



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 11:19 pm BST

PDB ID : 2DGL  
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](mailto: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.

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

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

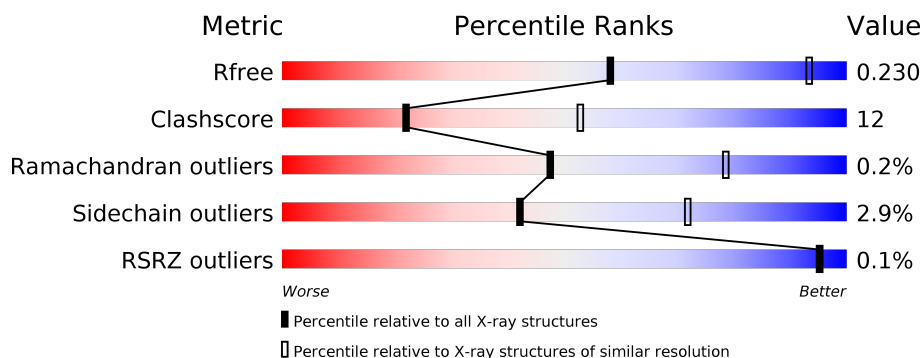
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.15 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))
$R_{free}$	130704	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	<div> <div>71%</div> <div>24%</div> <div>• •</div> </div>
1	B	466	<div> <div>73%</div> <div>23%</div> <div>• •</div> </div>
1	C	466	<div> <div>65%</div> <div>31%</div> <div>• •</div> </div>
1	D	466	<div> <div>71%</div> <div>24%</div> <div>• •</div> </div>
1	E	466	<div> <div>75%</div> <div>21%</div> <div>• •</div> </div>
1	F	466	<div> <div>74%</div> <div>22%</div> <div>• •</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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 (three-letter code: BR) (formula: Br).

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

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C<sub>8</sub>H<sub>10</sub>NO<sub>6</sub>P).



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 (three-letter code: ACY) (formula: C<sub>2</sub>H<sub>4</sub>O<sub>2</sub>).



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		

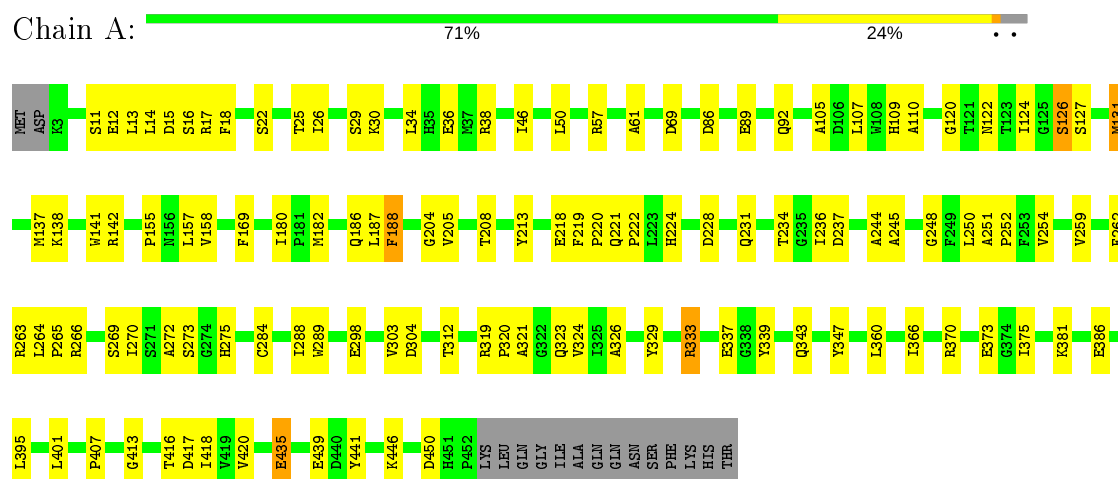
- Molecule 5 is water.

