



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 02:59 AM UTC

PDB ID : 2DGL / pdb_00002dgl
Title : Crystal structure of Escherichia coli GadB in complex with bromide
Authors : Gruetter, M.G.; Capitani, G.; Gut, H.
Deposited on : 2006-03-14
Resolution : 3.15 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

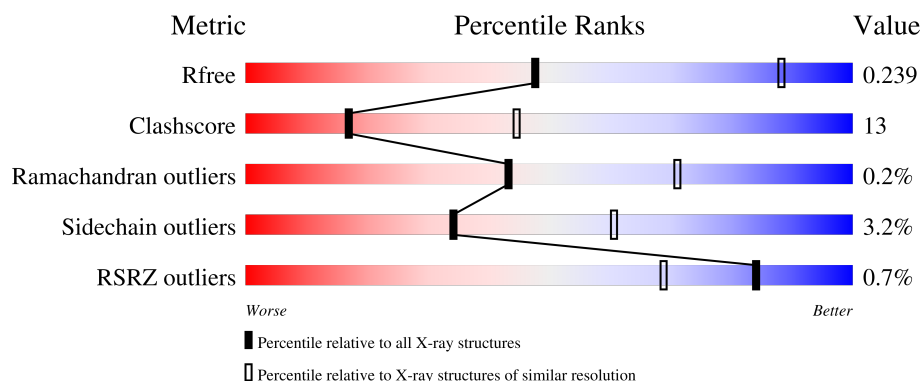
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (3.20-3.12)

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	466	% 69% 26% ..
1	B	466	% 71% 24% ..
1	C	466	% 63% 32% ..
1	D	466	 68% 28% ..
1	E	466	% 73% 22% ..

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Mol	Chain	Length	Quality of chain
1	F	466	

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
2	BR	B	469	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 21769 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.

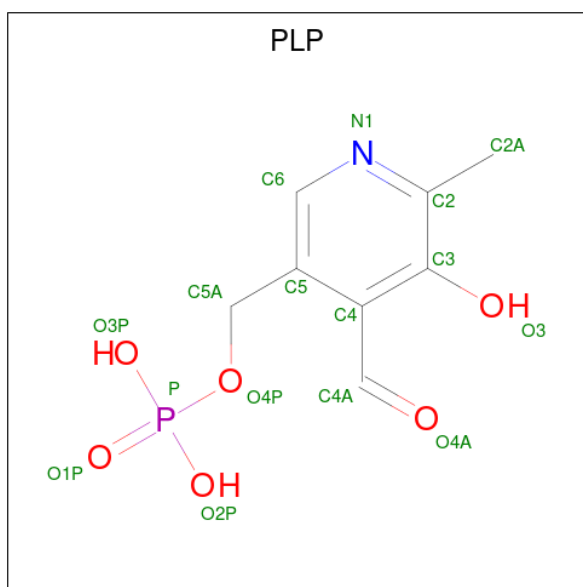
- Molecule 1 is a protein called Glutamate decarboxylase beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	450	Total	C	N	O	S	0	0	0
			3577	2283	610	660	24			
1	B	450	Total	C	N	O	S	0	0	0
			3577	2283	610	660	24			
1	C	451	Total	C	N	O	S	0	0	0
			3586	2289	612	661	24			
1	D	450	Total	C	N	O	S	0	0	0
			3577	2283	610	660	24			
1	E	452	Total	C	N	O	S	0	0	0
			3594	2295	613	662	24			
1	F	451	Total	C	N	O	S	0	0	0
			3586	2289	612	661	24			

- Molecule 2 is BROMIDE ION (CCD ID: BR) (formula: Br).

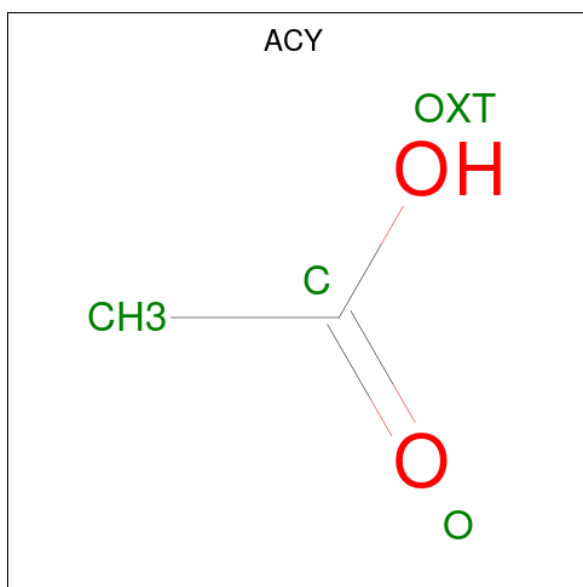
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	Br	0	0
			4	4		
2	B	5	Total	Br	0	0
			5	5		
2	C	4	Total	Br	0	0
			4	4		
2	D	3	Total	Br	0	0
			3	3		
2	E	4	Total	Br	0	0
			4	4		
2	F	4	Total	Br	0	0
			4	4		

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: C₈H₁₀NO₆P).



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

- Molecule 4 is ACETIC ACID (CCD ID: ACY) (formula: C₂H₄O₂).



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

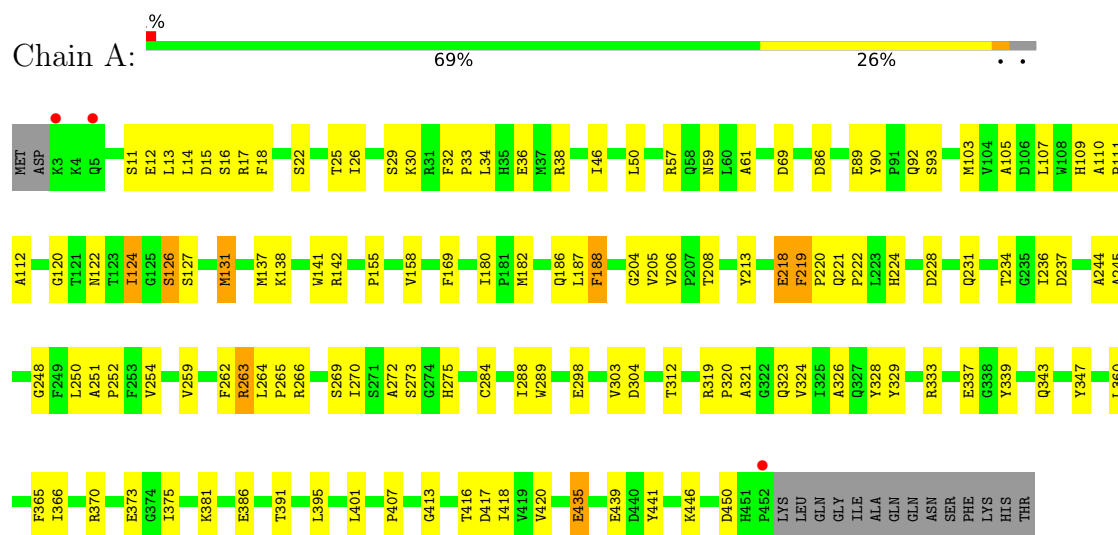
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	23	Total	O	0	0
			23	23		
5	B	33	Total	O	0	0
			33	33		
5	C	14	Total	O	0	0
			14	14		
5	D	13	Total	O	0	0
			13	13		
5	E	26	Total	O	0	0
			26	26		
5	F	25	Total	O	0	0
			25	25		

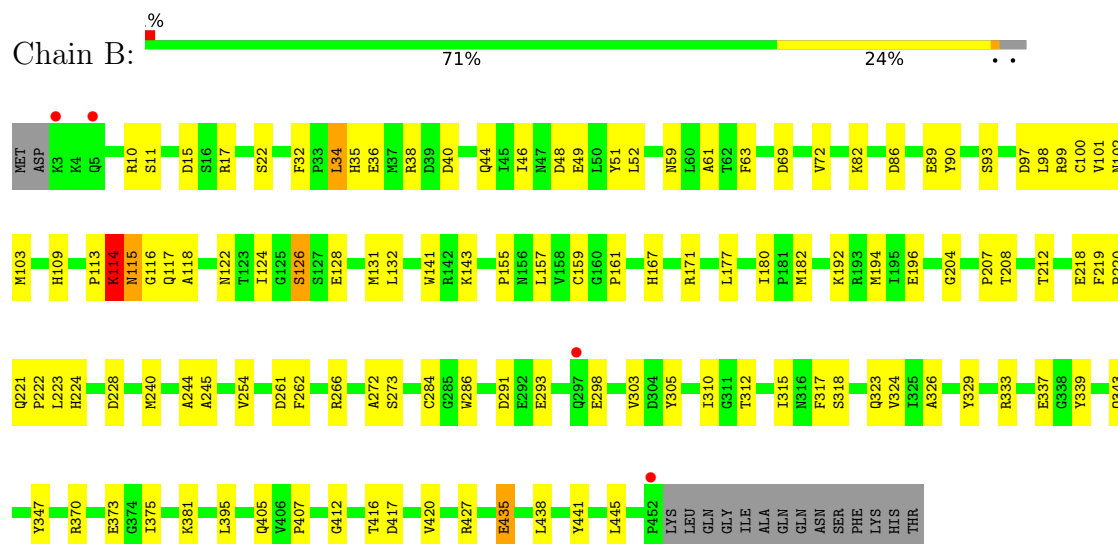
3 Residue-property plots [i](#)

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: Glutamate decarboxylase beta

