THR:O	2.16	0.45
1:C:340:MSE:HE2	1:C:362:ARG:HD2	1.97	0.45
1:D:35:LEU:HD11	1:D:87:ILE:HD13	1.97	0.45
1:D:58:GLU:HG2	1:D:257:HIS:C	2.41	0.45
1:D:486:LEU:N	1:D:486:LEU:CD1	2.78	0.45
1:A:77:ASP:O	1:A:78:VAL:HB	2.17	0.45
1:C:3:PHE:CE1	1:C:92:ARG:HD2	2.52	0.45
1:C:132:GLY:HA2	1:D:376:PHE:CE1	2.51	0.45
1:B:321:TYR:HA	1:B:324:ILE:HG12	1.98	0.45
1:B:404:LEU:C	1:B:404:LEU:HD23	2.41	0.45
1:C:83:TYR:HB2	1:C:84:PRO:HD3	1.97	0.45
1:D:423:ILE:HG23	1:D:558:GLU:OE1	2.17	0.45
1:D:555:THR:OG1	1:D:584:ASN:HA	2.17	0.45
1:A:542:LEU:HD13	1:A:542:LEU:C	2.42	0.45
1:D:429:GLN:H	1:D:429:GLN:CD	2.25	0.45
1:C:455:ASN:HD21	1:C:487:THR:H	1.62	0.45
1:C:556:VAL:HG13	1:C:611:MSE:CE	2.44	0.45
1:D:336:ASP:O	1:D:362:ARG:NH2	2.40	0.45
1:D:606:LEU:O	1:D:611:MSE:HE3	2.16	0.45
1:B:105:HIS:HA	1:B:594:GLN:HE21	1.81	0.45
1:C:340:MSE:CE	1:C:362:ARG:HD2	2.47	0.45
1:D:178:LEU:HD23	1:D:279:HIS:CD2	2.52	0.45
1:D:392:TYR:CD2	1:D:420:ARG:HG3	2.51	0.45
1:A:423:ILE:O	1:A:423:ILE:HG13	2.17	0.45
1:B:451:PRO:HG3	1:B:460:MSE:SE	2.67	0.45
1:A:156:THR:HG21	1:A:368:ILE:N	2.32	0.45
1:D:74:LEU:HD22	1:D:76:TRP:NE1	2.32	0.45
1:A:64:HIS:HD2	1:A:69:THR:OG1	1.99	0.45
1:A:153:GLY:O	1:A:368:ILE:HD12	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:GLU:OE1	1:A:485:GLU:HA	2.17	0.45
1:A:515:MSE:HB3	1:A:516:PRO:HD3	1.99	0.45
1:B:118:LEU:HD13	1:B:118:LEU:C	2.42	0.45
1:B:368:ILE:N	1:B:368:ILE:CD1	2.80	0.45
1:D:541:ALA:O	1:D:545:GLU:HG3	2.17	0.45
1:A:48:GLY:HA3	6:A:3067:HOH:O	2.16	0.44
1:C:401:ASP:OD1	1:D:122:HIS:CE1	2.70	0.44
1:D:11:LEU:HD23	1:D:11:LEU:C	2.42	0.44
1:D:70:PRO:HD3	1:D:115:TYR:CZ	2.52	0.44
1:D:404:LEU:CD1	1:D:443:ILE:HG23	2.47	0.44
1:A:3:PHE:CD2	1:A:3:PHE:C	2.95	0.44
1:B:484:VAL:HG12	1:B:485:GLU:H	1.81	0.44
1:D:89:THR:O	1:D:89:THR:CG2	2.65	0.44
1:B:118:LEU:HD13	1:B:119:SER:O	2.18	0.44
1:C:456:GLU:OE1	1:C:533:ARG:HD3	2.17	0.44
1:D:333:ALA:O	1:D:362:ARG:NH2	2.50	0.44
1:A:339:LEU:CD2	1:A:388:ILE:HD12	2.47	0.44
1:B:320:SER:O	1:B:323:LYS:HB3	2.16	0.44
1:A:131:ILE:HD11	1:A:167:ALA:HB2	1.99	0.44
1:A:354:GLU:CG	1:A:358:LYS:HE2	2.48	0.44
1:A:580:VAL:O	1:A:582:VAL:HG23	2.18	0.44
1:B:393:SER:HB3	1:B:433:GLY:HA3	1.99	0.44
1:C:72:ASP:OD2	1:C:270:ARG:NH1	2.50	0.44
1:D:84:PRO:O	1:D:87:ILE:HG22	2.17	0.44
1:B:30:LYS:O	1:B:34:GLU:HG3	2.17	0.44
1:B:596:THR:HG22	1:B:599:GLU:CB	2.45	0.44
1:C:320:SER:HA	1:C:480:ASN:HA	1.99	0.44
1:C:577:ARG:HG3	1:C:577:ARG:HH11	1.82	0.44
