



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 05:34 am BST

PDB ID : 6DNA
Title : Crystal structure of T110A mutant human Glutamate oxaloacetate transaminase 1 (GOT1)
Authors : Assar, Z.; Holt, M.C.; Stein, A.J.; Lairson, L.; Lyssiotis, C.A.
Deposited on : 2018-06-06
Resolution : 3.00 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

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

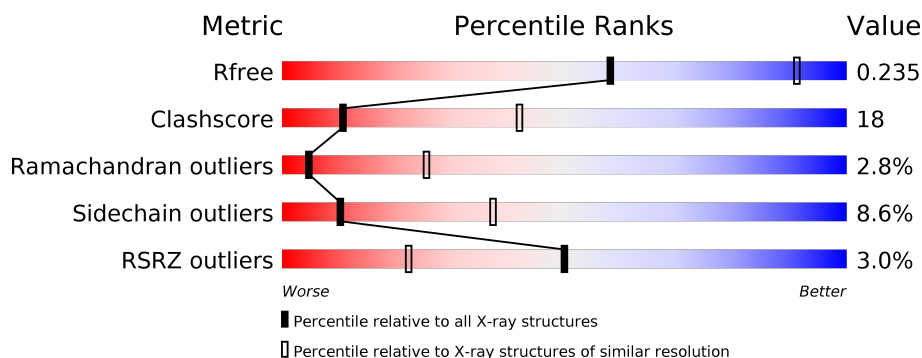
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	408	<div> <div>3%</div> <div> <div></div> <div>71%</div> <div>19%</div> <div>• • •</div> </div> </div>
1	B	408	<div> <div>3%</div> <div> <div></div> <div>73%</div> <div>18%</div> <div>5% • •</div> </div> </div>
1	C	408	<div> <div>%</div> <div> <div></div> <div>73%</div> <div>19%</div> <div>• • •</div> </div> </div>
1	D	408	<div> <div>4%</div> <div> <div></div> <div>72%</div> <div>20%</div> <div>• •</div> </div> </div>
1	E	408	<div> <div>4%</div> <div> <div></div> <div>69%</div> <div>21%</div> <div>5% • •</div> </div> </div>
1	F	408	<div> <div>2%</div> <div> <div></div> <div>67%</div> <div>21%</div> <div>5% • 6%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PLP	E	501	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 18520 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 Aspartate aminotransferase, cytoplasmic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	390	Total	C	N	O	S	0	2	0
			3029	1932	529	559	9			
1	B	395	Total	C	N	O	S	0	4	0
			3104	1985	537	573	9			
1	C	391	Total	C	N	O	S	0	2	0
			3049	1947	531	562	9			
1	D	396	Total	C	N	O	S	0	3	0
			3089	1968	542	570	9			
1	E	393	Total	C	N	O	S	0	3	0
			3095	1979	536	571	9			
1	F	383	Total	C	N	O	S	0	4	0
			3013	1925	523	556	9			

There are 24 discrepancies between the modelled and reference sequences:

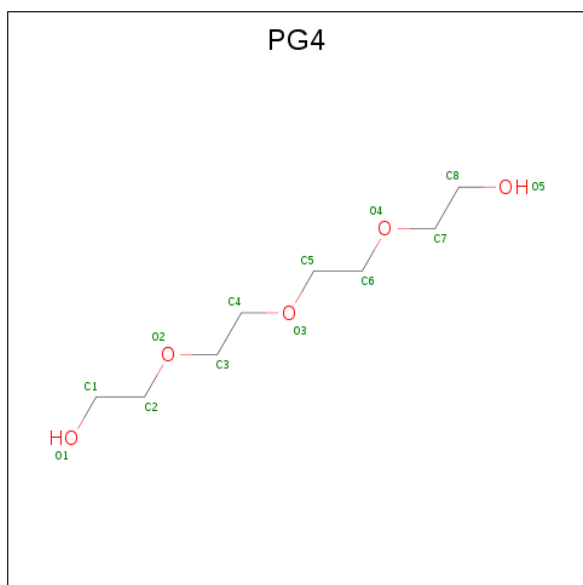
Chain	Residue	Modelled	Actual	Comment	Reference
A	110	ALA	THR	engineered mutation	UNP P17174
A	411	LYS	-	expression tag	UNP P17174
A	412	ILE	-	expression tag	UNP P17174
A	413	GLN	-	expression tag	UNP P17174
B	110	ALA	THR	engineered mutation	UNP P17174
B	411	LYS	-	expression tag	UNP P17174
B	412	ILE	-	expression tag	UNP P17174
B	413	GLN	-	expression tag	UNP P17174
C	110	ALA	THR	engineered mutation	UNP P17174
C	411	LYS	-	expression tag	UNP P17174
C	412	ILE	-	expression tag	UNP P17174
C	413	GLN	-	expression tag	UNP P17174
D	110	ALA	THR	engineered mutation	UNP P17174
D	411	LYS	-	expression tag	UNP P17174
D	412	ILE	-	expression tag	UNP P17174
D	413	GLN	-	expression tag	UNP P17174
E	110	ALA	THR	engineered mutation	UNP P17174

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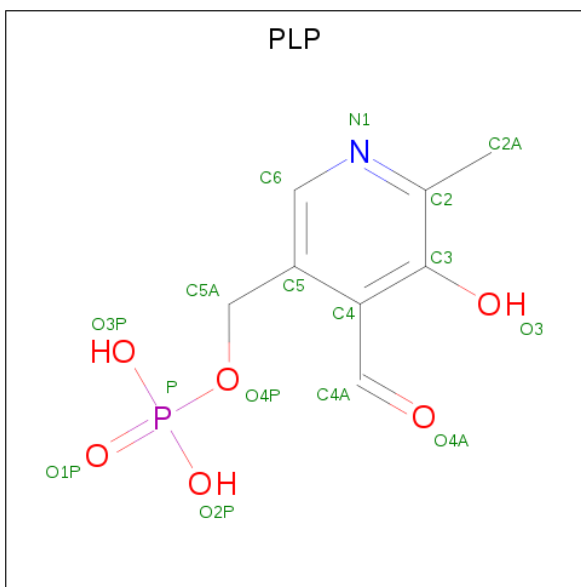
Chain	Residue	Modelled	Actual	Comment	Reference
E	411	LYS	-	expression tag	UNP P17174
E	412	ILE	-	expression tag	UNP P17174
E	413	GLN	-	expression tag	UNP P17174
F	110	ALA	THR	engineered mutation	UNP P17174
F	411	LYS	-	expression tag	UNP P17174
F	412	ILE	-	expression tag	UNP P17174
F	413	GLN	-	expression tag	UNP P17174

- Molecule 2 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	8	5		
2	B	1	Total	C	O	0	0
			10	6	4		
2	D	1	Total	C	O	0	0
			13	8	5		

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
3	B	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
3	C	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
3	D	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
3	E	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
3	F	1	Total	C	N	O	P	0	0
			16	8	1	6	1		

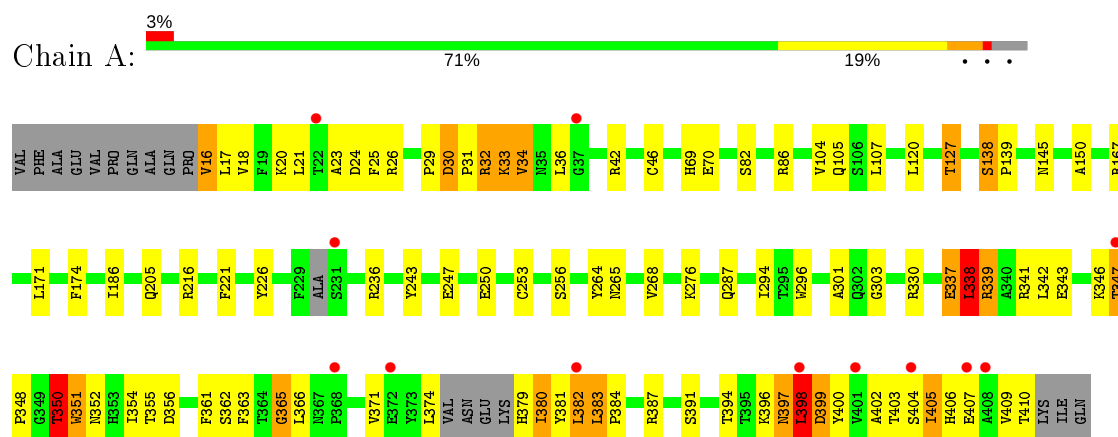
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	O	0	0
			1	1		
4	C	3	Total	O	0	0
			3	3		
4	E	3	Total	O	0	0
			3	3		
4	F	2	Total	O	0	0
			2	2		

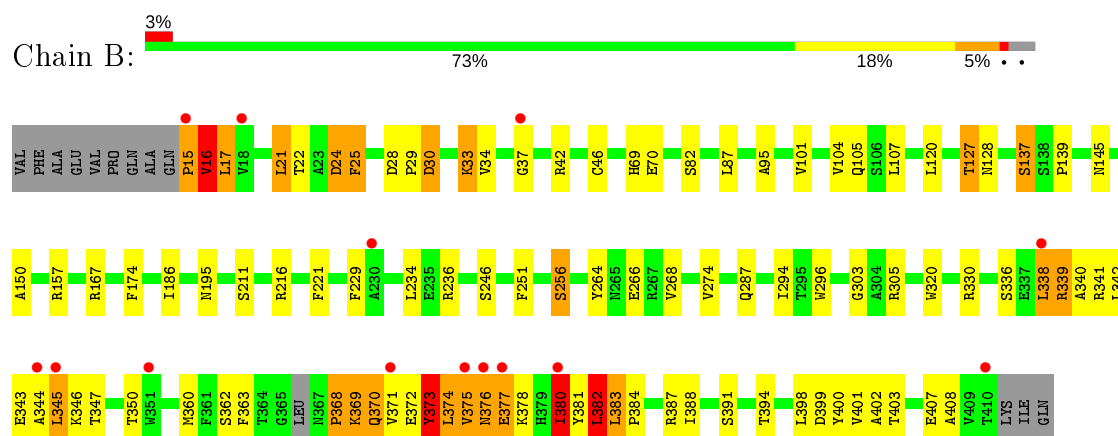
3 Residue-property plots [i](#)

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

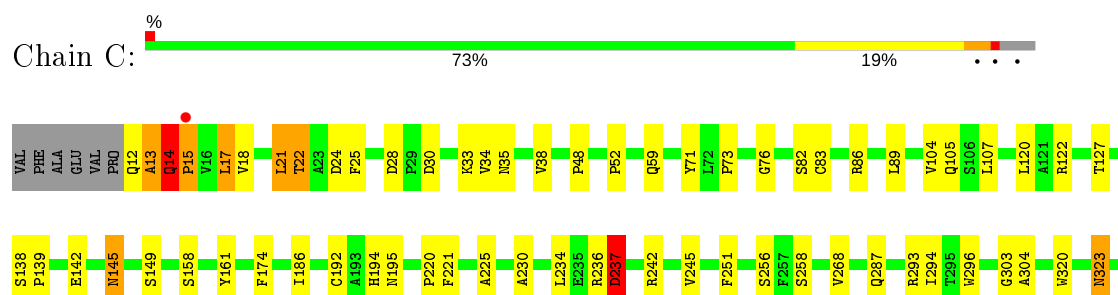
- Molecule 1: Aspartate aminotransferase, cytoplasmic