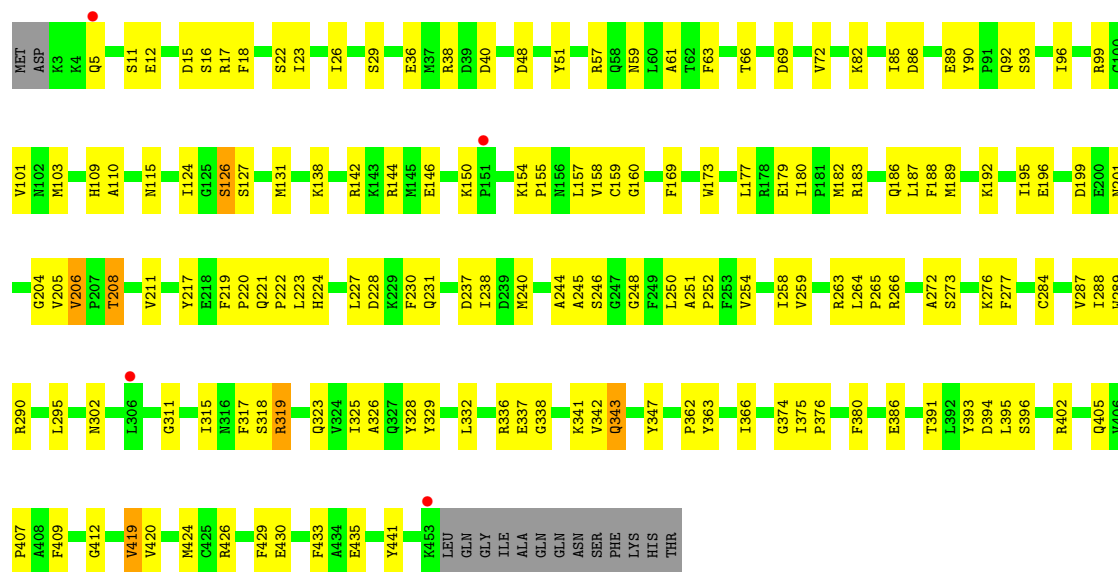


• Molecule 1: Glutamate decarboxylase beta



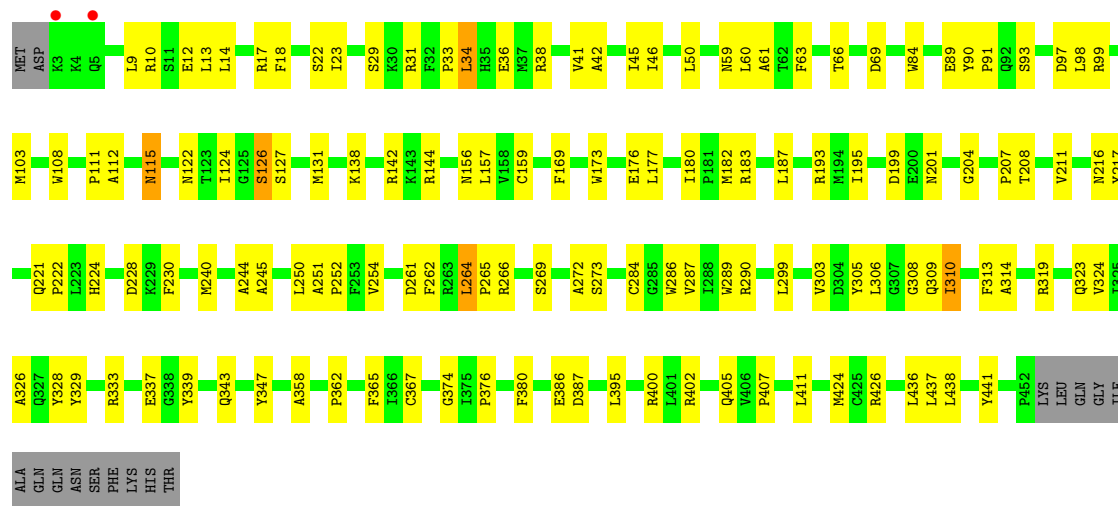
• Molecule 1: Glutamate decarboxylase beta





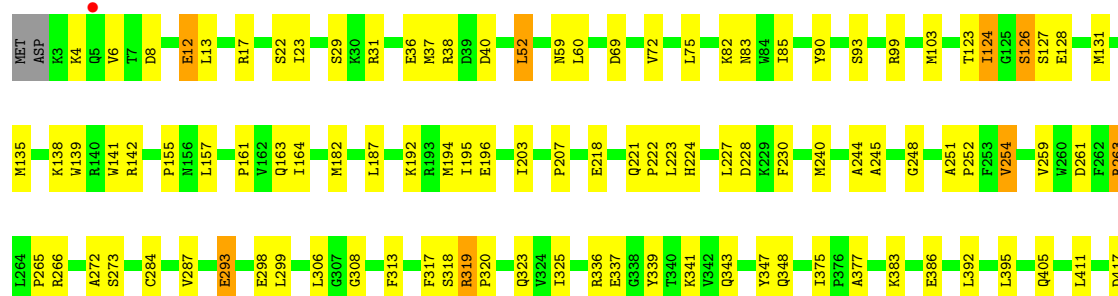
• Molecule 1: Glutamate decarboxylase beta

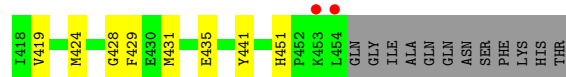
Chain D: 68% 28% . .



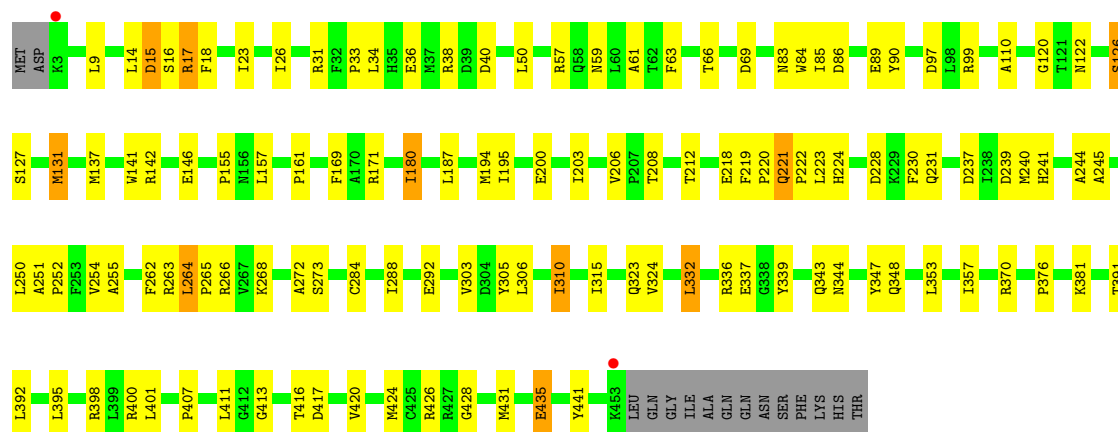
• Molecule 1: Glutamate decarboxylase beta

Chain E: 73% 22% . .





- Molecule 1: Glutamate decarboxylase beta



4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α , β , γ	297.05Å 297.05Å 233.73Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 3.15 40.00 – 3.15	Depositor EDS
% Data completeness (in resolution range)	99.6 (40.00-3.15) 99.6 (40.00-3.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.92 (at 3.12Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.218 , 0.248 0.212 , 0.239	Depositor DCC
R_{free} test set	2067 reflections (1.99%)	wwPDB-VP
Wilson B-factor (Å ²)	50.6	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 34.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	21769	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.49% 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: ACY, PLP, BR

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	0.50	0/3669	0.93	11/4974 (0.2%)
1	B	0.55	0/3669	0.95	4/4974 (0.1%)
1	C	0.46	0/3678	0.93	10/4985 (0.2%)
1	D	0.48	0/3669	0.94	10/4974 (0.2%)
1	E	0.52	0/3686	0.94	10/4996 (0.2%)
1	F	0.55	0/3678	0.93	8/4985 (0.2%)
All	All	0.51	0/22049	0.94	53/29888 (0.2%)

There are no bond length outliers.

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	90	TYR	CA-C-N	8.01	127.57	119.24
1	D	90	TYR	C-N-CA	8.01	127.57	119.24
1	C	90	TYR	CA-C-N	6.67	126.92	119.32
1	C	90	TYR	C-N-CA	6.67	126.92	119.32
1	B	90	TYR	CA-C-N	6.42	126.64	119.32
1	B	90	TYR	C-N-CA	6.42	126.64	119.32
1	E	319	ARG	CA-C-N	6.39	126.77	119.93
1	E	319	ARG	C-N-CA	6.39	126.77	119.93
1	C	429	PHE	N-CA-C	-6.35	100.84	109.54
1	A	90	TYR	CA-C-N	6.31	126.51	119.32
1	A	90	TYR	C-N-CA	6.31	126.51	119.32
1	E	90	TYR	CA-C-N	6.18	125.92	119.05
1	E	90	TYR	C-N-CA	6.18	125.92	119.05
1	F	90	TYR	CA-C-N	6.14	126.31	119.32
1	F	90	TYR	C-N-CA	6.14	126.31	119.32
1	B	93	SER	N-CA-C	-5.87	104.78	111.07
1	A	365	PHE	N-CA-C	5.80	118.12	109.25
1	E	451	HIS	CA-C-N	5.75	126.15	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	451	HIS	C-N-CA	5.75	126.15	119.47
1	F	264	LEU	CA-C-N	5.72	125.85	119.32
1	F	264	LEU	C-N-CA	5.72	125.85	119.32
1	C	319	ARG	CA-C-N	5.71	126.04	119.93
1	C	319	ARG	C-N-CA	5.71	126.04	119.93
1	D	319	ARG	CA-C-N	5.69	125.62	119.76
1	D	319	ARG	C-N-CA	5.69	125.62	119.76
1	C	93	SER	N-CA-C	-5.64	105.03	111.07
1	A	93	SER	N-CA-C	-5.61	105.17	111.28
1	E	93	SER	N-CA-C	-5.53	105.16	111.07
1	D	93	SER	N-CA-C	-5.52	105.16	111.07
1	D	264	LEU	CA-C-N	5.47	125.12	119.05
1	D	264	LEU	C-N-CA	5.47	125.12	119.05
1	F	255	ALA	CA-C-N	5.40	125.07	119.56
1	F	255	ALA	C-N-CA	5.40	125.07	119.56
1	E	263	ARG	N-CA-C	-5.37	105.98	112.54
1	F	206	VAL	N-CA-C	5.34	113.44	108.15
1	D	387	ASP	CA-C-N	5.30	126.14	120.47
1	D	387	ASP	C-N-CA	5.30	126.14	120.47
1	C	206	VAL	N-CA-C	5.24	113.33	108.15
1	A	32	PHE	CA-C-N	5.21	125.20	119.89
1	A	32	PHE	C-N-CA	5.21	125.20	119.89
1	E	429	PHE	N-CA-C	-5.19	101.22	108.54
1	D	314	ALA	N-CA-C	5.17	116.46	107.93
1	A	391	THR	N-CA-C	-5.15	101.53	109.52
1	B	167	HIS	N-CA-C	-5.11	105.71	111.28
1	F	263	ARG	N-CA-C	-5.11	106.31	112.54
1	C	115	ASN	N-CA-C	-5.11	107.00	113.18
1	A	206	VAL	N-CA-C	5.09	113.19	108.15
1	A	263	ARG	N-CA-C	-5.06	106.36	112.54
1	A	219	PHE	CA-C-N	5.05	124.54	119.19
1	A	219	PHE	C-N-CA	5.05	124.54	119.19
1	C	264	LEU	CA-C-N	5.03	125.06	119.32
1	C	264	LEU	C-N-CA	5.03	125.06	119.32
1	E	254	VAL	N-CA-C	5.01	117.71	112.90