1:A:413:PRO:HA	1:A:470:GLY:O	2.18	0.44
1:A:592:ILE:HA	1:A:593:PRO:HD3	1.85	0.44
1:B:74:LEU:HD13	1:B:75:ILE:N	2.32	0.44
1:B:429:GLN:HG3	1:B:592:ILE:O	2.17	0.44
1:C:579:PRO:HG3	1:D:581:PRO:HD3	1.99	0.44
1:D:75:ILE:HG23	1:D:118:LEU:HB3	2.00	0.44
1:D:175:LEU:HD11	1:D:278:LEU:HB2	2.00	0.44
1:B:407:VAL:CG1	1:B:471:PRO:HB3	2.48	0.43
1:C:501:ARG:HH11	1:C:523:GLU:CD	2.24	0.43
1:B:528:THR:CG2	1:B:550:HIS:NE2	2.80	0.43
1:D:77:ASP:CG	1:D:150:ILE:HG22	2.43	0.43
1:A:391:ILE:O	1:A:418:ILE:HA	2.18	0.43
1:A:404:LEU:O	1:A:408:ALA:HB3	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:491:LYS:HE3	6:B:4039:HOH:O	2.17	0.43
1:D:339:LEU:HD23	1:D:340:MSE:N	2.33	0.43
1:B:153:GLY:O	1:B:368:ILE:HD13	2.18	0.43
1:B:348:GLU:HG2	1:B:353:VAL:CG2	2.49	0.43
1:B:437:LEU:CD1	1:B:475:ARG:HH11	2.32	0.43
1:D:77:ASP:O	1:D:120:VAL:HB	2.18	0.43
1:D:170:ILE:HG13	1:D:172:PRO:HD3	1.99	0.43
1:D:454:GLU:OE2	1:D:483:GLY:N	2.48	0.43
1:C:341:ALA:HB3	1:C:355:PHE:CE2	2.53	0.43
1:C:501:ARG:NH1	1:C:523:GLU:CD	2.76	0.43
1:C:515:MSE:HB3	1:C:516:PRO:HD3	2.00	0.43
1:D:587:LEU:HA	1:D:588:PRO:HD3	1.81	0.43
1:B:392:TYR:HB2	1:B:395:PHE:CD2	2.54	0.43
1:D:147:VAL:HA	1:D:175:LEU:O	2.18	0.43
1:D:153:GLY:C	1:D:368:ILE:HD12	2.43	0.43
1:A:47:SER:OG	1:A:99:ARG:HG3	2.18	0.43
1:B:368:ILE:O	1:B:368:ILE:HG22	2.19	0.43
1:D:120:VAL:HG23	1:D:120:VAL:O	2.19	0.43
1:A:79:GLY:HA3	1:A:108:PRO:HD2	2.01	0.43
1:D:66:VAL:CG1	1:D:263:ILE:HG23	2.48	0.43
1:A:64:HIS:CE1	1:A:85:HIS:ND1	2.85	0.43
1:A:98:ILE:O	1:A:99:ARG:CB	2.66	0.43
1:A:339:LEU:HD13	1:A:340:MSE:N	2.33	0.43
1:B:36:ARG:O	1:B:40:LEU:HG	2.19	0.43
1:B:74:LEU:HD12	1:B:76:TRP:CD1	2.54	0.43
1:B:461:LEU:HD13	1:B:474:VAL:HG11	2.00	0.43
1:B:514:LEU:HB2	6:B:4016:HOH:O	2.18	0.43
1:B:74:LEU:HD13	1:B:74:LEU:C	2.44	0.43
1:C:250:TYR:HE1	1:C:252:GLY:HA2	1.84	0.43
1:D:424:VAL:HG22	1:D:432:GLN:OE1	2.18	0.43
1:A:382:ILE:CD1	1:B:118:LEU:HD23	2.48	0.42
1:B:429:GLN:HE21	1:B:429:GLN:N	2.16	0.42
1:C:151:GLY:HA3	4:C:3002:TPP:O2A	2.19	0.42
1:C:369:ALA:HB1	1:D:162:GLU:CD	2.44	0.42
1:D:256:GLY:HA3	1:D:280:ILE:CG2	2.48	0.42
1:A:78:VAL:HG22	1:A:123:SER:HB3	2.00	0.42
1:B:592:ILE:HA	1:B:593:PRO:HD3	1.80	0.42
1:D:17:THR:HG23	1:D:21:ARG:CZ	2.49	0.42
1:A:587:LEU:HA	1:A:588:PRO:HD3	1.81	0.42
1:B:73:GLN:NE2	1:B:117:VAL:HG13	2.33	0.42
1:B:342:ILE:HD11	1:B:380:LEU:HD12	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:394:THR:O	1:B:397:GLN:HB2	2.19	0.42
1:B:515:MSE:SE	1:B:529:LEU:HD21	2.69	0.42
