Full wwPDB X-ray Structure Validation Report (i)

Oct 17, 2023 – 01:38 PM EDT

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

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

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

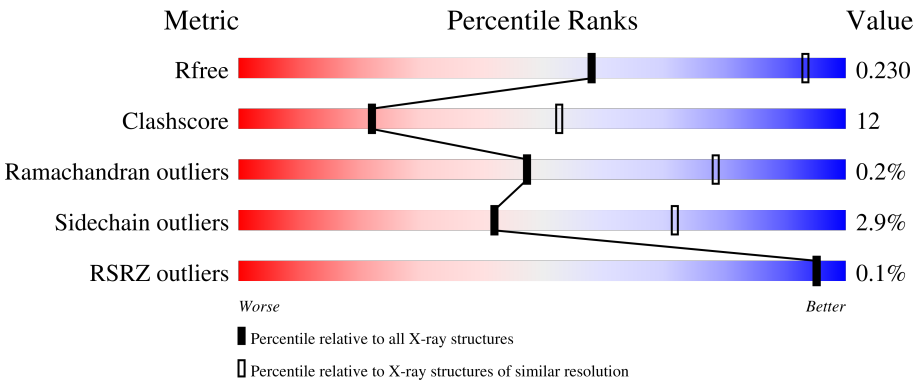
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	466	71% 24% • •
1	B	466	73% 23% • •
1	C	466	65% 31% • •
1	D	466	71% 24% • •
1	E	466	75% 21% • •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	466	74% 22%

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 (i)

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.

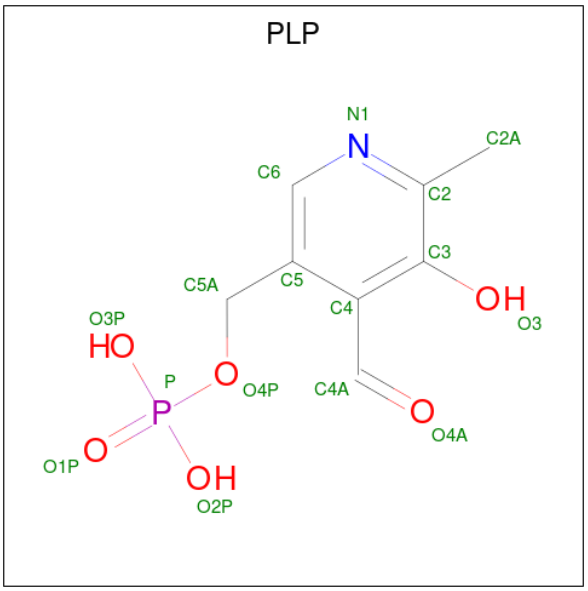
- Molecule 1 is a protein called Glutamate decarboxylase beta.

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

- Molecule 2 is BROMIDE ION (three-letter code: BR) (formula: Br).

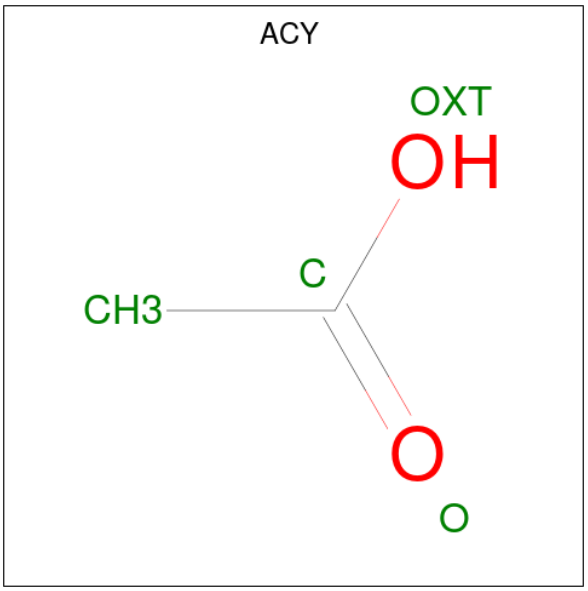
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Br		
2	A	4	4	4	0	0
2	B	5	5	5	0	0
2	C	4	4	4	0	0
2	D	3	3	3	0	0
2	E	4	4	4	0	0
2	F	4	4	4	0	0

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



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

- Molecule 4 is ACETIC ACID (three-letter code: ACY) (formula: $C_2H_4O_2$).



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

- Molecule 5 is water.