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	3577	0	3483	103	0
1	B	3577	0	3483	84	0
1	C	3586	0	3496	128	0
1	D	3577	0	3483	99	0
1	E	3594	0	3507	85	0
1	F	3586	0	3496	93	0
2	A	4	0	0	1	0
2	B	5	0	0	3	0
2	C	4	0	0	1	0
2	D	3	0	0	1	0
2	E	4	0	0	1	0
2	F	4	0	0	2	0
3	A	15	0	6	0	0
3	B	15	0	6	0	0
3	C	15	0	6	1	0
3	D	15	0	6	0	0
3	E	15	0	6	0	0
3	F	15	0	6	0	0
4	A	4	0	3	0	0
4	B	4	0	3	0	0
4	C	8	0	6	0	0
4	E	4	0	3	0	0
4	F	4	0	3	0	0
5	A	23	0	0	0	0
5	B	33	0	0	0	0
5	C	14	0	0	0	0
5	D	13	0	0	0	0
5	E	26	0	0	2	0
5	F	25	0	0	0	0
All	All	21769	0	21002	540	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 13.

All (540) 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:228:ASP:HA	1:A:266:ARG:HH21	1.24	1.01
1:C:221:GLN:HB3	1:C:222:PRO:HD3	1.44	0.99
1:D:182:MET:HE3	1:D:187:LEU:HB3	1.47	0.97
1:D:221:GLN:HB3	1:D:222:PRO:HD3	1.48	0.96
1:A:221:GLN:HB3	1:A:222:PRO:HD3	1.47	0.94
1:E:182:MET:HE3	1:E:187:LEU:HB3	1.52	0.92
1:C:103:MET:HE2	1:D:33:PRO:HD3	1.50	0.91
1:C:228:ASP:HA	1:C:266:ARG:HH21	1.34	0.90
1:B:221:GLN:HB3	1:B:222:PRO:HD3	1.54	0.89
1:A:126:SER:HB2	1:A:273:SER:OG	1.77	0.84
2:B:469:BR:BR	1:C:16:SER:OG	2.50	0.84
1:D:42:ALA:O	1:D:46:ILE:HD12	1.77	0.84
1:C:126:SER:HB2	1:C:273:SER:OG	1.79	0.82
1:A:103:MET:HE1	1:A:328:TYR:HE1	1.43	0.82
1:E:383:LYS:HB2	1:E:386:GLU:HG3	1.61	0.81
1:D:103:MET:HE1	1:D:328:TYR:HE1	1.44	0.81
1:A:228:ASP:HA	1:A:266:ARG:NH2	1.94	0.81
1:D:182:MET:HE1	1:D:411:LEU:HD22	1.64	0.80
1:A:122:ASN:ND2	1:A:319:ARG:HH22	1.80	0.79
1:A:182:MET:HE2	1:A:187:LEU:HB3	1.63	0.79
1:F:348:GLN:HE21	1:F:431:MET:HE3	1.47	0.79
1:B:291:ASP:OD2	1:B:293:GLU:HG2	1.83	0.78
1:E:207:PRO:HG2	1:E:240:MET:HE2	1.66	0.78
1:E:221:GLN:HB3	1:E:222:PRO:HD3	1.65	0.77
1:E:182:MET:CE	1:E:187:LEU:HB3	2.13	0.77
1:F:126:SER:HB2	1:F:273:SER:OG	1.84	0.77
1:F:336:ARG:HG3	1:F:336:ARG:HH11	1.50	0.77
1:C:250:LEU:HD12	1:C:375:ILE:HG22	1.68	0.75
1:F:348:GLN:HE21	1:F:431:MET:CE	1.99	0.74
1:E:182:MET:HE1	1:E:411:LEU:HD22	1.69	0.73
1:D:23:ILE:HG13	1:D:45:ILE:HD11	1.70	0.73
1:D:126:SER:HB2	1:D:273:SER:OG	1.89	0.73
1:D:103:MET:HE1	1:D:328:TYR:CE1	2.23	0.71
1:A:395:LEU:HD21	1:A:441:TYR:CZ	2.25	0.71
1:E:395:LEU:HD21	1:E:441:TYR:CZ	2.25	0.71
1:D:228:ASP:HA	1:D:266:ARG:HH21	1.56	0.71
1:C:395:LEU:HD21	1:C:441:TYR:CZ	2.26	0.70
1:C:17:ARG:HB2	2:C:468:BR:BR	2.48	0.69
1:A:339:TYR:O	1:A:343:GLN:HG2	1.93	0.68
1:E:348:GLN:HE21	1:E:431:MET:CE	2.06	0.68
1:F:221:GLN:HB3	1:F:222:PRO:HD3	1.75	0.68
1:B:17:ARG:HB2	2:B:468:BR:BR	2.49	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:ASP:HA	1:B:266:ARG:HH21	1.57	0.67
1:C:103:MET:CE	1:D:33:PRO:HD3	2.22	0.67
1:E:83:ASN:OD1	1:E:85:ILE:HG22	1.94	0.67
1:B:207:PRO:HG2	1:B:240:MET:HE2	1.75	0.67
1:E:348:GLN:HE21	1:E:431:MET:HE3	1.61	0.66
1:E:194:MET:SD	1:E:223:LEU:HD22	2.35	0.66
1:D:224:HIS:CE1	1:D:265:PRO:HD2	2.31	0.66
1:C:63:PHE:CE1	1:C:424:MET:HE3	2.31	0.66
1:F:231:GLN:NE2	1:F:237:ASP:HB2	2.11	0.65
1:C:338:GLY:O	1:C:342:VAL:HG23	1.95	0.65
1:D:216:ASN:HD21	1:D:367:CYS:HB2	1.61	0.65
1:E:339:TYR:O	1:E:343:GLN:HG2	1.97	0.65
1:E:251:ALA:HB3	1:E:252:PRO:HD3	1.79	0.64
1:A:259:VAL:HA	1:A:263:ARG:HH21	1.62	0.64
1:A:137:MET:CE	1:A:204:GLY:HA3	2.27	0.64
1:F:180:ILE:N	1:F:180:ILE:HD12	2.11	0.64
1:C:183:ARG:HD2	1:C:186:GLN:OE1	1.98	0.64
1:B:435:GLU:HG3	1:C:26:ILE:HD13	1.80	0.64
1:B:69:ASP:OD1	1:B:72:VAL:HG23	1.98	0.64
1:C:221:GLN:HB3	1:C:222:PRO:CD	2.26	0.63
1:C:228:ASP:HA	1:C:266:ARG:NH2	2.11	0.63
1:B:52:LEU:HD12	1:C:402:ARG:HH21	1.63	0.63
1:A:103:MET:HE1	1:A:328:TYR:CE1	2.32	0.63
1:A:137:MET:HE2	1:A:204:GLY:HA3	1.81	0.63
1:E:103:MET:HE2	1:F:33:PRO:HD3	1.80	0.62
1:E:126:SER:HB2	1:E:273:SER:OG	1.98	0.62
1:D:310:ILE:HD13	1:D:310:ILE:H	1.64	0.62
1:F:142:ARG:O	1:F:146:GLU:HG3	1.99	0.62
1:D:395:LEU:HD21	1:D:441:TYR:CZ	2.34	0.62
1:B:126:SER:HB2	1:B:273:SER:OG	1.99	0.62
1:B:370:ARG:HD3	1:B:373:GLU:OE2	2.00	0.61
1:D:305:TYR:CB	1:D:310:ILE:HD12	2.30	0.61
1:B:17:ARG:HD3	1:B:44:GLN:OE1	2.00	0.61
1:D:245:ALA:HA	1:D:272:ALA:HA	1.83	0.61
1:E:38:ARG:HB3	1:E:40:ASP:OD1	2.00	0.61
1:E:75:LEU:HD13	1:E:325:ILE:HG22	1.83	0.61
1:F:180:ILE:HD12	1:F:180:ILE:H	1.66	0.61
1:A:109:HIS:CD2	1:A:263:ARG:HD3	2.36	0.61
1:A:381:LYS:HB3	1:A:420:VAL:HG12	1.83	0.60
1:B:254:VAL:HG21	1:B:347:TYR:CE2	2.36	0.60
1:F:194:MET:SD	1:F:223:LEU:HD22	2.42	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:224:HIS:CE1	1:F:265:PRO:HD2	2.36	0.60
1:A:435:GLU:HG3	1:F:26:ILE:HD13	1.84	0.60
1:E:254:VAL:HG21	1:E:347:TYR:CE2	2.36	0.60
1:A:231:GLN:HE21	1:A:237:ASP:HB2	1.66	0.60
1:E:182:MET:HE2	1:E:187:LEU:HD22	1.83	0.60
1:C:183:ARG:HG3	1:C:186:GLN:HG3	1.83	0.60
1:E:17:ARG:HB2	2:E:469:BR:BR	2.57	0.60
1:C:224:HIS:CD2	1:C:266:ARG:HB2	2.37	0.60
1:C:224:HIS:CE1	1:C:265:PRO:HD2	2.36	0.60
1:C:245:ALA:HA	1:C:272:ALA:HA	1.84	0.59
1:C:180:ILE:N	1:C:180:ILE:HD12	2.18	0.59
1:C:158:VAL:HB	1:C:205:VAL:HG22	1.84	0.59
1:A:221:GLN:CB	1:A:222:PRO:HD3	2.28	0.59
1:D:69:ASP:C	1:D:69:ASP:OD1	2.46	0.59
1:D:305:TYR:HB3	1:D:310:ILE:HD12	1.85	0.59
1:F:57:ARG:HH11	1:F:57:ARG:HG3	1.68	0.58
1:E:336:ARG:HD2	1:F:34:LEU:HD23	1.84	0.58
1:A:36:GLU:HG2	1:B:337:GLU:OE1	2.04	0.58
1:C:183:ARG:CG	1:C:186:GLN:HG3	2.33	0.58
1:B:182:MET:CE	1:B:412:GLY:H	2.17	0.58
1:A:50:LEU:HD22	1:B:82:LYS:HE3	1.86	0.58
1:F:400:ARG:O	1:F:400:ARG:HD3	2.03	0.58
1:A:298:GLU:O	1:B:171:ARG:NH1	2.36	0.58
1:C:138:LYS:HE2	1:C:142:ARG:HH21	1.69	0.58
1:C:227:LEU:HD13	1:C:238:ILE:HG22	1.86	0.58
1:A:138:LYS:HE2	1:A:142:ARG:HH21	1.68	0.57
1:A:120:GLY:HA3	1:A:288:ILE:HD13	1.84	0.57
1:F:339:TYR:O	1:F:343:GLN:HG2	2.04	0.57
1:C:224:HIS:HE1	1:C:265:PRO:HD2	1.69	0.57
1:D:157:LEU:HD12	1:D:204:GLY:O	2.02	0.57
1:E:320:PRO:HB3	5:E:536:HOH:O	2.04	0.57
1:F:336:ARG:HG3	1:F:336:ARG:NH1	2.18	0.57
1:D:115:ASN:OD1	1:D:115:ASN:N	2.38	0.57
1:A:180:ILE:N	1:A:180:ILE:HD12	2.19	0.57
1:B:339:TYR:O	1:B:343:GLN:HG2	2.04	0.57
1:C:192:LYS:O	1:C:196:GLU:HG3	2.05	0.57
1:E:377:ALA:HB2	1:E:424:MET:HE1	1.87	0.57
1:F:395:LEU:HD21	1:F:441:TYR:CE1	2.40	0.57
1:C:393:TYR:HE2	1:C:419:VAL:HG21	1.70	0.56
1:E:224:HIS:CD2	1:E:266:ARG:HB2	2.41	0.56
1:F:17:ARG:HB2	2:F:469:BR:BR	2.60	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:ILE:HG12	1:A:319:ARG:HD2	1.88	0.56