1:B:600:MSE:O	1:B:604:LEU:HG	2.19	0.42
1:C:505:LYS:HE2	1:C:506:LEU:HD13	2.02	0.42
1:D:76:TRP:O	1:D:120:VAL:HG21	2.20	0.42
1:D:396:LEU:HD11	1:D:403:VAL:HG21	2.01	0.42
1:A:26:GLU:H	1:A:26:GLU:CD	2.27	0.42
1:C:47:SER:OG	1:C:99:ARG:HG3	2.20	0.42
1:C:118:LEU:HD13	1:C:118:LEU:C	2.44	0.42
1:D:60:THR:HG21	1:D:85:HIS:HA	2.01	0.42
1:D:386:LYS:HZ3	1:D:468:ASN:HD21	1.68	0.42
1:A:532:MSE:O	1:A:534:PHE:N	2.49	0.42
1:A:577:ARG:HG2	1:A:577:ARG:NH1	2.33	0.42
1:B:419:ASP:OD2	1:B:420:ARG:N	2.50	0.42
1:B:421:ALA:HB1	1:B:475:ARG:CZ	2.49	0.42
1:B:553:LEU:HD12	1:B:573:LEU:HD11	2.02	0.42
1:B:318:LEU:HD12	1:B:318:LEU:HA	1.91	0.42
1:C:154:ALA:C	1:C:156:THR:H	2.27	0.42
1:C:421:ALA:HB1	1:C:475:ARG:CZ	2.50	0.42
1:D:35:LEU:HD12	1:D:87:ILE:HD13	2.01	0.42
1:D:131:ILE:O	1:D:135:VAL:HG23	2.20	0.42
1:A:437:LEU:HD21	1:A:475:ARG:HD3	2.02	0.42
1:A:484:VAL:HG12	1:A:485:GLU:H	1.85	0.42
1:C:441:ARG:NH2	1:C:571:GLU:CD	2.78	0.42
1:C:456:GLU:OE1	1:C:533:ARG:CD	2.67	0.42
1:D:269:MSE:SE	1:D:278:LEU:HG	2.69	0.42
1:D:370:GLU:O	1:D:374:VAL:HG12	2.20	0.42
1:B:58:GLU:HG2	1:B:257:HIS:O	2.20	0.42
1:D:612:GLU:O	1:D:616:LYS:HD3	2.20	0.42
1:B:427:ASP:HB3	1:B:431:HIS:HB2	2.01	0.42
1:C:250:TYR:C	1:C:251:ILE:HD12	2.44	0.42
1:C:26:GLU:CD	1:C:26:GLU:N	2.72	0.42
1:A:67:TYR:CD2	1:A:270:ARG:HD2	2.55	0.41
1:B:441:ARG:NH2	1:B:571:GLU:OE1	2.53	0.41
1:C:86:LYS:O	1:C:91:ARG:HB2	2.20	0.41
1:C:99:ARG:HD3	6:C:3032:HOH:O	2.20	0.41
1:D:278:LEU:HD13	1:D:280:ILE:HG12	2.01	0.41
1:A:86:LYS:O	1:A:91:ARG:HB2	2.20	0.41
1:A:254:VAL:CG1	1:A:255:ASP:N	2.84	0.41
1:D:131:ILE:HD12	1:D:170:ILE:HD11	2.02	0.41
1:D:345:ALA:O	1:D:346:MSE:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:596:THR:HG22	1:D:598:GLU:N	2.35	0.41
1:B:8:TYR:N	1:B:9:PRO:CD	2.83	0.41
1:D:412:LEU:HA	1:D:413:PRO:HD3	1.79	0.41
1:D:592:ILE:HA	1:D:593:PRO:HD3	1.74	0.41
1:A:377:ALA:O	1:A:387:PRO:HG3	2.20	0.41
1:B:35:LEU:O	1:B:39:LEU:HG	2.20	0.41
1:B:77:ASP:O	1:B:78:VAL:CB	2.68	0.41
1:B:78:VAL:HG22	1:B:123:SER:HB3	2.03	0.41
1:B:393:SER:OG	1:B:436:ASP:HB2	2.19	0.41
1:C:291:ALA:C	1:C:478:ARG:NH1	2.76	0.41
1:B:354:GLU:HB2	6:B:4098:HOH:O	2.20	0.41
1:C:241:THR:O	1:C:245:GLU:HG2	2.20	0.41
1:B:180:ASP:O	1:B:281:MSE:HE3	2.20	0.41
1:B:577:ARG:C	1:B:579:PRO:HD3	2.46	0.41
1:D:28:LEU:HB2	1:D:29:PRO:HD3	2.01	0.41
1:A:320:SER:HA	1:A:480:ASN:HA	2.02	0.41
1:A:405:HIS:HA	1:A:409:ILE:HD12	2.03	0.41
1:C:372:HIS:HD2	1:D:128:SER:OG	2.02	0.41