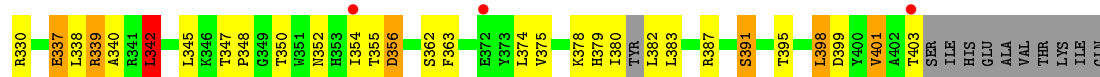


- Molecule 1: Aspartate aminotransferase, cytoplasmic

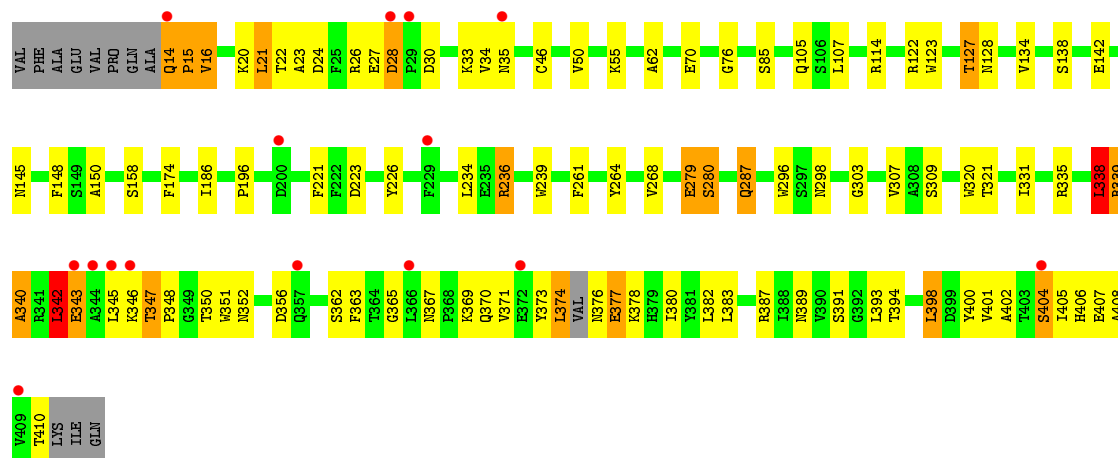
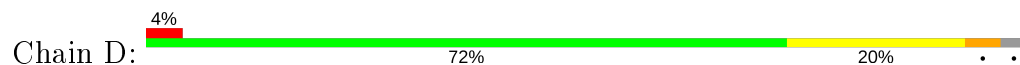


- Molecule 1: Aspartate aminotransferase, cytoplasmic

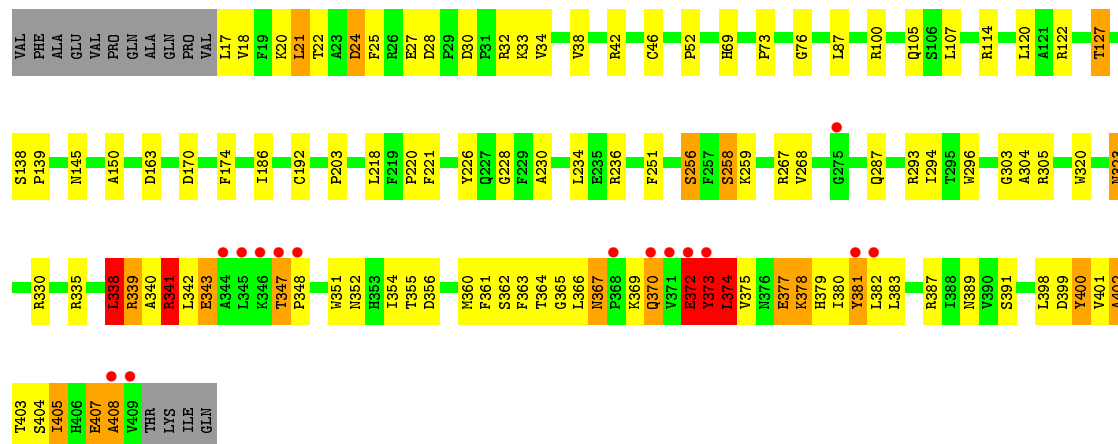




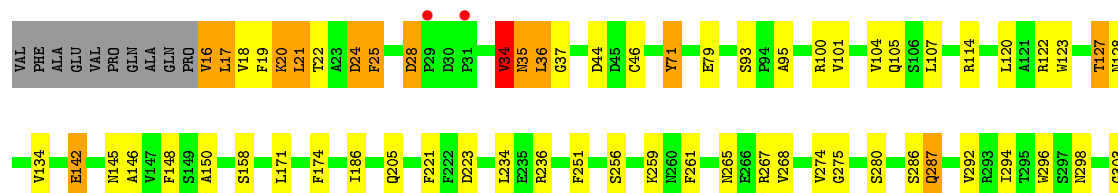
- Molecule 1: Aspartate aminotransferase, cytoplasmic

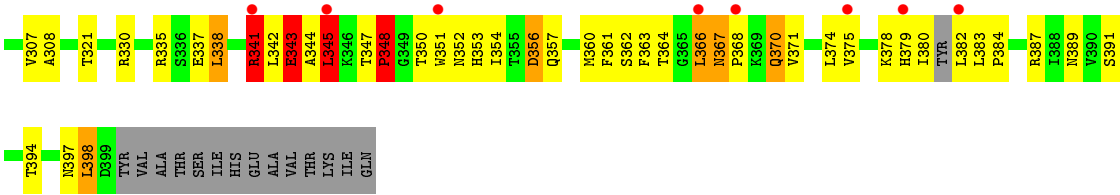


- Molecule 1: Aspartate aminotransferase, cytoplasmic



- Molecule 1: Aspartate aminotransferase, cytoplasmic





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	257.70Å 148.63Å 83.18Å 90.00° 89.98° 90.00°	Depositor
Resolution (Å)	48.70 – 3.00 48.70 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.70-3.00) 99.1 (48.70-3.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	65.47 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.184 , 0.211 0.206 , 0.235	Depositor DCC
R_{free} test set	3047 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	83.8	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 64.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.000 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.000 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.076 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.077 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.000 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	18520	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 3.52% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PG4, PLP

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	0.56	0/3108	0.77	0/4230
1	B	0.57	1/3192 (0.0%)	0.75	4/4343 (0.1%)
1	C	0.55	0/3129	0.73	1/4260 (0.0%)
1	D	0.54	0/3171	0.77	1/4315 (0.0%)
1	E	0.58	0/3180	0.76	1/4326 (0.0%)
1	F	0.53	0/3097	0.75	2/4211 (0.0%)
All	All	0.55	1/18877 (0.0%)	0.76	9/25685 (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	A	0	6
1	B	0	4
1	C	0	2
1	D	0	1
1	E	0	6
1	F	0	3
All	All	0	22

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	370	GLN	N-CA	5.35	1.57	1.46

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	373	TYR	CB-CG-CD2	6.77	125.06	121.00
1	B	373	TYR	CB-CG-CD1	-6.16	117.30	121.00
1	B	15	PRO	CA-N-CD	-6.07	103.00	111.50
1	C	242	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	F	71	TYR	CB-CG-CD1	5.76	124.46	121.00
1	F	71	TYR	CB-CG-CD2	-5.38	117.77	121.00
1	B	157	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	E	372	GLU	CB-CA-C	5.23	120.86	110.40
1	D	114	ARG	NE-CZ-NH2	-5.17	117.71	120.30

There are no chirality outliers.

All (22) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	167	ARG	Sidechain
1	A	216	ARG	Sidechain
1	A	236	ARG	Sidechain
1	A	350	THR	Peptide
1	A	365	GLY	Peptide
1	A	86	ARG	Sidechain
1	B	16	VAL	Peptide
1	B	167	ARG	Sidechain
1	B	236	ARG	Sidechain
1	B	369	LYS	Peptide
1	C	339	ARG	Sidechain
1	C	340	ALA	Peptide
1	D	28	ASP	Peptide
1	E	100	ARG	Sidechain
1	E	256	SER	Mainchain
1	E	27	GLU	Peptide
1	E	293	ARG	Sidechain
1	E	32	ARG	Sidechain
1	E	42	ARG	Sidechain
1	F	343	GLU	Peptide
1	F	348	PRO	Peptide
1	F	366	LEU	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	3029	0	2902	85	0
1	B	3104	0	2993	123	0
1	C	3049	0	2934	68	0
1	D	3089	0	2985	109	0
1	E	3095	0	2995	128	0
1	F	3013	0	2915	187	0
2	A	13	0	18	0	0
2	B	10	0	13	0	0
2	D	13	0	18	0	0
3	A	16	0	7	1	0
3	B	16	0	7	2	0
3	C	16	0	7	2	0
3	D	16	0	7	2	0
3	E	16	0	7	6	0
3	F	16	0	7	4	0
4	B	1	0	0	0	0
4	C	3	0	0	0	0
4	E	3	0	0	0	0
4	F	2	0	0	0	0
All	All	18520	0	17815	663	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 18.