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		

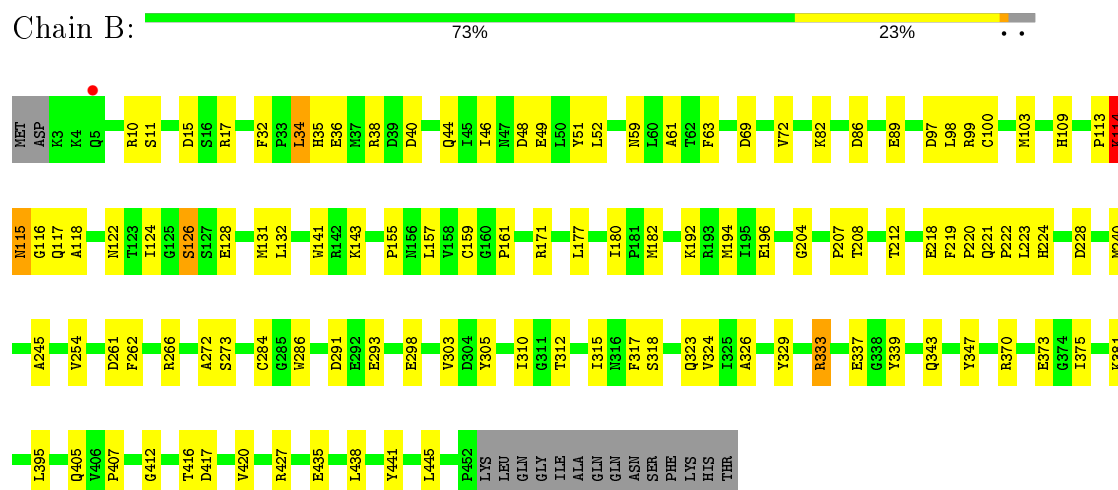
### 3 Residue-property plots

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

#### • Molecule 1: Glutamate decarboxylase beta

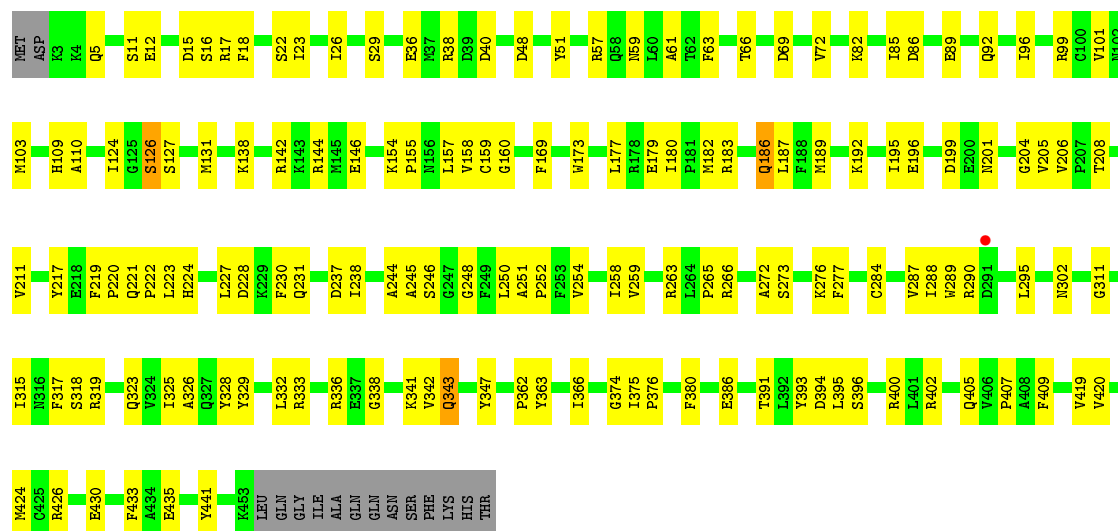


#### • Molecule 1: Glutamate decarboxylase beta



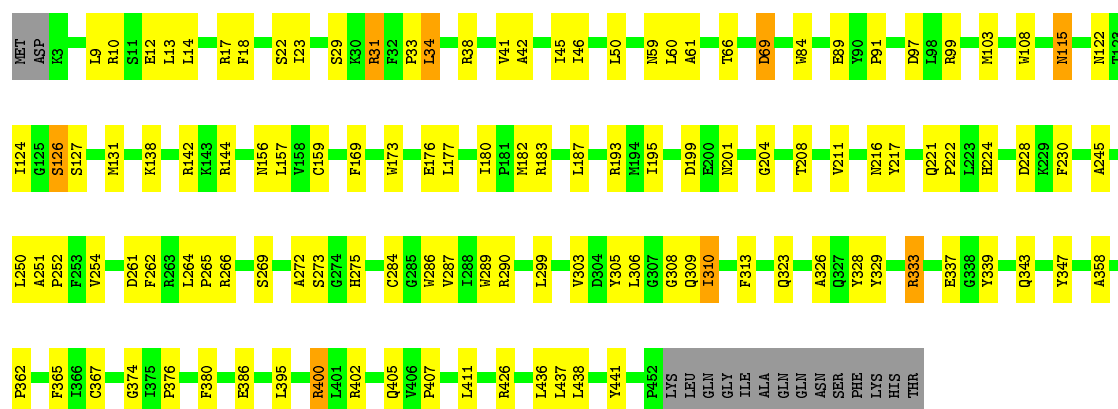
#### • Molecule 1: Glutamate decarboxylase beta