6:C:3116:HOH:O	1:D:371:GLN:HG3	2.20	0.41
1:D:84:PRO:HA	1:D:87:ILE:CG2	2.49	0.41
1:D:374:VAL:HG11	1:D:402:GLN:HB2	2.02	0.41
1:B:343:THR:OG1	1:B:352:MSE:HE1	2.20	0.41
1:B:539:ASP:CG	1:B:542:LEU:HB2	2.46	0.41
1:C:17:THR:CG2	1:C:21:ARG:NH1	2.79	0.41
1:C:101:LYS:HE3	1:C:603:GLU:HG3	2.01	0.41
1:D:400:TYR:CE2	1:D:443:ILE:HD11	2.55	0.41
1:D:432:GLN:HB2	6:D:4097:HOH:O	2.20	0.41
1:A:82:ALA:HA	6:A:3002:HOH:O	2.20	0.41
1:A:436:ASP:OD2	1:A:475:ARG:CD	2.68	0.41
1:A:449:MSE:HE3	1:A:474:VAL:HG22	2.03	0.41
1:A:455:ASN:OD1	1:A:486:LEU:HA	2.21	0.41
1:A:504:GLU:O	1:A:505:LYS:HB3	2.20	0.41
1:B:336:ASP:OD1	1:B:336:ASP:C	2.64	0.41
1:B:402:GLN:NE2	1:B:402:GLN:H	2.19	0.41
1:B:528:THR:HG21	1:B:550:HIS:NE2	2.36	0.41
1:C:156:THR:CG2	1:C:368:ILE:H	2.28	0.41
1:C:570:ASN:O	1:C:574:MSE:HG2	2.21	0.41
1:D:9:PRO:HB2	1:D:10:THR:H	1.71	0.41
1:D:391:ILE:O	1:D:418:ILE:HA	2.21	0.41
1:D:392:TYR:CE2	1:D:420:ARG:HG3	2.56	0.41
1:A:423:ILE:HD12	1:A:423:ILE:C	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:ASN:O	1:B:71:PHE:HB3	2.21	0.41
1:B:74:LEU:CD1	1:B:76:TRP:NE1	2.84	0.41
1:C:450:THR:HA	1:C:451:PRO:HD2	1.88	0.41
1:A:19:GLU:O	1:A:22:LEU:HB2	2.21	0.40
1:A:153:GLY:C	1:A:368:ILE:HD12	2.46	0.40
1:A:415:LEU:HD23	1:A:416:PHE:N	2.36	0.40
1:B:507:ALA:HA	1:B:528:THR:OG1	2.20	0.40
1:B:583:LEU:HB2	1:B:618:TRP:CE3	2.57	0.40
1:B:605:GLY:C	1:B:607:ASP:H	2.28	0.40
1:C:16:SER:OG	1:C:18:GLN:OE1	2.39	0.40
1:C:592:ILE:N	1:C:592:ILE:CD1	2.83	0.40
1:D:437:LEU:HD12	1:D:559:ASN:CB	2.51	0.40
1:A:254:VAL:HG11	6:A:3013:HOH:O	2.21	0.40
1:B:532:MSE:O	1:B:533:ARG:HB2	2.21	0.40
1:C:39:LEU:HD22	1:C:50:PHE:HB2	2.03	0.40
1:C:140:GLU:HB3	6:C:3086:HOH:O	2.21	0.40
1:B:82:ALA:HA	6:B:4080:HOH:O	2.22	0.40
1:B:501:ARG:HB3	1:B:529:LEU:HB3	2.03	0.40
1:A:376:PHE:CE1	1:B:132:GLY:HA2	2.57	0.40
1:A:439:TYR:CE2	1:A:440:LEU:HD13	2.56	0.40
1:A:581:PRO:HB2	1:A:618:TRP:CH2	2.57	0.40
1:B:84:PRO:HG2	6:B:4080:HOH:O	2.22	0.40
1:B:368:ILE:H	1:B:368:ILE:CD1	2.33	0.40
1:C:449:MSE:HG2	1:C:534:PHE:CE1	2.57	0.40
1:D:171:ARG:N	1:D:172:PRO:HD3	2.36	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	530/621 (85%)	501 (94%)	26 (5%)	3 (1%)	21 32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	483/621 (78%)	463 (96%)	19 (4%)	1 (0%)	43 58
1	C	530/621 (85%)	507 (96%)	19 (4%)	4 (1%)	16 25
1	D	477/621 (77%)	458 (96%)	18 (4%)	1 (0%)	43 58
All	All	2020/2484 (81%)	1929 (96%)	82 (4%)	9 (0%)	30 43