1:A:221:GLN:HB3	1:A:222:PRO:CD	2.29	0.56
1:A:259:VAL:HA	1:A:263:ARG:NH2	2.20	0.56
1:F:245:ALA:HA	1:F:272:ALA:HA	1.88	0.56
1:A:245:ALA:HA	1:A:272:ALA:HA	1.88	0.56
1:C:66:THR:HG23	1:C:426:ARG:HE	1.70	0.56
1:B:113:PRO:HB3	1:B:118:ALA:HA	1.87	0.56
1:E:207:PRO:CG	1:E:240:MET:HE2	2.34	0.56
1:A:250:LEU:HD12	1:A:375:ILE:HG22	1.88	0.55
1:C:251:ALA:HB3	1:C:252:PRO:HD3	1.87	0.55
1:D:343:GLN:HA	1:D:343:GLN:OE1	2.07	0.55
1:B:343:GLN:HA	1:B:343:GLN:OE1	2.05	0.55
1:E:377:ALA:HB2	1:E:424:MET:CE	2.37	0.55
1:B:122:ASN:HB2	1:B:286:TRP:CZ3	2.42	0.55
1:E:157:LEU:HD13	1:E:203:ILE:HD11	1.89	0.55
1:F:254:VAL:HG21	1:F:347:TYR:CE2	2.42	0.55
1:C:208:THR:HG22	1:C:208:THR:O	2.06	0.55
1:F:180:ILE:H	1:F:180:ILE:CD1	2.20	0.55
1:B:228:ASP:HA	1:B:266:ARG:NH2	2.22	0.55
1:C:250:LEU:HD13	1:C:376:PRO:HD3	1.88	0.55
1:D:180:ILE:N	1:D:180:ILE:HD12	2.21	0.55
1:D:41:VAL:O	1:D:45:ILE:HG12	2.07	0.54
1:D:221:GLN:HB3	1:D:222:PRO:CD	2.29	0.54
1:F:141:TRP:CZ3	1:F:155:PRO:HB3	2.42	0.54
1:C:289:TRP:CE2	1:C:295:LEU:HD13	2.42	0.54
1:F:381:LYS:HB3	1:F:420:VAL:HG12	1.89	0.54
1:E:284:CYS:HB2	1:E:323:GLN:HB3	1.89	0.54
1:A:284:CYS:HB2	1:A:323:GLN:HB3	1.88	0.54
1:D:262:PHE:CE1	1:D:290:ARG:HB3	2.42	0.54
1:A:188:PHE:N	1:A:188:PHE:CD1	2.76	0.54
1:B:427:ARG:HD2	2:B:469:BR:BR	2.63	0.54
1:C:250:LEU:HD21	1:C:277:PHE:CD1	2.43	0.53
1:E:123:THR:HB	1:E:128:GLU:OE1	2.08	0.53
1:D:122:ASN:HB2	1:D:286:TRP:CZ3	2.43	0.53
1:E:224:HIS:CE1	1:E:265:PRO:HD2	2.44	0.53
1:A:224:HIS:CD2	1:A:264:LEU:HB3	2.43	0.53
1:E:36:GLU:HG2	1:F:337:GLU:OE1	2.08	0.53
1:A:224:HIS:CE1	1:A:265:PRO:HD2	2.43	0.53
1:B:194:MET:SD	1:B:223:LEU:HD22	2.48	0.53
1:E:103:MET:CE	1:F:33:PRO:HD3	2.37	0.53
1:A:303:VAL:HG23	1:A:312:THR:HG23	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:245:ALA:HA	1:B:272:ALA:HA	1.90	0.53
1:B:395:LEU:HD21	1:B:441:TYR:CZ	2.43	0.53
1:F:284:CYS:HB2	1:F:323:GLN:HB3	1.91	0.53
1:E:37:MET:HE3	1:F:332:LEU:HB3	1.91	0.53
1:C:159:CYS:SG	1:C:177:LEU:HD11	2.49	0.53
1:C:182:MET:HE3	1:C:412:GLY:H	1.73	0.53
1:B:10:ARG:HA	1:D:9:LEU:HD11	1.91	0.52
1:C:386:GLU:HA	1:C:386:GLU:OE1	2.10	0.52
1:E:85:ILE:HG12	1:E:317:PHE:CD1	2.43	0.52
1:B:192:LYS:O	1:B:196:GLU:HG3	2.10	0.52
1:D:284:CYS:HB2	1:D:323:GLN:HB3	1.91	0.52
1:D:400:ARG:O	1:D:400:ARG:HD3	2.09	0.52
1:B:114:LYS:O	1:B:116:GLY:N	2.34	0.52
1:C:221:GLN:CB	1:C:222:PRO:HD3	2.28	0.52
1:E:293:GLU:HB2	5:E:542:HOH:O	2.09	0.52
1:C:393:TYR:O	1:C:396:SER:HB3	2.10	0.52
1:D:126:SER:HB2	1:D:273:SER:HG	1.73	0.52
1:E:99:ARG:O	1:E:103:MET:HG3	2.10	0.52
1:D:17:ARG:HB2	2:D:468:BR:BR	2.64	0.52
1:D:362:PRO:HB2	1:D:386:GLU:HG2	1.92	0.52
1:E:131:MET:HE3	1:F:315:ILE:O	2.09	0.52
1:E:337:GLU:HG2	1:E:341:LYS:HE3	1.92	0.52
1:F:250:LEU:HD13	1:F:376:PRO:HD3	1.93	0.52
1:C:393:TYR:CE2	1:C:419:VAL:HG21	2.45	0.51
1:E:182:MET:HG2	1:E:187:LEU:HA	1.92	0.51
1:B:143:LYS:HE3	1:B:298:GLU:OE1	2.10	0.51
1:E:245:ALA:HA	1:E:272:ALA:HA	1.92	0.51
1:E:254:VAL:HG21	1:E:347:TYR:HE2	1.74	0.51
1:F:38:ARG:HB3	1:F:40:ASP:OD1	2.11	0.51
1:D:89:GLU:C	1:D:91:PRO:HD3	2.36	0.51
1:A:321:ALA:O	1:A:324:VAL:HG12	2.10	0.51
1:D:254:VAL:HG21	1:D:347:TYR:CE2	2.46	0.51
1:E:29:SER:HB2	1:F:99:ARG:HG2	1.91	0.51
1:A:319:ARG:HB2	1:A:320:PRO:HD2	1.93	0.51
1:A:333:ARG:HD3	1:A:333:ARG:O	2.11	0.51
1:C:18:PHE:HA	1:C:23:ILE:HG21	1.92	0.51
1:B:128:GLU:HG3	1:B:315:ILE:HD13	1.92	0.51
1:E:221:GLN:CB	1:E:222:PRO:HD3	2.36	0.51
1:A:323:GLN:OE1	1:A:323:GLN:N	2.41	0.51
1:D:224:HIS:CD2	1:D:266:ARG:HB2	2.46	0.51
1:B:435:GLU:CG	1:C:26:ILE:HD13	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:180:ILE:HD12	1:C:180:ILE:H	1.75	0.50
1:C:199:ASP:OD1	1:C:201:ASN:N	2.43	0.50
1:E:306:LEU:C	1:E:308:GLY:H	2.18	0.50
1:A:92:GLN:HG2	1:B:49:GLU:O	2.12	0.50
1:D:60:LEU:CD1	1:D:437:LEU:HD22	2.41	0.50
1:E:139:TRP:CD2	1:E:299:LEU:HD11	2.45	0.50
1:F:228:ASP:HA	1:F:266:ARG:HH21	1.75	0.50
1:A:131:MET:HE2	1:A:169:PHE:HB2	1.93	0.50
1:B:254:VAL:HG21	1:B:347:TYR:HE2	1.76	0.50
1:F:57:ARG:HG3	1:F:57:ARG:NH1	2.26	0.50
1:A:343:GLN:OE1	1:A:343:GLN:HA	2.12	0.50
1:C:336:ARG:HD2	1:D:34:LEU:HD12	1.94	0.50
1:F:86:ASP:HB3	1:F:89:GLU:HB2	1.93	0.50
1:F:353:LEU:O	1:F:357:ILE:HG13	2.12	0.50
1:A:180:ILE:HD12	1:A:180:ILE:H	1.76	0.50
1:C:12:GLU:O	1:C:38:ARG:HD2	2.12	0.50
1:C:254:VAL:HG21	1:C:347:TYR:CE2	2.46	0.50
1:D:183:ARG:NH1	1:D:193:ARG:HD3	2.25	0.50
1:D:250:LEU:HD13	1:D:376:PRO:HD3	1.92	0.50
1:C:38:ARG:HB3	1:C:40:ASP:OD1	2.12	0.50
1:C:395:LEU:HD21	1:C:441:TYR:OH	2.10	0.50
1:B:86:ASP:HB3	1:B:89:GLU:HB2	1.93	0.50
1:C:366:ILE:HD12	1:C:420:VAL:HG11	1.94	0.50
1:A:446:LYS:HE3	1:A:450:ASP:OD2	2.12	0.49
1:A:188:PHE:N	1:A:188:PHE:HD1	2.09	0.49
1:C:109:HIS:O	1:C:110:ALA:C	2.55	0.49
1:C:250:LEU:CD1	1:C:375:ILE:HG22	2.41	0.49
1:D:310:ILE:HD13	1:D:310:ILE:N	2.26	0.49
1:F:161:PRO:HD2	1:F:218:GLU:OE2	2.11	0.49
1:B:221:GLN:HB3	1:B:222:PRO:CD	2.35	0.49
1:C:426:ARG:HG3	1:C:426:ARG:HH11	1.76	0.49
1:D:84:TRP:NE1	1:D:97:ASP:OD2	2.45	0.49
1:D:339:TYR:O	1:D:343:GLN:HG2	2.12	0.49
1:F:122:ASN:ND2	1:F:324:VAL:HG22	2.27	0.49
1:A:231:GLN:NE2	1:A:237:ASP:HB2	2.27	0.49
1:D:365:PHE:CD1	1:D:380:PHE:HB3	2.47	0.49
1:F:16:SER:HB2	2:F:468:BR:BR	2.68	0.49
1:C:169:PHE:CD1	1:C:173:TRP:CE3	3.01	0.49
1:B:161:PRO:HD2	1:B:218:GLU:OE2	2.13	0.49
1:B:182:MET:HE3	1:B:412:GLY:H	1.76	0.49
1:F:14:LEU:O	1:F:15:ASP:C	2.55	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:HIS:HD2	1:B:261:ASP:OD2	1.96	0.48
1:D:18:PHE:CE1	1:E:428:GLY:HA2	2.48	0.48
1:E:103:MET:HE2	1:F:31:ARG:O	2.13	0.48
1:A:26:ILE:CD1	1:F:435:GLU:HG3	2.43	0.48
1:A:186:GLN:O	1:A:186:GLN:HG3	2.13	0.48
1:B:63:PHE:HE2	1:B:375:ILE:CD1	2.26	0.48
1:E:138:LYS:HE2	1:E:142:ARG:HH22	1.76	0.48
1:A:29:SER:C	1:A:30:LYS:HD2	2.39	0.48
1:C:160:GLY:O	1:C:179:GLU:HG3	2.14	0.48
1:E:375:ILE:O	1:E:377:ALA:N	2.44	0.48
1:C:250:LEU:HD22	1:C:343:GLN:HG3	1.95	0.48
1:B:381:LYS:HB3	1:B:420:VAL:HG12	1.96	0.48
1:E:142:ARG:HG3	1:E:142:ARG:HH11	1.78	0.48
1:B:157:LEU:HD12	1:B:204:GLY:O	2.14	0.48
1:B:333:ARG:HD3	1:B:333:ARG:C	2.39	0.48
1:D:180:ILE:N	1:D:180:ILE:CD1	2.76	0.48
1:F:251:ALA:HB3	1:F:252:PRO:HD3	1.96	0.48
1:E:161:PRO:HD2	1:E:218:GLU:OE2	2.13	0.48
