



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:36 PM GMT

PDB ID : 1GC4
Title : THERMUS THERMOPHILUS ASPARTATE AMINOTRANSFERASE
TETRA MUTANT 2 COMPLEXED WITH ASPARTATE
Authors : Ura, H.; Nakai, T.; Hirotsu, K.; Kuramitsu, S.
Deposited on : 2000-07-19
Resolution : 3.30 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

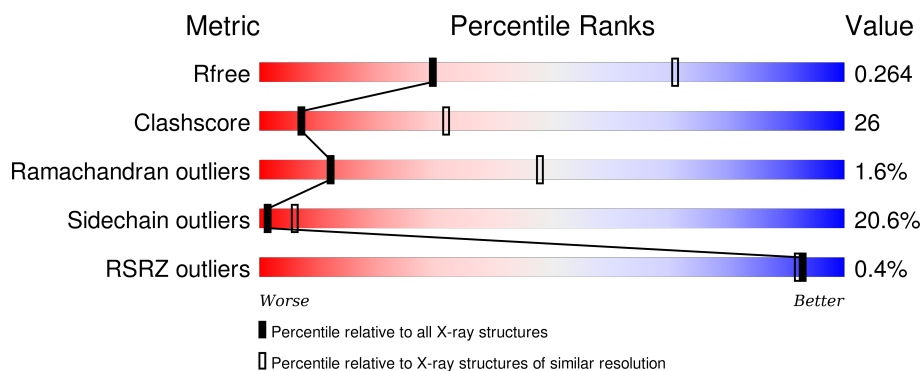
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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}	91344	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	385	<div> <div>%</div> <div> <div></div> <div>48%</div> <div>40%</div> <div>10%</div> <div>..</div> </div> </div>
1	B	385	<div> <div></div> <div> <div>49%</div> <div>40%</div> <div>10%</div> <div>..</div> </div> </div>
1	C	385	<div> <div>%</div> <div> <div></div> <div>47%</div> <div>40%</div> <div>11%</div> <div>.</div> </div> </div>
1	D	385	<div> <div></div> <div> <div>47%</div> <div>41%</div> <div>10%</div> <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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ASP	A	414	-	-	-	X
2	ASP	B	914	-	-	-	X
2	ASP	C	1414	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11888 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

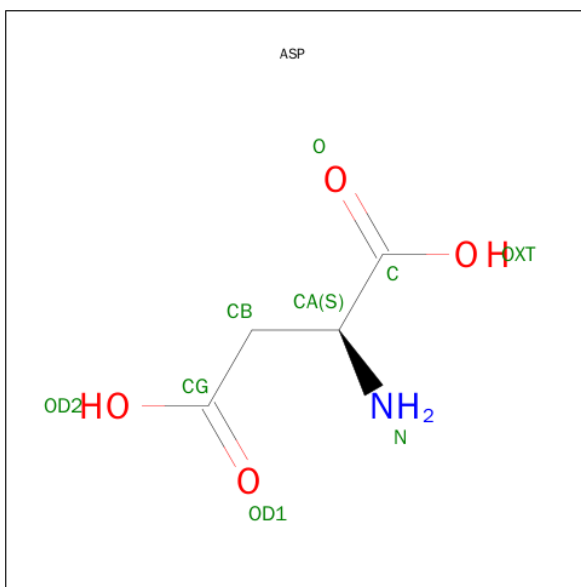
- Molecule 1 is a protein called ASPARTATE AMINOTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	382	Total	C	N	O	S	0	0	0
			2948	1866	523	551	8			
1	B	382	Total	C	N	O	S	0	0	0
			2948	1866	523	551	8			
1	C	382	Total	C	N	O	S	0	0	0
			2948	1866	523	551	8			
1	D	382	Total	C	N	O	S	0	0	0
			2948	1866	523	551	8			

There are 16 discrepancies between the modelled and reference sequences:

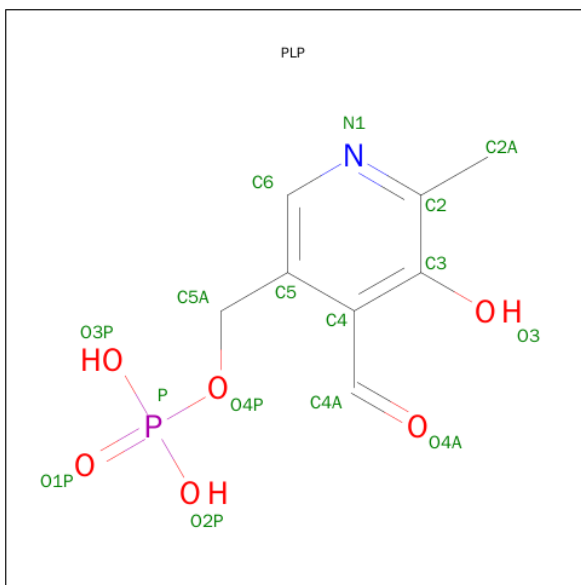
Chain	Residue	Modelled	Actual	Comment	Reference
A	14	ASP	SER	ENGINEERED	UNP Q56232
A	16	VAL	THR	ENGINEERED	UNP Q56232
A	101	SER	LYS	ENGINEERED	UNP Q56232
A	261	ARG	SER	ENGINEERED	UNP Q56232
B	514	ASP	SER	ENGINEERED	UNP Q56232
B	516	VAL	THR	ENGINEERED	UNP Q56232
B	601	SER	LYS	ENGINEERED	UNP Q56232
B	761	ARG	SER	ENGINEERED	UNP Q56232
C	1014	ASP	SER	ENGINEERED	UNP Q56232
C	1016	VAL	THR	ENGINEERED	UNP Q56232
C	1101	SER	LYS	ENGINEERED	UNP Q56232
C	1261	ARG	SER	ENGINEERED	UNP Q56232
D	1514	ASP	SER	ENGINEERED	UNP Q56232
D	1516	VAL	THR	ENGINEERED	UNP Q56232
D	1601	SER	LYS	ENGINEERED	UNP Q56232
D	1761	ARG	SER	ENGINEERED	UNP Q56232

- Molecule 2 is ASPARTIC ACID (three-letter code: ASP) (formula: C₄H₇NO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			9	4	1	4		
2	B	1	Total	C	N	O	0	0
			9	4	1	4		
2	C	1	Total	C	N	O	0	0
			9	4	1	4		
2	D	1	Total	C	N	O	0	0
			9	4	1	4		