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	252	GLY
1	A	48	GLY
1	C	505	LYS
1	D	77	ASP
1	C	48	GLY
1	B	78	VAL
1	A	121	GLY
1	C	121	GLY
1	A	579	PRO

5.3.2 Protein sidechains (i)

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	433/485 (89%)	413 (95%)	20 (5%)	24 41
1	B	401/485 (83%)	380 (95%)	21 (5%)	21 36
1	C	433/485 (89%)	410 (95%)	23 (5%)	20 36
1	D	395/485 (81%)	377 (95%)	18 (5%)	24 41
All	All	1662/1940 (86%)	1580 (95%)	82 (5%)	22 39

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	PHE
1	A	11	LEU

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Mol	Chain	Res	Type
1	A	39	LEU
1	A	74	LEU
1	A	118	LEU
1	A	124	SER
1	A	156	THR
1	A	178	LEU
1	A	264	THR
1	A	339	LEU
1	A	415	LEU
1	A	423	ILE
1	A	429	GLN
1	A	440	LEU
1	A	475	ARG
1	A	485	GLU
1	A	514	LEU
1	A	544	LEU
1	A	594	GLN
1	A	596	THR
1	B	11	LEU
1	B	15	ASP
1	B	74	LEU
1	B	124	SER
1	B	131	ILE
1	B	147	VAL
1	B	171	ARG
1	B	246	LEU
1	B	259	VAL
1	B	262	LEU
1	B	267	LYS
1	B	281	MSE
1	B	368	ILE
1	B	394	THR
1	B	410	GLN
1	B	429	GLN
1	B	441	ARG
1	B	461	LEU
1	B	530	VAL
1	B	542	LEU
1	B	574	MSE
1	C	3	PHE
1	C	11	LEU
1	C	17	THR

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Mol	Chain	Res	Type
1	C	19	GLU
1	C	26	GLU
1	C	31	LEU
1	C	39	LEU
1	C	66	VAL
1	C	118	LEU
1	C	156	THR
1	C	165	ASN
1	C	284	LYS
1	C	318	LEU
1	C	357	ARG
1	C	415	LEU
1	C	429	GLN
1	C	430	THR
1	C	437	LEU
1	C	501	ARG
1	C	530	VAL
1	C	577	ARG
1	C	594	GLN
1	C	603	GLU
1	D	17	THR
1	D	131	ILE
1	D	150	ILE
1	D	152	ASP
1	D	155	ILE
1	D	176	VAL
1	D	278	LEU
1	D	362	ARG
1	D	374	VAL
1	D	380	LEU
1	D	423	ILE
1	D	429	GLN
1	D	461	LEU
1	D	475	ARG
1	D	530	VAL
1	D	538	LEU
1	D	582	VAL
1	D	592	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	64	HIS
1	A	68	ASN
1	A	100	GLN
1	A	268	ASN
1	A	371	GLN
1	A	372	HIS
1	A	397	GLN
1	A	402	GLN
1	A	405	HIS
1	A	429	GLN
1	A	431	HIS
1	A	459	GLN
1	A	480	ASN
1	A	559	ASN
1	A	584	ASN
1	A	594	GLN
1	A	597	GLN
1	B	68	ASN
1	B	73	GLN
1	B	143	ASN
1	B	372	HIS
1	B	397	GLN
1	B	402	GLN
1	B	429	GLN
1	B	432	GLN
1	B	480	ASN
1	B	570	ASN
1	B	584	ASN
1	C	68	ASN
1	C	143	ASN
1	C	276	GLN
1	C	279	HIS
1	C	371	GLN
1	C	372	HIS
1	C	402	GLN
1	C	410	GLN
1	C	429	GLN
1	C	431	HIS
1	C	455	ASN
1	C	459	GLN
1	C	480	ASN
1	C	510	ASN

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Mol	Chain	Res	Type
1	C	584	ASN
1	D	64	HIS
1	D	68	ASN
1	D	165	ASN
1	D	181	ASN
1	D	249	ASN
1	D	371	GLN
1	D	372	HIS
1	D	405	HIS
1	D	429	GLN
1	D	431	HIS
1	D	468	ASN
1	D	480	ASN
1	D	510	ASN
1	D	584	ASN
1	D	597	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	DPO	D	4002	2	6,8,8	2.07	1 (16%)	12,13,13	0.99	1 (8%)
4	TPP	C	3002	2	26,27,27	1.58	5 (19%)	38,40,40	1.76	10 (26%)
5	DPO	B	4001	2	6,8,8	2.06	1 (16%)	12,13,13	0.96	1 (8%)
4	TPP	A	3001	2	26,27,27	1.43	3 (11%)	38,40,40	1.66	8 (21%)

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
5	DPO	D	4002	2	-	0/6/6/6	-
4	TPP	C	3002	2	-	2/17/17/17	0/2/2/2
5	DPO	B	4001	2	-	0/6/6/6	-
4	TPP	A	3001	2	-	2/17/17/17	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	4002	DPO	P2-O5	3.55	1.61	1.50
5	B	4001	DPO	P2-O5	3.54	1.61	1.50
4	C	3002	TPP	PB-O1B	3.52	1.61	1.50
4	C	3002	TPP	PA-O1A	3.03	1.61	1.50
4	A	3001	TPP	PA-O1A	3.02	1.61	1.50
4	A	3001	TPP	C4-N3	-2.77	1.34	1.39
4	C	3002	TPP	C4-N3	-2.71	1.34	1.39
4	A	3001	TPP	C5-C4	2.13	1.39	1.35
4	C	3002	TPP	C5-C4	2.11	1.39	1.35
4	C	3002	TPP	C5'-C4'	-2.04	1.39	1.42