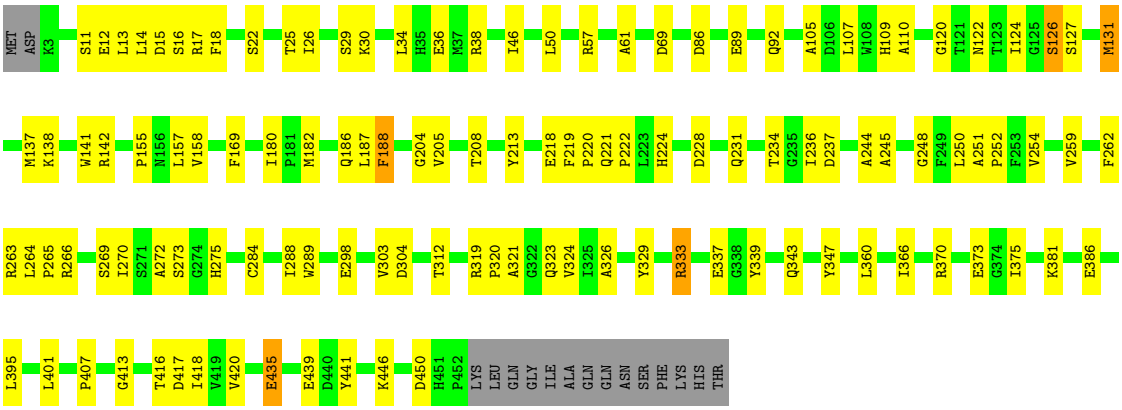
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	23	23	23	0	0
5	B	33	33	33	0	0
5	C	14	14	14	0	0
5	D	13	13	13	0	0
5	E	26	26	26	0	0
5	F	25	25	25	0	0

3 Residue-property plots (i)

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

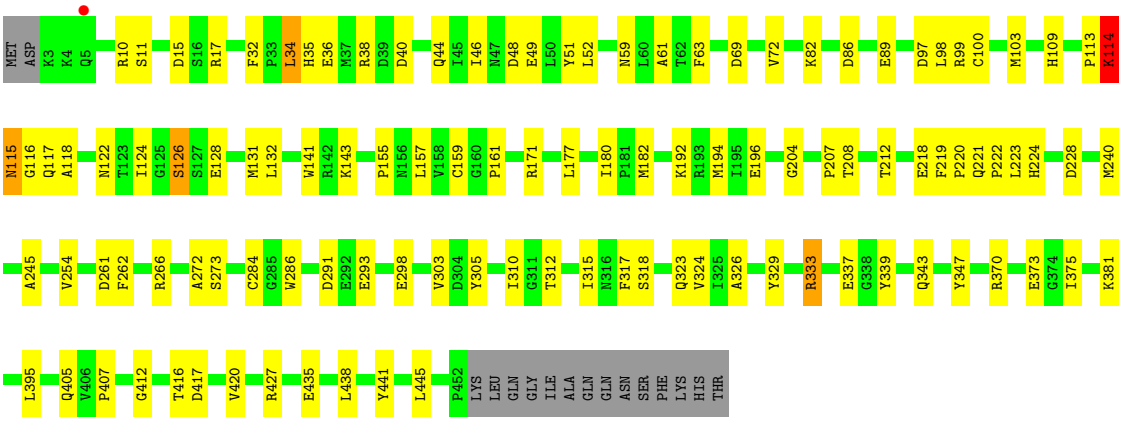
• Molecule 1: Glutamate decarboxylase beta

