



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 01:43 PM UTC

PDB ID : 2ZY4 / pdb_00002zy4
Title : dodecameric L-aspartate beta-decarboxylase
Authors : Chen, H.-J.; Ko, T.-P.; Lee, C.-Y.; Wang, N.-C.; Wang, A.H.-J.
Deposited on : 2009-01-13
Resolution : 2.00 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

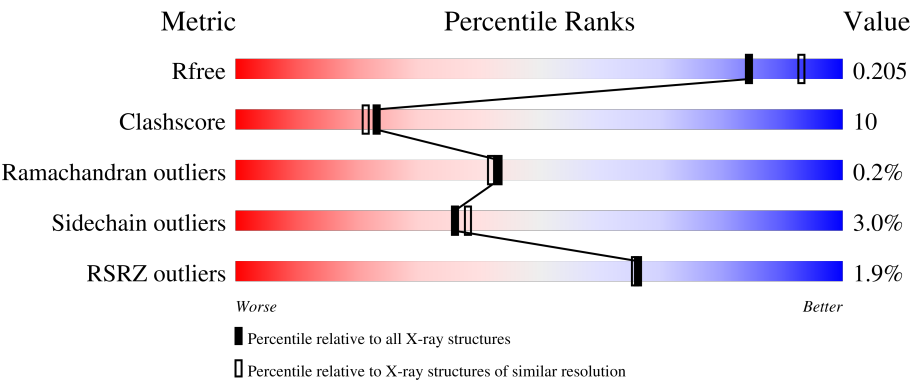
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.00 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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 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 $\leq 5\%$. 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	546	% 75% 19% . .
1	B	546	2% 73% 18% . 6%
1	C	546	2% 71% 21% . 6%
1	D	546	% 75% 18% . 6%
1	E	546	2% 68% 23% . 7%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	546	3% 75% 21% • •

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 27823 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 L-aspartate beta-decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	524	Total	C	N	O	S	0	0	0
			4131	2630	701	782	18			
1	B	512	Total	C	N	O	S	0	0	0
			4032	2567	687	761	17			
1	C	511	Total	C	N	O	S	0	0	0
			4019	2557	685	760	17			
1	D	515	Total	C	N	O	S	0	0	0
			4046	2573	692	764	17			
1	E	509	Total	C	N	O	S	0	0	0
			4007	2551	683	756	17			
1	F	535	Total	C	N	O	S	0	0	0
			4202	2675	716	794	17			

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	534	LYS	-	expression tag	UNP Q93QX0
A	535	LEU	-	expression tag	UNP Q93QX0
A	536	ALA	-	expression tag	UNP Q93QX0
A	537	ALA	-	expression tag	UNP Q93QX0
A	538	ALA	-	expression tag	UNP Q93QX0
A	539	LEU	-	expression tag	UNP Q93QX0
A	540	GLU	-	expression tag	UNP Q93QX0
A	541	HIS	-	expression tag	UNP Q93QX0
A	542	HIS	-	expression tag	UNP Q93QX0
A	543	HIS	-	expression tag	UNP Q93QX0
A	544	HIS	-	expression tag	UNP Q93QX0
A	545	HIS	-	expression tag	UNP Q93QX0
A	546	HIS	-	expression tag	UNP Q93QX0
B	534	LYS	-	expression tag	UNP Q93QX0
B	535	LEU	-	expression tag	UNP Q93QX0
B	536	ALA	-	expression tag	UNP Q93QX0
B	537	ALA	-	expression tag	UNP Q93QX0

Continued on next page...

Continued from previous page...

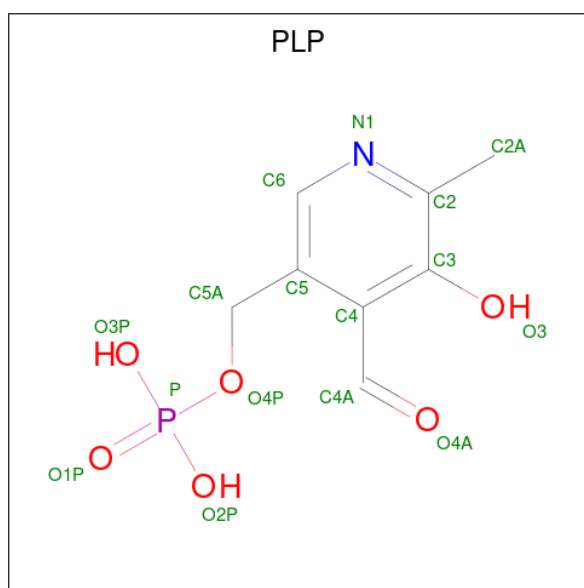
Chain	Residue	Modelled	Actual	Comment	Reference
B	538	ALA	-	expression tag	UNP Q93QX0
B	539	LEU	-	expression tag	UNP Q93QX0
B	540	GLU	-	expression tag	UNP Q93QX0
B	541	HIS	-	expression tag	UNP Q93QX0
B	542	HIS	-	expression tag	UNP Q93QX0
B	543	HIS	-	expression tag	UNP Q93QX0
B	544	HIS	-	expression tag	UNP Q93QX0
B	545	HIS	-	expression tag	UNP Q93QX0
B	546	HIS	-	expression tag	UNP Q93QX0
C	534	LYS	-	expression tag	UNP Q93QX0
C	535	LEU	-	expression tag	UNP Q93QX0
C	536	ALA	-	expression tag	UNP Q93QX0
C	537	ALA	-	expression tag	UNP Q93QX0
C	538	ALA	-	expression tag	UNP Q93QX0
C	539	LEU	-	expression tag	UNP Q93QX0
C	540	GLU	-	expression tag	UNP Q93QX0
C	541	HIS	-	expression tag	UNP Q93QX0
C	542	HIS	-	expression tag	UNP Q93QX0
C	543	HIS	-	expression tag	UNP Q93QX0
C	544	HIS	-	expression tag	UNP Q93QX0
C	545	HIS	-	expression tag	UNP Q93QX0
C	546	HIS	-	expression tag	UNP Q93QX0
D	534	LYS	-	expression tag	UNP Q93QX0
D	535	LEU	-	expression tag	UNP Q93QX0
D	536	ALA	-	expression tag	UNP Q93QX0
D	537	ALA	-	expression tag	UNP Q93QX0
D	538	ALA	-	expression tag	UNP Q93QX0
D	539	LEU	-	expression tag	UNP Q93QX0
D	540	GLU	-	expression tag	UNP Q93QX0
D	541	HIS	-	expression tag	UNP Q93QX0
D	542	HIS	-	expression tag	UNP Q93QX0
D	543	HIS	-	expression tag	UNP Q93QX0
D	544	HIS	-	expression tag	UNP Q93QX0
D	545	HIS	-	expression tag	UNP Q93QX0
D	546	HIS	-	expression tag	UNP Q93QX0
E	534	LYS	-	expression tag	UNP Q93QX0
E	535	LEU	-	expression tag	UNP Q93QX0
E	536	ALA	-	expression tag	UNP Q93QX0
E	537	ALA	-	expression tag	UNP Q93QX0
E	538	ALA	-	expression tag	UNP Q93QX0
E	539	LEU	-	expression tag	UNP Q93QX0
E	540	GLU	-	expression tag	UNP Q93QX0

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	541	HIS	-	expression tag	UNP Q93QX0
E	542	HIS	-	expression tag	UNP Q93QX0
E	543	HIS	-	expression tag	UNP Q93QX0
E	544	HIS	-	expression tag	UNP Q93QX0
E	545	HIS	-	expression tag	UNP Q93QX0
E	546	HIS	-	expression tag	UNP Q93QX0
F	534	LYS	-	expression tag	UNP Q93QX0
F	535	LEU	-	expression tag	UNP Q93QX0
F	536	ALA	-	expression tag	UNP Q93QX0
F	537	ALA	-	expression tag	UNP Q93QX0
F	538	ALA	-	expression tag	UNP Q93QX0
F	539	LEU	-	expression tag	UNP Q93QX0
F	540	GLU	-	expression tag	UNP Q93QX0
F	541	HIS	-	expression tag	UNP Q93QX0
F	542	HIS	-	expression tag	UNP Q93QX0
F	543	HIS	-	expression tag	UNP Q93QX0
F	544	HIS	-	expression tag	UNP Q93QX0
F	545	HIS	-	expression tag	UNP Q93QX0
F	546	HIS	-	expression tag	UNP Q93QX0

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: $C_8H_{10}NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	E	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	F	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		
3	B	1	Total	Cl	0	0
			1	1		
3	C	1	Total	Cl	0	0
			1	1		
3	D	1	Total	Cl	0	0
			1	1		
3	E	1	Total	Cl	0	0
			1	1		
3	F	1	Total	Cl	0	0
			1	1		

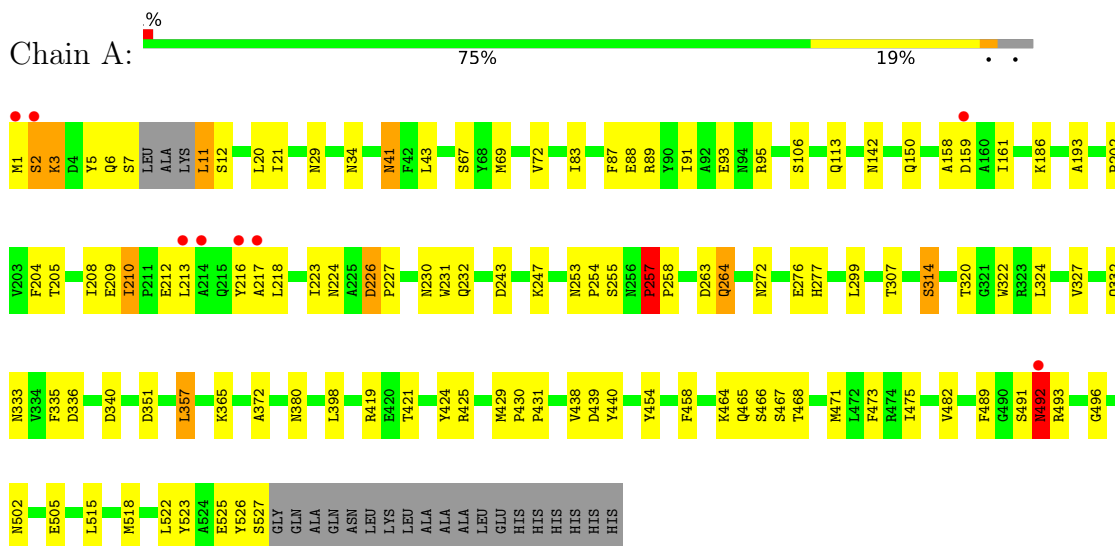
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	565	Total	O	0	0
			565	565		
4	B	611	Total	O	0	0
			611	611		
4	C	593	Total	O	0	0
			593	593		
4	D	573	Total	O	0	0
			573	573		
4	E	462	Total	O	0	0
			462	462		
4	F	486	Total	O	0	0
			486	486		