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

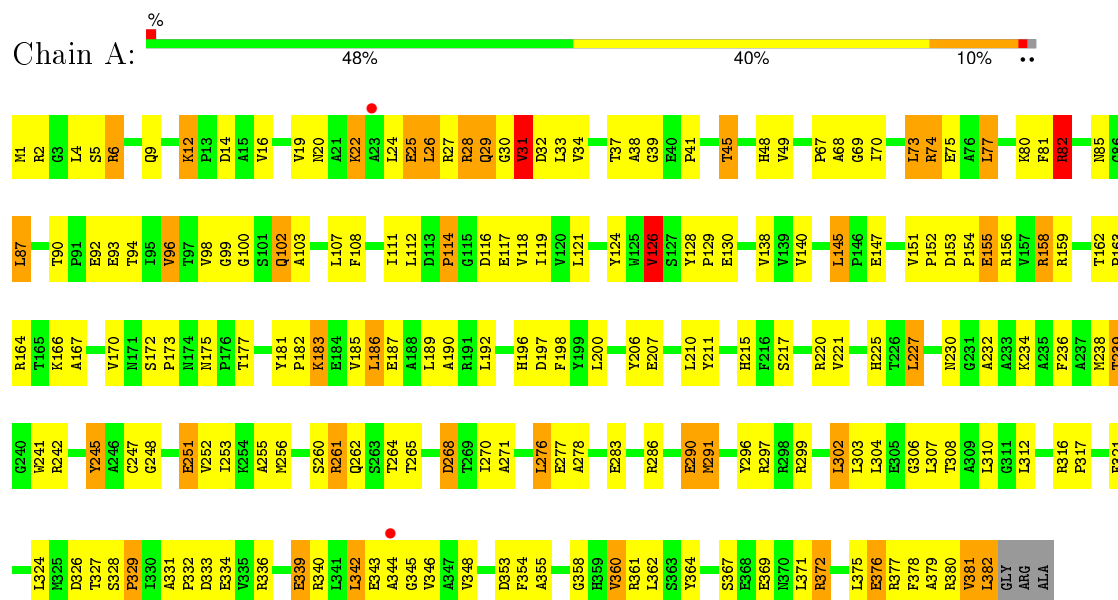


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

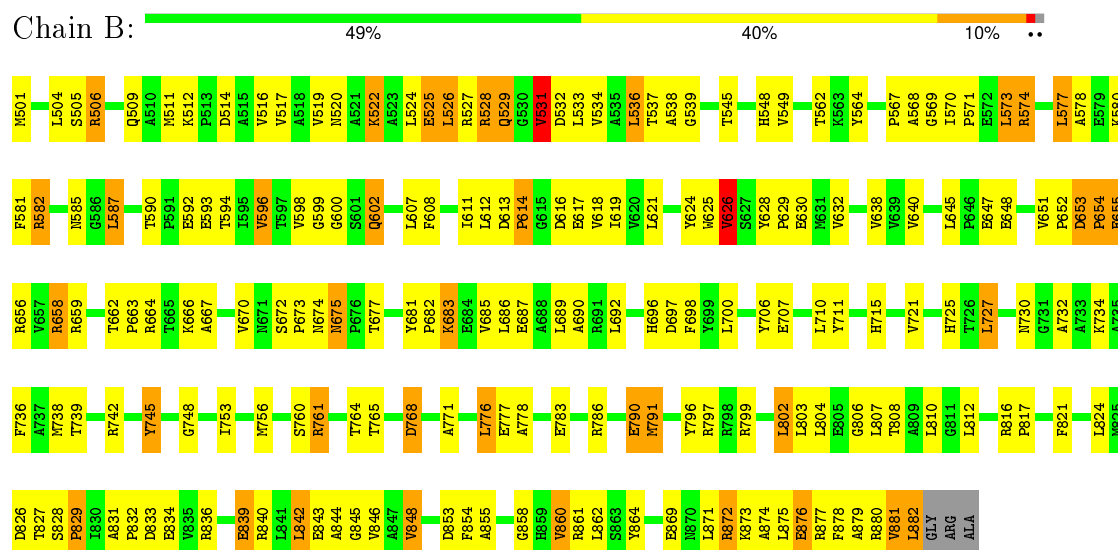
3 Residue-property plots

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

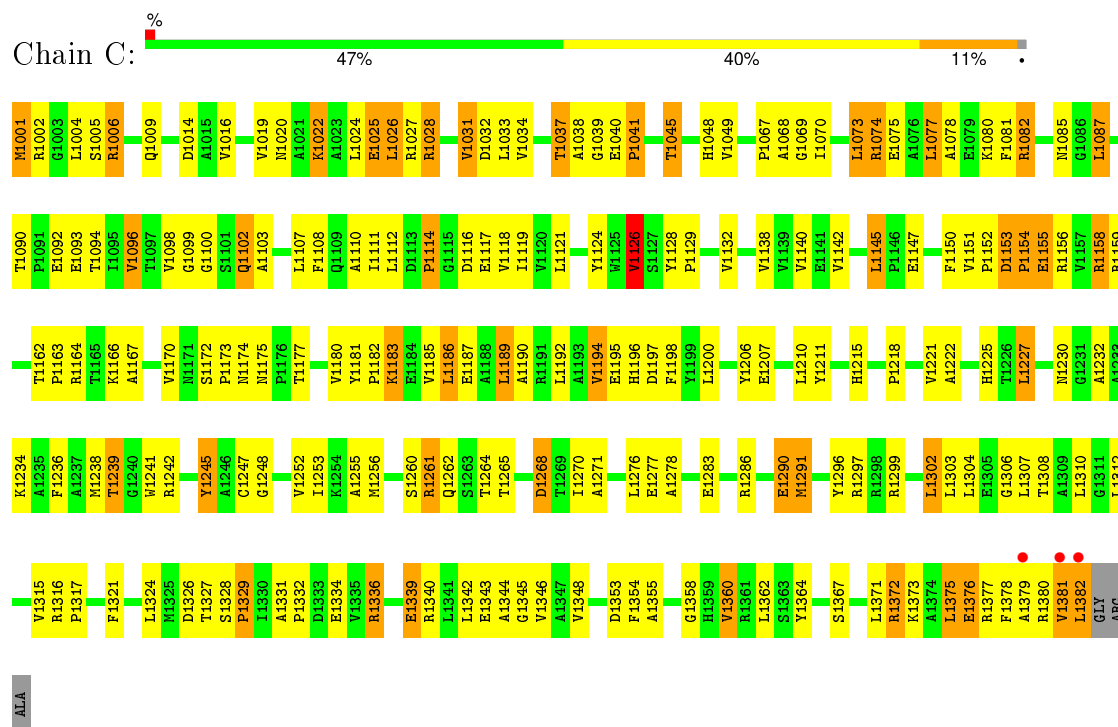
• Molecule 1: ASPARTATE AMINOTRANSFERASE



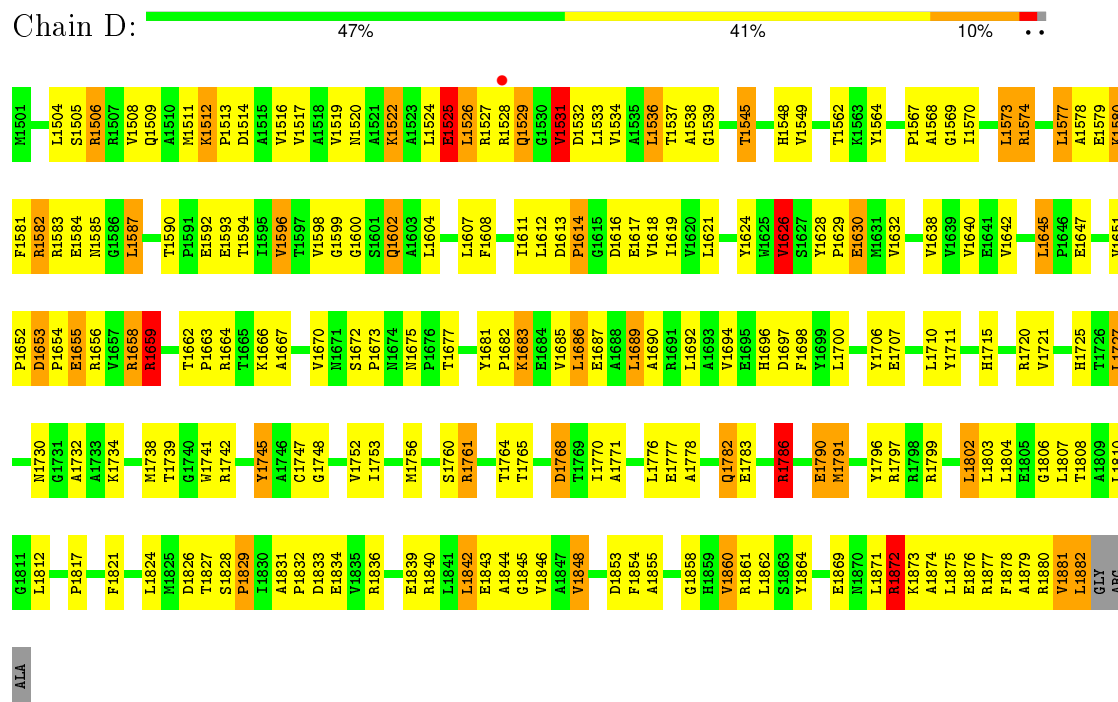
• Molecule 1: ASPARTATE AMINOTRANSFERASE



• Molecule 1: ASPARTATE AMINOTRANSFERASE



• Molecule 1: ASPARTATE AMINOTRANSFERASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.67Å 102.34Å 100.41Å 90.00° 112.14° 90.00°	Depositor
Resolution (Å)	8.00 – 3.30 45.29 – 3.30	Depositor EDS
% Data completeness (in resolution range)	97.0 (8.00-3.30) 97.1 (45.29-3.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 3.32Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.217 , 0.277 0.206 , 0.264	Depositor DCC
R_{free} test set	2094 reflections (9.92%)	DCC
Wilson B-factor (Å ²)	43.9	Xtriage
Anisotropy	0.526	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 57.6	EDS
Estimated twinning fraction	0.050 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Outliers	2 of 22777 reflections (0.009%)	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	11888	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.94% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: 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	0.43	0/3009	0.89	7/4092 (0.2%)
1	B	0.44	0/3009	0.87	5/4092 (0.1%)
1	C	0.42	0/3009	0.84	4/4092 (0.1%)
1	D	0.46	1/3009 (0.0%)	0.85	4/4092 (0.1%)
All	All	0.44	1/12036 (0.0%)	0.86	20/16368 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
1	C	0	1
1	D	0	4
All	All	0	8

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	1525	GLU	CG-CD	-7.27	1.41	1.51