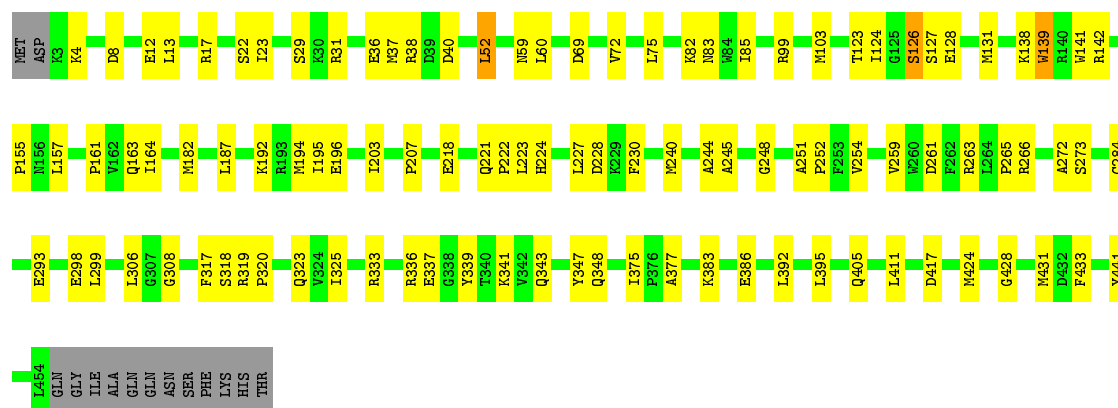
• Molecule 1: Glutamate decarboxylase beta

Chain D: 71% 24%



• Molecule 1: Glutamate decarboxylase beta

Chain E: 75% 21%



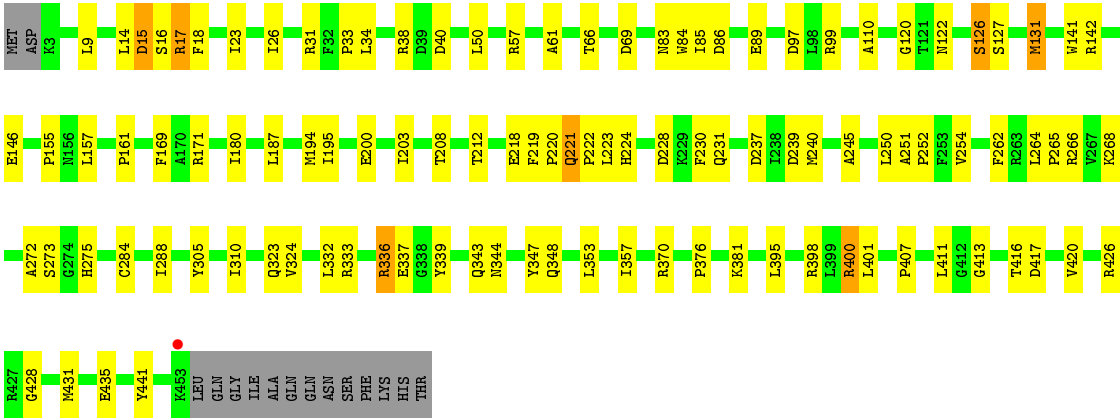
• Molecule 1: Glutamate decarboxylase beta



Chain F: 

74%

22%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	297.05Å 297.05Å 233.73Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 3.15 39.77 – 3.15	Depositor EDS
% Data completeness (in resolution range)	99.6 (40.00-3.15) 99.7 (39.77-3.15)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.13	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.92 (at 3.12Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.218 , 0.248 0.206 , 0.230	Depositor DCC
$R_{free}$ test set	2067 reflections (1.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	50.6	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 35.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.41	0/3669	0.63	1/4974 (0.0%)
1	B	0.45	0/3669	0.63	0/4974
1	C	0.40	0/3678	0.60	0/4985
1	D	0.40	0/3669	0.61	0/4974
1	E	0.42	0/3686	0.62	0/4996
1	F	0.44	0/3678	0.62	0/4985
All	All	0.42	0/22049	0.62	1/29888 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	157	LEU	CA-CB-CG	5.21	127.28	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3577	0	3483	94	0
1	B	3577	0	3483	79	0
1	C	3586	0	3496	123	0
1	D	3577	0	3483	92	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	3594	0	3507	79	0
1	F	3586	0	3496	86	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	505	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 12.