1:B:303:VAL:HG22	1:B:310:ILE:HG23	1.95	0.47
1:C:224:HIS:CD2	1:C:240:MET:HE2	2.49	0.47
1:C:124:ILE:HD11	1:C:319:ARG:HD2	1.96	0.47
1:E:141:TRP:CZ3	1:E:155:PRO:HB3	2.49	0.47
1:B:11:SER:O	1:B:15:ASP:HB2	2.14	0.47
1:C:343:GLN:OE1	1:C:343:GLN:HA	2.14	0.47
1:E:124:ILE:HG12	1:E:319:ARG:HD2	1.96	0.47
1:F:187:LEU:HD13	1:F:411:LEU:HD13	1.97	0.47
1:C:144:ARG:NH1	1:C:237:ASP:O	2.46	0.47
1:D:289:TRP:CH2	1:D:313:PHE:HD2	2.31	0.47
1:F:395:LEU:HD21	1:F:441:TYR:CZ	2.49	0.47
1:B:36:GLU:OE2	1:F:15:ASP:N	2.48	0.47
1:D:13:LEU:HG	1:D:14:LEU:HD23	1.97	0.47
1:D:169:PHE:HD1	1:D:173:TRP:CE3	2.33	0.47
1:D:305:TYR:CE1	1:D:306:LEU:HG	2.50	0.47
1:F:221:GLN:CB	1:F:222:PRO:HD3	2.44	0.47
1:D:10:ARG:HG2	1:D:10:ARG:NH1	2.30	0.47
1:D:251:ALA:HB3	1:D:252:PRO:HD3	1.96	0.47
1:A:366:ILE:HD12	1:A:420:VAL:HG11	1.95	0.47
1:D:10:ARG:HG2	1:D:10:ARG:HH11	1.78	0.47
1:F:63:PHE:CD2	1:F:424:MET:HE2	2.49	0.47
1:A:401:LEU:CD2	1:F:400:ARG:HB3	2.45	0.46
1:B:48:ASP:HA	1:B:51:TYR:CD2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:92:GLN:O	1:C:96:ILE:HG13	2.15	0.46
1:E:182:MET:HG2	1:E:187:LEU:CA	2.45	0.46
1:F:180:ILE:N	1:F:180:ILE:CD1	2.75	0.46
1:A:326:ALA:O	1:A:329:TYR:HB3	2.16	0.46
1:C:217:TYR:CD2	1:C:374:GLY:HA2	2.50	0.46
1:C:328:TYR:CE2	1:C:332:LEU:HD11	2.50	0.46
1:F:16:SER:O	1:F:17:ARG:C	2.57	0.46
1:B:97:ASP:O	1:B:100:CYS:HB2	2.16	0.46
1:C:325:ILE:HD13	1:D:50:LEU:HD21	1.98	0.46
1:D:333:ARG:O	1:D:333:ARG:HD3	2.15	0.46
1:E:17:ARG:HB2	1:E:17:ARG:HE	1.65	0.46
1:A:234:THR:OG1	1:A:236:ILE:HG13	2.16	0.46
1:A:329:TYR:HA	1:B:46:ILE:CD1	2.45	0.46
1:C:157:LEU:HD12	1:C:204:GLY:O	2.16	0.46
1:E:224:HIS:NE2	1:E:266:ARG:HB2	2.30	0.46
1:C:208:THR:HG21	1:C:211:VAL:HA	1.98	0.46
1:E:82:LYS:HE2	1:F:50:LEU:HD22	1.98	0.46
1:F:66:THR:HG21	1:F:426:ARG:NH2	2.31	0.46
1:C:180:ILE:H	1:C:180:ILE:CD1	2.29	0.46
1:C:289:TRP:CZ2	1:C:295:LEU:HD13	2.51	0.46
1:A:208:THR:O	1:A:218:GLU:HB2	2.15	0.46
1:F:305:TYR:CB	1:F:310:ILE:HG22	2.45	0.46
1:F:343:GLN:OE1	1:F:343:GLN:HA	2.15	0.46
1:C:59:ASN:HA	1:C:405:GLN:HB2	1.98	0.46
1:C:86:ASP:HB3	1:C:89:GLU:HB2	1.97	0.46
1:C:199:ASP:OD1	1:C:199:ASP:C	2.59	0.46
1:C:48:ASP:HA	1:C:51:TYR:CD2	2.52	0.46
1:F:224:HIS:CD2	1:F:264:LEU:HB3	2.51	0.46
1:C:219:PHE:HA	1:C:220:PRO:HD3	1.81	0.45
1:E:23:ILE:O	1:E:23:ILE:HG23	2.15	0.45
1:B:99:ARG:O	1:B:103:MET:HG3	2.15	0.45
1:C:273:SER:HB3	1:C:276:LYS:HG3	1.98	0.45
1:C:284:CYS:HB2	1:C:323:GLN:HB3	1.99	0.45
1:A:107:LEU:HD22	1:B:32:PHE:CE2	2.52	0.45
1:B:224:HIS:CD2	1:B:266:ARG:HB2	2.51	0.45
1:D:187:LEU:HD13	1:D:411:LEU:HD13	1.98	0.45
1:E:392:LEU:HD23	1:E:392:LEU:HA	1.73	0.45
1:F:110:ALA:HB2	1:F:262:PHE:CD2	2.52	0.45
1:B:17:ARG:NH1	1:B:40:ASP:HB2	2.32	0.45
1:C:82:LYS:HE3	1:D:50:LEU:HD22	1.99	0.45
1:C:302:ASN:HA	1:C:311:GLY:HA2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:83:ASN:OD1	1:F:85:ILE:HG22	2.16	0.45
1:A:57:ARG:HH11	1:A:57:ARG:HG3	1.82	0.45
1:A:105:ALA:HB2	1:A:288:ILE:HD12	1.99	0.45
1:A:124:ILE:HD13	1:A:124:ILE:HA	1.85	0.45
1:A:395:LEU:HD21	1:A:441:TYR:OH	2.16	0.45
1:B:34:LEU:HD23	1:B:35:HIS:CE1	2.52	0.45
1:B:284:CYS:HB2	1:B:323:GLN:HB3	1.99	0.45
1:C:409:PHE:CD1	1:C:409:PHE:N	2.84	0.45
1:D:305:TYR:CD1	1:D:306:LEU:HG	2.51	0.45
1:E:69:ASP:OD1	1:E:72:VAL:HG23	2.16	0.45
1:D:138:LYS:HE2	1:D:142:ARG:NH2	2.32	0.45
1:A:14:LEU:O	1:A:15:ASP:C	2.59	0.45
1:A:303:VAL:HG12	1:A:304:ASP:N	2.32	0.45
1:A:333:ARG:HD3	1:A:333:ARG:C	2.42	0.45
1:C:246:SER:HB3	1:C:375:ILE:HG21	1.99	0.45
1:C:347:TYR:CE1	1:C:376:PRO:HG3	2.52	0.45
1:A:269:SER:HB3	1:A:289:TRP:CD1	2.53	0.44
1:A:370:ARG:HD3	1:A:373:GLU:OE2	2.16	0.44
1:C:36:GLU:HG2	1:D:337:GLU:OE1	2.18	0.44
1:C:224:HIS:HD2	1:C:240:MET:HE2	1.82	0.44
1:D:333:ARG:HD3	1:D:333:ARG:C	2.42	0.44
1:F:219:PHE:HA	1:F:220:PRO:HD3	1.85	0.44
1:A:180:ILE:H	1:A:180:ILE:CD1	2.30	0.44
1:B:159:CYS:SG	1:B:177:LEU:HD11	2.58	0.44
1:D:61:ALA:HB2	1:D:407:PRO:HD3	1.99	0.44
1:D:195:ILE:HG23	1:D:230:PHE:CD1	2.52	0.44
1:C:273:SER:CB	1:C:276:LYS:HG3	2.47	0.44
1:C:318:SER:O	1:C:319:ARG:HB3	2.18	0.44
1:C:337:GLU:CD	1:D:36:GLU:HG2	2.42	0.44
1:D:299:LEU:HB3	1:D:313:PHE:CE1	2.53	0.44
1:D:358:ALA:HB2	1:D:365:PHE:CE2	2.53	0.44
1:A:395:LEU:HD21	1:A:441:TYR:CE1	2.52	0.44
1:C:69:ASP:OD1	1:C:69:ASP:C	2.60	0.44
1:E:194:MET:HE1	1:E:227:LEU:HG	1.99	0.44
1:F:84:TRP:NE1	1:F:97:ASP:OD2	2.48	0.44
1:F:131:MET:CE	1:F:169:PHE:HB2	2.48	0.44
1:A:435:GLU:O	1:A:439:GLU:HG3	2.18	0.44
1:B:182:MET:HE1	1:B:412:GLY:H	1.83	0.44
1:C:126:SER:HB3	3:C:501:PLP:O4P	2.17	0.44
1:C:287:VAL:O	1:C:288:ILE:HD13	2.18	0.44
1:A:137:MET:HE1	1:A:204:GLY:HA3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:435:GLU:HG2	1:F:26:ILE:HD11	1.98	0.44
1:B:208:THR:O	1:B:208:THR:HG22	2.17	0.44
1:C:189:MET:CE	1:C:223:LEU:HD13	2.48	0.44
1:C:366:ILE:O	1:C:366:ILE:HG22	2.18	0.44
1:D:250:LEU:CD1	1:D:376:PRO:HD3	2.48	0.44
1:E:395:LEU:HD21	1:E:441:TYR:OH	2.17	0.44
1:B:417:ASP:OD1	1:B:417:ASP:N	2.50	0.43
1:C:362:PRO:HB2	1:C:386:GLU:HG2	1.99	0.43
1:A:11:SER:HB3	1:A:15:ASP:OD1	2.18	0.43
1:A:110:ALA:HB2	1:A:262:PHE:CD2	2.53	0.43
1:B:101:VAL:O	1:B:102:ASN:C	2.61	0.43
1:B:132:LEU:HA	1:B:132:LEU:HD23	1.82	0.43
1:D:127:SER:O	1:D:131:MET:HG3	2.18	0.43
1:D:169:PHE:CD1	1:D:173:TRP:CE3	3.06	0.43
1:A:36:GLU:HG2	1:B:337:GLU:CD	2.44	0.43
1:C:430:GLU:HG2	1:C:433:PHE:H	1.83	0.43
1:F:398:ARG:HA	1:F:401:LEU:HD12	2.00	0.43
1:A:13:LEU:HD13	1:E:13:LEU:HD13	2.01	0.43
1:A:244:ALA:O	1:A:245:ALA:C	2.61	0.43
1:D:111:PRO:O	1:D:112:ALA:C	2.61	0.43
1:D:269:SER:HB3	1:D:289:TRP:CD1	2.53	0.43
1:E:192:LYS:O	1:E:196:GLU:HG3	2.18	0.43
1:A:57:ARG:HG3	1:A:57:ARG:NH1	2.34	0.43
1:B:261:ASP:HB2	1:B:262:PHE:H	1.60	0.43
1:C:258:ILE:O	1:C:263:ARG:NH2	2.51	0.43
1:D:261:ASP:HB2	1:D:262:PHE:H	1.67	0.43
1:A:18:PHE:CE1	1:F:428:GLY:HA2	2.54	0.43
1:B:36:GLU:OE2	1:F:15:ASP:HA	2.19	0.43
1:D:244:ALA:O	1:D:245:ALA:C	2.60	0.43
1:F:18:PHE:HA	1:F:23:ILE:HG21	2.00	0.43
1:A:213:TYR:CD1	1:A:213:TYR:N	2.86	0.43
1:A:254:VAL:HG21	1:A:347:TYR:CE2	2.54	0.43
1:B:219:PHE:HA	1:B:220:PRO:HD3	1.80	0.43
1:F:14:LEU:O	1:F:15:ASP:O	2.37	0.43
1:F:17:ARG:HB2	1:F:17:ARG:HE	1.61	0.43
1:F:413:GLY:O	1:F:416:THR:HG23	2.19	0.43
1:B:207:PRO:CG	1:B:240:MET:HE2	2.47	0.43