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	159	ARG	NE-CZ-NH2	-10.47	115.06	120.30
1	A	361	ARG	NE-CZ-NH1	-10.21	115.20	120.30
1	A	159	ARG	NE-CZ-NH1	9.66	125.13	120.30
1	B	659	ARG	NE-CZ-NH1	6.91	123.76	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	659	ARG	NE-CZ-NH2	-6.84	116.88	120.30
1	A	175	ASN	N-CA-C	-6.29	94.01	111.00
1	C	1175	ASN	N-CA-C	-6.26	94.09	111.00
1	D	1675	ASN	N-CA-C	-6.21	94.25	111.00
1	A	31	VAL	N-CA-C	6.12	127.51	111.00
1	A	82	ARG	NE-CZ-NH1	-5.76	117.42	120.30
1	B	861	ARG	NE-CZ-NH2	5.74	123.17	120.30
1	B	675	ASN	N-CA-C	-5.73	95.54	111.00
1	B	531	VAL	N-CA-C	5.38	125.54	111.00
1	D	1531	VAL	N-CA-C	5.35	125.44	111.00
1	D	1626	VAL	N-CA-C	5.30	125.31	111.00
1	A	145	LEU	N-CA-C	5.23	125.11	111.00
1	C	1037	THR	N-CA-C	5.11	124.78	111.00
1	C	1145	LEU	N-CA-C	5.06	124.67	111.00
1	C	1126	VAL	N-CA-C	5.04	124.62	111.00
1	D	1645	LEU	N-CA-C	5.02	124.54	111.00

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	82	ARG	Sidechain
1	B	528	ARG	Sidechain
1	B	872	ARG	Sidechain
1	C	1159	ARG	Sidechain
1	D	1659	ARG	Sidechain
1	D	1782	GLN	Mainchain
1	D	1786	ARG	Sidechain
1	D	1872	ARG	Sidechain

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	2948	0	2965	167	0
1	B	2948	0	2962	161	1
1	C	2948	0	2962	175	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2948	0	2962	162	1
2	A	9	0	3	0	0
2	B	9	0	3	3	0
2	C	9	0	3	0	0
2	D	9	0	3	0	0
3	A	15	0	6	1	0
3	B	15	0	6	2	0
3	C	15	0	6	1	0
3	D	15	0	6	1	0
All	All	11888	0	11887	622	1

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 26.