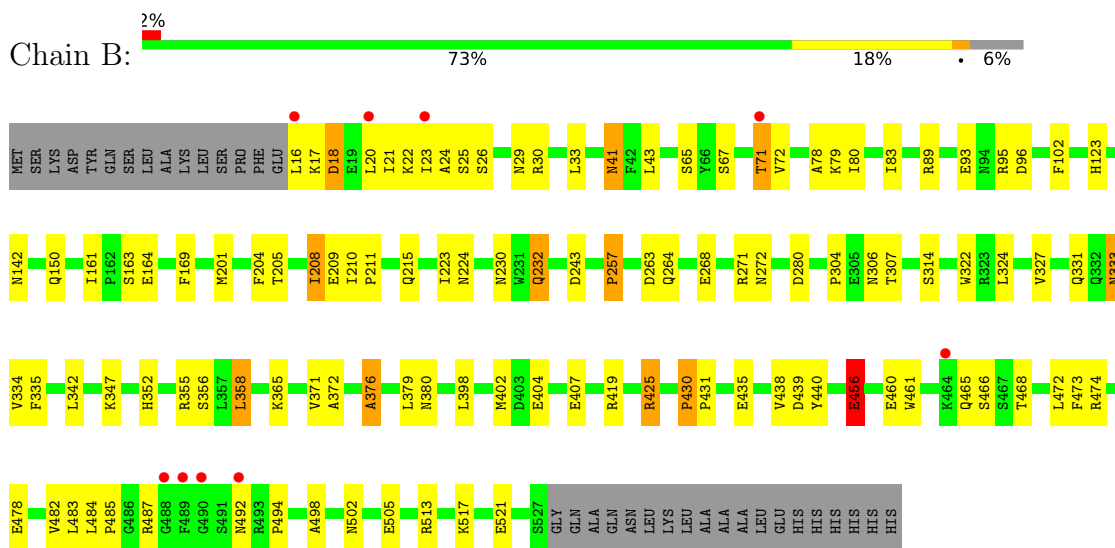
3 Residue-property plots [i](#)

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: L-aspartate beta-decarboxylase

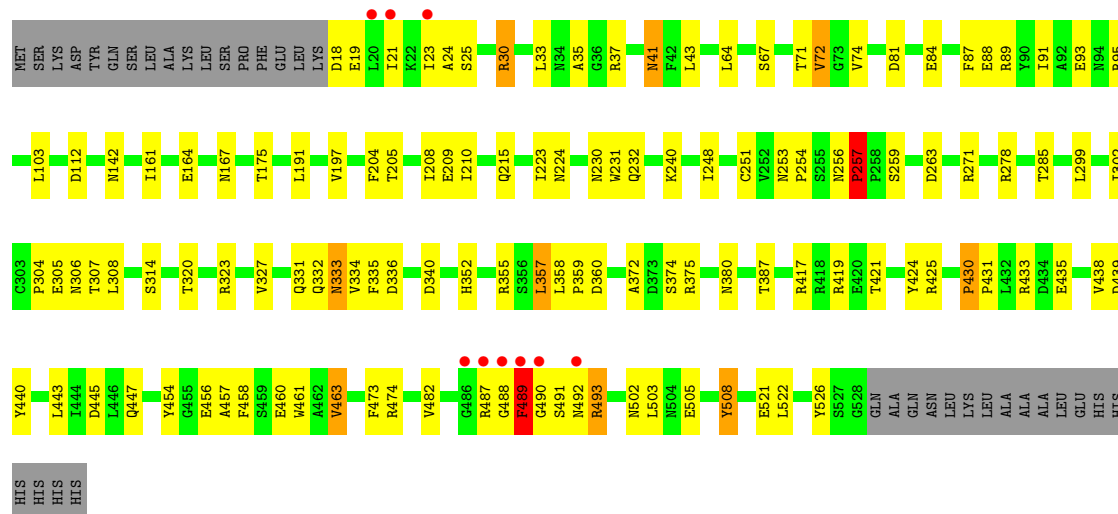


- Molecule 1: L-aspartate beta-decarboxylase



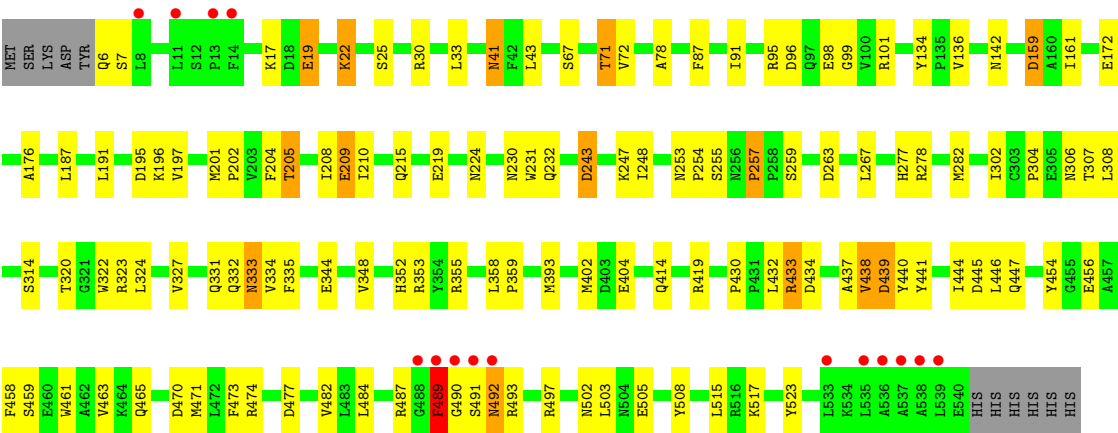
- Molecule 1: L-aspartate beta-decarboxylase





GLN
ALA
GLN
ASN
LEU
LYS
LEU
ALA
ALA
ALA
LEU
GLU
HIS
HIS
HIS
HIS
HIS

● Molecule 1: L-aspartate beta-decarboxylase



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	149.95Å 217.15Å 207.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00 30.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	94.7 (30.00-2.00) 94.7 (30.00-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 2.00Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.157 , 0.204 0.157 , 0.205	Depositor DCC
R_{free} test set	10656 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	19.3	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 62.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	27823	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.42% 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: PLP, CL

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	0.83	0/4215	1.10	32/5705 (0.6%)
1	B	0.84	0/4114	1.09	24/5571 (0.4%)
1	C	0.84	1/4101 (0.0%)	1.10	29/5554 (0.5%)
1	D	0.82	1/4128 (0.0%)	1.06	16/5591 (0.3%)
1	E	0.80	0/4089	1.12	22/5538 (0.4%)
1	F	0.86	3/4286 (0.1%)	1.10	22/5803 (0.4%)
All	All	0.83	5/24933 (0.0%)	1.10	145/33762 (0.4%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	402	MET	SD-CE	-10.14	1.54	1.79
1	C	210	ILE	CA-CB	6.40	1.57	1.54
1	F	210	ILE	CA-CB	6.23	1.57	1.54
1	F	402	MET	SD-CE	-5.14	1.66	1.79
1	F	393	MET	SD-CE	-5.08	1.66	1.79