All (505) 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:E:182:MET:HE3	1:E:187:LEU:HB3	1.17	1.16
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:103:MET:HE2	1:D:33:PRO:HD3	1.61	0.82
1:E:383:LYS:HB2	1:E:386:GLU:HG3	1.61	0.81
1:A:228:ASP:HA	1:A:266:ARG:NH2	1.94	0.81
1:A:122:ASN:ND2	1:A:319:ARG:HH22	1.80	0.79
1:D:182:MET:HE2	1:D:187:LEU:HB3	1.64	0.78
1:B:291:ASP:OD2	1:B:293:GLU:HG2	1.83	0.78
1:E:221:GLN:HB3	1:E:222:PRO:HD3	1.65	0.77
1:F:126:SER:HB2	1:F:273:SER:OG	1.84	0.77
1:F:336:ARG:HH11	1:F:336:ARG:HG3	1.50	0.77
1:F:348:GLN:HE21	1:F:431:MET:HE2	1.48	0.76
1:E:377:ALA:HB2	1:E:424:MET:HE1	1.68	0.75
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:D:126:SER:HB2	1:D:273:SER:OG	1.89	0.73
1:D:23:ILE:HG13	1:D:45:ILE:HD11	1.70	0.73
1:E:103:MET:HE2	1:F:33:PRO:HD3	1.70	0.72
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:C:103:MET:CE	1:D:33:PRO:HD3	2.22	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
1:B:228:ASP:HA	1:B:266:ARG:HH21	1.57	0.67
1:E:83:ASN:OD1	1:E:85:ILE:HG22	1.94	0.67
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: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:E:348:GLN:HE21	1:E:431:MET:HE3	1.62	0.64
1:A:137:MET:CE	1:A:204:GLY:HA3	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:180:ILE:HD12	1:F:180:ILE:N	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: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:75:LEU:HD13	1:E:325:ILE:HG22	1.83	0.61
1:E:38:ARG:HB3	1:E:40:ASP:OD1	2.00	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
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: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:HD12	1:C:180:ILE:N	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:LEU:HD22	1:B:82:LYS:HE3	1.86	0.58
1:F:400:ARG:HD3	1:F:400:ARG:O	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:A:137:MET:HE1	1:A:204:GLY:HA3	1.85	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:F:395:LEU:HD21	1:F:441:TYR:CE1	2.40	0.57
1:E:182:MET:HE2	1:E:411:LEU:HD13	1.86	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
1:A:124:ILE:HG12	1:A:319:ARG:HD2	1.88	0.56
1:A:259:VAL:HA	1:A:263:ARG:NH2	2.20	0.56
1:A:221:GLN:HB3	1:A:222:PRO:CD	2.29	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: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:OE1	1:B:343:GLN:HA	2.05	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:E:194:MET:HE1	1:E:227:LEU:HG	1.88	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:180:ILE:HD12	1:D:180:ILE:N	2.21	0.55
1:D:221:GLN:HB3	1:D:222:PRO:CD	2.29	0.54
1:D:41:VAL:O	1:D:45:ILE:HG12	2.07	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:D:69:ASP:C	1:D:69:ASP:OD1	2.46	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
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:C:159:CYS:SG	1:C:177:LEU:HD11	2.49	0.53
1:E:37:MET:HE3	1:F:332:LEU:HB3	1.91	0.53
1:C:386:GLU:OE1	1:C:386:GLU:HA	2.10	0.52
1:B:10:ARG:HA	1:D:9:LEU:HD11	1.91	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:HD3	1:D:400:ARG:O	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: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:337:GLU:HG2	1:E:341:LYS:HE3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:182:MET:HE1	1:D:411:LEU:HB3	1.93	0.51
1:E:254:VAL:HG21	1:E:347:TYR:HE2	1.74	0.51
1:E:245:ALA:HA	1:E:272:ALA:HA	1.92	0.51
1:F:38:ARG:HB3	1:F:40:ASP:OD1	2.11	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:D:182:MET:CE	1:D:187:LEU:HB3	2.38	0.51
1:E:182:MET:HE3	1:E:187:LEU:CB	2.12	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:N	1:A:323:GLN:OE1	2.41	0.51
1:D:224:HIS:CD2	1:D:266:ARG:HB2	2.46	0.51