All (622) 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:D:1653:ASP:HB3	1:D:1656:ARG:HH21	1.28	0.97
1:B:653:ASP:HB3	1:B:656:ARG:HH21	1.32	0.94
1:A:372:ARG:HG3	1:A:372:ARG:HH11	1.31	0.94
1:C:1372:ARG:HH11	1:C:1372:ARG:HG3	1.33	0.92
1:D:1653:ASP:HB3	1:D:1656:ARG:NH2	1.86	0.89
1:B:607:LEU:HD13	1:B:727:LEU:HD22	1.60	0.83
1:B:653:ASP:HB3	1:B:656:ARG:NH2	1.93	0.83
1:A:145:LEU:HD12	1:A:156:ARG:HH12	1.44	0.82
1:D:1682:PRO:HG2	1:D:1685:VAL:HG23	1.62	0.81
1:C:1182:PRO:HG2	1:C:1185:VAL:HG23	1.61	0.81
1:B:682:PRO:HG2	1:B:685:VAL:HG23	1.61	0.81
1:A:182:PRO:HG2	1:A:185:VAL:HG23	1.61	0.80
1:A:30:GLY:HA2	1:C:1340:ARG:HD2	1.63	0.80
1:C:1145:LEU:HD12	1:C:1156:ARG:HH12	1.48	0.79
1:A:286:ARG:O	1:A:290:GLU:HG2	1.82	0.78
1:D:1505:SER:OG	1:D:1508:VAL:HG12	1.85	0.77
1:B:577:LEU:HB3	1:B:594:THR:HG21	1.65	0.77
1:A:251:GLU:OE2	1:B:504:LEU:HD11	1.84	0.77
1:B:525:GLU:O	1:B:529:GLN:HG2	1.83	0.77
1:A:74:ARG:HH11	1:A:74:ARG:HG2	1.50	0.76
1:C:1077:LEU:HB3	1:C:1094:THR:HG21	1.68	0.76
1:A:77:LEU:HB3	1:A:94:THR:HG21	1.66	0.76
1:C:1340:ARG:NH2	1:C:1381:VAL:HG22	2.02	0.75
1:C:1074:ARG:HH11	1:C:1074:ARG:HG2	1.51	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:574:ARG:HH11	1:B:574:ARG:HG2	1.50	0.75
1:D:1607:LEU:HD13	1:D:1727:LEU:HD22	1.67	0.75
1:D:1574:ARG:HH11	1:D:1574:ARG:HG2	1.50	0.75
1:A:340:ARG:NH2	1:A:381:VAL:HG22	2.03	0.74
1:D:1525:GLU:O	1:D:1529:GLN:HG2	1.87	0.74
1:D:1577:LEU:HB3	1:D:1594:THR:HG21	1.70	0.74
1:D:1653:ASP:CB	1:D:1656:ARG:HH21	2.01	0.74
1:D:1582:ARG:HH11	1:D:1582:ARG:HG3	1.51	0.73
1:A:145:LEU:HD12	1:A:156:ARG:NH1	2.02	0.73
1:B:802:LEU:HD21	1:B:872:ARG:HD3	1.70	0.73
1:C:1145:LEU:HD12	1:C:1156:ARG:NH1	2.04	0.73
1:B:797:ARG:HH11	1:B:797:ARG:HG3	1.53	0.73
1:D:1797:ARG:HH11	1:D:1797:ARG:HG3	1.53	0.73
1:A:26:LEU:O	1:A:31:VAL:HB	1.88	0.73
1:C:1024:LEU:HB3	1:C:1028:ARG:NH1	2.04	0.72
1:D:1840:ARG:NH2	1:D:1881:VAL:HG22	2.03	0.72
1:C:1328:SER:HB3	1:C:1329:PRO:HD3	1.70	0.72
1:A:24:LEU:HB3	1:A:28:ARG:NH1	2.05	0.72
1:A:297:ARG:HG3	1:A:297:ARG:HH11	1.53	0.72
1:D:1828:SER:HB3	1:D:1829:PRO:HD3	1.70	0.72
1:A:328:SER:HB3	1:A:329:PRO:HD3	1.71	0.72
1:D:1833:ASP:OD1	1:D:1836:ARG:HD3	1.90	0.71
1:B:786:ARG:O	1:B:790:GLU:HG2	1.90	0.71
1:C:1297:ARG:HH11	1:C:1297:ARG:HG3	1.55	0.71
1:B:840:ARG:NH2	1:B:881:VAL:HG22	2.05	0.70
1:A:6:ARG:HH21	1:B:614:PRO:HD2	1.57	0.69
1:B:653:ASP:CB	1:B:656:ARG:HH21	2.06	0.68
1:A:25:GLU:O	1:A:29:GLN:HG2	1.93	0.68
1:B:828:SER:HB3	1:B:829:PRO:HD3	1.74	0.68
1:A:2:ARG:HG3	1:B:698:PHE:HA	1.75	0.68
1:C:1001:MET:O	1:D:1666:LYS:HD3	1.94	0.68
1:C:1006:ARG:HH21	1:D:1614:PRO:HD2	1.59	0.68
1:A:31:VAL:HG11	1:A:33:LEU:HD23	1.77	0.67
1:A:30:GLY:CA	1:C:1340:ARG:HD2	2.24	0.67
1:A:1:MET:O	1:B:666:LYS:HD3	1.96	0.66
1:B:578:ALA:O	1:B:582:ARG:HG3	1.95	0.66
1:A:372:ARG:HG3	1:A:372:ARG:NH1	2.09	0.66
1:D:1878:PHE:O	1:D:1882:LEU:HB2	1.95	0.66
1:C:1291:MET:C	1:C:1291:MET:SD	2.74	0.66
1:A:316:ARG:HH11	1:A:316:ARG:HG3	1.61	0.66
1:D:1768:ASP:HB3	1:D:1771:ALA:HB3	1.77	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:GLY:O	1:A:310:LEU:HD13	1.97	0.65
1:A:26:LEU:HB3	1:A:31:VAL:HG11	1.78	0.65
1:C:1306:GLY:O	1:C:1310:LEU:HD13	1.97	0.65
1:A:378:PHE:O	1:A:382:LEU:HB2	1.96	0.65
1:B:768:ASP:HB3	1:B:771:ALA:HB3	1.79	0.64
1:B:791:MET:C	1:B:791:MET:SD	2.75	0.64
1:B:878:PHE:O	1:B:882:LEU:HB2	1.97	0.64
1:A:268:ASP:HB3	1:A:271:ALA:HB3	1.78	0.64
1:D:1806:GLY:O	1:D:1810:LEU:HD13	1.98	0.64
1:C:1378:PHE:O	1:C:1382:LEU:HB2	1.98	0.63
1:A:74:ARG:HG2	1:A:74:ARG:NH1	2.13	0.63
1:A:291:MET:C	1:A:291:MET:SD	2.77	0.63
1:B:799:ARG:HB3	1:B:871:LEU:HD11	1.81	0.63
1:B:574:ARG:NH1	1:B:574:ARG:HG2	2.13	0.63
1:A:190:ALA:HA	1:A:200:LEU:HD12	1.80	0.63
1:C:1190:ALA:HA	1:C:1200:LEU:HD12	1.81	0.63
1:C:1026:LEU:HB3	1:C:1031:VAL:HG11	1.81	0.62
1:C:1316:ARG:HH11	1:C:1316:ARG:HG3	1.64	0.62
1:D:1690:ALA:HA	1:D:1700:LEU:HD12	1.81	0.62
1:C:1268:ASP:HB3	1:C:1271:ALA:HB3	1.79	0.62
1:C:1002:ARG:HG3	1:D:1698:PHE:HA	1.81	0.62
1:B:845:GLY:HA3	1:B:877:ARG:NH1	2.14	0.62
1:A:31:VAL:CG1	1:A:33:LEU:HD23	2.31	0.61
1:B:806:GLY:O	1:B:810:LEU:HD13	1.98	0.61
1:B:527:ARG:HA	1:B:531:VAL:O	2.00	0.61
1:C:1001:MET:HG2	1:C:1002:ARG:N	2.14	0.61
1:C:1299:ARG:HB3	1:C:1371:LEU:HD11	1.81	0.61
1:D:1617:GLU:HG2	1:D:1638:VAL:CG2	2.30	0.61
1:D:1791:MET:SD	1:D:1791:MET:C	2.78	0.61
1:C:1218:PRO:O	1:C:1221:VAL:HG13	2.00	0.61
1:C:1117:GLU:HG2	1:C:1138:VAL:CG2	2.30	0.61
1:D:1799:ARG:HB3	1:D:1871:LEU:HD11	1.82	0.61
1:B:619:ILE:HA	1:B:640:VAL:O	2.01	0.61
1:D:1598:VAL:HB	1:D:1602:GLN:HG3	1.82	0.61
1:C:1098:VAL:HB	1:C:1102:GLN:HG3	1.82	0.61
1:C:1119:ILE:HA	1:C:1140:VAL:O	2.01	0.61
1:B:598:VAL:HB	1:B:602:GLN:HG3	1.81	0.61
1:A:155:GLU:OE2	1:A:155:GLU:HA	2.01	0.61
1:A:98:VAL:HB	1:A:102:GLN:HG3	1.82	0.61
1:A:45:THR:HG21	1:A:241:TRP:HE1	1.66	0.60
1:D:1845:GLY:HA3	1:D:1877:ARG:NH1	2.16	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1839:GLU:O	1:D:1843:GLU:HG2	2.02	0.60
1:A:345:GLY:HA3	1:A:377:ARG:NH1	2.16	0.60
1:C:1031:VAL:HG11	1:C:1033:LEU:HD23	1.83	0.60
1:A:187:GLU:HG3	1:A:221:VAL:HG21	1.84	0.60