All (145) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	440	TYR	N-CA-C	-13.41	96.27	111.82
1	B	314	SER	N-CA-C	10.53	122.33	111.07
1	E	440	TYR	N-CA-C	-9.94	100.29	111.82
1	D	440	TYR	N-CA-C	-9.69	100.56	111.71
1	E	224	ASN	N-CA-C	9.48	124.04	108.96
1	F	314	SER	N-CA-C	9.10	122.03	111.11
1	E	314	SER	N-CA-C	8.93	121.82	111.11
1	C	314	SER	N-CA-C	8.65	121.49	111.11
1	B	440	TYR	N-CA-C	-8.34	102.12	111.71
1	C	505	GLU	N-CA-C	8.27	121.03	111.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	440	TYR	N-CA-C	-8.19	102.29	111.71
1	F	224	ASN	N-CA-C	8.17	122.74	109.76
1	A	210	ILE	CB-CA-C	-8.02	106.08	113.70
1	A	314	SER	N-CA-C	8.02	120.73	111.11
1	D	314	SER	N-CA-C	7.97	120.67	111.11
1	A	438	VAL	N-CA-C	-7.93	105.35	111.62
1	A	218	LEU	N-CA-C	7.93	121.68	110.50
1	A	440	TYR	N-CA-C	-7.91	102.65	111.82
1	C	223	ILE	N-CA-C	-7.66	95.97	106.85
1	C	257	PRO	N-CA-C	7.55	131.73	112.10
1	E	438	VAL	N-CA-C	-7.53	105.67	111.62
1	E	307	THR	N-CA-C	7.49	121.10	108.90
1	F	307	THR	N-CA-C	7.46	121.56	109.40
1	F	430	PRO	N-CA-C	7.23	117.41	110.47
1	C	430	PRO	CA-C-N	7.20	127.20	119.78
1	C	430	PRO	C-N-CA	7.20	127.20	119.78
1	B	257	PRO	N-CA-C	7.18	130.77	112.10
1	D	257	PRO	N-CA-C	7.16	130.71	112.10
1	C	438	VAL	N-CA-C	-6.94	106.14	111.62
1	E	209	GLU	N-CA-C	6.93	118.91	111.36
1	A	224	ASN	N-CA-C	6.88	120.70	109.76
1	C	209	GLU	N-CA-C	6.86	118.84	111.36
1	B	505	GLU	N-CA-C	6.79	119.25	111.11
1	D	299	LEU	N-CA-C	-6.78	104.11	112.38
1	B	438	VAL	N-CA-C	-6.74	106.30	111.62
1	B	307	THR	N-CA-C	6.74	119.88	108.90
1	F	327	VAL	N-CA-C	-6.71	98.78	108.17
1	D	307	THR	N-CA-C	6.71	120.39	109.59
1	D	502	ASN	N-CA-C	6.71	122.28	113.30
1	B	430	PRO	N-CA-C	6.70	118.88	110.70
1	F	257	PRO	N-CA-C	6.68	129.48	112.10
1	E	257	PRO	N-CA-C	6.67	129.45	112.10
1	E	142	ASN	N-CA-C	6.65	118.19	111.07
1	B	223	ILE	N-CA-C	-6.62	97.45	106.85
1	B	456	GLU	N-CA-C	6.62	118.49	111.28
1	A	67	SER	N-CA-C	6.60	121.34	113.16
1	E	354	TYR	N-CA-C	6.60	121.34	113.16
1	B	205	THR	N-CA-C	6.56	122.57	113.45
1	A	307	THR	N-CA-C	6.54	119.56	108.90
1	C	142	ASN	N-CA-C	6.51	118.03	111.07
1	D	430	PRO	N-CA-C	6.49	116.70	110.47
1	F	502	ASN	N-CA-C	6.49	122.00	113.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	505	GLU	N-CA-C	6.47	119.16	111.33
1	F	209	GLU	N-CA-C	6.43	118.37	111.36
1	B	142	ASN	N-CA-C	6.39	117.91	111.07
1	C	67	SER	N-CA-C	6.36	120.87	113.18
1	A	502	ASN	N-CA-C	6.34	121.06	112.88
1	E	505	GLU	N-CA-C	6.32	118.69	111.11
1	A	257	PRO	N-CA-C	6.28	128.43	112.10
1	A	83	ILE	N-CA-C	6.25	117.00	110.62
1	D	224	ASN	N-CA-C	6.25	118.90	108.96
1	A	2	SER	N-CA-C	6.25	120.17	111.74
1	C	224	ASN	N-CA-C	6.23	119.80	109.46
1	A	142	ASN	N-CA-C	6.18	117.68	111.07
1	A	205	THR	N-CA-C	6.17	122.03	113.45
1	B	376	ALA	N-CA-C	6.15	120.37	112.86
1	E	502	ASN	N-CA-C	6.04	120.67	112.88
1	C	299	LEU	N-CA-C	-6.03	105.18	112.54
1	A	226	ASP	CA-C-N	6.02	126.19	119.32
1	A	226	ASP	C-N-CA	6.02	126.19	119.32
1	B	439	ASP	N-CA-C	6.02	119.95	112.24
1	E	276	GLU	N-CA-C	6.01	120.23	113.01
1	F	67	SER	N-CA-C	6.00	120.60	113.28
1	E	255	SER	N-CA-C	6.00	118.45	110.53
1	C	307	THR	N-CA-C	5.99	118.67	108.90
1	E	430	PRO	N-CA-C	5.97	116.97	110.58
1	D	505	GLU	N-CA-C	5.96	118.26	111.11
1	D	438	VAL	N-CA-C	-5.91	106.95	111.62
1	A	208	ILE	N-CA-C	-5.89	104.58	111.00
1	F	491	SER	N-CA-C	-5.88	107.35	114.75
1	E	351	ASP	N-CA-C	-5.80	105.04	111.71
1	C	205	THR	N-CA-C	5.79	121.42	113.77
1	C	387	THR	CA-C-N	-5.77	113.07	119.19
1	C	387	THR	C-N-CA	-5.77	113.07	119.19
1	F	439	ASP	N-CA-C	5.76	119.61	112.24
1	E	223	ILE	N-CA-C	-5.75	97.57	106.72
1	C	112	ASP	N-CA-C	5.71	118.72	111.69
1	C	357	LEU	N-CA-C	5.70	118.70	111.69
1	B	224	ASN	N-CA-C	5.68	118.88	109.46
1	C	424	TYR	N-CA-C	5.67	120.19	113.16
1	B	208	ILE	N-CA-C	-5.66	104.37	112.35
1	A	223	ILE	N-CA-C	-5.65	98.83	106.85
1	A	439	ASP	N-CA-C	5.65	119.36	111.74
1	A	209	GLU	N-CA-C	5.64	117.50	111.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	439	ASP	N-CA-C	5.64	119.45	112.24
1	B	502	ASN	N-CA-C	5.61	120.12	112.88
1	F	142	ASN	N-CA-C	5.61	117.07	111.07
1	B	67	SER	N-CA-C	5.59	120.10	113.28
1	A	255	SER	N-CA-C	5.56	117.87	110.53
1	A	12	SER	N-CA-C	-5.54	102.22	110.20
1	D	67	SER	N-CA-C	5.53	120.01	113.16
1	F	505	GLU	N-CA-C	5.50	117.72	111.11
1	C	489	PHE	N-CA-C	-5.50	104.12	112.04
1	B	466	SER	N-CA-C	5.50	116.61	108.86
1	D	229	LEU	N-CA-C	-5.45	105.94	112.59
1	B	232	GLN	N-CA-C	-5.45	103.20	110.55
1	A	299	LEU	N-CA-C	-5.43	105.76	112.38
1	E	26	SER	N-CA-C	-5.41	100.85	109.07
1	E	439	ASP	N-CA-C	5.40	119.15	112.24
1	A	357	LEU	N-CA-C	5.40	118.33	111.69
1	E	67	SER	N-CA-C	5.38	119.84	113.16
1	C	208	ILE	N-CA-C	-5.38	105.14	111.00
1	E	290	GLY	N-CA-C	5.36	119.13	112.64
1	A	491	SER	N-CA-C	5.36	117.20	110.24
1	D	308	LEU	N-CA-C	-5.33	100.05	108.73
1	A	351	ASP	N-CA-C	-5.32	105.48	111.28
1	E	299	LEU	N-CA-C	-5.31	106.06	112.54
1	F	255	SER	N-CA-C	5.31	117.53	110.53
1	F	438	VAL	N-CA-C	-5.28	107.45	111.62
1	B	209	GLU	N-CA-C	5.28	117.12	111.36
1	B	83	ILE	N-CA-C	5.27	115.99	110.62
1	B	358	LEU	CA-C-N	5.22	124.66	119.24
1	B	358	LEU	C-N-CA	5.22	124.66	119.24
1	C	502	ASN	N-CA-C	5.22	120.29	113.30
1	A	492	ASN	N-CA-C	-5.21	106.43	112.89
1	E	424	TYR	N-CA-C	5.21	119.62	113.16
1	C	491	SER	N-CA-C	-5.20	108.19	114.75
1	A	424	TYR	N-CA-C	5.20	119.62	113.28
1	F	208	ILE	N-CA-C	-5.18	105.36	111.00
1	A	526	TYR	N-CA-C	-5.11	107.34	113.21
1	D	205	THR	N-CA-C	5.10	120.50	113.77
1	C	327	VAL	N-CA-C	-5.10	100.41	107.80
1	A	231	TRP	N-CA-C	5.10	118.76	112.24
1	D	369	ARG	N-CA-C	-5.09	105.81	112.23
1	C	278	ARG	N-CA-C	5.09	117.94	109.79
1	F	231	TRP	N-CA-C	5.08	118.78	112.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	493	ARG	N-CA-C	5.08	118.32	107.91
1	F	489	PHE	N-CA-C	-5.07	105.83	111.36
1	F	243	ASP	CA-C-N	5.07	125.35	119.47
1	F	243	ASP	C-N-CA	5.07	125.35	119.47
1	F	205	THR	N-CA-C	5.06	120.49	113.45
1	D	209	GLU	N-CA-C	5.05	116.86	111.36
1	C	508	TYR	N-CA-C	-5.04	105.87	111.36
1	A	327	VAL	N-CA-C	-5.00	101.17	108.17
1	B	327	VAL	N-CA-C	-5.00	100.55	107.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4131	0	4097	82	1
1	B	4032	0	4004	85	0
1	C	4019	0	3983	83	0
1	D	4046	0	4011	76	0
1	E	4007	0	3975	98	0
1	F	4202	0	4181	91	0
2	A	15	0	6	0	0
2	B	15	0	6	0	0
2	C	15	0	7	0	0
2	D	15	0	7	0	0
2	E	15	0	6	0	0
2	F	15	0	7	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
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	565	0	0	17	0
4	B	611	0	0	21	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	593	0	0	18	1
4	D	573	0	0	20	0
4	E	462	0	0	16	0
4	F	486	0	0	14	1
All	All	27823	0	24290	501	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (501) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:MET:HG3	4:A:2840:HOH:O	1.35	1.26
1:F:332:GLN:HG2	4:F:3116:HOH:O	1.54	1.08
1:E:26:SER:HB3	1:E:29:ASN:HB2	1.41	1.02
1:F:17:LYS:HE3	1:F:487:ARG:HH22	1.27	0.97
1:D:448:ASP:HB2	4:D:1323:HOH:O	1.64	0.94
1:E:359:PRO:HD2	4:E:2955:HOH:O	1.68	0.91
1:D:417:ARG:HH21	1:D:433:ARG:HH21	1.18	0.90
1:F:446:LEU:HB2	1:F:471:MET:HE1	1.54	0.89
1:D:417:ARG:NH2	1:D:433:ARG:HH21	1.70	0.89
1:A:29:ASN:HD21	1:A:482:VAL:H	1.20	0.87
1:C:306:ASN:ND2	1:C:334:VAL:HG11	1.89	0.87
1:B:333:ASN:HD22	1:B:335:PHE:H	1.23	0.86
1:B:41:ASN:HD21	1:B:419:ARG:HH22	1.23	0.86
1:F:447:GLN:HB3	1:F:493:ARG:HH21	1.41	0.86
1:B:96:ASP:HB3	4:B:2096:HOH:O	1.73	0.85
1:B:264:GLN:O	1:B:268:GLU:HG2	1.76	0.84
1:D:332:GLN:HG2	4:D:2937:HOH:O	1.75	0.83
1:A:7:SER:C	4:A:1922:HOH:O	2.21	0.83
1:B:24:ALA:HB3	1:B:482:VAL:HG23	1.59	0.83
1:E:64:LEU:HD23	4:E:2811:HOH:O	1.77	0.82
1:C:41:ASN:HD21	1:C:419:ARG:HH22	1.20	0.82
1:E:357:LEU:HD23	4:E:2634:HOH:O	1.79	0.81
1:F:17:LYS:HE3	1:F:487:ARG:NH2	1.94	0.81
1:C:490:GLY:HA3	4:C:3235:HOH:O	1.81	0.78
1:A:471:MET:HG3	1:A:518:MET:HE1	1.68	0.76
1:B:89:ARG:NH1	1:B:93:GLU:HG3	2.00	0.76
1:F:7:SER:N	4:F:2793:HOH:O	2.18	0.76
1:D:161:ILE:HD11	1:D:304:PRO:HG3	1.68	0.76
1:A:2:SER:H	1:A:34:ASN:ND2	1.83	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:TYR:OH	1:A:20:LEU:HD23	1.85	0.75
1:C:232:GLN:HE22	1:C:263:ASP:H	1.33	0.74
1:E:365:LYS:HE3	4:E:1522:HOH:O	1.88	0.74
1:B:435:GLU:HG2	4:B:3214:HOH:O	1.88	0.73
1:F:33:LEU:HD11	1:F:482:VAL:HG11	1.70	0.72
4:A:2061:HOH:O	1:B:71:THR:HB	1.88	0.72
1:E:333:ASN:HD22	1:E:335:PHE:H	1.37	0.72
1:F:446:LEU:HB2	1:F:471:MET:CE	2.20	0.72
1:B:232:GLN:HE22	1:B:263:ASP:H	1.38	0.71
1:E:201:MET:HE2	1:E:208:ILE:HD11	1.70	0.71
1:D:41:ASN:HD21	1:D:419:ARG:HH22	1.38	0.71
1:F:41:ASN:HD21	1:F:419:ARG:HH22	1.37	0.71
1:B:20:LEU:HB3	1:B:482:VAL:HG11	1.71	0.71
1:E:232:GLN:NE2	1:E:263:ASP:H	1.89	0.71
1:A:333:ASN:HD22	1:A:335:PHE:H	1.39	0.70
1:C:37:ARG:NH2	4:C:2971:HOH:O	2.15	0.70
1:F:490:GLY:HA2	4:F:2952:HOH:O	1.90	0.70
1:C:473:PHE:HD1	4:C:791:HOH:O	1.73	0.70
1:B:17:LYS:HE2	4:B:2886:HOH:O	1.91	0.70
1:C:232:GLN:NE2	1:C:263:ASP:H	1.88	0.70
1:E:456:GLU:H	1:E:456:GLU:CD	2.00	0.70
1:D:232:GLN:HE22	1:D:263:ASP:H	1.37	0.70
1:D:357:LEU:HD23	4:D:2261:HOH:O	1.92	0.69
1:D:365:LYS:NZ	4:D:1342:HOH:O	2.25	0.69
1:E:41:ASN:HD21	1:E:419:ARG:HH22	1.39	0.69
1:A:232:GLN:HE22	1:A:263:ASP:H	1.38	0.69
1:D:492:ASN:HB3	4:D:1370:HOH:O	1.91	0.69
1:E:24:ALA:HB3	1:E:482:VAL:CG2	2.22	0.69
1:E:201:MET:HE2	1:E:208:ILE:CD1	2.23	0.68
1:A:41:ASN:HD21	1:A:419:ARG:HH22	1.41	0.68
1:A:464:LYS:HG2	4:A:1914:HOH:O	1.93	0.68
1:D:26:SER:HB3	1:D:29:ASN:HB2	1.75	0.68
1:E:89:ARG:NH1	1:E:93:GLU:HG3	2.07	0.68
1:E:433:ARG:HD3	4:E:3024:HOH:O	1.92	0.68
1:B:468:THR:O	1:B:472:LEU:HG	1.94	0.68
1:C:333:ASN:HD22	1:C:335:PHE:H	1.39	0.68
1:C:87:PHE:CE2	1:C:91:ILE:HD11	2.30	0.67