1:D:217:TYR:CD2	1:D:374:GLY:HA2	2.54	0.43
1:B:305:TYR:HB3	1:B:310:ILE:HG22	2.00	0.43
1:C:169:PHE:HD1	1:C:173:TRP:CE3	2.36	0.43
1:C:363:TYR:HB3	1:C:380:PHE:HD2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:63:PHE:CE1	1:D:424:MET:HE3	2.54	0.43
1:E:69:ASP:OD1	1:E:69:ASP:C	2.61	0.43
1:F:120:GLY:HA3	1:F:288:ILE:HD13	2.00	0.43
1:D:12:GLU:O	1:D:38:ARG:HD3	2.19	0.42
1:E:261:ASP:OD1	1:E:263:ARG:HG3	2.19	0.42
1:A:29:SER:HB2	1:B:99:ARG:HG2	2.01	0.42
1:A:33:PRO:HD3	1:B:103:MET:HE2	2.01	0.42
1:A:124:ILE:CG1	1:A:319:ARG:HD2	2.49	0.42
1:A:262:PHE:CE2	1:A:270:ILE:HD12	2.54	0.42
1:B:244:ALA:O	1:B:245:ALA:C	2.60	0.42
1:C:11:SER:O	1:C:12:GLU:C	2.63	0.42
1:D:245:ALA:HA	1:D:273:SER:H	1.85	0.42
1:C:182:MET:SD	1:C:187:LEU:HB3	2.59	0.42
1:A:180:ILE:N	1:A:180:ILE:CD1	2.83	0.42
1:A:435:GLU:HG3	1:F:26:ILE:CD1	2.48	0.42
1:B:59:ASN:HA	1:B:405:GLN:HB2	2.01	0.42
1:B:326:ALA:O	1:B:329:TYR:HB3	2.20	0.42
1:C:11:SER:HB3	1:C:15:ASP:OD2	2.18	0.42
1:C:180:ILE:N	1:C:180:ILE:CD1	2.82	0.42
1:D:264:LEU:HA	1:D:265:PRO:HD3	1.89	0.42
1:D:436:LEU:HD13	1:E:52:LEU:HG	2.00	0.42
1:E:127:SER:O	1:E:131:MET:HG2	2.18	0.42
1:F:23:ILE:HG12	1:F:23:ILE:O	2.18	0.42
1:F:195:ILE:HD12	1:F:230:PHE:CD1	2.54	0.42
1:A:11:SER:C	1:A:13:LEU:N	2.75	0.42
1:A:61:ALA:HB2	1:A:407:PRO:HD3	2.00	0.42
1:E:4:LYS:HE2	1:E:8:ASP:OD2	2.20	0.42
1:F:157:LEU:HD12	1:F:203:ILE:HD11	2.00	0.42
1:A:413:GLY:O	1:A:416:THR:HG23	2.19	0.42
1:B:114:LYS:HB3	1:B:115:ASN:H	1.70	0.42
1:B:343:GLN:OE1	1:B:343:GLN:CA	2.67	0.42
1:C:69:ASP:OD1	1:C:72:VAL:HG23	2.19	0.42
1:C:99:ARG:HD3	1:D:29:SER:HB3	2.01	0.42
1:C:142:ARG:O	1:C:146:GLU:HG3	2.19	0.42
1:C:157:LEU:HD11	1:C:206:VAL:HG23	2.02	0.42
1:C:326:ALA:O	1:C:329:TYR:HB3	2.20	0.42
1:A:158:VAL:HB	1:A:205:VAL:HG22	2.02	0.42
1:A:219:PHE:HA	1:A:220:PRO:HD3	1.75	0.42
1:C:244:ALA:HB1	1:C:248:GLY:N	2.34	0.42
1:D:402:ARG:NH2	1:E:52:LEU:HD12	2.35	0.42
1:B:98:LEU:HB3	1:B:117:GLN:OE1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:188:PHE:CD1	1:C:188:PHE:C	2.97	0.42
1:D:287:VAL:O	1:D:287:VAL:HG13	2.20	0.42
1:E:244:ALA:O	1:E:245:ALA:C	2.61	0.42
1:E:298:GLU:O	1:F:171:ARG:HD3	2.19	0.42
1:F:370:ARG:HG2	1:F:370:ARG:HH11	1.84	0.42
1:B:52:LEU:HD12	1:C:402:ARG:NH2	2.33	0.42
1:C:231:GLN:OE1	1:C:237:ASP:HB2	2.19	0.42
1:E:259:VAL:O	1:E:259:VAL:HG12	2.20	0.42
1:A:337:GLU:OE1	1:B:36:GLU:HG2	2.20	0.42
1:D:66:THR:HG21	1:D:426:ARG:NH2	2.34	0.42
1:D:207:PRO:CG	1:D:240:MET:HE2	2.50	0.42
1:F:127:SER:O	1:F:131:MET:HG2	2.19	0.42
1:F:224:HIS:HD2	1:F:240:MET:CE	2.32	0.42
1:A:381:LYS:HD3	1:A:418:ILE:HG23	2.01	0.41
1:C:61:ALA:HB2	1:C:407:PRO:HD3	2.02	0.41
1:C:127:SER:O	1:C:131:MET:HG3	2.20	0.41
1:D:108:TRP:O	1:D:261:ASP:HB2	2.19	0.41
1:D:199:ASP:OD1	1:D:201:ASN:N	2.53	0.41
1:D:208:THR:HG21	1:D:211:VAL:HA	2.02	0.41
1:E:317:PHE:HB3	1:E:318:SER:H	1.66	0.41
1:C:29:SER:HB2	1:D:99:ARG:HG2	2.03	0.41
1:D:59:ASN:HA	1:D:405:GLN:HB2	2.02	0.41
1:D:199:ASP:OD1	1:D:199:ASP:C	2.63	0.41
1:A:251:ALA:HB3	1:A:252:PRO:HD3	2.01	0.41
1:C:66:THR:HG21	1:C:426:ARG:HH21	1.85	0.41
1:C:99:ARG:O	1:C:103:MET:HG3	2.20	0.41
1:E:195:ILE:HG23	1:E:230:PHE:CD1	2.56	0.41
1:E:343:GLN:OE1	1:E:343:GLN:HA	2.20	0.41
1:F:224:HIS:NE2	1:F:265:PRO:HD2	2.35	0.41
1:A:12:GLU:O	1:A:38:ARG:HD2	2.19	0.41
1:B:445:LEU:HD23	1:B:445:LEU:HA	1.91	0.41
1:D:10:ARG:HA	1:F:9:LEU:HD11	2.02	0.41
1:E:12:GLU:O	1:E:38:ARG:HD2	2.21	0.41
1:F:59:ASN:OD1	1:F:59:ASN:C	2.63	0.41
1:F:244:ALA:O	1:F:245:ALA:C	2.62	0.41
1:C:245:ALA:HA	1:C:273:SER:H	1.85	0.41
1:C:287:VAL:O	1:C:287:VAL:HG13	2.20	0.41
1:C:391:THR:HG23	1:C:394:ASP:OD2	2.21	0.41
1:E:59:ASN:HA	1:E:405:GLN:HB2	2.02	0.41
1:E:85:ILE:HG12	1:E:317:PHE:CE1	2.56	0.41
1:F:61:ALA:HB2	1:F:407:PRO:HD3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:305:TYR:HB2	1:F:310:ILE:HG22	2.02	0.41
1:B:61:ALA:HB2	1:B:407:PRO:HD3	2.03	0.41
1:C:315:ILE:HG23	1:D:131:MET:SD	2.61	0.41
1:D:156:ASN:HB3	1:D:176:GLU:HB3	2.03	0.41
1:E:337:GLU:CD	1:F:36:GLU:HG2	2.45	0.41
1:C:101:VAL:HG13	1:C:288:ILE:CD1	2.51	0.41
1:D:159:CYS:SG	1:D:177:LEU:HD11	2.61	0.41
1:A:435:GLU:CG	1:F:26:ILE:CD1	2.98	0.41
1:C:63:PHE:HB3	1:C:276:LYS:HD3	2.03	0.41
1:D:208:THR:O	1:D:208:THR:HG22	2.20	0.41
1:D:306:LEU:C	1:D:308:GLY:H	2.28	0.41
1:D:326:ALA:O	1:D:329:TYR:HB3	2.21	0.41
1:E:163:GLN:NE2	1:E:164:ILE:HG22	2.36	0.41
1:F:391:THR:O	1:F:392:LEU:C	2.63	0.41
1:A:46:ILE:CD1	1:B:329:TYR:HA	2.51	0.41
1:A:141:TRP:CZ3	1:A:155:PRO:HB3	2.55	0.41
1:C:85:ILE:HG12	1:C:317:PHE:CD1	2.56	0.41
1:A:264:LEU:HA	1:A:265:PRO:HD3	1.95	0.40
1:C:224:HIS:HD2	1:C:266:ARG:HB2	1.84	0.40
1:F:239:ASP:OD1	1:F:268:LYS:HE3	2.21	0.40
1:A:244:ALA:HB1	1:A:248:GLY:N	2.36	0.40
1:B:15:ASP:OD1	1:C:341:LYS:NZ	2.52	0.40
1:C:259:VAL:HA	1:C:263:ARG:NH2	2.36	0.40
1:D:308:GLY:O	1:D:309:GLN:HG3	2.22	0.40
1:E:60:LEU:HD23	1:E:60:LEU:HA	1.95	0.40
1:F:66:THR:HG23	1:F:426:ARG:HE	1.86	0.40
1:B:180:ILE:N	1:B:180:ILE:HD12	2.37	0.40
1:C:57:ARG:HG3	1:C:57:ARG:NH1	2.37	0.40
1:D:124:ILE:HD13	1:D:124:ILE:HA	1.97	0.40
1:E:135:MET:HE3	1:E:313:PHE:CZ	2.56	0.40
1:E:228:ASP:HA	1:E:266:ARG:HH21	1.86	0.40
1:E:244:ALA:HB1	1:E:248:GLY:N	2.37	0.40
1:F:69:ASP:OD1	1:F:69:ASP:C	2.64	0.40
1:F:137:MET:HE2	1:F:241:HIS:CB	2.52	0.40
1:F:344:ASN:HD22	1:F:344:ASN:HA	1.66	0.40
1:A:111:PRO:O	1:A:112:ALA:C	2.64	0.40
1:B:38:ARG:HB3	1:B:40:ASP:OD1	2.21	0.40
1:B:141:TRP:CZ3	1:B:155:PRO:HB3	2.57	0.40
1:C:195:ILE:HG23	1:C:230:PHE:CD1	2.57	0.40
1:C:224:HIS:CD2	1:C:266:ARG:HD2	2.57	0.40
1:C:244:ALA:O	1:C:245:ALA:C	2.62	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:ARG:HB2	2:A:468:BR:BR	2.77	0.40
1:A:59:ASN:OD1	1:A:59:ASN:C	2.65	0.40
1:A:86:ASP:HB3	1:A:89:GLU:HB2	2.03	0.40
1:A:127:SER:O	1:A:131:MET:HG3	2.22	0.40
1:B:317:PHE:HB3	1:B:318:SER:H	1.65	0.40
1:C:154:LYS:N	1:C:155:PRO:CD	2.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	448/466 (96%)	419 (94%)	28 (6%)	1 (0%)	43	71
1	B	448/466 (96%)	421 (94%)	25 (6%)	2 (0%)	30	59
1	C	449/466 (96%)	421 (94%)	28 (6%)	0	100	100
1	D	448/466 (96%)	419 (94%)	29 (6%)	0	100	100
1	E	450/466 (97%)	425 (94%)	25 (6%)	0	100	100
1	F	449/466 (96%)	424 (94%)	23 (5%)	2 (0%)	30	59
All	All	2692/2796 (96%)	2529 (94%)	158 (6%)	5 (0%)	43	71