1:A:119:ILE:HA	1:A:140:VAL:O	2.01	0.60
1:B:690:ALA:HA	1:B:700:LEU:HD12	1.83	0.60
1:D:1527:ARG:HA	1:D:1531:VAL:O	2.01	0.60
1:D:1619:ILE:HA	1:D:1640:VAL:O	2.02	0.60
1:C:1155:GLU:HA	1:C:1155:GLU:OE2	2.02	0.59
1:A:92:GLU:O	1:A:253:ILE:HG21	2.02	0.59
1:A:299:ARG:HB3	1:A:371:LEU:HD11	1.84	0.59
1:C:1345:GLY:HA3	1:C:1377:ARG:NH1	2.17	0.59
1:C:1077:LEU:HB3	1:C:1094:THR:CG2	2.33	0.59
1:B:504:LEU:HD12	1:B:504:LEU:H	1.67	0.59
1:A:6:ARG:HG3	1:B:613:ASP:OD1	2.02	0.59
1:D:1687:GLU:HG3	1:D:1721:VAL:HG21	1.84	0.59
1:B:617:GLU:HG2	1:B:638:VAL:CG2	2.32	0.59
1:A:117:GLU:HG2	1:A:138:VAL:CG2	2.32	0.59
1:B:687:GLU:HG3	1:B:721:VAL:HG21	1.83	0.59
1:A:107:LEU:HD21	1:A:227:LEU:HD13	1.83	0.59
1:C:1107:LEU:HD21	1:C:1227:LEU:HD13	1.85	0.59
1:B:577:LEU:HB3	1:B:594:THR:CG2	2.32	0.58
1:B:761:ARG:O	1:B:761:ARG:HD3	2.03	0.58
1:A:67:PRO:HA	1:A:265:THR:O	2.02	0.58
1:D:1786:ARG:O	1:D:1790:GLU:HG2	2.03	0.58
1:C:1099:GLY:HA3	1:C:1242:ARG:NH2	2.18	0.58
1:C:1067:PRO:HA	1:C:1265:THR:O	2.04	0.58
1:A:77:LEU:HB3	1:A:94:THR:CG2	2.34	0.58
1:D:1567:PRO:HA	1:D:1765:THR:O	2.03	0.58
1:A:177:THR:HG22	1:A:324:LEU:HD12	1.85	0.58
1:C:1025:GLU:HA	1:C:1028:ARG:HG2	1.86	0.58
1:B:675:ASN:ND2	2:B:914:ASP:O	2.37	0.58
1:A:372:ARG:HH11	1:A:372:ARG:CG	2.11	0.58
1:C:1074:ARG:HG2	1:C:1074:ARG:NH1	2.14	0.58
1:D:1677:THR:HG22	1:D:1824:LEU:HD12	1.85	0.58
1:C:1128:TYR:HB2	1:C:1129:PRO:HD3	1.85	0.58
1:A:107:LEU:HG	1:A:227:LEU:HD22	1.85	0.57
1:D:1574:ARG:NH1	1:D:1574:ARG:HG2	2.13	0.57
1:D:1578:ALA:O	1:D:1582:ARG:HB2	2.04	0.57
1:B:677:THR:HG22	1:B:824:LEU:HD12	1.86	0.57
1:B:567:PRO:HA	1:B:765:THR:O	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:TYR:HB2	1:A:129:PRO:HD3	1.86	0.57
1:D:1582:ARG:NH1	1:D:1582:ARG:HG3	2.18	0.57
1:C:1004:LEU:HD12	1:C:1004:LEU:H	1.69	0.57
1:D:1599:GLY:HA3	1:D:1742:ARG:NH2	2.19	0.57
1:A:261:ARG:HD3	1:A:261:ARG:O	2.05	0.57
1:B:599:GLY:HA3	1:B:742:ARG:NH2	2.19	0.57
1:A:27:ARG:HA	1:A:31:VAL:O	2.05	0.57
1:D:1504:LEU:HD12	1:D:1504:LEU:H	1.70	0.57
1:C:1177:THR:HG22	1:C:1324:LEU:HD12	1.85	0.57
1:D:1592:GLU:O	1:D:1753:ILE:HG21	2.05	0.57
1:B:625:TRP:HE1	2:B:914:ASP:HB3	1.68	0.56
1:C:1068:ALA:O	1:C:1096:VAL:HG23	2.05	0.56
1:A:99:GLY:HA3	1:A:242:ARG:NH2	2.20	0.56
1:A:22:LYS:O	1:A:26:LEU:HD22	2.05	0.56
1:C:1045:THR:HG21	1:C:1241:TRP:HE1	1.70	0.56
1:C:1174:ASN:ND2	1:C:1181:TYR:OH	2.37	0.56
1:D:1864:TYR:HA	1:D:1871:LEU:HD21	1.87	0.56
1:C:1031:VAL:CG1	1:C:1033:LEU:HD23	2.35	0.56
1:C:1262:GLN:HG3	1:D:1511:MET:HE1	1.88	0.56
1:B:592:GLU:O	1:B:753:ILE:HG21	2.05	0.56
1:D:1525:GLU:HG2	1:D:1526:LEU:N	2.20	0.56
1:B:568:ALA:O	1:B:596:VAL:HG23	2.06	0.56
1:C:1255:ALA:HB2	1:D:1504:LEU:HD23	1.86	0.56
1:A:68:ALA:O	1:A:96:VAL:HG23	2.06	0.55
1:A:85:ASN:CB	1:A:87:LEU:HD22	2.36	0.55
1:D:1568:ALA:O	1:D:1596:VAL:HG23	2.06	0.55
1:D:1522:LYS:O	1:D:1526:LEU:HD22	2.05	0.55
1:D:1577:LEU:HB3	1:D:1594:THR:CG2	2.35	0.55
1:A:25:GLU:HA	1:A:28:ARG:HG2	1.87	0.55
1:B:522:LYS:O	1:B:526:LEU:HD22	2.06	0.55
1:D:1585:ASN:CB	1:D:1587:LEU:HD22	2.36	0.55
1:C:1103:ALA:O	1:C:1107:LEU:HB2	2.07	0.55
1:C:1262:GLN:HG3	1:D:1511:MET:CE	2.37	0.55
1:B:833:ASP:OD2	1:B:836:ARG:HB3	2.07	0.55
1:D:1536:LEU:HD12	1:D:1848:VAL:HG13	1.88	0.55
1:C:1372:ARG:HH11	1:C:1372:ARG:CG	2.14	0.55
1:C:1006:ARG:HG3	1:D:1613:ASP:OD1	2.07	0.55
1:C:1364:TYR:HA	1:C:1371:LEU:HD21	1.89	0.55
1:D:1628:TYR:HB2	1:D:1629:PRO:HD3	1.88	0.55
1:C:1026:LEU:O	1:C:1031:VAL:HB	2.07	0.54
1:D:1608:PHE:O	1:D:1612:LEU:HB2	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:577:LEU:CB	1:B:594:THR:HG21	2.37	0.54
1:B:658:ARG:HH21	1:B:696:HIS:CE1	2.25	0.54
1:A:4:LEU:HD12	1:A:4:LEU:H	1.72	0.54
1:C:1372:ARG:HG3	1:C:1372:ARG:NH1	2.11	0.54
1:C:1331:ALA:HB1	1:C:1332:PRO:HD2	1.89	0.54
1:C:1092:GLU:O	1:C:1253:ILE:HG21	2.08	0.54
1:C:1085:ASN:CB	1:C:1087:LEU:HD22	2.38	0.54
1:D:1658:ARG:HB2	1:D:1692:LEU:HD11	1.89	0.54
1:C:1022:LYS:O	1:C:1026:LEU:HD22	2.08	0.54
1:A:24:LEU:HB3	1:A:28:ARG:HH12	1.70	0.54
1:C:1158:ARG:HH21	1:C:1196:HIS:CE1	2.26	0.54
1:A:107:LEU:O	1:A:111:ILE:HG12	2.07	0.54
1:B:628:TYR:HB2	1:B:629:PRO:HD3	1.89	0.54
1:A:158:ARG:HB2	1:A:192:LEU:HD11	1.89	0.53
1:C:1261:ARG:HD3	1:C:1261:ARG:O	2.07	0.53
1:C:1158:ARG:HB2	1:C:1192:LEU:HD11	1.90	0.53
1:A:364:TYR:HA	1:A:371:LEU:HD21	1.90	0.53
1:C:1107:LEU:HG	1:C:1227:LEU:HD22	1.90	0.53
1:D:1831:ALA:HB1	1:D:1832:PRO:HD2	1.90	0.53
1:A:333:ASP:OD2	1:A:336:ARG:HB3	2.09	0.53
1:C:1185:VAL:O	1:C:1189:LEU:HD22	2.08	0.53
1:A:69:GLY:HA3	1:A:96:VAL:CG2	2.39	0.53
1:B:658:ARG:HB2	1:B:692:LEU:HD11	1.90	0.53
1:C:1286:ARG:O	1:C:1290:GLU:HG2	2.08	0.53
1:B:536:LEU:HD12	1:B:848:VAL:HG13	1.89	0.53
1:A:77:LEU:CB	1:A:94:THR:HG21	2.38	0.53
1:B:585:ASN:CB	1:B:587:LEU:HD22	2.38	0.53
1:A:331:ALA:HB1	1:A:332:PRO:HD2	1.90	0.53
1:B:864:TYR:HA	1:B:871:LEU:HD21	1.89	0.53
1:C:1158:ARG:HH21	1:C:1196:HIS:HE1	1.57	0.53
1:C:1239:THR:HG22	1:D:1564:TYR:CZ	2.44	0.53
1:C:1102:GLN:HG3	1:D:1764:THR:HG22	1.91	0.52
1:C:1069:GLY:HA3	1:C:1096:VAL:CG2	2.40	0.52
1:C:1108:PHE:O	1:C:1112:LEU:HB2	2.08	0.52
1:C:1077:LEU:CB	1:C:1094:THR:HG21	2.38	0.52
1:A:102:GLN:HG3	1:B:764:THR:HG22	1.91	0.52