1:E:377:ALA:HB2	1:E:424:MET:CE	2.37	0.51
1:B:435:GLU:CG	1:C:26:ILE:HD13	2.40	0.51
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: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:B:254:VAL:HG21	1:B:347:TYR:HE2	1.76	0.50
1:F:57:ARG:NH1	1:F:57:ARG:HG3	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:A:137:MET:HE2	1:A:204:GLY:HA3	1.94	0.50
1:D:103:MET:HE1	1:D:328:TYR:HE1	1.77	0.50
1:F:353:LEU:O	1:F:357:ILE:HG13	2.12	0.50
1:A:180:ILE:H	1:A:180:ILE:HD12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:182:MET:HE1	1:B:412:GLY:H	1.77	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:339:TYR:O	1:D:343:GLN:HG2	2.12	0.49
1:D:84:TRP:NE1	1:D:97:ASP:OD2	2.45	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:A:131:MET:HE2	1:A:169:PHE:HB2	1.94	0.48
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: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:26:ILE:CD1	1:F:435:GLU:HG3	2.43	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:D:180:ILE:CD1	1:D:180:ILE:N	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: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:HA	1:C:343:GLN:OE1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:169:PHE:HD1	1:D:173:TRP:CE3	2.33	0.47
1:F:221:GLN:CB	1:F:222:PRO:HD3	2.44	0.47
1:F:348:GLN:NE2	1:F:431:MET:HE2	2.22	0.47
1:D:13:LEU:HG	1:D:14:LEU:HD23	1.97	0.47
1:D:305:TYR:CE1	1:D:306:LEU:HG	2.50	0.47
1:D:10:ARG:NH1	1:D:10:ARG:HG2	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:HH11	1:D:10:ARG:HG2	1.78	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
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:B:97:ASP:O	1:B:100:CYS:HB2	2.16	0.46
1:D:333:ARG:HD3	1:D:333:ARG:O	2.15	0.46
1:C:325:ILE:HD13	1:D:50:LEU:HD21	1.98	0.46
1:E:17:ARG:HB2	1:E:17:ARG:HE	1.65	0.46
1:E:306:LEU:C	1:E:308:GLY:H	2.18	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:HA	1:F:343:GLN:OE1	2.15	0.46
1:C:59:ASN:HA	1:C:405:GLN:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:86:ASP:HB3	1:C:89:GLU:HB2	1.97	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:B:224:HIS:CD2	1:B:266:ARG:HB2	2.51	0.45
1:A:107:LEU:HD22	1:B:32:PHE:CE2	2.52	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:302:ASN:HA	1:C:311:GLY:HA2	1.97	0.45
1:C:82:LYS:HE3	1:D:50:LEU:HD22	1.99	0.45
1:D:89:GLU:C	1:D:91:PRO:HD3	2.36	0.45
1:F:83:ASN:OD1	1:F:85:ILE:HG22	2.16	0.45
1:A:124:ILE:HA	1:A:124:ILE:HD13	1.85	0.45
1:A:105:ALA:HB2	1:A:288:ILE:HD12	1.99	0.45
1:A:395:LEU:HD21	1:A:441:TYR:OH	2.16	0.45
1:A:57:ARG:HG3	1:A:57:ARG:HH11	1.82	0.45
1:B:284:CYS:HB2	1:B:323:GLN:HB3	1.99	0.45
1:B:34:LEU:HD23	1:B:35:HIS:CE1	2.52	0.45
1:C:409:PHE:N	1:C:409:PHE:CD1	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:303:VAL:HG12	1:A:304:ASP:N	2.32	0.45
1:C:109:HIS:O	1:C:110:ALA:C	2.55	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: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:126:SER:HB2	1:D:273:SER:HG	1.82	0.44
1:D:195:ILE:HG23	1:D:230:PHE:CD1	2.52	0.44
1:D:61:ALA:HB2	1:D:407:PRO:HD3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:63:PHE:CZ	1:C:424:MET:HE1	2.52	0.44
1:F:14:LEU:O	1:F:15:ASP:C	2.55	0.44
1:F:131:MET:CE	1:F:169:PHE:HB2	2.48	0.44
1:F:84:TRP:NE1	1:F:97:ASP:OD2	2.48	0.44
1:A:435:GLU:O	1:A:439:GLU:HG3	2.18	0.44
1:C:287:VAL:O	1:C:288:ILE:HD13	2.18	0.44
1:C:126:SER:HB3	3:C:501:PLP:O4P	2.17	0.44
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:HG22	1:C:366:ILE:O	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:110:ALA:HB2	1:A:262:PHE:CD2	2.53	0.43
1:A:11:SER:HB3	1:A:15:ASP:OD1	2.18	0.43
1:A:29:SER:C	1:A:30:LYS:HD2	2.39	0.43
1:B:132:LEU:HA	1:B:132:LEU:HD23	1.82	0.43