Chain A: 71% 24%



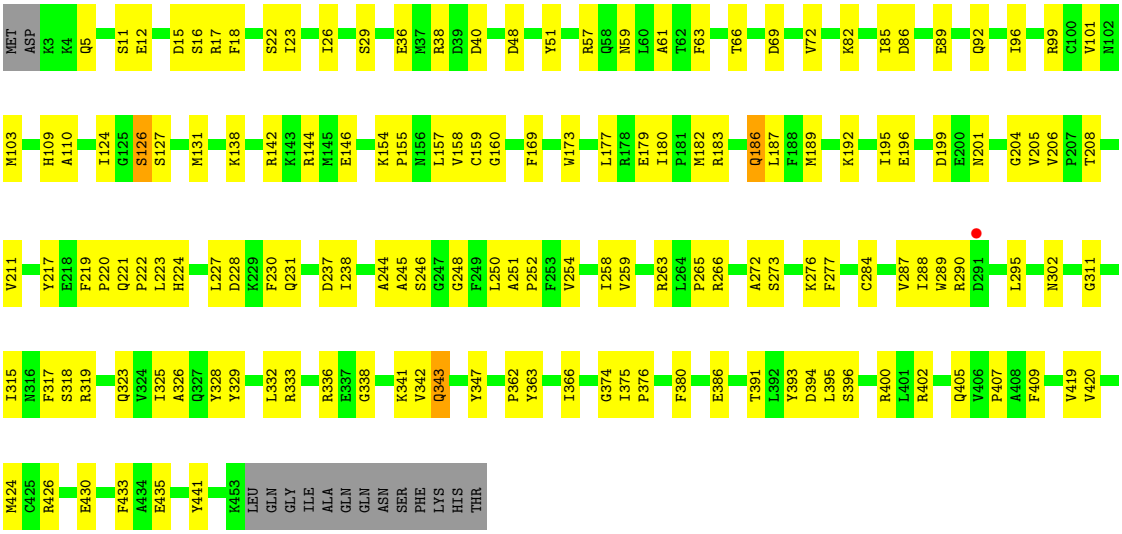
• Molecule 1: Glutamate decarboxylase beta

Chain B: 73% 23%



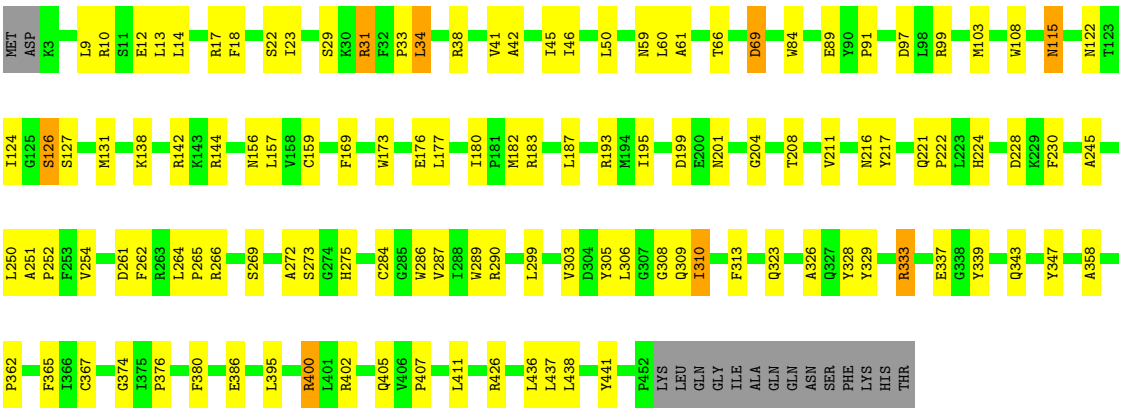
• Molecule 1: Glutamate decarboxylase beta

Chain C: 65% 31%



• Molecule 1: Glutamate decarboxylase beta

Chain D:



• Molecule 1: Glutamate decarboxylase beta

Chain E:

• Molecule 1: Glutamate decarboxylase beta

Chain F: 74% 22%

MET ASP K3 L9 L14 D15 S16 R17 F18 I23 I26 R31 F32 P33 L34 R38 D39 D40 L50 R57 A61 T66 D69 N83 W84 I85 D86 E89 D97 L98 R99 A110 G120 T121 N122 S126 S127 M131 W141 R142

E146 P155 N156 L157 P161 F169 A170 R171 I180 L187 M194 I195 E200 I203 T208 T212 E218 F219 P220 Q221 P222 L223 H224 D228 K229 F230 Q231 D237 I238 D239 M240 A245 L250 A251 P252 F253 V254 F262 R263 L264 P265 R266 V267 K268

A272 S273 G274 H275 C284 I288 Y305 I310 Q323 V324 L332 R333 R336 E337 G338 Y339 Q343 N344 Y347 Q348 L353 I357 R370 P376 K381 L395 R398 I399 R400 L401 P407 L411 G412 G413 T416 D417 V420 R426

R427 G428 M431 E435 Y441 K453 LEU GLN GLY ILE ALA GLN GLN ASN SER PHE LYS HIS THR

4 Data and refinement statistics (i)

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 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
$< I/\sigma(I) >$ [1]	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^2)	50.6	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 35.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	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.*

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

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(^{o})	Ideal(^{o})
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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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:HG3	1:F:336:ARG:HH11	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: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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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: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

Continued on next page...