1:C:1024:LEU:HB3	1:C:1028:ARG:HH12	1.75	0.52
1:D:1569:GLY:HA3	1:D:1596:VAL:CG2	2.40	0.52
1:C:1261:ARG:HD3	1:C:1261:ARG:C	2.30	0.52
1:D:1872:ARG:HA	1:D:1875:LEU:HD12	1.91	0.52
1:B:607:LEU:O	1:B:611:ILE:HG12	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:569:GLY:HA3	1:B:596:VAL:CG2	2.39	0.52
1:B:839:GLU:O	1:B:843:GLU:HG3	2.10	0.52
1:C:1093:GLU:HB3	1:C:1248:GLY:O	2.10	0.52
1:B:816:ARG:HG3	1:B:816:ARG:HH11	1.74	0.52
1:A:339:GLU:O	1:A:343:GLU:HG3	2.09	0.52
1:B:608:PHE:O	1:B:612:LEU:HB2	2.09	0.51
1:C:1078:ALA:O	1:C:1082:ARG:HB2	2.10	0.51
1:A:103:ALA:O	1:A:107:LEU:HB2	2.10	0.51
1:B:761:ARG:C	1:B:761:ARG:HD3	2.31	0.51
1:B:831:ALA:HB1	1:B:832:PRO:HD2	1.91	0.51
1:A:158:ARG:HH21	1:A:196:HIS:HE1	1.58	0.51
1:D:1812:LEU:HD21	1:D:1882:LEU:HD21	1.93	0.51
1:D:1685:VAL:O	1:D:1689:LEU:HD22	2.10	0.51
1:D:1577:LEU:CB	1:D:1594:THR:HG21	2.40	0.51
1:A:297:ARG:HG3	1:A:297:ARG:NH1	2.24	0.51
1:C:1334:GLU:HG3	1:C:1358:GLY:H	1.76	0.51
1:D:1834:GLU:HG3	1:D:1858:GLY:H	1.76	0.51
1:A:262:GLN:HG3	1:B:511:MET:CE	2.40	0.51
1:A:255:ALA:HB2	1:B:504:LEU:HD23	1.92	0.50
1:C:1027:ARG:HA	1:C:1031:VAL:O	2.11	0.50
1:A:264:THR:O	1:A:265:THR:HB	2.11	0.50
1:A:108:PHE:O	1:A:112:LEU:HB2	2.11	0.50
1:D:1607:LEU:O	1:D:1611:ILE:HG12	2.11	0.50
1:D:1653:ASP:N	1:D:1656:ARG:HH21	2.09	0.50
1:C:1297:ARG:NH1	1:C:1297:ARG:HG3	2.26	0.50
1:C:1316:ARG:NH1	1:C:1316:ARG:HG3	2.27	0.50
1:A:114:PRO:HD2	1:B:506:ARG:HH21	1.77	0.50
1:D:1681:TYR:N	1:D:1681:TYR:CD2	2.80	0.50
1:B:593:GLU:HB3	1:B:748:GLY:O	2.12	0.50
1:A:158:ARG:HH21	1:A:196:HIS:CE1	2.29	0.50
1:A:239:THR:HG22	1:B:564:TYR:CZ	2.46	0.50
1:B:655:GLU:OE2	1:B:658:ARG:HD2	2.11	0.50
1:A:316:ARG:NH1	1:A:316:ARG:HG3	2.27	0.50
1:C:1242:ARG:NH1	1:D:1564:TYR:HE1	2.10	0.50
1:C:1376:GLU:O	1:C:1379:ALA:HB3	2.11	0.50
1:B:797:ARG:HG3	1:B:797:ARG:NH1	2.24	0.49
1:B:645:LEU:HB2	1:B:648:GLU:HG3	1.94	0.49
1:B:872:ARG:HA	1:B:875:LEU:HD12	1.94	0.49
1:D:1658:ARG:HH21	1:D:1696:HIS:CE1	2.30	0.49
1:C:1253:ILE:HD12	1:C:1256:MET:HE3	1.94	0.49
1:C:1085:ASN:HB2	1:C:1087:LEU:HD22	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1593:GLU:HB3	1:D:1748:GLY:O	2.12	0.49
1:C:1033:LEU:HD12	1:C:1033:LEU:O	2.12	0.49
1:C:1339:GLU:O	1:C:1343:GLU:HG3	2.12	0.49
1:B:681:TYR:N	1:B:681:TYR:CD2	2.79	0.49
1:B:645:LEU:HD12	1:B:656:ARG:NH1	2.27	0.49
1:A:182:PRO:HG2	1:A:185:VAL:CG2	2.39	0.49
1:D:1536:LEU:HD12	1:D:1848:VAL:CG1	2.43	0.49
1:B:834:GLU:HG3	1:B:858:GLY:H	1.78	0.49
1:A:85:ASN:HB2	1:A:87:LEU:HD22	1.93	0.49
1:A:334:GLU:HG3	1:A:358:GLY:H	1.78	0.49
1:D:1537:THR:O	1:D:1861:ARG:NH2	2.41	0.49
1:C:1221:VAL:CG2	1:C:1222:ALA:N	2.75	0.49
1:D:1582:ARG:HA	1:D:1587:LEU:O	2.13	0.48
1:C:1264:THR:O	1:C:1265:THR:HB	2.13	0.48
1:C:1155:GLU:OE2	1:C:1158:ARG:HD2	2.13	0.48
1:A:261:ARG:C	1:A:261:ARG:HD3	2.33	0.48
1:A:155:GLU:OE2	1:A:158:ARG:HD2	2.14	0.48
1:A:312:LEU:HD21	1:A:382:LEU:HD21	1.96	0.48
1:D:1512:LYS:N	1:D:1630:GLU:OE2	2.45	0.48
1:D:1653:ASP:HB3	1:D:1656:ARG:CZ	2.42	0.48
1:A:241:TRP:HE1	1:B:562:THR:HB	1.78	0.48
1:C:1082:ARG:HA	1:C:1087:LEU:O	2.13	0.48
1:B:876:GLU:O	1:B:879:ALA:HB3	2.13	0.48
1:D:1761:ARG:O	1:D:1761:ARG:HD3	2.14	0.48
1:C:1182:PRO:HG2	1:C:1185:VAL:CG2	2.39	0.48
1:D:1585:ASN:HB3	1:D:1587:LEU:HD22	1.94	0.48
1:D:1797:ARG:NH1	1:D:1797:ARG:HG3	2.24	0.48
1:D:1876:GLU:O	1:D:1879:ALA:HB3	2.13	0.48
1:D:1585:ASN:HB2	1:D:1587:LEU:HD22	1.96	0.48
1:B:812:LEU:HD21	1:B:882:LEU:HD21	1.96	0.48
1:D:1519:VAL:HG12	1:D:1537:THR:HG21	1.96	0.48
1:B:577:LEU:HD23	1:B:594:THR:HG22	1.96	0.47
1:B:764:THR:O	1:B:765:THR:HB	2.14	0.47
1:C:1241:TRP:HE1	1:D:1562:THR:HB	1.79	0.47
1:A:181:TYR:CD2	1:A:181:TYR:N	2.82	0.47
1:B:512:LYS:N	1:B:630:GLU:OE2	2.47	0.47
1:D:1764:THR:O	1:D:1765:THR:HB	2.14	0.47
1:B:600:GLY:H	3:B:913:PLP:P	2.37	0.47
1:C:1180:VAL:HG13	1:C:1180:VAL:O	2.13	0.47
1:C:1232:ALA:HB2	1:C:1245:TYR:HE2	1.80	0.47
1:A:33:LEU:HD12	1:A:33:LEU:O	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:VAL:HG12	1:A:37:THR:HG21	1.96	0.47
1:A:93:GLU:HB3	1:A:248:GLY:O	2.14	0.47
1:D:1579:GLU:O	1:D:1583:ARG:HB3	2.13	0.47
1:B:585:ASN:HB3	1:B:587:LEU:HD22	1.97	0.47
1:D:1519:VAL:CG1	1:D:1537:THR:HG21	2.45	0.47
1:A:232:ALA:HB2	1:A:245:TYR:HE2	1.80	0.47
1:A:2:ARG:HG3	1:B:698:PHE:CA	2.44	0.47
1:C:1221:VAL:HG22	1:C:1222:ALA:N	2.28	0.47
1:D:1786:ARG:HD3	1:D:1790:GLU:CD	2.34	0.47
1:B:536:LEU:HD21	1:B:874:ALA:CB	2.45	0.47
1:A:5:SER:O	1:A:9:GLN:HB2	2.15	0.47
1:D:1545:THR:HG21	1:D:1741:TRP:HE1	1.79	0.47
1:B:505:SER:O	1:B:509:GLN:HB2	2.14	0.47
1:C:1039:GLY:O	1:C:1234:LYS:NZ	2.48	0.47
1:A:344:ALA:HB2	1:A:381:VAL:CG2	2.45	0.47
1:D:1617:GLU:HG2	1:D:1638:VAL:HG22	1.95	0.47
1:D:1834:GLU:HG3	1:D:1858:GLY:N	2.30	0.47
1:C:1114:PRO:HD2	1:D:1506:ARG:HH21	1.80	0.47
1:B:533:LEU:O	1:B:533:LEU:HD12	2.15	0.47
1:D:1711:TYR:OH	1:D:1796:TYR:HB3	2.15	0.46
1:A:210:LEU:HD13	1:A:215:HIS:HB2	1.97	0.46
1:B:824:LEU:HD23	1:B:824:LEU:HA	1.75	0.46
1:C:1181:TYR:N	1:C:1181:TYR:CD2	2.81	0.46
1:B:536:LEU:HD11	1:B:846:VAL:CG1	2.44	0.46
1:C:1077:LEU:HD23	1:C:1094:THR:HG22	1.96	0.46
1:D:1529:GLN:O	1:D:1531:VAL:HG23	2.15	0.46