1:B:182:MET:HE3	1:B:412:GLY:H	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:182:MET:CE	1:A:187:LEU:HB3	2.48	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: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:NH1	1:A:57:ARG:HG3	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:333:ARG:HD3	1:B:333:ARG:C	2.39	0.43
1:B:36:GLU:OE2	1:F:15:ASP:HA	2.19	0.43
1:F:18:PHE:HA	1:F:23:ILE:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:16:SER:O	1:F:17:ARG:C	2.57	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:C:103:MET:HE2	1:D:31:ARG:O	2.18	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
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:262:PHE:CE2	1:A:270:ILE:HD12	2.54	0.42
1:A:124:ILE:CG1	1:A:319:ARG:HD2	2.49	0.42
1:A:29:SER:HB2	1:B:99:ARG:HG2	2.01	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:326:ALA:O	1:B:329:TYR:HB3	2.20	0.42
1:B:59:ASN:HA	1:B:405:GLN:HB2	2.01	0.42
1:C:11:SER:HB3	1:C:15:ASP:OD2	2.18	0.42
1:C:180:ILE:CD1	1:C:180:ILE:N	2.82	0.42
1:C:63:PHE:CE1	1:C:424:MET:HE3	2.54	0.42
1:D:264:LEU:HA	1:D:265:PRO:HD3	1.89	0.42
1:E:127:SER:O	1:E:131:MET:HG2	2.18	0.42
1:D:436:LEU:HD13	1:E:52:LEU:HG	2.00	0.42
1:F:195:ILE:HD12	1:F:230:PHE:CD1	2.54	0.42
1:F:23:ILE:HG12	1:F:23:ILE:O	2.18	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:D:287:VAL:O	1:D:287:VAL:HG13	2.20	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: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:127:SER:O	1:C:131:MET:HG3	2.20	0.41
1:C:61:ALA:HB2	1:C:407:PRO:HD3	2.02	0.41
1:D:108:TRP:O	1:D:261:ASP:HB2	2.19	0.41
1:E:207:PRO:HG2	1:E:240:MET:CE	2.50	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:E:103:MET:HE2	1:F:31:ARG:O	2.21	0.41
1:D:59:ASN:HA	1:D:405:GLN:HB2	2.02	0.41
1:C:29:SER:HB2	1:D:99:ARG:HG2	2.03	0.41
1:A:251:ALA:HB3	1:A:252:PRO:HD3	2.01	0.41
1:C:99:ARG:O	1:C:103:MET:HG3	2.20	0.41
1:C:66:THR:HG21	1:C:426:ARG:HH21	1.85	0.41
1:E:195:ILE:HG23	1:E:230:PHE:CD1	2.56	0.41
1:E:207:PRO:HG2	1:E:240:MET:HE1	2.03	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:E:12:GLU:O	1:E:38:ARG:HD2	2.21	0.41
1:D:10:ARG:HA	1:F:9:LEU:HD11	2.02	0.41
1:B:207:PRO:HG2	1:B:240:MET:HE2	2.02	0.41
1:C:245:ALA:HA	1:C:273:SER:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:305:TYR:HB2	1:F:310:ILE:HG22	2.02	0.41
1:F:61:ALA:HB2	1:F:407:PRO:HD3	2.03	0.41
1:B:61:ALA:HB2	1:B:407:PRO:HD3	2.03	0.41
1:C:199:ASP:OD1	1:C:199:ASP:C	2.59	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: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:14:LEU:O	1:A:15:ASP:C	2.59	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:HG22	1:D:208:THR:O	2.20	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:A:141:TRP:CZ3	1:A:155:PRO:HB3	2.55	0.41
1:A:46:ILE:CD1	1:B:329:TYR:HA	2.51	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:HD12	1:B:180:ILE:N	2.37	0.40
1:C:57:ARG:HG3	1:C:57:ARG:NH1	2.37	0.40
1:D:124:ILE:HA	1:D:124:ILE:HD13	1.97	0.40
1:E:244:ALA:HB1	1:E:248:GLY:N	2.37	0.40
1:E:228:ASP:HA	1:E:266:ARG:HH21	1.86	0.40
1:F:344:ASN:HA	1:F:344:ASN:HD22	1.66	0.40
1:B:141:TRP:CZ3	1:B:155:PRO:HB3	2.57	0.40
1:B:38:ARG:HB3	1:B:40:ASP:OD1	2.21	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:63:PHE:CE1	1:C:424:MET:CE	3.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:SER:O	1:A:131:MET:HG3	2.22	0.40
1:A:17:ARG:HB2	2:A:468:BR:BR	2.77	0.40
1:A:86:ASP:HB3	1:A:89:GLU:HB2	2.03	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%)	47	78
1	B	448/466 (96%)	421 (94%)	25 (6%)	2 (0%)	34	68
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%)	34	68
All	All	2692/2796 (96%)	2529 (94%)	158 (6%)	5 (0%)	47	78