All (663) 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:F:21:LEU:HA	1:F:25:PHE:CD2	1.41	1.56
1:B:382:LEU:CD2	1:B:388:ILE:HG23	1.49	1.41
1:F:21:LEU:HA	1:F:25:PHE:CE2	1.59	1.37
1:F:17:LEU:O	1:F:20:LYS:CD	1.76	1.33
1:F:17:LEU:O	1:F:20:LYS:CE	1.74	1.32
1:B:373:TYR:C	1:B:381:TYR:CE1	1.88	1.29
1:F:20:LYS:N	1:F:24:ASP:OD2	1.63	1.29
1:F:34:VAL:HG21	1:F:380:ILE:CG2	1.63	1.28
1:F:20:LYS:O	1:F:25:PHE:CE2	1.89	1.25
1:F:34:VAL:HG21	1:F:380:ILE:CB	1.67	1.24
1:F:44:ASP:O	1:F:394:THR:HG21	1.33	1.22
1:B:373:TYR:C	1:B:381:TYR:HE1	1.03	1.21
1:F:21:LEU:CA	1:F:25:PHE:CD2	2.22	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:44:ASP:O	1:F:394:THR:CG2	1.90	1.20
1:F:34:VAL:CG2	1:F:380:ILE:HA	1.78	1.14
1:F:21:LEU:N	1:F:24:ASP:OD2	1.79	1.14
1:F:34:VAL:HG21	1:F:380:ILE:HG23	1.18	1.14
1:B:382:LEU:HD23	1:B:388:ILE:CG2	1.78	1.13
1:C:22:THR:OG1	1:C:35:ASN:ND2	1.81	1.13
1:B:381:TYR:O	1:B:382:LEU:O	1.64	1.13
1:F:20:LYS:O	1:F:25:PHE:HE2	1.22	1.11
1:E:34:VAL:O	1:E:380:ILE:O	1.67	1.10
1:F:20:LYS:C	1:F:25:PHE:HE2	1.56	1.10
1:A:337:GLU:O	1:A:399:ASP:OD1	1.69	1.09
1:E:87:LEU:HD11	1:E:234:LEU:CD1	1.83	1.08
1:B:30:ASP:OD1	1:B:377:GLU:OE2	1.69	1.08
1:D:22:THR:HG23	1:D:35:ASN:HD21	1.16	1.07
1:F:34:VAL:CG2	1:F:380:ILE:HG23	1.84	1.06
1:F:342:LEU:O	1:F:344:ALA:N	1.86	1.05
1:F:17:LEU:O	1:F:20:LYS:HE2	1.51	1.05
1:D:352:ASN:O	1:D:356:ASP:CG	1.94	1.04
1:F:34:VAL:CG2	1:F:380:ILE:HD12	1.85	1.03
1:A:33:LYS:O	1:A:34:VAL:HG23	1.59	1.03
1:F:34:VAL:HG22	1:F:380:ILE:CD1	1.89	1.02
1:A:366:LEU:HD12	1:A:381:TYR:OH	1.60	1.01
1:B:382:LEU:CD2	1:B:388:ILE:CG2	2.34	1.01
1:F:21:LEU:O	1:F:25:PHE:CD2	2.14	1.01
1:A:21:LEU:HD21	1:A:382:LEU:O	1.61	1.01
1:D:22:THR:CG2	1:D:35:ASN:HD21	1.75	1.00
1:A:30:ASP:O	1:A:32:ARG:N	1.92	1.00
1:A:394:THR:OG1	1:A:397:ASN:HB3	1.59	0.99
1:D:373:TYR:OH	1:D:407:GLU:OE1	1.77	0.99
1:F:21:LEU:CA	1:F:25:PHE:CE2	2.40	0.99
1:A:371:VAL:HG11	1:A:384:PRO:HA	1.43	0.99
1:F:21:LEU:O	1:F:25:PHE:HD2	1.45	0.99
1:F:17:LEU:O	1:F:20:LYS:HD2	1.59	0.98
1:B:374:LEU:HB2	1:B:381:TYR:CZ	1.97	0.98
1:B:339:ARG:O	1:B:343:GLU:OE1	1.76	0.98
1:D:22:THR:HG23	1:D:35:ASN:ND2	1.78	0.98
1:F:34:VAL:CG1	1:F:380:ILE:HD12	1.93	0.98
1:F:21:LEU:C	1:F:25:PHE:HD2	1.66	0.97
1:D:352:ASN:O	1:D:356:ASP:OD1	1.81	0.96
1:B:195:ASN:ND2	3:B:502:PLP:O3	1.98	0.95
1:D:373:TYR:HD1	1:D:374:LEU:HD22	1.32	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:339:ARG:O	1:B:343:GLU:CD	2.04	0.95
1:A:347:THR:CG2	1:A:410:THR:HA	1.98	0.94
1:B:374:LEU:HB2	1:B:381:TYR:CE2	2.02	0.94
1:B:341:ARG:O	1:B:346:LYS:NZ	2.00	0.94
1:F:20:LYS:CA	1:F:24:ASP:OD2	2.14	0.94
1:F:34:VAL:CG2	1:F:380:ILE:CD1	2.45	0.94
1:F:371:VAL:HG13	1:F:382:LEU:HG	1.49	0.92
1:E:87:LEU:HD11	1:E:234:LEU:HD13	1.50	0.92
1:F:374:LEU:CD1	1:F:380:ILE:O	2.18	0.92
1:B:368:PRO:O	1:B:371:VAL:HG23	1.69	0.92
1:F:20:LYS:C	1:F:24:ASP:OD2	2.08	0.92
1:B:374:LEU:C	1:B:381:TYR:CE1	2.44	0.91
1:A:347:THR:HG21	1:A:410:THR:HA	1.51	0.91
1:A:30:ASP:OD1	1:A:32:ARG:HB3	1.71	0.91
1:B:340:ALA:O	1:B:343:GLU:OE2	1.55	0.91
1:F:34:VAL:HG22	1:F:380:ILE:HD12	1.48	0.90
1:F:34:VAL:HG13	1:F:380:ILE:HD12	1.54	0.88
1:E:339:ARG:O	1:E:341:ARG:NH1	2.05	0.88
1:F:34:VAL:HG21	1:F:380:ILE:CA	2.03	0.88
1:E:370:GLN:HA	1:E:374:LEU:HD23	1.53	0.88
1:D:14:GLN:NE2	1:D:14:GLN:O	2.07	0.88
1:F:366:LEU:HB2	1:F:370:GLN:HE21	1.37	0.87
1:D:373:TYR:HA	1:D:377:GLU:OE2	1.73	0.87
1:B:372:GLU:O	1:B:373:TYR:O	1.91	0.87
1:F:34:VAL:CB	1:F:380:ILE:HD12	2.05	0.87
1:D:226:TYR:OH	3:D:502:PLP:O4A	1.93	0.87
1:F:347:THR:N	1:F:348:PRO:HD2	1.89	0.87
1:E:379:HIS:O	1:E:381:TYR:CE1	2.29	0.86
1:D:389:ASN:OD1	1:D:391:SER:OG	1.92	0.86
1:F:34:VAL:CG2	1:F:380:ILE:CA	2.53	0.86
1:A:374:LEU:C	1:A:380:ILE:HA	1.97	0.85
1:B:375:VAL:HG23	1:B:380:ILE:HA	1.58	0.85
1:B:369:LYS:O	1:B:373:TYR:CG	2.07	0.85
1:B:374:LEU:CB	1:B:381:TYR:CZ	2.46	0.84
1:D:134:VAL:HG22	1:D:186:ILE:HD12	1.59	0.84
1:E:338:LEU:HD12	1:E:354:ILE:HG21	1.59	0.84
1:A:350:THR:O	1:A:351:TRP:HB2	1.78	0.83
1:D:287[B]:GLN:HA	1:D:287[B]:GLN:OE1	1.75	0.83
1:F:374:LEU:HD11	1:F:380:ILE:HB	1.61	0.83
1:B:374:LEU:O	1:B:381:TYR:CE1	2.31	0.83
1:D:234:LEU:HD12	1:D:321:THR:HG22	1.61	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:344:ALA:O	1:F:345:LEU:HB2	1.77	0.83
1:B:373:TYR:O	1:B:381:TYR:HE1	1.61	0.82
1:F:342:LEU:C	1:F:344:ALA:N	2.29	0.82
1:F:374:LEU:CD1	1:F:380:ILE:HB	2.09	0.82
1:B:374:LEU:O	1:B:381:TYR:CD1	2.31	0.82
1:A:406:HIS:O	1:A:410:THR:OG1	1.98	0.82
1:B:382:LEU:HD23	1:B:388:ILE:HG23	0.82	0.81
1:D:22:THR:CG2	1:D:35:ASN:ND2	2.41	0.81
1:E:351:TRP:CZ2	1:E:405:ILE:HD12	2.15	0.81
1:D:128:ASN:OD1	1:F:127:THR:HG22	1.81	0.81
1:F:21:LEU:CD1	1:F:380:ILE:C	2.48	0.81
1:F:379:HIS:O	1:F:380:ILE:HD13	1.81	0.81
1:C:22:THR:HG1	1:C:35:ASN:ND2	1.78	0.81
1:F:35:ASN:ND2	1:F:37:GLY:H	1.78	0.81
1:A:402:ALA:HB3	1:A:405:ILE:HA	1.63	0.81
1:F:21:LEU:C	1:F:25:PHE:CD2	2.48	0.80
1:F:338:LEU:O	1:F:338:LEU:HD22	1.82	0.80
1:E:377:GLU:N	1:E:377:GLU:OE2	2.13	0.80
1:F:20:LYS:C	1:F:25:PHE:CE2	2.47	0.80
1:F:34:VAL:CG2	1:F:380:ILE:CB	2.56	0.80
1:B:256:SER:OG	3:B:502:PLP:O1P	2.00	0.80
1:E:339:ARG:HB2	1:E:341:ARG:HD2	1.64	0.80
1:A:21:LEU:CD2	1:A:382:LEU:O	2.30	0.79
1:C:192:CYS:SG	1:C:237:ASP:OD1	2.39	0.79
1:E:351:TRP:CE2	1:E:405:ILE:HD12	2.17	0.79
1:C:25:PHE:O	1:C:25:PHE:CD1	2.36	0.79
1:A:347:THR:HB	1:A:348:PRO:HD3	1.65	0.79
1:E:354:ILE:HD11	1:E:364:THR:HG22	1.65	0.78
1:F:20:LYS:O	1:F:25:PHE:CZ	2.35	0.78
1:D:23:ALA:O	1:D:27:GLU:N	2.16	0.78
1:E:338:LEU:CD1	1:E:354:ILE:HG21	2.14	0.78
1:E:373:TYR:CE1	1:E:408:ALA:HB1	2.19	0.78
1:F:366:LEU:HB2	1:F:370:GLN:NE2	1.97	0.78
1:E:343:GLU:O	1:E:405:ILE:CG2	2.32	0.78
1:F:21:LEU:HD13	1:F:375:VAL:HG22	1.64	0.78
1:B:373:TYR:CA	1:B:381:TYR:CE1	2.66	0.77
1:E:52:PRO:HD2	1:E:323:ASN:OD1	1.84	0.77
1:F:35:ASN:CG	1:F:36:LEU:H	1.88	0.77
1:B:22:THR:HG21	1:B:37:GLY:HA3	1.66	0.77
1:B:342:LEU:HD12	1:B:347:THR:OG1	1.84	0.77
1:D:127:THR:HG22	1:F:128:ASN:OD1	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:35:ASN:HD21	1:F:37:GLY:H	1.33	0.77
1:E:373:TYR:CD1	1:E:408:ALA:CB	2.69	0.76
1:F:374:LEU:HD13	1:F:380:ILE:O	1.86	0.76
1:B:382:LEU:CG	1:B:388:ILE:CG2	2.64	0.76
1:F:374:LEU:HD11	1:F:380:ILE:CG2	2.15	0.76
1:E:343:GLU:O	1:E:405:ILE:HG21	1.85	0.76
1:B:343:GLU:OE2	1:B:343:GLU:N	2.19	0.75
1:E:367:ASN:HB3	1:E:372:GLU:CG	2.17	0.75
1:F:35:ASN:O	1:F:36:LEU:HG	1.86	0.75
1:B:342:LEU:N	1:B:343:GLU:OE2	2.20	0.75
1:F:374:LEU:CD2	1:F:380:ILE:HB	2.17	0.75
1:F:389:ASN:ND2	1:F:391:SER:OG	2.20	0.75
1:F:374:LEU:HD11	1:F:380:ILE:CB	2.17	0.74
1:F:371:VAL:HG21	1:F:384:PRO:HA	1.70	0.74
1:D:400:TYR:O	1:D:404:SER:HB3	1.88	0.74
1:E:20:LYS:O	1:E:24:ASP:HB2	1.88	0.74
1:D:338:LEU:O	1:D:342:LEU:CD2	2.36	0.74
1:E:17:LEU:O	1:E:21:LEU:N	2.20	0.74
1:E:367:ASN:ND2	1:E:372:GLU:N	2.35	0.74
1:C:339:ARG:HB2	1:C:355:THR:HG23	1.69	0.73
1:F:21:LEU:HD13	1:F:380:ILE:C	2.09	0.73
1:F:34:VAL:HG21	1:F:380:ILE:CG1	2.19	0.73
1:E:347:THR:H	1:E:348:PRO:CD	2.02	0.73
1:E:372:GLU:HG3	1:E:373:TYR:CD2	2.24	0.73
1:F:21:LEU:O	1:F:25:PHE:CB	2.37	0.73
1:E:256:SER:OG	3:E:501:PLP:O3P	2.06	0.73
1:F:21:LEU:CA	1:F:25:PHE:HD2	1.81	0.73
1:B:374:LEU:O	1:B:381:TYR:CG	2.42	0.72
1:F:342:LEU:HD22	1:F:342:LEU:O	1.88	0.72