1:A:242:ARG:NH1	1:B:564:TYR:HE1	2.14	0.46
1:C:1334:GLU:HG3	1:C:1358:GLY:N	2.31	0.46
1:D:1842:LEU:HA	1:D:1842:LEU:HD23	1.84	0.46
1:D:1533:LEU:HD12	1:D:1533:LEU:O	2.15	0.46
1:C:1372:ARG:NH1	1:C:1372:ARG:CG	2.77	0.46
1:B:682:PRO:HG2	1:B:685:VAL:CG2	2.39	0.46
1:A:232:ALA:O	1:A:238:MET:HB2	2.16	0.46
1:B:617:GLU:HG2	1:B:638:VAL:HG22	1.97	0.46
1:D:1710:LEU:HD13	1:D:1715:HIS:HB2	1.96	0.46
1:C:1019:VAL:HG12	1:C:1037:THR:HG21	1.98	0.46
1:A:77:LEU:HD21	1:A:245:TYR:HB3	1.98	0.46
1:D:1577:LEU:HD23	1:D:1594:THR:HG22	1.98	0.46
1:B:844:ALA:HB2	1:B:881:VAL:CG2	2.45	0.46
1:B:655:GLU:HA	1:B:655:GLU:OE2	2.14	0.46
1:B:519:VAL:HG12	1:B:537:THR:HG21	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:529:GLN:O	1:B:531:VAL:HG23	2.15	0.46
1:C:1117:GLU:HG2	1:C:1138:VAL:HG22	1.96	0.46
1:A:252:VAL:O	1:A:256:MET:HG3	2.16	0.46
1:C:1100:GLY:N	3:C:1413:PLP:O3P	2.48	0.46
1:C:1172:SER:HA	1:C:1173:PRO:C	2.36	0.46
1:C:1210:LEU:HD13	1:C:1215:HIS:HB2	1.97	0.46
1:B:526:LEU:C	1:B:528:ARG:N	2.66	0.46
1:A:28:ARG:CG	1:A:28:ARG:HH11	2.29	0.46
1:C:1025:GLU:HG2	1:C:1026:LEU:N	2.31	0.46
1:A:241:TRP:NE1	1:B:562:THR:HB	2.31	0.46
1:C:1334:GLU:CG	1:C:1358:GLY:H	2.29	0.46
1:B:600:GLY:N	3:B:913:PLP:O3P	2.49	0.46
1:C:1049:VAL:HG21	1:C:1278:ALA:HB2	1.97	0.46
1:A:172:SER:HA	1:A:173:PRO:C	2.35	0.46
1:D:1539:GLY:O	1:D:1734:LYS:NZ	2.49	0.46
1:C:1344:ALA:HB2	1:C:1381:VAL:CG2	2.46	0.46
1:B:710:LEU:HD13	1:B:715:HIS:HB2	1.97	0.46
1:D:1505:SER:O	1:D:1509:GLN:HB2	2.16	0.46
1:A:25:GLU:HG2	1:A:26:LEU:N	2.31	0.46
1:D:1844:ALA:HB2	1:D:1881:VAL:CG2	2.46	0.46
1:A:85:ASN:HB3	1:A:87:LEU:HD22	1.97	0.46
1:A:70:ILE:HG13	1:A:73:LEU:H	1.81	0.46
1:D:1655:GLU:O	1:D:1659:ARG:HB2	2.15	0.46
1:B:525:GLU:HG2	1:B:526:LEU:N	2.32	0.45
1:D:1525:GLU:HG3	1:D:1529:GLN:HE21	1.80	0.45
1:D:1645:LEU:HD12	1:D:1656:ARG:NH1	2.30	0.45
1:B:732:ALA:HB2	1:B:745:TYR:HE2	1.80	0.45
1:D:1732:ALA:HB2	1:D:1745:TYR:HE2	1.80	0.45
1:B:585:ASN:HB2	1:B:587:LEU:HD22	1.96	0.45
1:D:1761:ARG:C	1:D:1761:ARG:HD3	2.36	0.45
1:D:1672:SER:HA	1:D:1673:PRO:C	2.37	0.45
1:A:39:GLY:O	1:A:234:LYS:NZ	2.50	0.45
1:B:842:LEU:HD23	1:B:842:LEU:HA	1.81	0.45
1:A:312:LEU:HA	1:A:312:LEU:HD23	1.80	0.45
1:A:117:GLU:HG2	1:A:138:VAL:HG22	1.97	0.45
1:D:1753:ILE:HD12	1:D:1756:MET:HE3	1.98	0.45
1:D:1549:VAL:HG21	1:D:1778:ALA:HB2	1.97	0.45
1:B:539:GLY:O	1:B:734:LYS:NZ	2.48	0.45
1:A:166:LYS:O	1:A:198:PHE:HB2	2.16	0.45
1:B:653:ASP:N	1:B:656:ARG:HH21	2.13	0.45
1:D:1577:LEU:HD21	1:D:1745:TYR:HB3	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1085:ASN:HB3	1:C:1087:LEU:HD22	1.99	0.45
1:B:536:LEU:HD12	1:B:848:VAL:CG1	2.46	0.45
1:C:1150:PHE:CE1	1:C:1315:VAL:HG21	2.51	0.45
1:C:1070:ILE:HG13	1:C:1073:LEU:H	1.80	0.45
1:C:1344:ALA:HB2	1:C:1381:VAL:HG21	1.98	0.45
1:A:26:LEU:HB3	1:A:31:VAL:CG1	2.45	0.45
1:A:253:ILE:HD12	1:A:256:MET:HE3	1.97	0.45
1:C:1255:ALA:HB2	1:D:1504:LEU:CD2	2.46	0.45
1:C:1255:ALA:CB	1:D:1504:LEU:HD23	2.46	0.45
1:C:1049:VAL:CG2	1:C:1278:ALA:HB2	2.46	0.45
1:C:1005:SER:O	1:C:1009:GLN:HB2	2.17	0.45
1:B:626:VAL:HG22	1:B:853:ASP:HB3	1.99	0.45
1:B:618:VAL:HG13	1:B:667:ALA:HB3	1.99	0.45
1:D:1802:LEU:O	1:D:1802:LEU:HD22	2.17	0.45
1:A:344:ALA:HB2	1:A:381:VAL:HG21	1.99	0.45
1:A:45:THR:HG21	1:A:241:TRP:NE1	2.29	0.45
1:A:19:VAL:CG1	1:A:37:THR:HG21	2.46	0.45
1:D:1626:VAL:HG22	1:D:1853:ASP:HB3	1.99	0.45
1:C:1312:LEU:HD21	1:C:1382:LEU:HD21	1.98	0.45
1:C:1152:PRO:HD3	1:C:1181:TYR:CZ	2.52	0.45
1:C:1107:LEU:O	1:C:1111:ILE:HG12	2.17	0.45
1:C:1241:TRP:NE1	1:D:1562:THR:HB	2.32	0.45
1:B:834:GLU:HG3	1:B:858:GLY:N	2.32	0.45
1:C:1001:MET:CG	1:C:1002:ARG:N	2.80	0.44
1:A:262:GLN:HG3	1:B:511:MET:HE1	1.99	0.44
1:D:1804:LEU:HD11	1:D:1817:PRO:HD2	2.00	0.44
1:B:549:VAL:HG21	1:B:778:ALA:HB2	1.97	0.44
1:B:753:ILE:HD12	1:B:756:MET:HE3	2.00	0.44
1:A:334:GLU:HG3	1:A:358:GLY:N	2.32	0.44
1:A:49:VAL:HG21	1:A:278:ALA:HB2	2.00	0.44
1:B:732:ALA:O	1:B:738:MET:HB2	2.18	0.44
1:A:232:ALA:HB2	1:A:245:TYR:CE2	2.53	0.44
1:A:82:ARG:HA	1:A:87:LEU:O	2.18	0.44
1:C:1093:GLU:O	1:C:1247:CYS:HB2	2.18	0.44
1:A:302:LEU:HD22	1:A:302:LEU:O	2.16	0.44
1:A:100:GLY:N	3:A:413:PLP:O3P	2.49	0.44
1:C:1264:THR:HG22	1:D:1602:GLN:HG3	1.99	0.44
1:C:1121:LEU:HD13	1:C:1152:PRO:HB3	2.00	0.44
1:C:1166:LYS:O	1:C:1198:PHE:HB2	2.18	0.44
1:C:1126:VAL:HG22	1:C:1353:ASP:HB3	1.98	0.44
1:A:286:ARG:HB3	1:A:286:ARG:CZ	2.47	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:582:ARG:HA	1:B:587:LEU:O	2.18	0.44
1:A:93:GLU:O	1:A:247:CYS:HB2	2.17	0.44
1:A:372:ARG:HA	1:A:375:LEU:HD12	1.98	0.44
1:B:732:ALA:HB2	1:B:745:TYR:CE2	2.52	0.44
1:C:1236:PHE:O	1:C:1238:MET:HG3	2.18	0.44
1:B:844:ALA:HB2	1:B:881:VAL:HG21	1.99	0.44
1:B:666:LYS:O	1:B:698:PHE:HB2	2.17	0.44
1:B:834:GLU:CG	1:B:858:GLY:H	2.31	0.44
1:A:198:PHE:O	1:A:225:HIS:HB3	2.18	0.44
1:C:1194:VAL:HG12	1:C:1195:GLU:N	2.32	0.44
1:B:577:LEU:HD21	1:B:745:TYR:HB3	2.00	0.44
1:C:1211:TYR:OH	1:C:1296:TYR:HB3	2.17	0.44
1:D:1698:PHE:O	1:D:1725:HIS:HB3	2.18	0.44
1:D:1824:LEU:HD23	1:D:1824:LEU:HA	1.76	0.44
1:C:1151:VAL:HG23	1:C:1152:PRO:HD2	2.00	0.44
1:A:118:VAL:HG13	1:A:167:ALA:HB3	2.00	0.44