1:B:41:ASN:ND2	1:B:419:ARG:HH22	1.92	0.66
1:A:492:ASN:HD22	1:A:492:ASN:N	1.94	0.66
1:C:430:PRO:HD3	4:C:1175:HOH:O	1.95	0.66
1:A:11:LEU:N	1:A:11:LEU:HD23	2.11	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:433:ARG:HD3	1:F:434:ASP:O	1.95	0.66
1:B:24:ALA:HB3	1:B:482:VAL:CG2	2.25	0.66
1:B:232:GLN:NE2	1:B:263:ASP:H	1.93	0.66
1:B:23:ILE:HD13	1:B:473:PHE:CD1	2.30	0.65
1:A:88:GLU:OE1	4:A:2810:HOH:O	2.13	0.65
1:F:447:GLN:HG3	1:F:459:SER:OG	1.97	0.65
1:E:232:GLN:HE22	1:E:263:ASP:H	1.45	0.65
1:A:272:ASN:ND2	1:A:276:GLU:HG3	2.11	0.65
1:C:23:ILE:HD13	1:C:473:PHE:CE1	2.31	0.65
1:C:435:GLU:HG2	4:C:3182:HOH:O	1.97	0.65
1:B:487:ARG:HD2	4:B:3209:HOH:O	1.95	0.64
1:F:25:SER:OG	1:F:30:ARG:NH2	2.29	0.64
1:A:272:ASN:HD21	1:A:276:GLU:HG3	1.63	0.64
1:E:23:ILE:HG23	4:E:2651:HOH:O	1.97	0.64
1:D:417:ARG:CZ	1:D:433:ARG:HE	2.11	0.64
1:E:25:SER:HB2	1:E:30:ARG:HH21	1.63	0.63
1:F:19:GLU:O	1:F:22:LYS:HB3	1.98	0.63
1:A:475:ILE:HD11	1:A:515:LEU:HD13	1.79	0.63
1:B:425:ARG:HD2	4:B:2205:HOH:O	1.98	0.63
1:B:41:ASN:HD21	1:B:419:ARG:NH2	1.94	0.63
1:A:3:LYS:HE2	1:B:356:SER:HB3	1.79	0.63
1:C:443:LEU:HD21	1:C:489:PHE:HZ	1.63	0.63
1:C:447:GLN:HB2	1:C:463:VAL:HG21	1.80	0.63
1:D:465:GLN:HG2	4:D:3012:HOH:O	1.99	0.63
1:B:333:ASN:HD22	1:B:335:PHE:N	1.93	0.62
1:C:433:ARG:HG2	1:C:433:ARG:HH11	1.64	0.62
1:D:30:ARG:HG3	1:D:30:ARG:HH11	1.65	0.62
1:B:306:ASN:ND2	1:B:334:VAL:HG11	2.15	0.62
1:E:234:PRO:HG2	1:E:237:GLU:HG2	1.80	0.62
1:D:417:ARG:NH2	1:D:433:ARG:NH2	2.46	0.61
1:E:344:GLU:O	1:E:348:VAL:HG23	2.00	0.61
1:A:11:LEU:N	4:A:1924:HOH:O	2.32	0.61
1:D:89:ARG:O	1:D:93:GLU:HG2	2.01	0.61
1:D:232:GLN:NE2	1:D:263:ASP:H	1.98	0.61
1:C:333:ASN:HD22	1:C:335:PHE:N	1.97	0.61
1:E:81:ASP:HB3	4:E:2541:HOH:O	1.99	0.61
1:D:417:ARG:NH2	1:D:433:ARG:HE	1.97	0.61
1:B:89:ARG:O	1:B:93:GLU:HG2	2.01	0.61
1:F:257:PRO:HB2	1:F:497:ARG:HD2	1.82	0.61
1:A:106:SER:HB2	1:A:398:LEU:HD13	1.83	0.61
1:C:305:GLU:HG2	1:C:332:GLN:O	2.01	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:343:GLN:HB2	1:E:346:GLU:HG3	1.83	0.60
1:B:16:LEU:CA	4:B:3287:HOH:O	2.48	0.60
1:F:195:ASP:CG	1:F:247:LYS:HD3	2.27	0.60
1:F:71:THR:HA	4:F:2778:HOH:O	2.01	0.60
1:B:18:ASP:O	1:B:22:LYS:HG2	2.01	0.60
1:F:433:ARG:HG2	1:F:437:ALA:CB	2.32	0.60
1:C:421:THR:O	1:C:425:ARG:HG3	2.02	0.59
1:C:35:ALA:HB1	1:C:37:ARG:HH11	1.67	0.59
1:D:333:ASN:HD22	1:D:335:PHE:H	1.50	0.59
1:D:474:ARG:O	1:D:478:GLU:HG3	2.02	0.59
1:B:372:ALA:HA	1:B:380:ASN:HD22	1.66	0.59
1:C:25:SER:OG	1:C:30:ARG:NH2	2.35	0.59
1:F:333:ASN:HD22	1:F:335:PHE:H	1.51	0.59
1:A:232:GLN:NE2	1:A:263:ASP:H	1.99	0.59
1:E:487:ARG:NE	4:E:3271:HOH:O	2.34	0.59
1:A:89:ARG:NH1	1:A:93:GLU:HG3	2.17	0.59
1:C:340:ASP:OD1	4:C:2983:HOH:O	2.17	0.59
1:D:28:GLY:HA2	4:D:2319:HOH:O	2.01	0.59
1:A:158:ALA:HB1	1:A:161:ILE:HD12	1.85	0.58
1:B:306:ASN:HA	1:B:334:VAL:HG22	1.85	0.58
1:A:492:ASN:N	1:A:492:ASN:ND2	2.50	0.58
1:C:41:ASN:ND2	1:C:419:ARG:HH22	1.98	0.58
1:A:333:ASN:HD22	1:A:335:PHE:N	2.01	0.58
1:F:433:ARG:HG2	1:F:437:ALA:HB3	1.86	0.58
1:A:2:SER:HA	1:A:34:ASN:HD22	1.69	0.57
1:B:483:LEU:HD22	1:B:498:ALA:HB2	1.85	0.57
1:F:232:GLN:HE22	1:F:263:ASP:H	1.50	0.57
1:D:425:ARG:NH1	1:F:159:ASP:O	2.38	0.57
1:F:159:ASP:CG	4:F:3108:HOH:O	2.47	0.57
1:A:333:ASN:ND2	1:A:336:ASP:H	2.03	0.57
1:B:474:ARG:O	1:B:478:GLU:HG3	2.04	0.57
1:E:81:ASP:CB	4:E:2541:HOH:O	2.51	0.57
1:A:340:ASP:OD1	4:A:2035:HOH:O	2.17	0.57
1:A:6:GLN:HA	1:A:6:GLN:NE2	2.20	0.56
1:B:268:GLU:OE1	1:B:271:ARG:NH1	2.39	0.56
1:A:2:SER:CB	1:A:21:ILE:HD13	2.36	0.56
1:B:271:ARG:NH1	4:B:604:HOH:O	2.27	0.56
1:B:16:LEU:N	4:B:3287:HOH:O	2.37	0.56
1:D:425:ARG:CZ	1:F:159:ASP:O	2.54	0.56
1:E:19:GLU:HA	1:E:22:LYS:NZ	2.21	0.56
1:E:333:ASN:HD22	1:E:335:PHE:N	2.03	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:GLN:HE22	1:E:425:ARG:HH22	1.53	0.56
1:B:25:SER:OG	1:B:30:ARG:NH1	2.39	0.56
1:F:445:ASP:OD2	1:F:493:ARG:NH2	2.39	0.56
1:E:41:ASN:ND2	1:E:419:ARG:HH22	2.04	0.56
1:A:3:LYS:HE2	1:B:356:SER:CB	2.36	0.55
1:C:473:PHE:C	1:C:473:PHE:CD2	2.84	0.55
1:E:271:ARG:HB2	1:E:302:ILE:CG2	2.36	0.55
1:B:20:LEU:HB3	1:B:482:VAL:CG1	2.36	0.55
1:C:167:ASN:HD21	1:C:331:GLN:HE21	1.53	0.55
1:F:33:LEU:CD1	1:F:482:VAL:HG11	2.34	0.55
1:B:365:LYS:NZ	4:B:572:HOH:O	2.39	0.55
1:C:41:ASN:HD21	1:C:419:ARG:NH2	1.97	0.55
1:C:33:LEU:HD11	1:C:482:VAL:HG11	1.88	0.55
1:E:70:THR:OG1	1:E:72:VAL:HG23	2.05	0.55
1:D:527:SER:O	1:D:531:GLN:HG3	2.07	0.55
1:B:358:LEU:N	1:B:358:LEU:HD23	2.22	0.54
1:F:187:LEU:HD13	1:F:353:ARG:NH2	2.23	0.54
1:B:333:ASN:ND2	1:B:335:PHE:H	1.98	0.54
1:D:461:TRP:CH2	1:D:465:GLN:HG3	2.42	0.54
1:F:474:ARG:HH21	1:F:517:LYS:HE3	1.71	0.54
1:B:65:SER:OG	1:B:79:LYS:HE2	2.07	0.54
1:A:159:ASP:O	1:E:425:ARG:HG2	2.08	0.54
1:A:322:TRP:HB3	1:A:324:LEU:HG	1.90	0.54
1:E:343:GLN:O	1:E:346:GLU:N	2.40	0.54
1:F:454:TYR:HB2	1:F:458:PHE:CD2	2.43	0.54
1:F:333:ASN:HD22	1:F:335:PHE:N	2.06	0.54
1:A:193:ALA:HA	1:A:217:ALA:HB3	1.89	0.53
1:D:41:ASN:ND2	1:D:419:ARG:HH22	2.06	0.53
1:F:358:LEU:HD23	1:F:358:LEU:N	2.23	0.53
1:D:89:ARG:NH1	1:D:93:GLU:HG3	2.23	0.53
1:E:497:ARG:HD2	4:E:3256:HOH:O	2.07	0.53
1:B:95:ARG:NH2	4:B:2815:HOH:O	2.39	0.53
1:F:344:GLU:O	1:F:348:VAL:HG23	2.07	0.53
1:F:253:ASN:HA	1:F:254:PRO:C	2.33	0.53
1:F:306:ASN:ND2	1:F:334:VAL:HG11	2.23	0.53
1:A:89:ARG:O	1:A:93:GLU:HG2	2.09	0.53
1:A:41:ASN:ND2	1:A:419:ARG:HH22	2.05	0.53
1:D:417:ARG:HH21	1:D:433:ARG:NH2	1.98	0.53
1:E:41:ASN:HD21	1:E:419:ARG:NH2	2.06	0.53
1:F:96:ASP:HB2	4:F:969:HOH:O	2.08	0.53
1:E:461:TRP:HH2	1:E:525:GLU:HG3	1.74	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:41:ASN:ND2	1:F:419:ARG:HH22	2.05	0.52
1:F:447:GLN:OE1	1:F:463:VAL:HG21	2.09	0.52
1:A:6:GLN:HA	1:A:6:GLN:HE21	1.74	0.52
1:B:164:GLU:CD	1:B:164:GLU:H	2.18	0.52
1:B:487:ARG:NH1	4:B:2086:HOH:O	2.42	0.52
1:E:474:ARG:HG3	1:E:518:MET:CE	2.40	0.52
1:D:333:ASN:HD22	1:D:335:PHE:N	2.08	0.52
1:D:136:VAL:HA	1:D:137:PRO:C	2.34	0.52
1:A:365:LYS:HE3	4:A:3167:HOH:O	2.08	0.52
1:C:253:ASN:HA	1:C:254:PRO:C	2.35	0.52
1:C:445:ASP:OD1	1:C:493:ARG:NH2	2.43	0.52
1:D:41:ASN:HD21	1:D:419:ARG:NH2	2.08	0.52
1:C:240:LYS:NZ	4:C:2370:HOH:O	2.43	0.52
1:A:41:ASN:HD21	1:A:419:ARG:NH2	2.06	0.51
1:C:474:ARG:HH22	1:C:521:GLU:CD	2.18	0.51
1:F:243:ASP:OD1	1:F:243:ASP:C	2.54	0.51
1:D:268:GLU:HG2	4:D:1337:HOH:O	2.10	0.51
1:A:471:MET:HE1	1:A:496:GLY:N	2.26	0.51
1:C:490:GLY:HA2	4:C:1092:HOH:O	2.09	0.51
1:F:254:PRO:HB3	1:F:438:VAL:HG21	1.93	0.51
1:C:503:LEU:HB2	1:C:508:TYR:CZ	2.46	0.51
1:E:525:GLU:O	1:E:526:TYR:C	2.54	0.51
1:B:331:GLN:NE2	4:B:578:HOH:O	2.34	0.51
1:E:136:VAL:HA	1:E:137:PRO:C	2.36	0.51
1:D:333:ASN:ND2	1:D:336:ASP:H	2.09	0.50
1:F:322:TRP:HB3	1:F:324:LEU:HG	1.93	0.50
1:A:429:MET:CG	4:A:2840:HOH:O	2.19	0.50
1:C:161:ILE:HD13	1:C:304:PRO:HB3	1.93	0.50
1:C:461:TRP:CZ3	1:C:526:TYR:HB2	2.46	0.50
1:C:21:ILE:HG13	1:C:33:LEU:HD12	1.94	0.50
1:E:89:ARG:O	1:E:93:GLU:HG2	2.12	0.50
1:D:158:ALA:HB1	1:D:161:ILE:HD12	1.92	0.50
1:D:425:ARG:NE	1:F:159:ASP:O	2.45	0.50
1:A:11:LEU:N	1:A:11:LEU:CD2	2.75	0.50
1:E:253:ASN:HA	1:E:254:PRO:C	2.35	0.50
1:C:333:ASN:ND2	1:C:336:ASP:H	2.10	0.50
1:A:186:LYS:HD2	1:A:216:TYR:CD2	2.47	0.50
1:B:513:ARG:NH1	4:B:2931:HOH:O	2.44	0.50
1:C:358:LEU:HB2	1:C:359:PRO:HD2	1.93	0.50
1:D:167:ASN:HD21	1:D:331:GLN:HE21	1.60	0.49
1:E:306:ASN:ND2	1:E:334:VAL:HG11	2.27	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:78:ALA:HB1	4:F:2674:HOH:O	2.12	0.49
1:F:161:ILE:CD1	1:F:304:PRO:HB3	2.42	0.49
1:C:487:ARG:HD2	4:C:2039:HOH:O	2.11	0.49
1:D:320:THR:O	1:D:323:ARG:HD2	2.12	0.49
1:B:26:SER:OG	1:B:29:ASN:HB2	2.12	0.49
1:F:41:ASN:HD21	1:F:419:ARG:NH2	2.08	0.49
1:C:95:ARG:NH1	4:C:967:HOH:O	2.44	0.49
1:D:253:ASN:HA	1:D:254:PRO:C	2.37	0.49
1:C:89:ARG:HD2	4:F:899:HOH:O	2.13	0.49
1:B:484:LEU:HD22	1:B:487:ARG:HH22	1.77	0.49
1:E:398:LEU:HB3	1:E:402:MET:HE2	1.95	0.49
1:A:525:GLU:C	1:A:527:SER:H	2.21	0.48
1:C:89:ARG:O	1:C:93:GLU:HG2	2.13	0.48
1:E:106:SER:HB2	1:E:398:LEU:HD13	1.95	0.48
1:E:269:ARG:O	1:E:273:ILE:HG13	2.12	0.48
1:E:474:ARG:HG3	1:E:474:ARG:NH1	2.27	0.48
1:E:236:SER:HB2	4:E:3099:HOH:O	2.12	0.48
1:A:458:PHE:CE1	1:A:523:TYR:HA	2.49	0.48
1:C:41:ASN:C	1:C:41:ASN:HD22	2.21	0.48
1:B:33:LEU:HD11	1:B:482:VAL:HG11	1.95	0.48
1:C:161:ILE:CD1	1:C:304:PRO:HB3	2.43	0.48
1:B:517:LYS:O	1:B:521:GLU:HG3	2.14	0.48
1:D:304:PRO:HD2	4:D:2498:HOH:O	2.14	0.48
1:F:358:LEU:HB2	1:F:359:PRO:HD2	1.96	0.48
1:D:429:MET:HG2	4:D:2514:HOH:O	2.14	0.48
1:D:433:ARG:HD2	4:D:3034:HOH:O	2.13	0.48
1:E:19:GLU:HA	1:E:22:LYS:HZ3	1.78	0.48
1:E:352:HIS:CE1	1:E:355:ARG:HH12	2.32	0.48
1:E:474:ARG:HG3	1:E:474:ARG:HH11	1.78	0.48
1:B:483:LEU:CD2	1:B:498:ALA:HB2	2.43	0.47
1:C:334:VAL:HG12	4:C:2359:HOH:O	2.14	0.47
1:E:32:MET:O	1:E:484:LEU:HD21	2.14	0.47
1:F:232:GLN:NE2	1:F:263:ASP:H	2.10	0.47
1:B:322:TRP:HB3	1:B:324:LEU:HG	1.95	0.47
1:E:461:TRP:CH2	1:E:525:GLU:HG3	2.49	0.47
1:F:332:GLN:HA	1:F:332:GLN:NE2	2.28	0.47
1:F:333:ASN:HD22	1:F:333:ASN:C	2.23	0.47
1:F:447:GLN:HB2	1:F:463:VAL:CG2	2.44	0.47
1:A:43:LEU:C	1:A:43:LEU:HD12	2.40	0.47
1:E:20:LEU:HB3	1:E:482:VAL:HG11	1.95	0.47
1:A:2:SER:OG	1:A:21:ILE:CG2	2.62	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:30:ARG:HG3	1:D:30:ARG:NH1	2.28	0.47
1:E:208:ILE:O	1:E:220:GLU:OE2	2.33	0.47
1:A:340:ASP:CG	4:A:735:HOH:O	2.57	0.47
1:C:87:PHE:HZ	1:C:103:LEU:HB3	1.80	0.47
1:F:489:PHE:CE2	1:F:493:ARG:HD3	2.50	0.47
1:D:96:ASP:HB3	4:D:1231:HOH:O	2.14	0.47
1:D:254:PRO:HB3	1:D:438:VAL:HG21	1.95	0.47
1:E:243:ASP:C	1:E:243:ASP:OD1	2.56	0.47
1:F:247:LYS:HG3	4:F:2700:HOH:O	2.15	0.47
1:A:468:THR:HB	1:A:489:PHE:HA	1.97	0.47