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	114	LYS
1	F	15	ASP
1	F	17	ARG
1	A	16	SER
1	B	115	ASN

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	376/390 (96%)	362 (96%)	14 (4%)	30	58
1	B	376/390 (96%)	364 (97%)	12 (3%)	34	61
1	C	377/390 (97%)	368 (98%)	9 (2%)	43	66
1	D	376/390 (96%)	365 (97%)	11 (3%)	37	63
1	E	378/390 (97%)	366 (97%)	12 (3%)	34	61
1	F	377/390 (97%)	363 (96%)	14 (4%)	30	58
All	All	2260/2340 (97%)	2188 (97%)	72 (3%)	34	61

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	SER
1	A	25	THR
1	A	34	LEU
1	A	69	ASP
1	A	124	ILE
1	A	126	SER
1	A	131	MET
1	A	188	PHE
1	A	218	GLU
1	A	275	HIS
1	A	360	LEU
1	A	386	GLU
1	A	417	ASP
1	A	435	GLU
1	B	22	SER
1	B	34	LEU
1	B	114	LYS
1	B	124	ILE
1	B	126	SER
1	B	131	MET
1	B	212	THR
1	B	312	THR

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Mol	Chain	Res	Type
1	B	324	VAL
1	B	416	THR
1	B	435	GLU
1	B	438	LEU
1	C	5	GLN
1	C	22	SER
1	C	126	SER
1	C	150	LYS
1	C	208	THR
1	C	290	ARG
1	C	343	GLN
1	C	419	VAL
1	C	435	GLU
1	D	22	SER
1	D	31	ARG
1	D	34	LEU
1	D	98	LEU
1	D	115	ASN
1	D	126	SER
1	D	144	ARG
1	D	303	VAL
1	D	310	ILE
1	D	324	VAL
1	D	438	LEU
1	E	6	VAL
1	E	12	GLU
1	E	22	SER
1	E	31	ARG
1	E	52	LEU
1	E	124	ILE
1	E	126	SER
1	E	287	VAL
1	E	293	GLU
1	E	417	ASP
1	E	419	VAL
1	E	435	GLU
1	F	126	SER
1	F	131	MET
1	F	180	ILE
1	F	200	GLU
1	F	208	THR
1	F	212	THR

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Mol	Chain	Res	Type
1	F	221	GLN
1	F	292	GLU
1	F	303	VAL
1	F	306	LEU
1	F	310	ILE
1	F	332	LEU
1	F	417	ASP
1	F	435	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	HIS
1	A	122	ASN
1	A	221	GLN
1	A	231	GLN
1	A	302	ASN
1	A	344	ASN
1	B	5	GLN
1	B	109	HIS
1	B	167	HIS
1	B	302	ASN
1	B	344	ASN
1	B	348	GLN
1	B	405	GLN
1	C	5	GLN
1	C	35	HIS
1	C	71	ASN
1	C	201	ASN
1	C	302	ASN
1	C	344	ASN
1	D	186	GLN
1	D	201	ASN
1	D	216	ASN
1	D	297	GLN
1	D	302	ASN
1	D	348	GLN
1	D	405	GLN
1	D	451	HIS
1	E	216	ASN
1	E	309	GLN
1	E	316	ASN