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	3001	TPP	S1-C2-N3	-3.52	107.84	112.30
4	C	3002	TPP	S1-C2-N3	-3.51	107.85	112.30
4	C	3002	TPP	N1'-C2'-N3'	-3.39	119.89	125.53
4	A	3001	TPP	N1'-C2'-N3'	-3.30	120.04	125.53
4	A	3001	TPP	C6'-N1'-C2'	3.13	121.21	116.07
4	C	3002	TPP	C6'-N1'-C2'	3.13	121.21	116.07
4	C	3002	TPP	C4-C5-S1	-2.80	106.20	110.56
4	C	3002	TPP	O3B-PB-O3A	2.68	113.63	104.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	3001	TPP	C2-S1-C5	2.66	92.98	91.22
4	A	3001	TPP	C4-C5-S1	-2.64	106.44	110.56
4	C	3002	TPP	C2-S1-C5	2.56	92.91	91.22
4	A	3001	TPP	CM2-C2'-N1'	2.48	119.84	117.20
4	C	3002	TPP	CM2-C2'-N1'	2.47	119.83	117.20
4	C	3002	TPP	CM4-C4-C5	-2.37	121.68	127.75
4	A	3001	TPP	CM4-C4-C5	-2.35	121.74	127.75
5	D	4002	DPO	O7-P2-O4	2.32	112.43	104.64
5	B	4001	DPO	O7-P2-O4	2.25	112.19	104.64
4	C	3002	TPP	N4'-C4'-N3'	2.11	119.87	117.03
4	C	3002	TPP	CM2-C2'-N3'	2.10	120.28	117.13
4	A	3001	TPP	C2-N3-C4	2.00	116.76	114.06

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	3002	TPP	C4'-C5'-C7'-N3
4	A	3001	TPP	PB-O3A-PA-O7
4	A	3001	TPP	C4'-C5'-C7'-N3
4	C	3002	TPP	C6'-C5'-C7'-N3

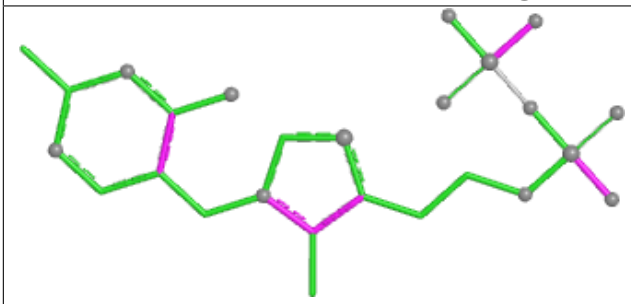
There are no ring outliers.

2 monomers are involved in 5 short contacts:

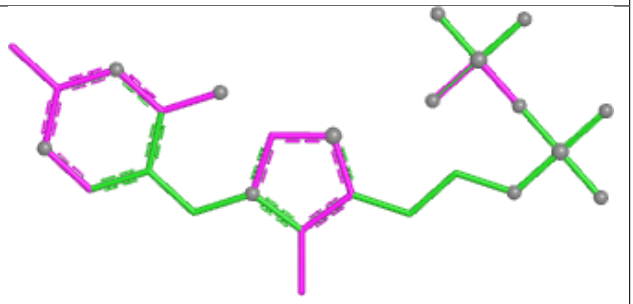
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	3002	TPP	3	0
4	A	3001	TPP	2	0