1:E:242:LYS:O	1:E:244:PRO:HD3	2.15	0.47
1:B:474:ARG:HH22	1:B:521:GLU:CD	2.23	0.47
1:E:100:VAL:HG12	4:E:2547:HOH:O	2.16	0.47
1:F:41:ASN:C	1:F:41:ASN:HD22	2.22	0.47
1:A:430:PRO:HA	1:A:431:PRO:HD3	1.79	0.46
1:C:430:PRO:HA	1:C:431:PRO:HD3	1.76	0.46
1:F:444:ILE:HG21	1:F:515:LEU:CD1	2.44	0.46
1:C:489:PHE:CD2	1:C:493:ARG:HD3	2.50	0.46
1:A:2:SER:HB2	1:A:21:ILE:HD13	1.97	0.46
1:B:280:ASP:HB3	4:B:676:HOH:O	2.14	0.46
1:C:271:ARG:HB2	1:C:302:ILE:CG2	2.46	0.46
1:B:71:THR:O	1:B:71:THR:HG23	2.15	0.46
1:E:472:LEU:HD23	1:E:472:LEU:N	2.31	0.46
1:B:150:GLN:NE2	1:B:163:SER:OG	2.49	0.46
1:E:27:ASP:HA	1:E:30:ARG:NH1	2.31	0.46
1:E:293:ALA:HB2	1:E:438:VAL:HG22	1.97	0.46
1:A:230:ASN:CG	4:A:1872:HOH:O	2.58	0.46
1:C:357:LEU:HD11	1:C:372:ALA:HB2	1.96	0.46
1:D:359:PRO:HG2	4:D:797:HOH:O	2.15	0.46
1:F:196:LYS:HE2	1:F:219:GLU:OE2	2.16	0.46
1:A:210:ILE:HD11	1:B:379:LEU:HD11	1.97	0.46
1:A:454:TYR:HB2	1:A:458:PHE:CD2	2.50	0.46
1:C:175:THR:HG22	1:D:375:ARG:HD2	1.98	0.46
1:A:202:PRO:HG2	1:A:258:PRO:CG	2.46	0.46
1:A:113:GLN:HE22	1:E:504:ASN:ND2	2.13	0.45
1:B:398:LEU:O	1:B:402:MET:HG3	2.16	0.45
1:D:414:GLN:HG2	4:D:2509:HOH:O	2.15	0.45
1:B:23:ILE:HD13	1:B:473:PHE:CE1	2.51	0.45
1:B:352:HIS:O	1:B:355:ARG:HG2	2.15	0.45
1:D:333:ASN:ND2	1:D:335:PHE:HB2	2.32	0.45
1:E:21:ILE:HG12	1:E:33:LEU:CD1	2.47	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:234:PRO:HG2	1:E:237:GLU:CG	2.45	0.45
1:E:474:ARG:HG3	1:E:518:MET:HE3	1.97	0.45
1:A:276:GLU:HB2	1:A:277:HIS:HD2	1.82	0.45
1:C:72:VAL:HG12	1:C:74:VAL:HG23	1.98	0.45
1:D:461:TRP:CZ2	1:D:465:GLN:HG3	2.51	0.45
1:A:87:PHE:O	1:A:91:ILE:HG12	2.17	0.45
1:C:215:GLN:NE2	4:C:2354:HOH:O	2.47	0.45
1:B:23:ILE:HD13	1:B:473:PHE:HD1	1.77	0.45
1:B:24:ALA:CB	1:B:482:VAL:HG23	2.38	0.45
1:C:23:ILE:HD13	1:C:473:PHE:HE1	1.80	0.45
1:B:468:THR:OG1	1:B:494:PRO:HA	2.17	0.45
1:C:355:ARG:HE	1:C:355:ARG:HB2	1.63	0.45
1:D:432:LEU:HD23	4:D:3244:HOH:O	2.17	0.45
1:C:443:LEU:HD21	1:C:489:PHE:CZ	2.48	0.45
1:E:345:SER:HB2	4:E:2629:HOH:O	2.16	0.45
1:E:454:TYR:HB2	1:E:458:PHE:CD2	2.52	0.45
1:F:458:PHE:CE1	1:F:523:TYR:HA	2.52	0.45
1:A:421:THR:O	1:A:425:ARG:HG3	2.17	0.44
1:F:461:TRP:O	1:F:465:GLN:HG2	2.17	0.44
1:A:213:LEU:HD11	1:B:376:ALA:O	2.17	0.44
1:C:352:HIS:O	1:C:355:ARG:HG2	2.16	0.44
1:C:357:LEU:HD21	1:C:380:ASN:CB	2.47	0.44
1:B:243:ASP:OD1	1:B:243:ASP:C	2.59	0.44
1:E:183:GLU:HG3	1:E:187:LEU:HD11	1.98	0.44
1:F:33:LEU:HD11	1:F:482:VAL:CG1	2.44	0.44
1:F:95:ARG:O	1:F:101:ARG:HD3	2.17	0.44
4:A:2061:HOH:O	1:B:71:THR:CB	2.57	0.44
1:D:316:TYR:OH	1:D:409:LYS:HB2	2.17	0.44
1:D:358:LEU:N	1:D:358:LEU:HD23	2.32	0.44
1:A:226:ASP:HA	1:A:227:PRO:HD3	1.84	0.44
1:C:320:THR:O	1:C:323:ARG:HD2	2.18	0.44
1:C:334:VAL:CG1	4:C:2359:HOH:O	2.65	0.44
1:D:197:VAL:HG23	1:D:248:ILE:HG23	1.99	0.44
1:D:240:LYS:NZ	4:D:3067:HOH:O	2.19	0.44
1:A:522:LEU:HD23	1:A:522:LEU:HA	1.87	0.44
1:B:215:GLN:HB2	4:B:2123:HOH:O	2.18	0.44
1:E:243:ASP:HA	1:E:244:PRO:HD2	1.86	0.44
1:A:464:LYS:HE3	4:A:1914:HOH:O	2.16	0.43
1:B:161:ILE:HD11	1:B:304:PRO:HB3	2.00	0.43
1:E:454:TYR:O	1:E:458:PHE:HB3	2.17	0.43
1:F:95:ARG:HA	4:F:2290:HOH:O	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:GLN:HE22	1:B:263:ASP:N	2.12	0.43
1:D:184:SER:CB	1:D:370:LEU:HD23	2.48	0.43
1:E:257:PRO:HG2	1:E:258:PRO:HD3	2.00	0.43
1:A:253:ASN:HA	1:A:254:PRO:C	2.44	0.43
1:B:342:LEU:O	1:B:347:LYS:HE3	2.18	0.43
1:E:254:PRO:HB3	1:E:438:VAL:HG21	1.99	0.43
1:F:267:LEU:HB3	1:F:302:ILE:HG13	2.00	0.43
1:F:484:LEU:HB2	1:F:497:ARG:HB2	2.00	0.43
1:C:256:ASN:HA	1:C:257:PRO:HA	1.90	0.43
1:C:374:SER:O	1:C:375:ARG:HD3	2.18	0.43
1:F:98:GLU:O	1:F:99:GLY:C	2.62	0.43
1:F:473:PHE:O	1:F:477:ASP:HB2	2.18	0.43
1:D:322:TRP:HB3	1:D:324:LEU:HG	2.01	0.43
1:E:343:GLN:O	1:E:344:GLU:C	2.60	0.43
1:B:102:PHE:CE1	1:B:402:MET:CE	3.01	0.43
1:F:439:ASP:HA	1:F:441:TYR:O	2.18	0.43
1:A:264:GLN:HE21	1:A:264:GLN:HB2	1.56	0.43
1:F:444:ILE:HG21	1:F:515:LEU:HD13	2.00	0.43
1:B:210:ILE:HB	1:B:211:PRO:HD3	2.01	0.43
1:C:191:LEU:HD23	1:C:191:LEU:HA	1.76	0.43
1:C:358:LEU:N	1:C:358:LEU:HD23	2.34	0.43
1:E:23:ILE:HD13	1:E:473:PHE:CD1	2.54	0.43
1:E:429:MET:CE	4:E:564:HOH:O	2.67	0.43
1:F:432:LEU:HA	1:F:432:LEU:HD12	1.80	0.43
1:B:407:GLU:HG2	4:B:732:HOH:O	2.18	0.43
1:C:231:TRP:CZ3	1:C:488:GLY:HA3	2.54	0.43
1:E:25:SER:HB2	1:E:30:ARG:NH2	2.33	0.43
1:F:503:LEU:HB2	1:F:508:TYR:CZ	2.53	0.43
1:B:272:ASN:ND2	4:B:666:HOH:O	2.47	0.42
4:C:920:HOH:O	1:F:404:GLU:HB3	2.19	0.42
1:D:226:ASP:HB2	1:D:234:PRO:HG3	2.01	0.42
1:D:234:PRO:HD2	1:D:237:GLU:HB2	2.01	0.42
1:D:468:THR:HG23	1:D:495:SER:O	2.18	0.42
1:E:467:SER:O	1:E:468:THR:C	2.61	0.42
1:E:139:ARG:HG3	1:E:169:PHE:HA	2.01	0.42
1:F:161:ILE:HD13	1:F:304:PRO:HB3	2.00	0.42
1:F:446:LEU:HD13	1:F:471:MET:HE2	2.01	0.42
1:B:201:MET:HE2	4:B:633:HOH:O	2.18	0.42
1:D:41:ASN:C	1:D:41:ASN:HD22	2.26	0.42
1:C:72:VAL:HG12	1:C:74:VAL:CG2	2.49	0.42
1:F:6:GLN:HA	4:F:2793:HOH:O	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:25:SER:CB	1:F:30:ARG:HH21	2.30	0.42
1:A:247:LYS:HA	1:A:247:LYS:HD3	1.70	0.42
1:A:276:GLU:HB2	1:A:277:HIS:CD2	2.55	0.42
1:D:474:ARG:HH22	1:D:521:GLU:CD	2.27	0.42
1:E:352:HIS:CE1	1:E:355:ARG:NH1	2.87	0.42
1:A:357:LEU:HD23	4:A:816:HOH:O	2.19	0.42
1:C:522:LEU:HD23	1:C:522:LEU:HA	1.88	0.42
1:C:84:GLU:O	1:C:88:GLU:HG3	2.20	0.42
1:D:308:LEU:HD23	1:D:308:LEU:HA	1.92	0.42
1:D:430:PRO:HD3	4:D:2513:HOH:O	2.20	0.42
1:B:169:PHE:CD1	1:B:371:VAL:HG22	2.55	0.42
1:C:24:ALA:HB3	1:C:482:VAL:HG23	2.01	0.42
1:C:417:ARG:HA	1:C:417:ARG:HD3	1.81	0.42
1:D:242:LYS:O	1:D:244:PRO:HD3	2.20	0.42
1:D:448:ASP:CB	4:D:1323:HOH:O	2.44	0.42
1:E:162:PRO:HG2	1:E:165:SER:OG	2.20	0.42
1:E:352:HIS:CD2	1:E:355:ARG:NH1	2.88	0.42
1:A:257:PRO:CD	1:A:258:PRO:HD3	2.50	0.42
1:E:23:ILE:CG2	4:E:2651:HOH:O	2.63	0.42
1:F:87:PHE:O	1:F:91:ILE:HG12	2.20	0.42
1:F:461:TRP:CH2	1:F:465:GLN:HG3	2.54	0.42
1:A:493:ARG:HB3	4:A:1910:HOH:O	2.19	0.42
1:B:80:ILE:HG13	1:B:123:HIS:HB2	2.01	0.42
1:B:456:GLU:O	1:B:460:GLU:HG3	2.19	0.42
1:C:308:LEU:HD23	1:C:308:LEU:HA	1.97	0.42
1:C:456:GLU:O	1:C:460:GLU:HG3	2.20	0.42
1:D:425:ARG:NH1	1:F:161:ILE:O	2.49	0.42
1:E:20:LEU:O	1:E:23:ILE:HB	2.19	0.42
1:F:205:THR:O	1:F:209:GLU:HG3	2.19	0.42
1:F:308:LEU:HD23	1:F:308:LEU:HA	1.92	0.42
1:A:492:ASN:ND2	4:A:2794:HOH:O	2.53	0.41
1:B:404:GLU:HG3	1:F:414:GLN:HG2	2.02	0.41
1:D:445:ASP:CG	1:D:493:ARG:HH21	2.27	0.41
1:B:21:ILE:HD11	4:B:2058:HOH:O	2.20	0.41
1:B:215:GLN:CB	4:B:2123:HOH:O	2.69	0.41
1:D:187:LEU:HD13	1:D:353:ARG:NH2	2.35	0.41
1:D:410:HIS:HD2	4:D:2733:HOH:O	2.03	0.41
1:E:220:GLU:HG3	4:E:3092:HOH:O	2.20	0.41
1:E:358:LEU:HB2	1:E:359:PRO:CD	2.51	0.41
1:E:429:MET:HB3	1:E:430:PRO:HD2	2.03	0.41
1:C:251:CYS:O	1:C:285:THR:HA	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:269:ARG:O	1:D:273:ILE:HG13	2.20	0.41
1:D:428:GLY:O	1:D:429:MET:HB2	2.21	0.41
1:F:134:TYR:O	1:F:136:VAL:HG23	2.20	0.41
1:B:78:ALA:HB1	4:B:2100:HOH:O	2.20	0.41
1:C:64:LEU:HD11	4:F:873:HOH:O	2.20	0.41
1:C:454:TYR:HB2	1:C:458:PHE:CD2	2.56	0.41
1:C:457:ALA:HB3	4:C:1194:HOH:O	2.19	0.41
1:E:500:LEU:HD23	1:E:500:LEU:HA	1.92	0.41
1:A:95:ARG:HA	4:A:1985:HOH:O	2.21	0.41
1:C:164:GLU:CG	4:C:1035:HOH:O	2.67	0.41
1:E:372:ALA:HA	1:E:380:ASN:HD22	1.85	0.41
1:E:454:TYR:O	1:E:455:GLY:O	2.39	0.41
1:A:243:ASP:OD1	1:A:243:ASP:C	2.64	0.41
1:A:466:SER:HB3	1:A:467:SER:H	1.71	0.41
1:E:270:VAL:O	1:E:274:VAL:HG23	2.21	0.41
1:B:461:TRP:CH2	1:B:465:GLN:HG3	2.56	0.41
1:D:81:ASP:HB2	4:D:849:HOH:O	2.20	0.41
1:E:21:ILE:HG12	1:E:33:LEU:HD12	2.03	0.41
1:E:350:LEU:HA	1:E:350:LEU:HD23	1.78	0.41
1:A:69:MET:HE1	1:D:399:PHE:CD1	2.55	0.41
1:A:212:GLU:OE2	1:A:212:GLU:HA	2.21	0.41
1:B:306:ASN:HA	1:B:334:VAL:CG2	2.50	0.41
1:C:18:ASP:N	4:C:3289:HOH:O	2.52	0.41
1:C:359:PRO:HG2	1:C:360:ASP:H	1.85	0.41
1:D:192:LYS:NZ	1:D:346:GLU:OE1	2.53	0.41
1:E:205:THR:O	1:E:206:PRO:C	2.63	0.41
1:F:172:GLU:HB2	1:F:176:ALA:HB2	2.03	0.41
1:F:191:LEU:HD23	1:F:191:LEU:HA	1.95	0.41
1:F:248:ILE:HA	1:F:282:MET:O	2.20	0.41
1:F:333:ASN:ND2	1:F:335:PHE:H	2.16	0.41
1:B:355:ARG:HG3	1:B:356:SER:N	2.36	0.41
1:C:35:ALA:HB1	1:C:37:ARG:NH1	2.33	0.41
1:E:342:LEU:O	1:E:347:LYS:HE3	2.20	0.41
1:E:410:HIS:O	1:E:414:GLN:HG3	2.21	0.41
1:F:358:LEU:N	1:F:358:LEU:CD2	2.84	0.41
1:A:1:MET:HE2	1:A:1:MET:HB2	1.95	0.40
1:A:464:LYS:HA	1:A:464:LYS:HD3	1.78	0.40
1:D:272:ASN:O	1:D:276:GLU:HG2	2.21	0.40
1:E:434:ASP:OD1	1:E:434:ASP:C	2.64	0.40
1:F:6:GLN:NE2	4:F:2766:HOH:O	2.53	0.40
1:A:314:SER:HB3	1:A:320:THR:HG22	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:430:PRO:HA	1:B:431:PRO:HD3	1.98	0.40
1:C:95:ARG:HA	1:C:95:ARG:HD2	1.96	0.40
1:E:232:GLN:HE22	1:E:262:MET:HA	1.87	0.40
1:E:250:PHE:CD1	1:E:284:LEU:HD23	2.56	0.40
1:E:294:ASP:O	1:E:295:ASP:C	2.64	0.40
1:F:461:TRP:CZ2	1:F:465:GLN:HG3	2.56	0.40
1:A:41:ASN:HD21	1:A:419:ARG:HH12	1.68	0.40
1:A:372:ALA:HA	1:A:380:ASN:HD22	1.86	0.40
1:C:197:VAL:HG23	1:C:248:ILE:HG23	2.02	0.40
1:D:87:PHE:O	1:D:91:ILE:HG12	2.21	0.40
1:E:428:GLY:O	1:E:429:MET:HB2	2.21	0.40
1:C:19:GLU:HG3	4:C:791:HOH:O	2.22	0.40
1:C:357:LEU:HD11	1:C:372:ALA:CB	2.52	0.40
1:F:320:THR:O	1:F:323:ARG:HD2	2.22	0.40
1:F:352:HIS:O	1:F:355:ARG:HG2	2.22	0.40
1:A:20:LEU:HD11	1:A:473:PHE:HA	2.04	0.40
1:B:472:LEU:HD11	1:B:485:PRO:HA	2.03	0.40
1:E:336:ASP:HA	1:E:339:LEU:HD12	2.03	0.40
1:F:201:MET:HA	1:F:202:PRO:C	2.46	0.40
1:F:277:HIS:O	1:F:278:ARG:HD2	2.21	0.40
1:F:456:GLU:OE1	4:F:3261:HOH:O	2.22	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:1730:HOH:O	4:F:1730:HOH:O[4_566]	2.09	0.11
1:A:425:ARG:NH2	4:C:1033:HOH:O[4_566]	2.15	0.05