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%)	363 (96%)	13 (4%)	36	67
1	B	376/390 (96%)	365 (97%)	11 (3%)	42	72
1	C	377/390 (97%)	368 (98%)	9 (2%)	49	76
1	D	376/390 (96%)	363 (96%)	13 (4%)	36	67
1	E	378/390 (97%)	370 (98%)	8 (2%)	53	78
1	F	377/390 (97%)	365 (97%)	12 (3%)	39	70
All	All	2260/2340 (97%)	2194 (97%)	66 (3%)	42	72

All (66) 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	126	SER
1	A	131	MET
1	A	188	PHE
1	A	275	HIS
1	A	333	ARG
1	A	360	LEU
1	A	386	GLU
1	A	417	ASP
1	A	435	GLU
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
1	B	324	VAL
1	B	333	ARG

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Mol	Chain	Res	Type
1	B	416	THR
1	B	438	LEU
1	C	5	GLN
1	C	22	SER
1	C	126	SER
1	C	186	GLN
1	C	290	ARG
1	C	333	ARG
1	C	343	GLN
1	C	400	ARG
1	C	435	GLU
1	D	22	SER
1	D	31	ARG
1	D	34	LEU
1	D	69	ASP
1	D	115	ASN
1	D	126	SER
1	D	144	ARG
1	D	275	HIS
1	D	303	VAL
1	D	310	ILE
1	D	333	ARG
1	D	400	ARG
1	D	438	LEU
1	E	22	SER
1	E	31	ARG
1	E	52	LEU
1	E	126	SER
1	E	139	TRP
1	E	333	ARG
1	E	417	ASP
1	E	433	PHE
1	F	69	ASP
1	F	126	SER
1	F	131	MET
1	F	200	GLU
1	F	208	THR
1	F	212	THR
1	F	221	GLN
1	F	275	HIS
1	F	333	ARG
1	F	336	ARG

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Mol	Chain	Res	Type
1	F	400	ARG
1	F	417	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	HIS
1	A	122	ASN
1	A	231	GLN
1	A	344	ASN
1	B	81	ASN
1	B	109	HIS
1	B	302	ASN
1	B	344	ASN
1	B	348	GLN
1	C	5	GLN
1	C	216	ASN
1	C	316	ASN
1	C	344	ASN
1	D	186	GLN
1	D	201	ASN
1	D	216	ASN
1	D	316	ASN
1	D	451	HIS
1	E	216	ASN
1	E	348	GLN
1	F	81	ASN
1	F	221	GLN
1	F	344	ASN
1	F	348	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

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	D	501	1	15,15,16	0.73	0	20,22,23	1.44	4 (20%)
3	PLP	C	501	1	15,15,16	0.91	0	20,22,23	1.39	5 (25%)
4	ACY	C	538	-	1,3,3	2.57	1 (100%)	0,3,3	0.00	-
3	PLP	E	502	1	15,15,16	0.92	0	20,22,23	1.34	5 (25%)
3	PLP	B	500	1	15,15,16	1.02	0	20,22,23	1.34	5 (25%)
4	ACY	F	528	-	1,3,3	2.08	1 (100%)	0,3,3	0.00	-
4	ACY	C	548	-	1,3,3	2.76	1 (100%)	0,3,3	0.00	-
4	ACY	A	568	-	1,3,3	3.19	1 (100%)	0,3,3	0.00	-
3	PLP	A	500	1	15,15,16	0.98	1 (6%)	20,22,23	1.42	5 (25%)
3	PLP	F	502	1	15,15,16	0.89	0	20,22,23	1.40	3 (15%)
4	ACY	B	558	-	1,3,3	3.48	1 (100%)	0,3,3	0.00	-
4	ACY	E	518	-	1,3,3	2.88	1 (100%)	0,3,3	0.00	-

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PLP	F	502	1	-	1/6/6/8	0/1/1/1
3	PLP	A	500	1	-	2/6/6/8	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	558	ACY	CH3-C	3.48	1.53	1.48
4	A	568	ACY	CH3-C	3.19	1.52	1.48
4	E	518	ACY	CH3-C	2.88	1.52	1.48
4	C	548	ACY	CH3-C	2.76	1.52	1.48
4	C	538	ACY	CH3-C	2.57	1.52	1.48
3	A	500	PLP	C3-C2	2.20	1.43	1.40
4	F	528	ACY	CH3-C	2.08	1.51	1.48

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	501	PLP	C6-N1-C2	2.70	124.17	119.17
3	A	500	PLP	C4A-C4-C5	2.70	123.71	120.94
3	D	501	PLP	C6-N1-C2	2.67	124.11	119.17
3	B	500	PLP	C6-N1-C2	2.67	124.11	119.17
3	D	501	PLP	C4A-C4-C5	2.66	123.68	120.94
3	F	502	PLP	C4A-C4-C5	2.62	123.63	120.94
3	E	502	PLP	C6-N1-C2	2.61	124.01	119.17
3	A	500	PLP	C6-N1-C2	2.54	123.87	119.17
3	F	502	PLP	C6-N1-C2	2.48	123.77	119.17
3	D	501	PLP	C3-C2-N1	-2.46	117.58	120.77
3	C	501	PLP	C3-C2-N1	-2.41	117.66	120.77
3	A	500	PLP	C3-C2-N1	-2.39	117.68	120.77
3	C	501	PLP	C2A-C2-C3	2.38	123.83	120.89
3	A	500	PLP	C2A-C2-C3	2.31	123.75	120.89
3	E	502	PLP	C3-C2-N1	-2.28	117.82	120.77
3	E	502	PLP	C4A-C4-C5	2.27	123.28	120.94
3	C	501	PLP	C4A-C4-C5	2.26	123.26	120.94
3	B	500	PLP	C3-C2-N1	-2.22	117.90	120.77
3	B	500	PLP	C2A-C2-C3	2.21	123.61	120.89
3	C	501	PLP	O3P-P-O1P	2.18	119.23	110.68
3	F	502	PLP	C3-C2-N1	-2.18	117.95	120.77
3	D	501	PLP	C2A-C2-C3	2.18	123.58	120.89
3	B	500	PLP	C4A-C4-C5	2.16	123.16	120.94
3	E	502	PLP	C2A-C2-C3	2.12	123.51	120.89
3	B	500	PLP	O3P-P-O1P	2.08	118.84	110.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	500	PLP	O3P-P-O1P	2.07	118.78	110.68
3	E	502	PLP	O3P-P-O1P	2.06	118.73	110.68