1:F:44:ASP:HA	1:F:394:THR:HG23	1.72	0.72
1:E:25:PHE:CG	1:E:381:TYR:CZ	2.77	0.72
1:C:352:ASN:O	1:C:356:ASP:OD1	2.07	0.72
1:D:352:ASN:O	1:D:356:ASP:OD2	2.08	0.72
1:A:394:THR:OG1	1:A:397:ASN:CB	2.38	0.72
1:C:145[A]:ASN:HD22	1:C:145[A]:ASN:C	1.93	0.72
1:B:374:LEU:HD13	1:B:378:LYS:HG2	1.72	0.71
1:D:371:VAL:CG1	1:D:382:LEU:O	2.38	0.71
1:B:339:ARG:O	1:B:343:GLU:CG	2.37	0.71
1:E:367:ASN:ND2	1:E:372:GLU:HB3	2.05	0.71
1:E:367:ASN:ND2	1:E:372:GLU:H	1.87	0.71
1:B:374:LEU:CA	1:B:381:TYR:CE1	2.51	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:373:TYR:CA	1:B:381:TYR:HE1	1.98	0.71
1:F:343:GLU:OE2	1:F:351:TRP:CD2	2.44	0.71
1:F:24:ASP:HB2	1:F:25:PHE:CE2	2.25	0.71
1:B:342:LEU:HD21	1:B:402:ALA:HB1	1.72	0.70
1:C:12:GLN:O	1:C:13:ALA:HB2	1.91	0.70
1:F:20:LYS:N	1:F:24:ASP:CG	2.43	0.70
1:A:338:LEU:HD22	1:A:338:LEU:O	1.91	0.70
1:D:21:LEU:C	1:D:21:LEU:HD12	2.12	0.70
1:F:17:LEU:O	1:F:20:LYS:HD3	1.90	0.70
1:C:345:LEU:HD12	1:C:401:VAL:HG22	1.74	0.70
1:E:352:ASN:O	1:E:356:ASP:OD1	2.09	0.70
1:A:347:THR:HG22	1:A:410:THR:HA	1.73	0.70
1:F:19:PHE:C	1:F:24:ASP:CG	2.50	0.70
1:C:24:ASP:O	1:C:28:ASP:HB2	1.92	0.69
1:D:122:ARG:HD2	1:D:128:ASN:ND2	2.08	0.69
1:E:46:CYS:O	1:E:46:CYS:SG	2.50	0.69
1:C:59:GLN:NE2	1:D:62:ALA:O	2.24	0.69
1:B:382:LEU:HG	1:B:388:ILE:HG22	1.75	0.69
1:F:352:ASN:O	1:F:356:ASP:OD1	2.10	0.69
1:E:18:VAL:O	1:E:22:THR:OG1	2.05	0.69
1:B:28:ASP:CB	1:B:33:LYS:NZ	2.57	0.68
1:F:374:LEU:HD11	1:F:380:ILE:HG22	1.74	0.68
1:B:377:GLU:O	1:B:377:GLU:CD	2.32	0.68
1:B:371:VAL:N	1:B:373:TYR:CZ	2.57	0.68
1:F:259:LYS:NZ	3:F:501:PLP:O4A	2.27	0.68
1:C:25:PHE:O	1:C:25:PHE:CG	2.46	0.68
1:A:396:LYS:C	1:A:398:LEU:H	1.97	0.68
1:B:22:THR:HG21	1:B:37:GLY:CA	2.24	0.68
1:F:21:LEU:O	1:F:25:PHE:HB2	1.93	0.68
1:C:52:PRO:HD2	1:C:323:ASN:OD1	1.94	0.67
1:A:348:PRO:HG2	1:A:409:VAL:HG12	1.75	0.67
1:A:34:VAL:CG1	1:A:36:LEU:HG	2.24	0.67
1:B:382:LEU:HG	1:B:388:ILE:CG2	2.22	0.67
1:F:19:PHE:C	1:F:24:ASP:OD1	2.32	0.67
1:B:374:LEU:O	1:B:381:TYR:CZ	2.46	0.67
1:E:372:GLU:O	1:E:373:TYR:C	2.33	0.67
1:B:374:LEU:C	1:B:381:TYR:CZ	2.58	0.66
1:F:374:LEU:HD21	1:F:380:ILE:HB	1.75	0.66
1:B:369:LYS:O	1:B:373:TYR:CD1	2.33	0.66
1:A:347:THR:CB	1:A:348:PRO:HD3	2.26	0.66
1:A:366:LEU:HD12	1:A:381:TYR:HH	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:LYS:O	1:A:347:THR:OG1	2.13	0.66
1:A:294:ILE:HD12	1:B:150:ALA:HB2	1.78	0.66
1:F:21:LEU:HD11	1:F:380:ILE:C	2.16	0.66
1:F:17:LEU:O	1:F:20:LYS:NZ	2.29	0.66
1:E:407:GLU:N	1:E:407:GLU:OE1	2.30	0.65
1:F:34:VAL:HG13	1:F:380:ILE:CD1	2.25	0.65
1:F:19:PHE:C	1:F:24:ASP:OD2	2.33	0.65
1:C:25:PHE:CD1	1:C:33:LYS:CB	2.80	0.65
1:B:382:LEU:CG	1:B:388:ILE:HG23	2.23	0.65
1:B:371:VAL:HG13	1:B:384:PRO:HA	1.77	0.64
1:F:21:LEU:N	1:F:25:PHE:CE2	2.65	0.64
1:F:21:LEU:N	1:F:25:PHE:HE2	1.95	0.64
1:B:87:LEU:HD11	1:B:234:LEU:HD23	1.79	0.64
1:B:377:GLU:O	1:B:377:GLU:OE2	2.16	0.64
1:D:373:TYR:CD2	1:D:377:GLU:OE2	2.50	0.64
1:F:34:VAL:HG22	1:F:380:ILE:HD13	1.74	0.64
1:A:348:PRO:HG3	1:A:410:THR:O	1.97	0.64
1:D:339:ARG:HG3	1:D:351:TRP:O	1.97	0.64
1:D:343:GLU:OE2	1:D:343:GLU:HA	1.97	0.64
1:A:30:ASP:OD1	1:A:32:ARG:CB	2.45	0.64
1:D:34:VAL:HG21	1:D:380:ILE:HD11	1.79	0.64
1:B:374:LEU:CD1	1:B:407:GLU:OE1	2.46	0.64
1:B:22:THR:O	1:B:380:ILE:HD13	1.98	0.63
3:E:501:PLP:O2P	1:F:71:TYR:OH	2.14	0.63
1:B:399:ASP:O	1:B:403:THR:HG23	1.98	0.63
1:D:122:ARG:CD	1:D:128:ASN:HD21	2.12	0.63
1:D:24:ASP:O	1:D:27:GLU:CG	2.46	0.63
1:F:34:VAL:HG23	1:F:380:ILE:HA	1.76	0.63
1:F:34:VAL:CG1	1:F:380:ILE:CD1	2.74	0.63
1:E:120:LEU:HD13	1:E:186:ILE:HD13	1.80	0.63
1:E:258:SER:OG	3:E:501:PLP:O3P	2.16	0.63
1:F:236:ARG:O	1:F:236:ARG:NH1	2.32	0.63
1:F:35:ASN:ND2	1:F:36:LEU:N	2.46	0.63
1:B:28:ASP:CB	1:B:33:LYS:HZ3	2.12	0.63
1:B:374:LEU:O	1:B:381:TYR:CD2	2.52	0.63
1:F:34:VAL:HG22	1:F:380:ILE:HA	1.76	0.62
1:F:44:ASP:CA	1:F:394:THR:HG23	2.28	0.62
1:E:369:LYS:O	1:E:374:LEU:HB3	1.98	0.62
1:E:25:PHE:CD2	1:E:381:TYR:CE1	2.86	0.62
1:B:15:PRO:HB3	1:B:21:LEU:HD23	1.82	0.62
1:F:337:GLU:O	1:F:341:ARG:HG2	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:134:VAL:HG11	1:D:148:PHE:CD2	2.35	0.62
1:F:17:LEU:C	1:F:20:LYS:HE2	2.20	0.62
1:E:87:LEU:HD11	1:E:234:LEU:HD11	1.77	0.62
1:E:352:ASN:O	1:E:356:ASP:CG	2.37	0.62
1:B:341:ARG:HD2	1:B:398:LEU:CD2	2.30	0.62
1:A:381:TYR:O	1:A:383:LEU:N	2.32	0.61
1:D:234:LEU:CD1	1:D:321:THR:HG22	2.28	0.61
1:B:127:THR:HG23	1:E:127:THR:HG23	1.82	0.61
1:E:367:ASN:CG	1:E:372:GLU:H	2.03	0.61
1:F:21:LEU:O	1:F:25:PHE:CG	2.54	0.61
1:D:373:TYR:CE2	1:D:377:GLU:OE1	2.52	0.61
1:C:89:LEU:HD22	1:C:245:VAL:HG21	1.83	0.61
1:D:122:ARG:HD2	1:D:128:ASN:HD21	1.63	0.61
1:E:354:ILE:CD1	1:E:364:THR:HG22	2.31	0.61
1:A:33:LYS:O	1:A:34:VAL:CG2	2.43	0.61
1:F:17:LEU:C	1:F:20:LYS:CE	2.64	0.61
1:F:374:LEU:HD12	1:F:382:LEU:HD22	1.81	0.61
1:F:374:LEU:O	1:F:374:LEU:HD22	2.01	0.61
1:A:30:ASP:OD1	1:A:32:ARG:HG2	2.00	0.61
1:A:347:THR:HB	1:A:348:PRO:CD	2.31	0.61
1:D:234:LEU:HD11	1:D:320:TRP:CZ3	2.35	0.60
1:E:373:TYR:CE1	1:E:408:ALA:CB	2.83	0.60
1:F:34:VAL:CB	1:F:380:ILE:HG23	2.31	0.60
1:E:25:PHE:CG	1:E:381:TYR:CE1	2.89	0.60
1:B:34:VAL:O	1:B:380:ILE:HB	2.02	0.60
1:D:373:TYR:CD1	1:D:374:LEU:HD22	2.24	0.60
3:F:501:PLP:H4A	3:F:501:PLP:O4P	2.00	0.60
1:B:374:LEU:HD12	1:B:407:GLU:OE1	2.01	0.60
1:E:256:SER:OG	1:E:258:SER:OG	2.15	0.60
1:F:123:TRP:CZ2	1:F:287[B]:GLN:NE2	2.70	0.60
1:B:127:THR:CG2	1:E:127:THR:HG23	2.32	0.60
1:D:46:CYS:SG	1:D:46:CYS:O	2.60	0.59
1:A:394:THR:OG1	1:A:397:ASN:N	2.32	0.59
1:B:381:TYR:C	1:B:382:LEU:O	2.39	0.59
1:F:374:LEU:HD12	1:F:382:LEU:CD2	2.33	0.59
1:B:374:LEU:CG	1:B:381:TYR:OH	2.43	0.59
1:C:145[A]:ASN:ND2	1:C:145[A]:ASN:O	2.35	0.59
1:E:367:ASN:HB3	1:E:372:GLU:HG3	1.83	0.59
1:F:44:ASP:C	1:F:394:THR:CG2	2.67	0.59
1:E:367:ASN:CB	1:E:372:GLU:HB3	2.33	0.59
1:A:394:THR:HG1	1:A:397:ASN:H	1.51	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:338:LEU:HD13	1:E:338:LEU:O	2.02	0.59
1:D:371:VAL:HG13	1:D:382:LEU:HD23	1.85	0.58
1:B:127:THR:HG23	1:E:127:THR:CG2	2.33	0.58
1:C:145[A]:ASN:C	1:C:145[A]:ASN:ND2	2.56	0.58
1:B:373:TYR:HB2	1:B:381:TYR:CZ	2.39	0.58
1:E:339:ARG:HB2	1:E:341:ARG:CD	2.32	0.58
1:B:137:SER:OG	1:B:139:PRO:O	2.21	0.58
1:E:373:TYR:O	1:E:374:LEU:O	2.21	0.58
1:F:17:LEU:HA	1:F:20:LYS:HE2	1.84	0.58
1:F:17:LEU:C	1:F:20:LYS:HZ3	2.07	0.58
1:F:44:ASP:C	1:F:394:THR:HG21	2.18	0.58
1:E:367:ASN:CB	1:E:372:GLU:CB	2.82	0.58
1:F:134:VAL:HG11	1:F:148:PHE:CD2	2.38	0.58
1:D:261:PHE:CE2	1:D:307:VAL:HG13	2.38	0.57
1:A:150:ALA:HB2	1:B:294:ILE:HD12	1.85	0.57
1:E:69:HIS:HA	1:F:265:ASN:ND2	2.19	0.57
1:F:234:LEU:HD11	1:F:321:THR:HG22	1.86	0.57
1:B:120:LEU:HD13	1:B:186:ILE:HD13	1.86	0.57
1:F:34:VAL:CG2	1:F:380:ILE:CG1	2.81	0.57
1:C:347:THR:CG2	1:C:403:THR:C	2.73	0.57
1:F:347:THR:N	1:F:348:PRO:CD	2.65	0.57
1:A:366:LEU:HD12	1:A:381:TYR:CZ	2.38	0.57
1:F:335:ARG:NH1	1:F:354:ILE:O	2.36	0.57
1:E:351:TRP:NE1	1:E:405:ILE:HD12	2.19	0.57
1:F:25:PHE:O	1:F:28:ASP:HB2	2.05	0.57
1:E:87:LEU:CD1	1:E:234:LEU:HD13	2.28	0.56
1:F:348:PRO:HA	1:F:351:TRP:CD1	2.40	0.56
1:E:367:ASN:HD22	1:E:372:GLU:HB3	1.70	0.56
1:A:339:ARG:HB3	1:A:355:THR:HG23	1.86	0.56
1:B:382:LEU:HB3	1:B:387:ARG:O	2.06	0.56
1:B:374:LEU:O	1:B:381:TYR:CE2	2.59	0.56