Continued from previous page...

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: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: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: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: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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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

Continued on next page...

Continued from previous page...

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: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: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:29:SER:HB2	1:F:99:ARG:HG2	1.91	0.51
1:E:182:MET:HE3	1:E:187:LEU:CB	2.12	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: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: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: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: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

Continued on next page...

Continued from previous page...

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: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: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: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: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: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: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

Continued on next page...

Continued from previous page...

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: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:F:348:GLN:NE2	1:F:431:MET:HE2	2.22	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: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: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: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:OE1	1:F:343:GLN:HA	2.15	0.46
1:C:59:ASN:HA	1:C:405:GLN:HB2	1.98	0.46

Continued on next page...

Continued from previous page...

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: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
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: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: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:61:ALA:HB2	1:D:407:PRO:HD3	1.99	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

Continued on next page...

Continued from previous page...

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: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: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: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:29:SER:C	1:A:30:LYS:HD2	2.39	0.43
1:A:110:ALA:HB2	1:A:262:PHE:CD2	2.53	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: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:B:333:ARG:HD3	1:B:333:ARG:C	2.39	0.43
1:F:18:PHE:HA	1:F:23:ILE:HG21	2.00	0.43

Continued on next page...

Continued from previous page...

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:29:SER:HB2	1:B:99:ARG:HG2	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: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:63:PHE:CE1	1:C:424:MET:HE3	2.54	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:287:VAL:HG13	1:D:287:VAL:O	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: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: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:103:MET:HE2	1:F:31:ARG:O	2.21	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: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: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: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: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

Continued on next page...

Continued from previous page...

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:61:ALA:HB2	1:F:407:PRO:HD3	2.03	0.41
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: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:O	1:D:208:THR:HG22	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: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: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:344:ASN:HD22	1:F:344:ASN:HA	1.66	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:63:PHE:CE1	1:C:424:MET:CE	3.04	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

Continued on next page...

Continued from previous page...

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: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%)	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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Sometimes 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 (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 monosaccharides 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	$\#\|Z\| > 2$
4	ACY	A	568	-	3,3,3	1.26	0	3,3,3	1.66	1 (33%)
3	PLP	A	500	1	15,15,16	0.98	1 (6%)	20,22,23	1.42	5 (25%)
3	PLP	C	501	1	15,15,16	0.91	0	20,22,23	1.39	5 (25%)
4	ACY	F	528	-	3,3,3	1.09	0	3,3,3	1.77	1 (33%)
3	PLP	D	501	1	15,15,16	0.73	0	20,22,23	1.44	4 (20%)
4	ACY	C	538	-	3,3,3	1.26	1 (33%)	3,3,3	1.68	1 (33%)
4	ACY	B	558	-	3,3,3	1.33	0	3,3,3	1.57	1 (33%)
4	ACY	C	548	-	3,3,3	1.16	0	3,3,3	1.72	1 (33%)
3	PLP	E	502	1	15,15,16	0.92	0	20,22,23	1.34	5 (25%)
4	ACY	E	518	-	3,3,3	1.30	1 (33%)	3,3,3	1.66	1 (33%)
3	PLP	B	500	1	15,15,16	1.02	0	20,22,23	1.34	5 (25%)
3	PLP	F	502	1	15,15,16	0.89	0	20,22,23	1.40	3 (15%)

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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	500	PLP	C3-C2	2.20	1.43	1.40
4	E	518	ACY	O-C	2.05	1.31	1.22
4	C	538	ACY	O-C	2.01	1.31	1.22

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
4	F	528	ACY	O-C-CH3	-2.43	112.87	122.33
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
4	C	548	ACY	O-C-CH3	-2.36	113.14	122.33
3	A	500	PLP	C2A-C2-C3	2.31	123.75	120.89
4	C	538	ACY	O-C-CH3	-2.30	113.39	122.33
4	A	568	ACY	O-C-CH3	-2.28	113.44	122.33
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
4	E	518	ACY	O-C-CH3	-2.26	113.52	122.33
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
4	B	558	ACY	O-C-CH3	-2.15	113.96	122.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
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	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
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, 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%)	-0.52	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 monosaccharides in this entry.

6.4 Ligands (i)

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

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

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

6.5 Other polymers (i)

There are no such residues in this entry.