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	501	PLP	C4-C5-C5A-O4P
3	C	501	PLP	C5A-O4P-P-O2P
3	A	500	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
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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	450/466 (96%)	-0.52	0 100 100	15, 34, 61, 79	0
1	B	450/466 (96%)	-0.63	1 (0%) 95 94	11, 30, 56, 82	0
1	C	451/466 (96%)	-0.48	1 (0%) 95 94	14, 37, 64, 80	0
1	D	450/466 (96%)	-0.57	0 100 100	16, 35, 60, 85	0
1	E	452/466 (96%)	-0.62	0 100 100	12, 31, 57, 77	0
1	F	451/466 (96%)	-0.61	1 (0%) 95 94	12, 30, 56, 84	0
All	All	2704/2796 (96%)	-0.57	3 (0%) 95 95	11, 33, 60, 85	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	5	GLN	2.4
1	F	453	LYS	2.1
1	C	291	ASP	2.0

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,



median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	BR	D	469	1/1	0.90	0.26	121,121,121,121	0
2	BR	B	471	1/1	0.90	0.19	83,83,83,83	0
4	ACY	B	558	4/4	0.91	0.25	42,42,42,44	0
2	BR	C	470	1/1	0.92	0.18	117,117,117,117	0
2	BR	B	468	1/1	0.92	0.07	78,78,78,78	0
4	ACY	C	538	4/4	0.93	0.22	72,73,73,73	0
4	ACY	C	548	4/4	0.93	0.23	48,49,49,49	0
4	ACY	E	518	4/4	0.93	0.31	68,69,69,69	0
4	ACY	F	528	4/4	0.94	0.16	43,43,43,45	0
2	BR	D	467	1/1	0.95	0.07	67,67,67,67	0
2	BR	E	470	1/1	0.95	0.15	93,93,93,93	0
2	BR	D	468	1/1	0.95	0.06	66,66,66,66	0
2	BR	A	468	1/1	0.95	0.10	75,75,75,75	0
2	BR	C	467	1/1	0.95	0.08	76,76,76,76	0
2	BR	A	470	1/1	0.96	0.17	98,98,98,98	0
4	ACY	A	568	4/4	0.96	0.14	28,29,30,31	0
2	BR	B	467	1/1	0.96	0.12	69,69,69,69	0
2	BR	F	468	1/1	0.96	0.06	67,67,67,67	0
3	PLP	A	500	15/16	0.97	0.17	27,37,42,43	0
3	PLP	D	501	15/16	0.97	0.16	26,31,34,35	0
2	BR	C	468	1/1	0.97	0.11	58,58,58,58	0
2	BR	E	467	1/1	0.97	0.09	70,70,70,70	1
2	BR	E	468	1/1	0.97	0.07	62,62,62,62	0
2	BR	F	469	1/1	0.97	0.09	90,90,90,90	0
3	PLP	C	501	15/16	0.97	0.21	36,43,44,45	0
3	PLP	E	502	15/16	0.98	0.16	25,27,28,29	0
2	BR	E	469	1/1	0.98	0.08	64,64,64,64	0
2	BR	B	470	1/1	0.98	0.07	65,65,65,65	0
3	PLP	B	500	15/16	0.98	0.14	22,27,28,28	0
3	PLP	F	502	15/16	0.98	0.21	21,26,28,30	0
2	BR	C	469	1/1	0.98	0.07	84,84,84,84	0
2	BR	B	469	1/1	0.98	0.06	56,56,56,56	0
2	BR	A	467	1/1	0.99	0.07	66,66,66,66	0
2	BR	A	469	1/1	0.99	0.06	67,67,67,67	0
2	BR	F	470	1/1	0.99	0.11	100,100,100,100	0
2	BR	F	467	1/1	0.99	0.10	58,58,58,58	1

## 6.5 Other polymers ⓘ

There are no such residues in this entry.