1:D:373:TYR:CD2	1:D:377:GLU:OE1	2.58	0.56
1:D:223:ASP:OD2	3:D:502:PLP:N1	2.39	0.56
1:D:373:TYR:CD2	1:D:377:GLU:CD	2.80	0.56
1:E:360:MET:HE3	1:E:389:ASN:HD21	1.71	0.56
1:A:339:ARG:CB	1:A:355:THR:HG23	2.36	0.56
1:C:293:ARG:NH1	1:D:142:GLU:OE1	2.37	0.56
1:E:22:THR:OG1	1:E:38:VAL:HB	2.06	0.56
1:D:127:THR:CG2	1:F:128:ASN:OD1	2.52	0.56
1:A:398:LEU:C	1:A:400:TYR:N	2.59	0.55
1:B:370:GLN:HG2	1:B:408:ALA:CB	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:120:LEU:HD13	1:F:186:ILE:HD13	1.88	0.55
1:A:352:ASN:ND2	1:A:356:ASP:OD2	2.39	0.55
1:F:25:PHE:HB3	1:F:28:ASP:OD1	2.06	0.55
1:F:371:VAL:HG13	1:F:382:LEU:CG	2.32	0.55
1:B:400:TYR:O	1:B:403:THR:OG1	2.24	0.55
1:F:24:ASP:HB2	1:F:25:PHE:CD2	2.41	0.55
1:A:34:VAL:HG12	1:A:36:LEU:HG	1.88	0.55
1:E:323:ASN:HD22	1:E:323:ASN:N	2.04	0.55
1:F:25:PHE:CD2	1:F:25:PHE:N	2.74	0.55
1:F:347:THR:H	1:F:348:PRO:HD2	1.69	0.55
1:C:48:PRO:HB3	1:D:70:GLU:OE2	2.06	0.55
1:D:338:LEU:O	1:D:342:LEU:HD23	2.05	0.54
1:F:21:LEU:CD1	1:F:375:VAL:HG22	2.34	0.54
1:B:21:LEU:O	1:B:24:ASP:OD1	2.25	0.54
1:C:34:VAL:HB	1:C:380:ILE:HG12	1.89	0.54
1:E:367:ASN:CG	1:E:372:GLU:N	2.61	0.54
1:A:20:LYS:HE2	1:A:23:ALA:HB3	1.90	0.54
1:C:195:ASN:ND2	3:C:501:PLP:O3	2.40	0.54
1:E:379:HIS:O	1:E:381:TYR:CD1	2.61	0.54
1:B:373:TYR:O	1:B:381:TYR:CE1	2.46	0.54
1:D:346:LYS:O	1:D:347:THR:C	2.45	0.54
1:A:342:LEU:HD11	1:A:406:HIS:HE2	1.73	0.53
1:C:12:GLN:O	1:C:13:ALA:CB	2.54	0.53
1:A:34:VAL:HG11	1:A:36:LEU:HG	1.90	0.53
1:E:367:ASN:HB3	1:E:372:GLU:CB	2.38	0.53
1:B:268:VAL:HG22	1:B:303:GLY:HA3	1.91	0.53
1:C:339:ARG:O	1:C:342:LEU:N	2.33	0.53
1:F:21:LEU:O	1:F:25:PHE:N	2.41	0.53
1:D:373:TYR:CA	1:D:377:GLU:OE2	2.51	0.53
1:F:18:VAL:HG23	1:F:142:GLU:OE2	2.08	0.53
1:A:250:GLU:CD	1:A:276:LYS:HG2	2.29	0.53
1:B:46:CYS:SG	1:B:394:THR:HG21	2.48	0.53
1:F:19:PHE:HB3	1:F:24:ASP:OD1	2.08	0.53
1:D:15:PRO:O	1:D:16:VAL:HG13	2.09	0.52
1:E:335:ARG:O	1:E:355:THR:HG22	2.09	0.52
1:D:127:THR:HG23	1:F:127:THR:CG2	2.39	0.52
1:D:34:VAL:CG2	1:D:380:ILE:HD11	2.39	0.52
1:D:405:ILE:HG23	1:D:406:HIS:CD2	2.44	0.52
1:E:367:ASN:CG	1:E:372:GLU:CA	2.77	0.52
1:F:348:PRO:HA	1:F:351:TRP:NE1	2.24	0.52
1:D:402:ALA:O	1:D:405:ILE:HG22	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:234:LEU:HD11	1:C:320:TRP:CH2	2.44	0.52
1:C:83:CYS:SG	1:C:86:ARG:NH2	2.83	0.52
1:D:21:LEU:O	1:D:21:LEU:HD12	2.10	0.52
1:B:338:LEU:HD22	1:B:338:LEU:O	2.10	0.52
1:E:259:LYS:NZ	3:E:501:PLP:O4A	2.42	0.52
1:E:25:PHE:HD1	1:E:28:ASP:CB	2.22	0.52
1:A:264:TYR:HB2	1:B:69:HIS:O	2.10	0.52
1:C:236:ARG:HD2	1:C:236:ARG:C	2.30	0.52
1:F:374:LEU:HD11	1:F:380:ILE:O	2.09	0.52
1:C:347:THR:HG22	1:C:403:THR:C	2.30	0.52
1:E:367:ASN:CB	1:E:372:GLU:CG	2.88	0.51
1:E:343:GLU:O	1:E:405:ILE:HG23	2.09	0.51
1:D:128:ASN:OD1	1:F:127:THR:CG2	2.54	0.51
1:E:338:LEU:O	1:E:338:LEU:HD22	2.10	0.51
1:D:371:VAL:HG13	1:D:382:LEU:CD2	2.40	0.51
1:E:373:TYR:CD1	1:E:408:ALA:HB1	2.41	0.51
1:E:294:ILE:HD12	1:F:150:ALA:HB2	1.93	0.51
1:F:34:VAL:CG2	1:F:380:ILE:CG2	2.53	0.51
1:B:234:LEU:HD12	1:B:234:LEU:H	1.75	0.51
1:B:382:LEU:CG	1:B:388:ILE:HG22	2.35	0.51
1:D:369:LYS:C	1:D:371:VAL:H	2.14	0.51
1:D:398:LEU:O	1:D:401:VAL:N	2.44	0.51
1:F:223:ASP:OD2	3:F:501:PLP:N1	2.44	0.51
1:A:30:ASP:OD1	1:A:32:ARG:CG	2.59	0.51
1:E:367:ASN:CG	1:E:372:GLU:HB3	2.32	0.51
1:B:128:ASN:OD1	1:E:127:THR:HG22	2.11	0.51
1:F:367:ASN:HB2	1:F:368:PRO:HD2	1.93	0.51
1:F:367:ASN:O	1:F:370:GLN:HG2	2.11	0.50
1:C:323:ASN:N	1:C:323:ASN:HD22	2.09	0.50
1:D:268:VAL:HG22	1:D:303:GLY:HA3	1.92	0.50
1:D:339:ARG:HA	1:D:342:LEU:HD21	1.93	0.50
1:C:395:THR:HA	1:C:398:LEU:HB2	1.93	0.50
1:F:348:PRO:HA	1:F:351:TRP:HE1	1.76	0.50
1:C:71:TYR:CE2	1:D:264:TYR:CD2	2.99	0.50
1:D:393:LEU:CD2	1:D:401:VAL:HG21	2.42	0.50
1:A:120:LEU:HD13	1:A:186:ILE:HD13	1.93	0.50
1:C:337:GLU:CB	1:C:398:LEU:HD21	2.42	0.50
1:F:35:ASN:O	1:F:36:LEU:CG	2.58	0.50
1:E:25:PHE:HA	1:E:28:ASP:HB2	1.94	0.50
1:D:34:VAL:HB	1:D:380:ILE:HG12	1.93	0.50
1:E:25:PHE:CB	1:E:381:TYR:CZ	2.95	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:339:ARG:NH2	1:D:345:LEU:HD21	2.27	0.49
1:F:35:ASN:ND2	1:F:36:LEU:H	2.06	0.49
1:A:371:VAL:O	1:A:374:LEU:O	2.29	0.49
1:B:370:GLN:HG2	1:B:408:ALA:HB3	1.94	0.49
1:B:128:ASN:OD1	1:E:127:THR:CG2	2.60	0.49
1:E:294:ILE:HG21	1:F:146:ALA:HB1	1.94	0.49
1:A:347:THR:CG2	1:A:348:PRO:HD3	2.42	0.49
1:A:226:TYR:OH	3:A:502:PLP:O4A	2.31	0.49
1:C:105:GLN:NE2	1:C:304:ALA:HB2	2.28	0.49
1:C:374:LEU:HA	1:C:378:LYS:HB2	1.94	0.49
1:D:50:VAL:HG11	1:D:55:LYS:HE3	1.94	0.49
1:E:25:PHE:CD1	1:E:28:ASP:CB	2.96	0.49
1:E:351:TRP:CZ2	1:E:405:ILE:CD1	2.93	0.49
1:F:17:LEU:CA	1:F:20:LYS:HE2	2.42	0.49
1:A:402:ALA:CB	1:A:405:ILE:HA	2.39	0.49
1:E:373:TYR:CZ	1:E:408:ALA:HB1	2.46	0.49
1:F:261:PHE:CE2	1:F:307:VAL:HG13	2.47	0.49
1:B:234:LEU:HD12	1:B:234:LEU:N	2.27	0.49
1:F:267:ARG:HH22	3:F:501:PLP:P	2.36	0.49
1:E:401:VAL:O	1:E:402:ALA:HB2	2.13	0.49
1:D:374:LEU:HD21	1:D:408:ALA:HB2	1.95	0.49
1:C:107:LEU:HD11	1:D:107:LEU:HD11	1.95	0.48
1:D:342:LEU:H	1:D:342:LEU:HD23	1.76	0.48
1:D:400:TYR:O	1:D:404:SER:N	2.45	0.48
1:C:17:LEU:HD22	1:C:142:GLU:OE2	2.13	0.48
1:D:279:GLU:HG2	1:D:280:SER:N	2.25	0.48
1:F:122:ARG:HD2	1:F:128:ASN:HD21	1.78	0.48
1:A:268:VAL:HG22	1:A:303:GLY:HA3	1.94	0.48
1:A:339:ARG:O	1:A:342:LEU:N	2.33	0.48
1:C:71:TYR:CE2	1:D:264:TYR:HD2	2.31	0.48
1:D:127:THR:HB	1:F:122:ARG:NH2	2.29	0.48
1:F:122:ARG:CD	1:F:128:ASN:HD21	2.26	0.48
1:B:372:GLU:O	1:B:373:TYR:C	2.50	0.48
1:A:32:ARG:NE	1:A:32:ARG:O	2.46	0.48
1:D:14:GLN:N	1:D:15:PRO:HD3	2.28	0.48
1:A:406:HIS:HA	1:A:409:VAL:HB	1.96	0.48
1:F:35:ASN:O	1:F:36:LEU:CB	2.61	0.48
1:C:14:GLN:O	1:C:15:PRO:O	2.32	0.48
1:E:18:VAL:CG1	1:E:383:LEU:HD21	2.44	0.48
1:E:347:THR:H	1:E:348:PRO:HD2	1.76	0.48
1:D:339:ARG:HD3	1:D:345:LEU:HD11	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:340:ALA:H	1:D:342:LEU:HD21	1.79	0.48
1:E:379:HIS:O	1:E:381:TYR:CZ	2.66	0.48
1:A:32:ARG:CD	1:A:32:ARG:O	2.61	0.47
1:C:258:SER:OG	3:C:501:PLP:O1P	2.26	0.47
1:F:122:ARG:HD2	1:F:128:ASN:ND2	2.28	0.47
1:A:32:ARG:HB2	1:A:32:ARG:CZ	2.44	0.47
1:D:26:ARG:C	1:D:28:ASP:H	2.17	0.47
1:E:163:ASP:HB2	1:E:170:ASP:HB2	1.96	0.47
1:D:122:ARG:CD	1:D:128:ASN:ND2	2.74	0.47
1:F:344:ALA:O	1:F:345:LEU:CB	2.54	0.47
1:D:342:LEU:HD13	1:D:351:TRP:CD1	2.49	0.47
1:B:234:LEU:HD21	1:B:320:TRP:CH2	2.50	0.47
1:A:107:LEU:HD23	1:A:296:TRP:CE2	2.49	0.47
1:A:397:ASN:O	1:A:397:ASN:OD1	2.32	0.47
1:A:70:GLU:OE1	1:B:42:ARG:NH1	2.47	0.47
1:B:362:SER:O	1:B:387:ARG:HA	2.15	0.47
1:B:341:ARG:HD2	1:B:398:LEU:HD22	1.96	0.47
1:D:338:LEU:HD23	1:D:398:LEU:HD11	1.97	0.47
1:D:402:ALA:O	1:D:405:ILE:CG2	2.63	0.47
1:E:330:ARG:NH2	1:E:391:SER:O	2.47	0.47
1:F:171:LEU:HD22	1:F:205:GLN:HG2	1.96	0.47
1:A:409:VAL:O	1:A:410:THR:C	2.53	0.47
1:D:14:GLN:O	1:D:15:PRO:O	2.33	0.47
1:F:107:LEU:HD23	1:F:296:TRP:CE2	2.50	0.47
1:B:21:LEU:HD13	1:B:21:LEU:O	2.13	0.47
1:F:19:PHE:CA	1:F:24:ASP:OD1	2.63	0.47
1:A:400:TYR:HA	1:A:405:ILE:HD11	1.96	0.47
1:B:382:LEU:N	1:B:382:LEU:HD12	2.30	0.47
1:B:342:LEU:CD2	1:B:402:ALA:HB1	2.44	0.47
1:C:362:SER:O	1:C:387:ARG:HA	2.14	0.47
1:E:25:PHE:CE1	1:E:28:ASP:OD2	2.68	0.47
1:F:367:ASN:CB	1:F:368:PRO:HD2	2.45	0.46
1:F:371:VAL:HG11	1:F:383:LEU:C	2.35	0.46