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	520/546 (95%)	509 (98%)	11 (2%)	0	100	100
1	B	510/546 (93%)	500 (98%)	9 (2%)	1 (0%)	43	42
1	C	509/546 (93%)	493 (97%)	15 (3%)	1 (0%)	43	42
1	D	513/546 (94%)	504 (98%)	8 (2%)	1 (0%)	43	42
1	E	507/546 (93%)	481 (95%)	24 (5%)	2 (0%)	30	27
1	F	533/546 (98%)	522 (98%)	10 (2%)	1 (0%)	43	42
All	All	3092/3276 (94%)	3009 (97%)	77 (2%)	6 (0%)	43	42

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	492	ASN
1	D	492	ASN
1	E	455	GLY
1	C	492	ASN
1	F	492	ASN
1	E	377	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	439/455 (96%)	429 (98%)	10 (2%)	44	49
1	B	427/455 (94%)	415 (97%)	12 (3%)	38	41
1	C	425/455 (93%)	412 (97%)	13 (3%)	35	37
1	D	426/455 (94%)	416 (98%)	10 (2%)	44	49
1	E	424/455 (93%)	410 (97%)	14 (3%)	33	34
1	F	444/455 (98%)	426 (96%)	18 (4%)	27	26
All	All	2585/2730 (95%)	2508 (97%)	77 (3%)	36	38