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

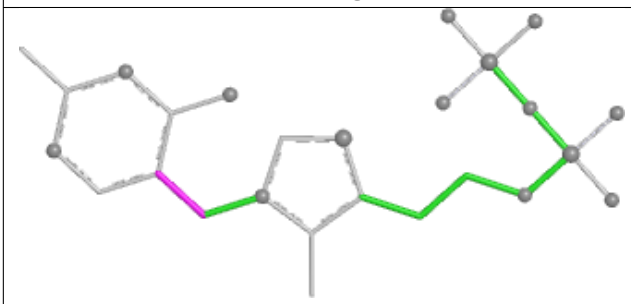
Ligand TPP C 3002



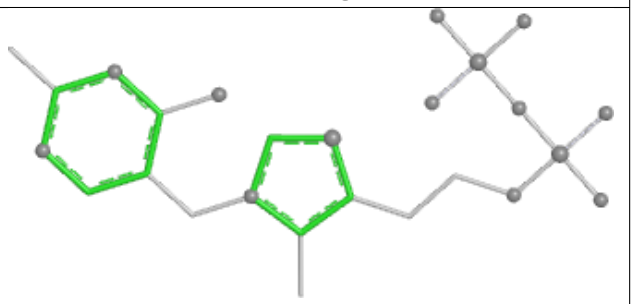
Bond lengths



Bond angles

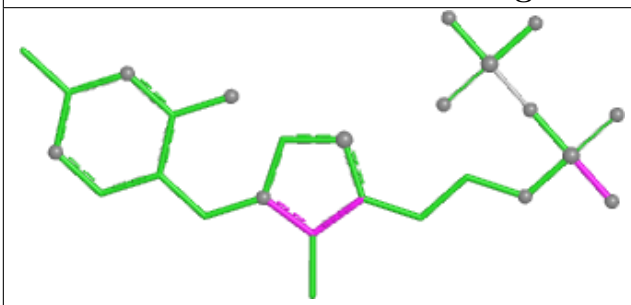


Torsions

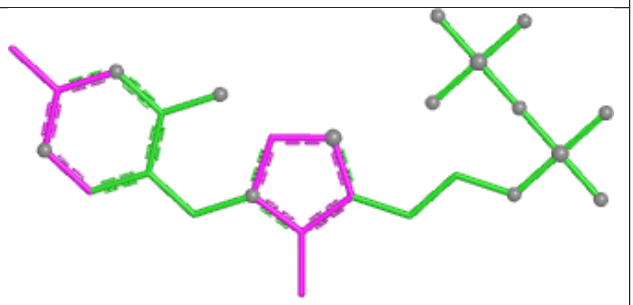


Rings

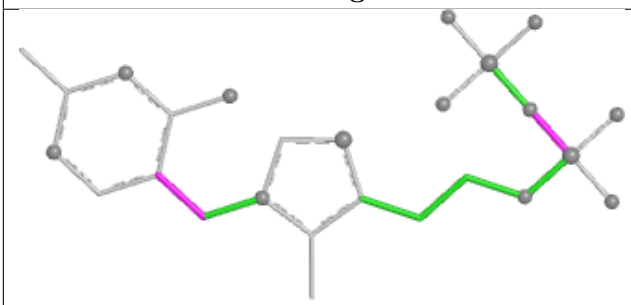
Ligand TPP A 3001



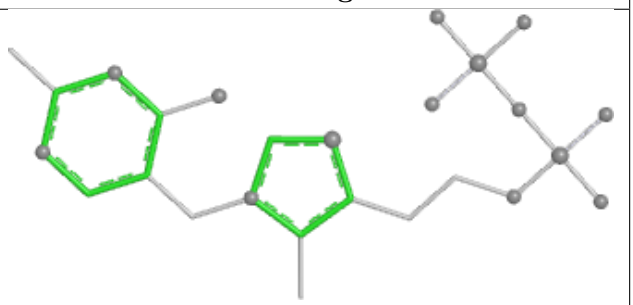
Bond lengths



Bond angles



Torsions



Rings

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	518/621 (83%)	-0.45	3 (0%)	85	83	3, 14, 31, 43	0
1	B	475/621 (76%)	-0.11	19 (4%)	42	38	3, 17, 53, 62	0
1	C	518/621 (83%)	-0.44	4 (0%)	82	80	4, 13, 30, 42	0
1	D	469/621 (75%)	-0.05	19 (4%)	41	37	5, 19, 45, 58	0
All	All	1980/2484 (79%)	-0.27	45 (2%)	61	57	3, 15, 40, 62	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	252	GLY	3.9
1	B	78	VAL	3.5
1	B	106	PRO	3.5
1	B	109	TRP	3.5
1	D	13	LEU	3.4
1	B	115	TYR	3.3
1	D	9	PRO	3.3
1	B	81	GLN	3.1
1	D	15	ASP	3.1
1	D	115	TYR	3.1
1	B	107	PHE	3.0
1	B	116	ASP	3.0
1	A	47	SER	3.0
1	B	14	VAL	3.0
1	D	78	VAL	3.0
1	D	119	SER	2.9
1	B	108	PRO	2.9
1	D	283	LYS	2.9
1	B	105	HIS	2.8
1	A	239	PRO	2.7
1	B	80	HIS	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	113	SER	2.5
1	D	121	GLY	2.5
1	C	3	PHE	2.4
1	D	427	ASP	2.4
1	B	83	TYR	2.4
1	B	89	THR	2.4
1	D	120	VAL	2.4
1	D	426	ALA	2.4
1	D	428	GLY	2.3
1	A	289	GLU	2.3
1	D	90	GLY	2.2
1	D	39	LEU	2.2
1	D	87	ILE	2.2
1	B	18	GLN	2.2
1	B	22	LEU	2.2
1	D	18	GLN	2.1
1	D	81	GLN	2.1
1	C	579	PRO	2.1
1	D	14	VAL	2.1
1	B	39	LEU	2.1
1	B	113	SER	2.1
1	C	182	GLU	2.1
1	B	15	ASP	2.1
1	B	607	ASP	2.0

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

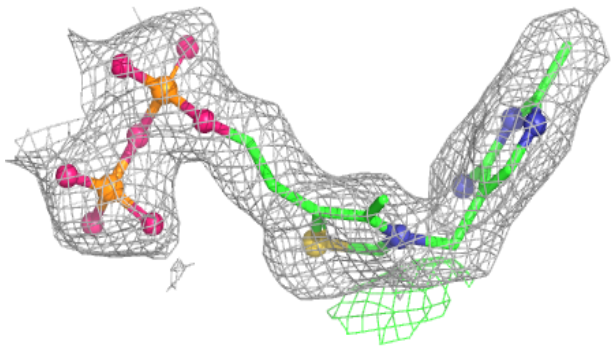
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