1:B:17:LEU:HG	1:B:383:LEU:HD11	1.96	0.46
1:C:35:ASN:HD21	1:C:38:VAL:HG12	1.79	0.46
1:E:407:GLU:N	1:E:407:GLU:CD	2.68	0.46
1:D:400:TYR:O	1:D:404:SER:CB	2.62	0.46
1:A:330:ARG:NH2	1:A:391:SER:O	2.48	0.46
1:A:42:ARG:NH1	1:B:70:GLU:OE1	2.46	0.46
1:A:69:HIS:O	1:B:264:TYR:HB2	2.16	0.46
1:A:32:ARG:O	1:A:32:ARG:CG	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:362:SER:O	1:E:387:ARG:HA	2.14	0.46
1:F:17:LEU:C	1:F:20:LYS:NZ	2.69	0.46
1:E:17:LEU:O	1:E:21:LEU:HB2	2.15	0.46
1:F:342:LEU:O	1:F:342:LEU:HD13	2.16	0.46
1:B:398:LEU:HD23	1:B:399:ASP:N	2.31	0.46
1:E:400:TYR:C	1:E:400:TYR:CD2	2.88	0.46
1:E:192:CYS:SG	1:E:230:ALA:HB2	2.56	0.46
1:E:377:GLU:HG2	1:E:378:LYS:HD2	1.98	0.46
1:E:18:VAL:HG12	1:E:383:LEU:HD21	1.98	0.46
1:D:20:LYS:O	1:D:24:ASP:HB2	2.16	0.45
1:E:366:LEU:HA	1:E:373:TYR:HB2	1.97	0.45
1:B:107:LEU:HD23	1:B:296:TRP:CE2	2.51	0.45
1:B:383:LEU:HG	1:B:384:PRO:HD2	1.98	0.45
1:D:362:SER:O	1:D:387:ARG:HA	2.16	0.45
1:E:25:PHE:HD1	1:E:28:ASP:HB3	1.81	0.45
1:E:347:THR:N	1:E:348:PRO:CD	2.75	0.45
1:E:367:ASN:HB3	1:E:372:GLU:C	2.37	0.45
1:B:398:LEU:O	1:B:401:VAL:N	2.50	0.45
1:D:338:LEU:HD23	1:D:398:LEU:CD1	2.47	0.45
1:D:394:THR:O	1:D:398:LEU:HD22	2.16	0.45
1:A:404:SER:O	1:A:405:ILE:HB	2.17	0.45
1:C:330:ARG:NH2	1:C:391:SER:O	2.50	0.45
1:F:394:THR:O	1:F:398:LEU:HD22	2.17	0.45
1:A:347:THR:HG22	1:A:348:PRO:HD3	1.99	0.45
1:A:301:ALA:HB3	1:B:266:GLU:OE2	2.17	0.45
1:C:230:ALA:HB3	1:C:237:ASP:OD1	2.16	0.45
1:C:21:LEU:HD11	1:C:382:LEU:N	2.32	0.45
1:D:107:LEU:HD23	1:D:296:TRP:CE2	2.51	0.45
1:E:339:ARG:HD2	1:E:341:ARG:HD2	1.99	0.45
1:F:362:SER:O	1:F:387:ARG:HA	2.16	0.44
1:B:376:ASN:HD22	1:B:376:ASN:H	1.65	0.44
1:B:377:GLU:CD	1:B:377:GLU:C	2.75	0.44
1:C:25:PHE:HA	1:C:28:ASP:HB2	1.99	0.44
1:D:22:THR:HG22	1:D:35:ASN:ND2	2.29	0.44
1:A:107:LEU:HD11	1:B:107:LEU:HD11	1.99	0.44
1:E:366:LEU:CD1	1:E:382:LEU:HD11	2.47	0.44
1:B:229:PHE:CE2	1:B:360:MET:HE2	2.53	0.44
1:A:104:VAL:O	1:A:105:GLN:C	2.55	0.44
1:E:69:HIS:HA	1:F:265:ASN:HD21	1.83	0.44
1:D:122:ARG:NH2	1:F:127:THR:HB	2.33	0.44
1:A:243:TYR:CE1	1:A:247:GLU:HG3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:ASN:HD21	1:B:305:ARG:HH22	1.65	0.44
1:F:374:LEU:O	1:F:374:LEU:HD13	2.18	0.44
1:B:127:THR:HB	1:E:122:ARG:NH2	2.32	0.43
1:B:373:TYR:HB2	1:B:381:TYR:CE1	2.53	0.43
1:E:145[A]:ASN:N	1:E:145[A]:ASN:OD1	2.50	0.43
1:F:100:ARG:HD2	1:F:275:GLY:O	2.18	0.43
1:F:330:ARG:NH2	1:F:391:SER:O	2.50	0.43
1:A:16:VAL:O	1:A:18:VAL:N	2.51	0.43
1:D:236:ARG:O	1:D:239:TRP:N	2.45	0.43
1:F:35:ASN:ND2	1:F:37:GLY:N	2.58	0.43
1:B:342:LEU:C	1:B:343:GLU:OE2	2.57	0.43
1:D:389:ASN:CG	1:D:391:SER:OG	2.54	0.43
1:F:356:ASP:OD1	1:F:356:ASP:N	2.51	0.43
1:F:44:ASP:O	1:F:394:THR:HG23	2.01	0.43
1:E:21:LEU:HA	1:E:24:ASP:HB2	2.00	0.43
1:E:228:GLY:CA	1:E:234:LEU:HD23	2.48	0.43
1:B:330:ARG:NH2	1:B:391:SER:O	2.51	0.43
1:A:171:LEU:HD22	1:A:205:GLN:HG2	2.00	0.43
1:E:150:ALA:HB2	1:F:294:ILE:HD12	2.01	0.43
1:A:362:SER:O	1:A:387:ARG:HA	2.19	0.43
1:B:95:ALA:HB1	1:B:101:VAL:CG2	2.49	0.43
1:C:294:ILE:HD12	1:D:150:ALA:HB2	2.00	0.43
1:F:268:VAL:HG22	1:F:303:GLY:HA3	2.01	0.43
1:F:44:ASP:C	1:F:394:THR:HG23	2.38	0.43
1:C:107:LEU:HD23	1:C:296:TRP:CE2	2.54	0.43
1:B:234:LEU:CD1	1:B:234:LEU:H	2.31	0.42
1:D:338:LEU:O	1:D:342:LEU:HD21	2.16	0.42
1:F:374:LEU:HD21	1:F:380:ILE:CG1	2.49	0.42
1:A:339:ARG:HB2	1:A:354:ILE:HB	2.01	0.42
1:B:17:LEU:HA	1:B:17:LEU:HD12	1.85	0.42
1:D:342:LEU:N	1:D:342:LEU:HD23	2.33	0.42
1:E:267:ARG:NH2	3:E:501:PLP:O1P	2.43	0.42
1:C:268:VAL:HG22	1:C:303:GLY:HA3	2.00	0.42
1:D:123:TRP:CE2	1:D:287[B]:GLN:HG3	2.53	0.42
1:D:196:PRO:CB	1:D:387:ARG:HD3	2.49	0.42
1:E:373:TYR:CD1	1:E:408:ALA:HB2	2.52	0.42
1:E:73:PRO:HB2	1:E:76:GLY:H	1.83	0.42
1:F:104:VAL:O	1:F:105:GLN:C	2.58	0.42
1:F:95:ALA:HB1	1:F:101:VAL:CG2	2.49	0.42
1:C:347:THR:HG23	1:C:403:THR:CA	2.49	0.42
1:D:21:LEU:HD21	1:D:383:LEU:HD22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:393:LEU:HD22	1:D:401:VAL:HG21	2.02	0.42
1:E:25:PHE:HE1	1:E:28:ASP:OD2	2.03	0.42
1:E:105:GLN:NE2	1:E:304:ALA:HB2	2.34	0.42
1:C:356:ASP:N	1:C:356:ASP:OD1	2.52	0.42
1:D:26:ARG:C	1:D:28:ASP:N	2.73	0.42
1:D:331:ILE:O	1:D:335:ARG:HG3	2.19	0.42
1:B:371:VAL:HG13	1:B:384:PRO:CA	2.48	0.42
1:F:342:LEU:C	1:F:342:LEU:HD13	2.40	0.42
1:F:353:HIS:NE2	1:F:364:THR:O	2.53	0.42
1:C:138:SER:HA	1:C:139:PRO:HA	1.92	0.42
1:C:337:GLU:O	1:C:398:LEU:HD21	2.20	0.42
1:B:370:GLN:HG2	1:B:408:ALA:HB1	2.01	0.42
1:C:59:GLN:NE2	1:D:62:ALA:HB1	2.34	0.42
1:B:403:THR:O	1:B:407:GLU:HG3	2.20	0.42
1:E:378:LYS:HG2	1:E:400:TYR:OH	2.19	0.42
1:F:335:ARG:HH12	1:F:357:GLN:HB2	1.85	0.42
1:B:345:LEU:HD23	1:B:345:LEU:O	2.19	0.41
1:D:138:SER:HB2	1:D:158:SER:HB3	2.01	0.41
1:E:220:PRO:O	1:E:251:PHE:HB2	2.19	0.41
1:E:33:LYS:HB3	1:E:381:TYR:OH	2.20	0.41
1:D:371:VAL:HG11	1:D:382:LEU:O	2.19	0.41
1:E:107:LEU:HD23	1:E:296:TRP:CE2	2.55	0.41
1:F:343:GLU:OE2	1:F:351:TRP:CG	2.72	0.41
1:A:226:TYR:OH	1:A:361:PHE:HE2	2.03	0.41
1:D:76:GLY:HA3	1:D:105:GLN:HB3	2.03	0.41
1:E:30:ASP:HB3	1:E:379:HIS:CE1	2.54	0.41
1:F:360:MET:SD	1:F:361:PHE:CZ	3.14	0.41
1:B:251:PHE:CZ	1:B:274:VAL:HG21	2.55	0.41
1:A:127:THR:HB	1:C:122:ARG:NH2	2.36	0.41
1:C:375:VAL:HG22	1:C:380:ILE:O	2.19	0.41
1:E:234:LEU:HD11	1:E:320:TRP:CH2	2.55	0.41
1:F:16:VAL:C	1:F:20:LYS:HZ1	2.24	0.41
1:C:25:PHE:CE1	1:C:33:LYS:CB	3.03	0.41
1:D:393:LEU:HD21	1:D:401:VAL:HG11	2.02	0.41
1:F:394:THR:N	1:F:397:ASN:OD1	2.54	0.41
1:B:104:VAL:O	1:B:105:GLN:C	2.59	0.41
1:C:225:ALA:HA	1:C:256:SER:HB3	2.01	0.41
1:C:339:ARG:CB	1:C:355:THR:HG23	2.47	0.41
1:E:258:SER:OG	3:E:501:PLP:P	2.79	0.41
1:E:268:VAL:HG22	1:E:303:GLY:HA3	2.03	0.41
1:F:251:PHE:CZ	1:F:274:VAL:HG21	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:SER:HA	1:A:139:PRO:HA	1.92	0.41
1:C:18:VAL:HG12	1:C:383:LEU:HD21	2.01	0.41
1:C:120:LEU:HD13	1:C:186:ILE:HD13	2.03	0.41
1:E:226:TYR:OH	1:E:361:PHE:HE2	2.04	0.41
1:E:114:ARG:NH2	1:F:114:ARG:NH2	2.68	0.41
1:C:354:ILE:H	1:C:354:ILE:HD12	1.86	0.41
1:D:236:ARG:C	1:D:236:ARG:CD	2.90	0.41
1:A:30:ASP:C	1:A:32:ARG:N	2.62	0.41
1:B:374:LEU:HG	1:B:381:TYR:OH	2.21	0.41
1:C:220:PRO:O	1:C:251:PHE:HB2	2.21	0.41
1:C:30:ASP:HB2	1:C:379:HIS:CE1	2.56	0.41
1:D:398:LEU:HD13	1:D:398:LEU:HA	1.85	0.41
1:E:305:ARG:HH22	1:F:265:ASN:HD21	1.69	0.41
1:F:79[B]:GLU:CD	1:F:308:ALA:HB1	2.41	0.41
1:C:161:TYR:CE2	1:C:194:HIS:CD2	3.09	0.40
1:C:236:ARG:CD	1:C:236:ARG:C	2.89	0.40
1:D:279:GLU:CG	1:D:280:SER:N	2.83	0.40
1:E:340:ALA:O	1:E:341:ARG:NH1	2.54	0.40
1:E:399:ASP:O	1:E:400:TYR:HB3	2.21	0.40
1:F:34:VAL:HB	1:F:35:ASN:H	1.52	0.40
1:F:374:LEU:HD21	1:F:380:ILE:CB	2.47	0.40
1:A:371:VAL:HG21	1:A:384:PRO:O	2.21	0.40
1:A:348:PRO:CG	1:A:409:VAL:HG12	2.47	0.40
1:B:342:LEU:HA	1:B:346:LYS:HE3	2.02	0.40
1:B:229:PHE:CE2	1:B:360:MET:CE	3.05	0.40
1:C:104:VAL:O	1:C:105:GLN:C	2.60	0.40
1:E:138:SER:HA	1:E:139:PRO:HA	1.92	0.40
1:F:292:VAL:HG13	1:F:296:TRP:NE1	2.36	0.40
1:F:374:LEU:HA	1:F:378:LYS:CB	2.50	0.40
1:C:395:THR:HG22	1:C:398:LEU:HD12	2.03	0.40
1:C:73:PRO:HB2	1:C:76:GLY:H	1.86	0.40
1:E:372:GLU:HG3	1:E:373:TYR:CE2	2.56	0.40
1:A:396:LYS:C	1:A:398:LEU:N	2.69	0.40
1:B:25:PHE:HE1	1:B:33:LYS:HB2	1.86	0.40
1:E:347:THR:CG2	1:E:348:PRO:HD3	2.52	0.40