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	11	LEU
1	A	41	ASN
1	A	72	VAL
1	A	204	PHE
1	A	257	PRO
1	A	264	GLN
1	A	332	GLN
1	A	465	GLN
1	A	492	ASN
1	B	18	ASP
1	B	41	ASN
1	B	43	LEU
1	B	71	THR
1	B	72	VAL
1	B	204	PHE
1	B	208	ILE
1	B	230	ASN
1	B	257	PRO
1	B	333	ASN
1	B	425	ARG
1	B	456	GLU
1	C	30	ARG
1	C	41	ASN
1	C	43	LEU
1	C	71	THR
1	C	72	VAL
1	C	81	ASP
1	C	204	PHE
1	C	230	ASN
1	C	257	PRO
1	C	259	SER
1	C	333	ASN
1	C	463	VAL
1	C	489	PHE
1	D	29	ASN
1	D	41	ASN
1	D	72	VAL
1	D	201	MET
1	D	204	PHE
1	D	230	ASN
1	D	259	SER
1	D	333	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	513	ARG
1	D	534	LYS
1	E	30	ARG
1	E	41	ASN
1	E	43	LEU
1	E	72	VAL
1	E	136	VAL
1	E	159	ASP
1	E	163	SER
1	E	197	VAL
1	E	204	PHE
1	E	236	SER
1	E	259	SER
1	E	333	ASN
1	E	425	ARG
1	E	474	ARG
1	F	19	GLU
1	F	22	LYS
1	F	41	ASN
1	F	43	LEU
1	F	71	THR
1	F	72	VAL
1	F	159	ASP
1	F	197	VAL
1	F	204	PHE
1	F	215	GLN
1	F	230	ASN
1	F	259	SER
1	F	331	GLN
1	F	333	ASN
1	F	433	ARG
1	F	470	ASP
1	F	489	PHE
1	F	492	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (87) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	29	ASN
1	A	34	ASN
1	A	41	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	142	ASN
1	A	150	GLN
1	A	167	ASN
1	A	232	GLN
1	A	264	GLN
1	A	272	ASN
1	A	277	HIS
1	A	331	GLN
1	A	332	GLN
1	A	333	ASN
1	A	352	HIS
1	A	380	ASN
1	A	381	HIS
1	A	392	GLN
1	A	492	ASN
1	B	34	ASN
1	B	41	ASN
1	B	97	GLN
1	B	150	GLN
1	B	215	GLN
1	B	232	GLN
1	B	306	ASN
1	B	333	ASN
1	B	380	ASN
1	B	447	GLN
1	B	504	ASN
1	C	34	ASN
1	C	41	ASN
1	C	133	ASN
1	C	142	ASN
1	C	150	GLN
1	C	230	ASN
1	C	232	GLN
1	C	306	ASN
1	C	331	GLN
1	C	332	GLN
1	C	333	ASN
1	C	343	GLN
1	C	392	GLN
1	C	410	HIS
1	C	447	GLN
1	D	29	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	34	ASN
1	D	41	ASN
1	D	97	GLN
1	D	150	GLN
1	D	167	ASN
1	D	230	ASN
1	D	232	GLN
1	D	332	GLN
1	D	333	ASN
1	D	352	HIS
1	D	380	ASN
1	D	410	HIS
1	D	504	ASN
1	E	34	ASN
1	E	41	ASN
1	E	142	ASN
1	E	150	GLN
1	E	215	GLN
1	E	232	GLN
1	E	306	ASN
1	E	331	GLN
1	E	333	ASN
1	E	380	ASN
1	E	381	HIS
1	E	504	ASN
1	F	6	GLN
1	F	34	ASN
1	F	41	ASN
1	F	142	ASN
1	F	167	ASN
1	F	230	ASN
1	F	232	GLN
1	F	264	GLN
1	F	277	HIS
1	F	306	ASN
1	F	332	GLN
1	F	333	ASN
1	F	380	ASN
1	F	381	HIS
1	F	465	GLN
1	F	504	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 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$
2	PLP	C	900	1	15,15,16	2.25	7 (46%)	21,22,23	1.63	3 (14%)
2	PLP	D	900	1	15,15,16	2.33	6 (40%)	21,22,23	2.01	4 (19%)
2	PLP	B	900	1	15,15,16	2.27	6 (40%)	21,22,23	1.68	5 (23%)
2	PLP	F	900	1	15,15,16	2.79	6 (40%)	21,22,23	2.05	5 (23%)
2	PLP	A	900	1	15,15,16	2.61	6 (40%)	21,22,23	1.88	5 (23%)
2	PLP	E	900	1	15,15,16	2.96	7 (46%)	21,22,23	1.44	2 (9%)