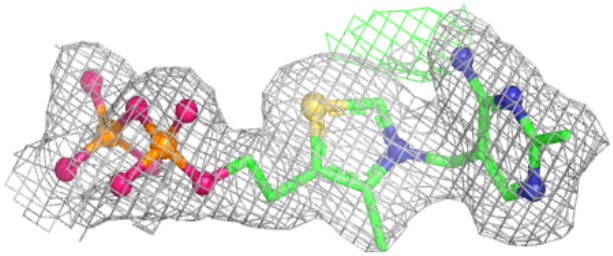
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MG	C	1003	1/1	0.81	0.13	26,26,26,26	0
2	MG	B	1002	1/1	0.85	0.10	48,48,48,48	0
2	MG	D	1004	1/1	0.85	0.16	61,61,61,61	0
5	DPO	B	4001	9/9	0.85	0.13	50,51,55,56	0
5	DPO	D	4002	9/9	0.86	0.13	50,51,54,54	0
3	K	D	2004	1/1	0.96	0.06	34,34,34,34	0
3	K	B	2002	1/1	0.97	0.05	14,14,14,14	0
4	TPP	A	3001	26/26	0.98	0.06	5,13,16,16	0
4	TPP	C	3002	26/26	0.98	0.05	4,13,16,18	0
2	MG	A	1001	1/1	0.98	0.06	9,9,9,9	0
3	K	A	2001	1/1	0.98	0.03	23,23,23,23	0
3	K	C	2003	1/1	0.99	0.03	24,24,24,24	0

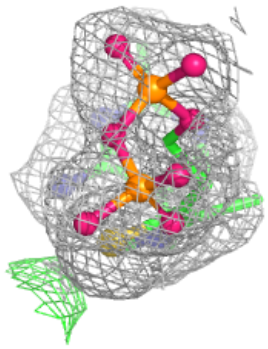
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TPP A 3001:

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

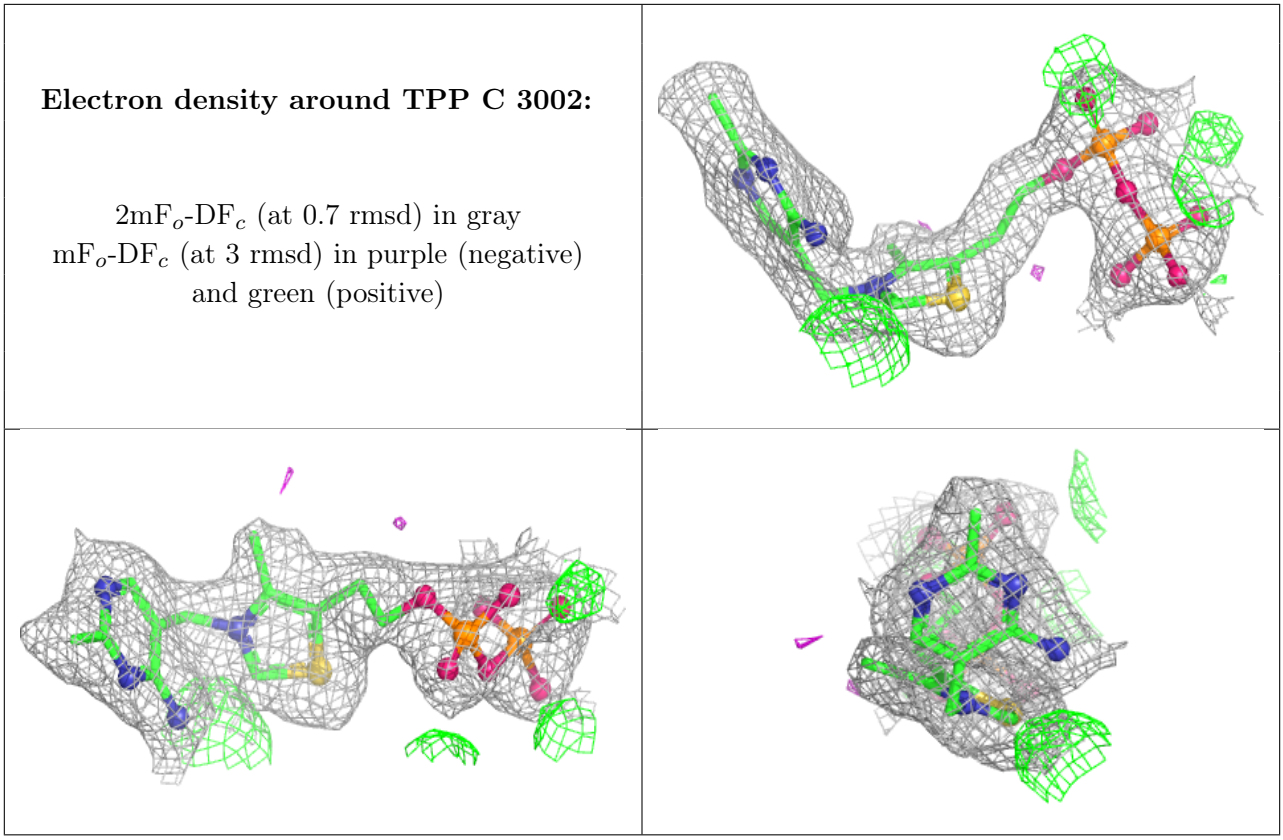






Electron density around TPP C 3002:

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



6.5 Other polymers (i)

There are no such residues in this entry.