There are no symmetry-related clashes.

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	385/408 (94%)	344 (89%)	22 (6%)	19 (5%)	2	13
1	B	395/408 (97%)	358 (91%)	28 (7%)	9 (2%)	6	30
1	C	389/408 (95%)	355 (91%)	25 (6%)	9 (2%)	6	30
1	D	395/408 (97%)	355 (90%)	31 (8%)	9 (2%)	6	30
1	E	394/408 (97%)	347 (88%)	35 (9%)	12 (3%)	4	24
1	F	383/408 (94%)	353 (92%)	23 (6%)	7 (2%)	8	37
All	All	2341/2448 (96%)	2112 (90%)	164 (7%)	65 (3%)	5	25

All (65) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	17	LEU
1	A	26	ARG
1	A	29	PRO
1	A	33	LYS
1	A	347	THR
1	A	351	TRP
1	A	380	ILE
1	A	382	LEU
1	A	405	ILE
1	B	373	TYR
1	B	375	VAL
1	B	382	LEU
1	C	13	ALA
1	C	15	PRO
1	C	237	ASP
1	C	342	LEU
1	D	342	LEU
1	D	348	PRO
1	E	342	LEU
1	E	347	THR

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Mol	Chain	Res	Type
1	E	374	LEU
1	E	400	TYR
1	E	402	ALA
1	F	36	LEU
1	F	341	ARG
1	F	343	GLU
1	F	345	LEU
1	F	348	PRO
1	A	25	PHE
1	A	338	LEU
1	A	398	LEU
1	A	399	ASP
1	B	368	PRO
1	B	380	ILE
1	D	338	LEU
1	D	340	ALA
1	E	341	ARG
1	E	373	TYR
1	E	404	SER
1	F	35	ASN
1	A	31	PRO
1	B	16	VAL
1	B	29	PRO
1	B	344	ALA
1	C	337	GLU
1	C	338	LEU
1	D	15	PRO
1	D	370	GLN
1	E	338	LEU
1	A	403	THR
1	C	14	GLN
1	E	408	ALA
1	B	17	LEU
1	D	343	GLU
1	D	347	THR
1	E	365	GLY
1	E	405	ILE
1	F	34	VAL
1	A	34	VAL
1	A	350	THR
1	A	365	GLY
1	A	397	ASN

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Mol	Chain	Res	Type
1	C	348	PRO
1	D	365	GLY
1	C	401	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	313/346 (90%)	288 (92%)	25 (8%)	12	40
1	B	324/346 (94%)	291 (90%)	33 (10%)	7	28
1	C	316/346 (91%)	293 (93%)	23 (7%)	14	44
1	D	321/346 (93%)	290 (90%)	31 (10%)	8	31
1	E	323/346 (93%)	294 (91%)	29 (9%)	9	35
1	F	315/346 (91%)	281 (89%)	34 (11%)	6	26
All	All	1912/2076 (92%)	1737 (91%)	175 (9%)	10	34

All (175) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	VAL
1	A	24	ASP
1	A	30	ASP
1	A	32	ARG
1	A	46	CYS
1	A	82	SER
1	A	127	THR
1	A	138	SER
1	A	145	ASN
1	A	174	PHE
1	A	221	PHE
1	A	253	CYS
1	A	256	SER
1	A	287[A]	GLN
1	A	287[B]	GLN

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Mol	Chain	Res	Type
1	A	337	GLU
1	A	338	LEU
1	A	339	ARG
1	A	341	ARG
1	A	343	GLU
1	A	363	PHE
1	A	379	HIS
1	A	383	LEU
1	A	398	LEU
1	A	407	GLU
1	B	16	VAL
1	B	21	LEU
1	B	24	ASP
1	B	25	PHE
1	B	30	ASP
1	B	33	LYS
1	B	82	SER
1	B	127	THR
1	B	137	SER
1	B	145[A]	ASN
1	B	145[B]	ASN
1	B	174	PHE
1	B	211	SER
1	B	216	ARG
1	B	221	PHE
1	B	246	SER
1	B	256	SER
1	B	287[A]	GLN
1	B	287[B]	GLN
1	B	336[A]	SER
1	B	336[B]	SER
1	B	338	LEU
1	B	339	ARG
1	B	345	LEU
1	B	350	THR
1	B	363	PHE
1	B	373	TYR
1	B	374	LEU
1	B	376	ASN
1	B	377	GLU
1	B	380	ILE
1	B	382	LEU

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Mol	Chain	Res	Type
1	B	383	LEU
1	C	14	GLN
1	C	17	LEU
1	C	21	LEU
1	C	22	THR
1	C	82	SER
1	C	127	THR
1	C	145[A]	ASN
1	C	145[B]	ASN
1	C	149	SER
1	C	158	SER
1	C	174	PHE
1	C	221	PHE
1	C	237	ASP
1	C	287[A]	GLN
1	C	287[B]	GLN
1	C	323	ASN
1	C	342	LEU
1	C	350	THR
1	C	356	ASP
1	C	363	PHE
1	C	391	SER
1	C	398	LEU
1	C	399	ASP
1	D	14	GLN
1	D	16	VAL
1	D	21	LEU
1	D	30	ASP
1	D	33	LYS
1	D	85	SER
1	D	127	THR
1	D	145[A]	ASN
1	D	145[B]	ASN
1	D	174	PHE
1	D	221	PHE
1	D	236	ARG
1	D	279	GLU
1	D	280	SER
1	D	287[A]	GLN
1	D	287[B]	GLN
1	D	298	ASN
1	D	309	SER

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Mol	Chain	Res	Type
1	D	338	LEU
1	D	339	ARG
1	D	342	LEU
1	D	350	THR
1	D	363	PHE
1	D	367	ASN
1	D	374	LEU
1	D	376	ASN
1	D	377	GLU
1	D	378	LYS
1	D	398	LEU
1	D	404	SER
1	D	410	THR
1	E	21	LEU
1	E	24	ASP
1	E	127	THR
1	E	174	PHE
1	E	203	PRO
1	E	218	LEU
1	E	221	PHE
1	E	236	ARG
1	E	258	SER
1	E	287[A]	GLN
1	E	287[B]	GLN
1	E	323	ASN
1	E	338	LEU
1	E	339	ARG
1	E	341	ARG
1	E	343	GLU
1	E	363	PHE
1	E	367	ASN
1	E	370	GLN
1	E	372	GLU
1	E	373	TYR
1	E	374	LEU
1	E	375	VAL
1	E	377	GLU
1	E	378	LYS
1	E	381	TYR
1	E	398	LEU
1	E	403	THR
1	E	407	GLU

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Mol	Chain	Res	Type
1	F	16	VAL
1	F	17	LEU
1	F	20	LYS
1	F	21	LEU
1	F	22	THR
1	F	24	ASP
1	F	25	PHE
1	F	28	ASP
1	F	34	VAL
1	F	46	CYS
1	F	93	SER
1	F	127	THR
1	F	142	GLU
1	F	145[A]	ASN
1	F	145[B]	ASN
1	F	158	SER
1	F	174	PHE
1	F	221	PHE
1	F	256	SER
1	F	280	SER
1	F	286	SER
1	F	287[A]	GLN
1	F	287[B]	GLN
1	F	298	ASN
1	F	338	LEU
1	F	341	ARG
1	F	345	LEU
1	F	348	PRO
1	F	350	THR
1	F	356	ASP
1	F	363	PHE
1	F	367	ASN
1	F	370	GLN
1	F	398	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	145	ASN
1	A	323	ASN
1	B	180	ASN
1	B	323	ASN

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Mol	Chain	Res	Type
1	B	376	ASN
1	C	14	GLN
1	C	65	ASN
1	C	128	ASN
1	C	379	HIS
1	D	65	ASN
1	D	270	ASN
1	D	283	GLN
1	D	298	ASN
1	D	323	ASN
1	D	379	HIS
1	D	406	HIS
1	E	128	ASN
1	E	283	GLN
1	E	323	ASN
1	E	367	ASN
1	E	379	HIS
1	F	35	ASN
1	F	265	ASN
1	F	298	ASN
1	F	302	GLN
1	F	389	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](#)

9 ligands are modelled in this entry.