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
2	PLP	C	900	1	-	0/6/6/8	0/1/1/1
2	PLP	D	900	1	-	0/6/6/8	0/1/1/1
2	PLP	B	900	1	-	0/6/6/8	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PLP	F	900	1	-	0/6/6/8	0/1/1/1
2	PLP	A	900	1	-	1/6/6/8	0/1/1/1
2	PLP	E	900	1	-	0/6/6/8	0/1/1/1

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	900	PLP	C2A-C2	7.33	1.62	1.50
2	A	900	PLP	C3-C2	-5.86	1.34	1.41
2	F	900	PLP	C4A-C4	5.60	1.62	1.51
2	F	900	PLP	C5-C4	5.25	1.46	1.40
2	D	900	PLP	C2-N1	4.80	1.42	1.33
2	B	900	PLP	C4A-C4	4.66	1.60	1.51
2	F	900	PLP	C2A-C2	4.61	1.57	1.50
2	A	900	PLP	O4P-C5A	4.51	1.61	1.44
2	E	900	PLP	C5-C4	4.48	1.45	1.40
2	C	900	PLP	O4P-C5A	4.47	1.61	1.44
2	B	900	PLP	O4P-C5A	4.21	1.60	1.44
2	A	900	PLP	C5A-C5	4.16	1.61	1.50
2	F	900	PLP	C6-N1	3.96	1.42	1.34
2	E	900	PLP	C2-N1	3.84	1.40	1.33
2	C	900	PLP	C5A-C5	3.66	1.60	1.50
2	D	900	PLP	C2A-C2	3.38	1.55	1.50
2	D	900	PLP	C5-C4	3.34	1.44	1.40
2	D	900	PLP	C5A-C5	3.23	1.59	1.50
2	D	900	PLP	O4P-C5A	3.16	1.56	1.44
2	E	900	PLP	C6-N1	3.14	1.40	1.34
2	B	900	PLP	P-O3P	-3.13	1.43	1.54
2	E	900	PLP	C4A-C4	2.96	1.57	1.51
2	A	900	PLP	P-O3P	-2.95	1.43	1.54
2	C	900	PLP	C6-N1	2.74	1.40	1.34
2	C	900	PLP	C2A-C2	2.69	1.54	1.50
2	A	900	PLP	C2A-C2	2.65	1.54	1.50
2	B	900	PLP	C5A-C5	2.60	1.57	1.50
2	C	900	PLP	C3-C2	-2.57	1.38	1.41
2	B	900	PLP	C6-N1	2.57	1.39	1.34
2	C	900	PLP	P-O2P	-2.51	1.45	1.54
2	A	900	PLP	P-O4P	-2.42	1.52	1.60
2	E	900	PLP	P-O4P	-2.35	1.52	1.60
2	C	900	PLP	C2-N1	2.24	1.37	1.33
2	F	900	PLP	P-O3P	-2.20	1.46	1.54
2	F	900	PLP	O4P-C5A	2.17	1.52	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	900	PLP	P-O4P	-2.11	1.53	1.60
2	E	900	PLP	P-O3P	-2.11	1.47	1.54
2	D	900	PLP	O3-C3	2.02	1.41	1.36

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	900	PLP	C4A-C4-C5	6.91	128.07	120.94
2	D	900	PLP	C4A-C4-C5	5.40	126.51	120.94
2	A	900	PLP	C4A-C4-C5	5.24	126.34	120.94
2	B	900	PLP	C4A-C4-C5	5.00	126.09	120.94
2	C	900	PLP	C4A-C4-C5	4.86	125.95	120.94
2	D	900	PLP	C6-C5-C4	3.86	121.26	118.10
2	F	900	PLP	C4A-C4-C3	-3.85	114.10	120.52
2	A	900	PLP	C5A-C5-C6	-3.84	113.11	119.36
2	D	900	PLP	C4A-C4-C3	-3.69	114.37	120.52
2	D	900	PLP	C5A-C5-C6	-3.40	113.81	119.36
2	E	900	PLP	C4A-C4-C5	2.96	123.99	120.94
2	E	900	PLP	C5A-C5-C6	-2.90	114.64	119.36
2	C	900	PLP	C4A-C4-C3	-2.89	115.71	120.52
2	F	900	PLP	C5A-C5-C6	-2.87	114.68	119.36
2	C	900	PLP	C5A-C5-C6	-2.67	115.02	119.36
2	F	900	PLP	C5A-C5-C4	2.46	127.49	122.64
2	A	900	PLP	C4A-C4-C3	-2.45	116.43	120.52
2	B	900	PLP	C4A-C4-C3	-2.41	116.51	120.52
2	B	900	PLP	C5A-C5-C6	-2.33	115.56	119.36
2	B	900	PLP	O3P-P-O2P	2.29	116.39	107.80
2	F	900	PLP	O4P-C5A-C5	-2.17	105.30	109.36
2	A	900	PLP	C5A-C5-C4	2.13	126.84	122.64
2	B	900	PLP	O2P-P-O4P	-2.07	101.26	106.67
2	A	900	PLP	O3P-P-O1P	2.02	118.69	110.83

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	900	PLP	C6-C5-C5A-O4P

There are no ring outliers.

No monomer is involved in short contacts.

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	524/546 (95%)	-0.49	8 (1%) 72 71	10, 20, 42, 65	0
1	B	512/546 (93%)	-0.53	9 (1%) 67 67	9, 19, 43, 81	0
1	C	511/546 (93%)	-0.52	9 (1%) 67 67	9, 20, 46, 76	0
1	D	515/546 (94%)	-0.53	8 (1%) 70 70	9, 21, 43, 76	0
1	E	509/546 (93%)	-0.11	11 (2%) 62 61	11, 25, 57, 88	0
1	F	535/546 (97%)	-0.33	15 (2%) 55 54	9, 22, 52, 78	0
All	All	3106/3276 (94%)	-0.42	60 (1%) 66 66	9, 21, 48, 88	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	490	GLY	4.8
1	F	539	LEU	4.4
1	E	489	PHE	4.3
1	D	28	GLY	4.3
1	F	490	GLY	4.3
1	E	490	GLY	4.1
1	D	490	GLY	3.9
1	B	71	THR	3.8
1	E	71	THR	3.8
1	F	14	PHE	3.7
1	C	490	GLY	3.6
1	F	491	SER	3.6
1	A	2	SER	3.5
1	E	20	LEU	3.4
1	E	21	ILE	3.4
1	F	536	ALA	3.3
1	F	538	ALA	3.3
1	B	489	PHE	3.3
1	C	489	PHE	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	489	PHE	3.2
1	F	488	GLY	3.2
1	D	536	ALA	3.1
1	A	213	LEU	3.1
1	E	486	GLY	3.0
1	E	24	ALA	3.0
1	B	492	ASN	2.8
1	E	473	PHE	2.8
1	A	217	ALA	2.8
1	F	11	LEU	2.7
1	C	21	ILE	2.7
1	A	492	ASN	2.6
1	E	23	ILE	2.6
1	F	537	ALA	2.6
1	D	492	ASN	2.5
1	D	26	SER	2.5
1	F	8	LEU	2.5
1	C	492	ASN	2.5
1	C	487	ARG	2.5
1	C	23	ILE	2.4
1	E	488	GLY	2.3
1	D	538	ALA	2.3
1	A	1	MET	2.3
1	F	13	PRO	2.3
1	D	537	ALA	2.3
1	C	486	GLY	2.3
1	D	533	LEU	2.3
1	E	455	GLY	2.2
1	F	492	ASN	2.2
1	A	214	ALA	2.2
1	A	159	ASP	2.2
1	B	488	GLY	2.1
1	C	488	GLY	2.1
1	B	20	LEU	2.1
1	F	535	LEU	2.1
1	B	23	ILE	2.1
1	B	464	LYS	2.1
1	B	16	LEU	2.1
1	F	533	LEU	2.1
1	C	20	LEU	2.0
1	A	216	TYR	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($\text{\AA}^2$)	Q<0.9
2	PLP	E	900	15/16	0.98	0.05	17,21,23,24	0
3	CL	B	4002	1/1	0.98	0.04	20,20,20,20	0
3	CL	E	4005	1/1	0.98	0.05	20,20,20,20	0
3	CL	F	4006	1/1	0.98	0.06	24,24,24,24	0
2	PLP	A	900	15/16	0.99	0.04	14,15,18,18	0
2	PLP	F	900	15/16	0.99	0.04	13,15,18,18	0
3	CL	A	4001	1/1	0.99	0.02	18,18,18,18	0
2	PLP	B	900	15/16	0.99	0.03	12,15,17,18	0
3	CL	D	4004	1/1	0.99	0.04	21,21,21,21	0
2	PLP	C	900	15/16	0.99	0.04	13,15,17,17	0
2	PLP	D	900	15/16	0.99	0.04	14,16,17,18	0
3	CL	C	4003	1/1	1.00	0.02	19,19,19,19	0

6.5 Other polymers [i](#)

There are no such residues in this entry.