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Mol	Chain	Res	Type
1	E	348	GLN
1	E	405	GLN
1	F	35	HIS
1	F	316	ASN
1	F	344	ASN
1	F	348	GLN
1	F	405	GLN

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 36 ligands modelled in this entry, 24 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PLP	C	501	1	15,15,16	0.93	0	21,22,23	1.40	5 (23%)
3	PLP	B	500	1	15,15,16	1.04	1 (6%)	21,22,23	1.35	5 (23%)
3	PLP	F	502	1	15,15,16	0.90	0	21,22,23	1.40	4 (19%)
4	ACY	C	538	-	3,3,3	1.34	1 (33%)	3,3,3	1.65	1 (33%)
4	ACY	C	548	-	3,3,3	1.23	0	3,3,3	1.69	1 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ACY	B	558	-	3,3,3	1.41	1 (33%)	3,3,3	1.55	1 (33%)
4	ACY	F	528	-	3,3,3	1.16	0	3,3,3	1.74	1 (33%)
4	ACY	E	518	-	3,3,3	1.38	1 (33%)	3,3,3	1.63	1 (33%)
4	ACY	A	568	-	3,3,3	1.34	1 (33%)	3,3,3	1.63	1 (33%)
3	PLP	E	502	1	15,15,16	0.93	0	21,22,23	1.36	5 (23%)
3	PLP	A	500	1	15,15,16	0.97	1 (6%)	21,22,23	1.43	5 (23%)
3	PLP	D	501	1	15,15,16	0.74	0	21,22,23	1.45	4 (19%)

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	C	501	1	-	4/6/6/8	0/1/1/1
3	PLP	B	500	1	-	0/6/6/8	0/1/1/1
3	PLP	F	502	1	-	1/6/6/8	0/1/1/1
3	PLP	E	502	1	-	5/6/6/8	0/1/1/1
3	PLP	A	500	1	-	2/6/6/8	0/1/1/1
3	PLP	D	501	1	-	5/6/6/8	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	518	ACY	O-C	2.17	1.31	1.22
4	C	538	ACY	O-C	2.13	1.31	1.22
4	B	558	ACY	O-C	2.11	1.31	1.22
3	B	500	PLP	C3-C4	2.09	1.44	1.40
4	A	568	ACY	O-C	2.08	1.31	1.22
3	A	500	PLP	C3-C2	2.05	1.43	1.41

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	501	PLP	C6-N1-C2	2.74	124.17	119.20
3	D	501	PLP	C6-N1-C2	2.71	124.11	119.20
3	B	500	PLP	C6-N1-C2	2.71	124.11	119.20
3	A	500	PLP	C4A-C4-C5	2.69	123.71	120.94
3	D	501	PLP	C3-C2-N1	-2.68	117.58	120.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	501	PLP	C4A-C4-C5	2.66	123.68	120.94
3	E	502	PLP	C6-N1-C2	2.65	124.01	119.20
3	C	501	PLP	C3-C2-N1	-2.62	117.66	120.96
3	F	502	PLP	C4A-C4-C5	2.61	123.63	120.94
3	A	500	PLP	C3-C2-N1	-2.60	117.68	120.96
3	C	501	PLP	C2A-C2-C3	2.59	123.83	120.80
3	A	500	PLP	C6-N1-C2	2.58	123.87	119.20
3	A	500	PLP	C2A-C2-C3	2.52	123.75	120.80
3	F	502	PLP	C6-N1-C2	2.52	123.77	119.20
3	E	502	PLP	C3-C2-N1	-2.49	117.82	120.96
3	B	500	PLP	C3-C2-N1	-2.43	117.90	120.96
3	B	500	PLP	C2A-C2-C3	2.41	123.61	120.80
3	F	502	PLP	C3-C2-N1	-2.39	117.95	120.96
3	D	501	PLP	C2A-C2-C3	2.37	123.58	120.80
4	F	528	ACY	O-C-CH3	-2.36	112.87	122.53
3	E	502	PLP	C2A-C2-C3	2.31	123.51	120.80
4	C	548	ACY	O-C-CH3	-2.29	113.14	122.53
3	E	502	PLP	C4A-C4-C5	2.27	123.28	120.94
3	C	501	PLP	C4A-C4-C5	2.25	123.26	120.94
4	C	538	ACY	O-C-CH3	-2.23	113.39	122.53
4	A	568	ACY	O-C-CH3	-2.22	113.44	122.53
4	E	518	ACY	O-C-CH3	-2.20	113.52	122.53
3	F	502	PLP	C2A-C2-C3	2.18	123.35	120.80
3	C	501	PLP	O3P-P-O1P	2.16	119.23	110.83
3	B	500	PLP	C4A-C4-C5	2.15	123.16	120.94
4	B	558	ACY	O-C-CH3	-2.09	113.96	122.53
3	B	500	PLP	O3P-P-O1P	2.05	118.84	110.83
3	A	500	PLP	O3P-P-O1P	2.04	118.78	110.83
3	E	502	PLP	O3P-P-O1P	2.03	118.73	110.83

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	500	PLP	C5A-O4P-P-O2P
3	C	501	PLP	C4-C5-C5A-O4P
3	C	501	PLP	C5A-O4P-P-O2P
3	D	501	PLP	C5A-O4P-P-O1P
3	D	501	PLP	C5A-O4P-P-O2P
3	D	501	PLP	C5A-O4P-P-O3P
3	E	502	PLP	C5A-O4P-P-O1P
3	E	502	PLP	C5A-O4P-P-O2P

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Mol	Chain	Res	Type	Atoms
3	E	502	PLP	C5A-O4P-P-O3P
3	C	501	PLP	C5A-O4P-P-O1P
3	F	502	PLP	C5A-O4P-P-O1P
3	D	501	PLP	C6-C5-C5A-O4P
3	A	500	PLP	C5A-O4P-P-O3P
3	D	501	PLP	C4-C5-C5A-O4P
3	E	502	PLP	C4-C5-C5A-O4P
3	C	501	PLP	C6-C5-C5A-O4P
3	E	502	PLP	C6-C5-C5A-O4P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	501	PLP	1	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	450/466 (96%)	-0.20	3 (0%) 84 69	15, 34, 61, 79	0
1	B	450/466 (96%)	-0.32	4 (0%) 81 64	11, 30, 56, 82	0
1	C	451/466 (96%)	-0.11	4 (0%) 81 64	14, 37, 64, 80	0
1	D	450/466 (96%)	-0.26	2 (0%) 88 78	16, 35, 60, 85	0
1	E	452/466 (96%)	-0.31	3 (0%) 84 69	12, 31, 57, 77	0
1	F	451/466 (96%)	-0.38	2 (0%) 88 78	12, 30, 56, 84	0
All	All	2704/2796 (96%)	-0.26	18 (0%) 84 69	11, 33, 60, 85	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	5	GLN	3.6
1	A	3	LYS	3.5
1	D	3	LYS	3.4
1	F	453	LYS	3.1
1	B	5	GLN	3.0
1	E	454	LEU	2.9
1	E	453	LYS	2.9
1	D	5	GLN	2.6
1	B	452	PRO	2.5
1	C	453	LYS	2.4
1	B	297	GLN	2.4
1	B	3	LYS	2.3
1	E	5	GLN	2.3
1	A	5	GLN	2.3
1	C	151	PRO	2.2
1	F	3	LYS	2.2
1	A	452	PRO	2.2
1	C	306	LEU	2.1

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	BR	E	470	1/1	0.91	0.10	93,93,93,93	0
4	ACY	E	518	4/4	0.92	0.25	68,69,69,69	0
4	ACY	C	538	4/4	0.93	0.18	72,73,73,73	0
2	BR	A	470	1/1	0.94	0.09	98,98,98,98	0
3	PLP	C	501	15/16	0.95	0.10	36,43,44,45	0
2	BR	D	468	1/1	0.95	0.08	66,66,66,66	0
2	BR	D	467	1/1	0.95	0.06	67,67,67,67	0
2	BR	E	468	1/1	0.96	0.07	62,62,62,62	0
2	BR	C	467	1/1	0.96	0.10	76,76,76,76	0
2	BR	F	470	1/1	0.96	0.09	100,100,100,100	0
2	BR	B	468	1/1	0.96	0.08	78,78,78,78	0
4	ACY	A	568	4/4	0.96	0.10	28,29,30,31	0
4	ACY	B	558	4/4	0.96	0.12	42,42,42,44	0
2	BR	B	471	1/1	0.96	0.10	83,83,83,83	0
2	BR	D	469	1/1	0.96	0.10	121,121,121,121	0
2	BR	B	467	1/1	0.97	0.05	69,69,69,69	0
3	PLP	D	501	15/16	0.97	0.07	26,31,34,35	0
2	BR	F	468	1/1	0.97	0.04	67,67,67,67	0
2	BR	F	469	1/1	0.97	0.09	90,90,90,90	0
2	BR	A	468	1/1	0.97	0.08	75,75,75,75	0
4	ACY	C	548	4/4	0.97	0.12	48,49,49,49	0
3	PLP	A	500	15/16	0.97	0.09	27,37,42,43	0
4	ACY	F	528	4/4	0.97	0.11	43,43,43,45	0
3	PLP	E	502	15/16	0.98	0.07	25,27,28,29	0
3	PLP	F	502	15/16	0.98	0.07	21,26,28,30	0
2	BR	C	470	1/1	0.98	0.09	117,117,117,117	0
2	BR	B	470	1/1	0.98	0.10	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	BR	A	469	1/1	0.98	0.06	67,67,67,67	0
2	BR	B	469	1/1	0.98	0.04	56,56,56,56	0
2	BR	C	468	1/1	0.98	0.09	58,58,58,58	0
2	BR	C	469	1/1	0.98	0.06	84,84,84,84	0
2	BR	A	467	1/1	0.99	0.04	66,66,66,66	0
2	BR	E	469	1/1	0.99	0.07	64,64,64,64	0
2	BR	E	467	1/1	0.99	0.06	70,70,70,70	1
2	BR	F	467	1/1	0.99	0.10	58,58,58,58	1
3	PLP	B	500	15/16	0.99	0.06	22,27,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.