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	PLP	F	501	-	16,16,16	2.73	3 (18%)	20,23,23	1.81	7 (35%)
3	PLP	C	501	-	16,16,16	2.80	3 (18%)	20,23,23	1.60	6 (30%)
2	PG4	A	501	-	12,12,12	0.64	0	11,11,11	0.35	0
3	PLP	B	502	-	16,16,16	2.90	3 (18%)	20,23,23	1.45	2 (10%)
3	PLP	A	502	-	16,16,16	2.90	3 (18%)	20,23,23	1.81	5 (25%)
3	PLP	E	501	-	16,16,16	2.75	3 (18%)	20,23,23	2.01	5 (25%)
3	PLP	D	502	-	16,16,16	2.42	3 (18%)	20,23,23	1.93	6 (30%)
2	PG4	B	501	-	9,9,12	0.64	0	8,8,11	0.48	0
2	PG4	D	501	-	12,12,12	0.54	0	11,11,11	0.26	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PLP	F	501	-	-	5/8/8/8	0/1/1/1
3	PLP	C	501	-	-	3/8/8/8	0/1/1/1
2	PG4	A	501	-	-	4/10/10/10	-
3	PLP	B	502	-	-	3/8/8/8	0/1/1/1
3	PLP	A	502	-	-	0/8/8/8	0/1/1/1
3	PLP	E	501	-	-	2/8/8/8	0/1/1/1
3	PLP	D	502	-	-	1/8/8/8	0/1/1/1
2	PG4	B	501	-	-	5/7/7/10	-
2	PG4	D	501	-	-	5/10/10/10	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	PLP	C3-C2	8.11	1.49	1.40
3	A	502	PLP	C3-C2	7.93	1.48	1.40
3	F	501	PLP	C3-C2	7.60	1.48	1.40
3	E	501	PLP	C3-C2	7.49	1.48	1.40
3	C	501	PLP	C3-C2	6.73	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	501	PLP	C4-C5	6.20	1.49	1.42
3	A	502	PLP	C4-C5	6.11	1.49	1.42
3	D	502	PLP	C3-C2	5.94	1.46	1.40
3	B	502	PLP	C4-C5	5.88	1.49	1.42
3	D	502	PLP	C4-C5	5.81	1.49	1.42
3	E	501	PLP	C4-C5	5.71	1.49	1.42
3	C	501	PLP	C4-C3	5.70	1.49	1.40
3	F	501	PLP	C4-C3	5.35	1.48	1.40
3	B	502	PLP	C4-C3	5.22	1.48	1.40
3	E	501	PLP	C4-C3	5.16	1.48	1.40
3	F	501	PLP	C4-C5	4.99	1.48	1.42
3	A	502	PLP	C4-C3	4.74	1.47	1.40
3	D	502	PLP	C4-C3	4.31	1.47	1.40

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	PLP	O4P-C5A-C5	5.04	118.96	109.35
3	E	501	PLP	C4-C3-C2	-4.87	117.18	120.19
3	D	502	PLP	O4P-C5A-C5	4.74	118.38	109.35
3	F	501	PLP	O4P-C5A-C5	4.53	117.98	109.35
3	E	501	PLP	O4P-C5A-C5	4.11	117.19	109.35
3	B	502	PLP	C3-C4-C5	-3.73	115.40	118.26
3	E	501	PLP	C5A-C5-C6	-3.25	114.02	119.37
3	D	502	PLP	C2A-C2-C3	-3.25	116.87	120.89
3	E	501	PLP	O4A-C4A-C4	-3.21	117.91	124.91
3	F	501	PLP	C6-N1-C2	3.06	124.84	119.17
3	D	502	PLP	C2A-C2-N1	3.03	123.58	117.67
3	D	502	PLP	C4-C3-C2	-2.79	118.46	120.19
3	B	502	PLP	O4A-C4A-C4	-2.70	119.03	124.91
3	C	501	PLP	C4-C3-C2	-2.63	118.56	120.19
3	F	501	PLP	C4-C3-C2	-2.63	118.56	120.19
3	E	501	PLP	C6-N1-C2	2.62	124.02	119.17
3	F	501	PLP	O4A-C4A-C4	-2.58	119.28	124.91
3	C	501	PLP	C6-N1-C2	2.58	123.94	119.17
3	D	502	PLP	C6-N1-C2	2.53	123.85	119.17
3	C	501	PLP	C2A-C2-N1	2.52	122.60	117.67
3	A	502	PLP	C6-N1-C2	2.36	123.54	119.17
3	A	502	PLP	O4A-C4A-C4	-2.34	119.81	124.91
3	F	501	PLP	C3-C2-N1	-2.33	117.76	120.77
3	C	501	PLP	C2A-C2-C3	-2.29	118.06	120.89
3	C	501	PLP	O4P-C5A-C5	2.29	113.72	109.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	PLP	C2A-C2-N1	2.25	122.07	117.67
3	C	501	PLP	O4A-C4A-C4	-2.18	120.17	124.91
3	A	502	PLP	C3-C4-C5	-2.17	116.59	118.26
3	F	501	PLP	C2A-C2-N1	2.16	121.90	117.67
3	F	501	PLP	O3P-P-O2P	2.15	115.86	107.64
3	D	502	PLP	O4A-C4A-C4	-2.13	120.26	124.91

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	501	PLP	C4-C5-C5A-O4P
3	F	501	PLP	C6-C5-C5A-O4P
3	F	501	PLP	C5A-O4P-P-O2P
3	F	501	PLP	C5A-O4P-P-O3P
3	C	501	PLP	C5A-O4P-P-O2P
3	E	501	PLP	C4-C5-C5A-O4P
3	E	501	PLP	C6-C5-C5A-O4P
3	B	502	PLP	C5A-O4P-P-O1P
3	B	502	PLP	C5A-O4P-P-O2P
3	B	502	PLP	C5A-O4P-P-O3P
2	D	501	PG4	O3-C5-C6-O4
2	A	501	PG4	O2-C3-C4-O3
2	B	501	PG4	O3-C5-C6-O4
2	D	501	PG4	O4-C7-C8-O5
2	B	501	PG4	O2-C3-C4-O3
2	A	501	PG4	O3-C5-C6-O4
2	D	501	PG4	C1-C2-O2-C3
3	F	501	PLP	C5A-O4P-P-O1P
3	C	501	PLP	C5A-O4P-P-O3P
2	B	501	PG4	C6-C5-O3-C4
2	D	501	PG4	C8-C7-O4-C6
2	A	501	PG4	C1-C2-O2-C3
2	D	501	PG4	C6-C5-O3-C4
3	C	501	PLP	C5A-O4P-P-O1P
3	D	502	PLP	C5A-O4P-P-O1P
2	B	501	PG4	C3-C4-O3-C5
2	A	501	PG4	O4-C7-C8-O5
2	B	501	PG4	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	501	PLP	4	0
3	C	501	PLP	2	0
3	B	502	PLP	2	0
3	A	502	PLP	1	0
3	E	501	PLP	6	0
3	D	502	PLP	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	390/408 (95%)	-0.11	12 (3%)	49	21	38, 68, 113, 168	2 (0%)
1	B	395/408 (96%)	-0.04	14 (3%)	44	18	38, 75, 128, 228	1 (0%)
1	C	391/408 (95%)	-0.17	4 (1%)	82	59	37, 72, 109, 156	1 (0%)
1	D	396/408 (97%)	-0.11	15 (3%)	40	16	42, 70, 124, 208	1 (0%)
1	E	393/408 (96%)	-0.04	15 (3%)	40	16	40, 75, 123, 213	0
1	F	383/408 (93%)	-0.06	10 (2%)	56	27	35, 77, 126, 159	1 (0%)
All	All	2348/2448 (95%)	-0.09	70 (2%)	50	22	35, 73, 120, 228	6 (0%)

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	409	VAL	16.6
1	A	382	LEU	13.4
1	A	347	THR	12.8
1	E	347	THR	11.8
1	D	344	ALA	7.9
1	D	345	LEU	6.8
1	E	348	PRO	6.2
1	E	344	ALA	6.2
1	A	408	ALA	6.1
1	E	370	GLN	5.9
1	D	372	GLU	5.1
1	B	376	ASN	5.1
1	B	375	VAL	5.0
1	E	346	LYS	4.8
1	E	371	VAL	4.7
1	B	351	TRP	4.6
1	A	404	SER	4.6
1	A	372	GLU	4.4
1	A	407	GLU	4.3

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Mol	Chain	Res	Type	RSRZ
1	D	409	VAL	4.2
1	E	408	ALA	4.1
1	B	230	ALA	3.6
1	B	377	GLU	3.5
1	C	15	PRO	3.5
1	F	31	PRO	3.5
1	D	366	LEU	3.4
1	B	344	ALA	3.4
1	D	343	GLU	3.3
1	D	35	ASN	3.3
1	F	379	HIS	3.2
1	E	368	PRO	3.1
1	D	14	GLN	3.1
1	A	398	LEU	3.1
1	B	345	LEU	3.1
1	B	37	GLY	3.0
1	E	345	LEU	3.0
1	D	404	SER	2.9
1	B	371	VAL	2.9
1	E	381	TYR	2.9
1	F	366	LEU	2.9
1	C	403	THR	2.8
1	C	372	GLU	2.8
1	A	22	THR	2.7
1	F	375	VAL	2.7
1	D	346	LYS	2.6
1	A	37	GLY	2.5
1	C	354	ILE	2.5
1	F	351	TRP	2.5
1	D	28	ASP	2.5
1	F	368	PRO	2.5
1	A	231	SER	2.4
1	B	15	PRO	2.4
1	D	357	GLN	2.4
1	D	200	ASP	2.4
1	E	275	GLY	2.4
1	B	338	LEU	2.3
1	B	380	ILE	2.3
1	E	382	LEU	2.2
1	F	382	LEU	2.2
1	A	368	PRO	2.2
1	B	410	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	229	PHE	2.2
1	E	372	GLU	2.2
1	D	29	PRO	2.1
1	F	345	LEU	2.1
1	F	341	ARG	2.1
1	E	373	TYR	2.1
1	B	18	VAL	2.1
1	A	401	VAL	2.0
1	F	29	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	PG4	A	501	13/13	0.80	0.24	87,99,115,123	0
3	PLP	B	502	16/16	0.80	0.47	101,111,159,163	10
3	PLP	A	502	16/16	0.81	0.56	96,121,141,145	10
3	PLP	E	501	16/16	0.81	0.37	102,116,133,137	16
3	PLP	C	501	16/16	0.81	0.46	122,136,158,166	10
2	PG4	B	501	10/13	0.88	0.22	75,81,88,91	0
2	PG4	D	501	13/13	0.88	0.18	85,99,107,108	0
3	PLP	D	502	16/16	0.90	0.28	78,101,143,148	10
3	PLP	F	501	16/16	0.92	0.35	75,90,106,110	10

6.5 Other polymers [i](#)

There are no such residues in this entry.