1:A:77:LEU:HD23	1:A:94:THR:HG22	1.98	0.44
1:D:1666:LYS:O	1:D:1698:PHE:HB2	2.18	0.44
1:A:256:MET:O	1:A:260:SER:HB2	2.18	0.44
1:D:1683:LYS:O	1:D:1687:GLU:HB2	2.18	0.44
1:C:1252:VAL:O	1:C:1256:MET:HG3	2.18	0.44
1:C:1173:PRO:HB2	1:C:1206:TYR:HB2	2.00	0.44
1:A:34:VAL:O	1:A:346:VAL:HA	2.18	0.44
1:B:520:ASN:HD21	1:B:538:ALA:HB2	1.83	0.44
1:C:1028:ARG:HH11	1:C:1028:ARG:CG	2.31	0.43
1:D:1834:GLU:CG	1:D:1858:GLY:H	2.30	0.43
1:D:1549:VAL:CG2	1:D:1778:ALA:HB2	2.48	0.43
1:D:1520:ASN:HD21	1:D:1538:ALA:HB2	1.83	0.43
1:B:736:PHE:O	1:B:738:MET:HG3	2.18	0.43
1:A:2:ARG:CZ	1:B:725:HIS:CD2	3.01	0.43
1:B:658:ARG:HH21	1:B:696:HIS:HE1	1.65	0.43
1:B:651:VAL:HG23	1:B:652:PRO:HD2	1.99	0.43
1:B:607:LEU:HD13	1:B:727:LEU:CD2	2.40	0.43
1:D:1844:ALA:HB2	1:D:1881:VAL:HG21	2.00	0.43
1:C:1190:ALA:HB3	1:C:1221:VAL:HG21	2.01	0.43
1:B:756:MET:O	1:B:760:SER:HB2	2.18	0.43
1:C:1256:MET:O	1:C:1260:SER:HB2	2.18	0.43
1:A:151:VAL:HG23	1:A:152:PRO:HD2	2.01	0.43
1:B:519:VAL:CG1	1:B:537:THR:HG21	2.47	0.43
1:A:12:LYS:HB2	1:A:130:GLU:OE2	2.18	0.43
1:B:827:THR:CG2	1:B:860:VAL:HB	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1232:ALA:HB2	1:C:1245:TYR:CE2	2.52	0.43
1:D:1526:LEU:O	1:D:1531:VAL:HB	2.19	0.43
1:A:324:LEU:HA	1:A:324:LEU:HD23	1.77	0.43
1:D:1536:LEU:HD11	1:D:1846:VAL:CG1	2.49	0.43
1:A:121:LEU:HD13	1:A:152:PRO:HB3	2.01	0.43
1:B:549:VAL:CG2	1:B:778:ALA:HB2	2.48	0.43
1:A:49:VAL:CG2	1:A:278:ALA:HB2	2.47	0.43
1:D:1600:GLY:H	3:D:1913:PLP:P	2.41	0.43
1:B:672:SER:HA	1:B:673:PRO:C	2.39	0.43
1:D:1593:GLU:O	1:D:1747:CYS:HB2	2.19	0.43
1:B:570:ILE:HG13	1:B:573:LEU:H	1.82	0.43
1:D:1621:LEU:HD13	1:D:1652:PRO:HB3	2.00	0.43
1:B:711:TYR:OH	1:B:796:TYR:HB3	2.18	0.43
1:D:1580:LYS:HZ3	1:D:1584:GLU:HB2	1.84	0.43
1:C:1183:LYS:O	1:C:1187:GLU:HB2	2.19	0.43
1:A:145:LEU:CD1	1:A:156:ARG:NH1	2.77	0.43
1:D:1732:ALA:O	1:D:1738:MET:HB2	2.19	0.43
1:D:1732:ALA:HB2	1:D:1745:TYR:CE2	2.53	0.43
1:C:1026:LEU:HB3	1:C:1031:VAL:CG1	2.46	0.43
1:C:1306:GLY:HA3	1:C:1375:LEU:HD21	2.01	0.43
1:C:1354:PHE:O	1:C:1355:ALA:HB3	2.18	0.43
1:B:854:PHE:O	1:B:855:ALA:HB3	2.18	0.43
1:C:1290:GLU:H	1:C:1290:GLU:HG2	1.51	0.43
1:C:1302:LEU:HD22	1:C:1302:LEU:O	2.19	0.43
1:C:1232:ALA:O	1:C:1238:MET:HB2	2.19	0.43
1:B:802:LEU:O	1:B:802:LEU:HD22	2.18	0.43
1:A:45:THR:HG22	1:B:562:THR:OG1	2.18	0.43
1:C:1327:THR:CG2	1:C:1360:VAL:HB	2.49	0.43
1:B:548:HIS:O	1:B:777:GLU:HG2	2.19	0.43
1:C:1118:VAL:HG21	1:C:1132:VAL:HG22	2.01	0.43
1:A:24:LEU:O	1:A:27:ARG:HB2	2.19	0.42
1:A:26:LEU:C	1:A:31:VAL:HB	2.38	0.42
1:A:20:ASN:HD21	1:A:38:ALA:HB2	1.84	0.42
1:A:264:THR:HG22	1:B:602:GLN:HG3	2.01	0.42
1:C:1019:VAL:CG1	1:C:1037:THR:HG21	2.48	0.42
1:D:1827:THR:CG2	1:D:1860:VAL:HB	2.49	0.42
1:C:1304:LEU:HD11	1:C:1317:PRO:HD2	2.01	0.42
1:D:1570:ILE:HG13	1:D:1573:LEU:H	1.83	0.42
1:B:648:GLU:OE2	1:B:656:ARG:NH2	2.53	0.42
1:A:354:PHE:O	1:A:355:ALA:HB3	2.18	0.42
1:A:211:TYR:OH	1:A:296:TYR:HB3	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:845:GLY:HA3	1:B:877:ARG:HH12	1.84	0.42
1:A:217:SER:HB2	1:A:220:ARG:HD2	2.02	0.42
1:C:1145:LEU:CD1	1:C:1156:ARG:NH1	2.78	0.42
1:B:698:PHE:O	1:B:725:HIS:HB3	2.19	0.42
1:C:1190:ALA:HA	1:C:1200:LEU:CD1	2.49	0.42
1:D:1752:VAL:O	1:D:1756:MET:HG3	2.19	0.42
1:D:1756:MET:O	1:D:1760:SER:HB2	2.20	0.42
1:A:81:PHE:O	1:A:87:LEU:HB2	2.19	0.42
1:C:1180:VAL:CG1	1:C:1180:VAL:O	2.67	0.42
1:D:1651:VAL:HG23	1:D:1652:PRO:HD2	2.01	0.42
1:D:1548:HIS:O	1:D:1777:GLU:HG2	2.20	0.42
1:A:126:VAL:HG22	1:A:353:ASP:HB3	2.01	0.42
1:D:1662:THR:HB	1:D:1663:PRO:CD	2.50	0.42
1:C:1020:ASN:HD21	1:C:1038:ALA:HB2	1.84	0.42
1:C:1040:GLU:HA	1:C:1041:PRO:HD3	1.95	0.42
1:A:186:LEU:HD12	1:A:186:LEU:HA	1.80	0.42
1:C:1336:ARG:HD2	1:C:1336:ARG:HA	1.73	0.42
1:A:152:PRO:HD3	1:A:181:TYR:CZ	2.54	0.42
1:C:1077:LEU:HD21	1:C:1245:TYR:HB3	2.01	0.42
1:A:236:PHE:O	1:A:238:MET:HG3	2.20	0.42
1:B:711:TYR:HB3	1:B:797:ARG:NH1	2.35	0.42
1:A:28:ARG:HG2	1:A:28:ARG:HH11	1.85	0.42
1:D:1845:GLY:HA3	1:D:1877:ARG:HH12	1.85	0.42
1:A:183:LYS:O	1:A:187:GLU:HB2	2.19	0.42
1:C:1121:LEU:HA	1:C:1142:VAL:O	2.20	0.42
1:D:1534:VAL:O	1:D:1846:VAL:HA	2.20	0.42
1:C:1186:LEU:HD12	1:C:1186:LEU:HA	1.79	0.42
1:D:1536:LEU:HD21	1:D:1874:ALA:CB	2.50	0.42
1:C:1081:PHE:O	1:C:1087:LEU:HB2	2.19	0.42
1:C:1198:PHE:O	1:C:1225:HIS:HB3	2.20	0.42
1:C:1118:VAL:HG13	1:C:1167:ALA:HB3	2.02	0.42
1:D:1690:ALA:O	1:D:1694:VAL:HG23	2.20	0.41
1:D:1604:LEU:O	1:D:1608:PHE:CD1	2.73	0.41
1:B:536:LEU:HD11	1:B:846:VAL:HG11	2.01	0.41
1:B:673:PRO:HB2	1:B:706:TYR:HB2	2.02	0.41
1:D:1621:LEU:HA	1:D:1642:VAL:O	2.20	0.41
1:A:304:LEU:HD11	1:A:317:PRO:HD2	2.02	0.41
1:A:376:GLU:O	1:A:379:ALA:HB3	2.19	0.41
1:C:1162:THR:HB	1:C:1163:PRO:CD	2.50	0.41
1:C:1045:THR:HG22	1:D:1562:THR:OG1	2.20	0.41
1:C:1110:ALA:HA	1:D:1508:VAL:HG11	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1373:LYS:O	1:C:1377:ARG:HG2	2.20	0.41
1:A:69:GLY:HA3	1:A:96:VAL:HG23	2.02	0.41
1:A:334:GLU:CG	1:A:358:GLY:H	2.32	0.41
1:D:1682:PRO:HG2	1:D:1685:VAL:CG2	2.39	0.41
1:D:1711:TYR:HB3	1:D:1797:ARG:NH1	2.36	0.41
1:B:625:TRP:NE1	2:B:914:ASP:HB3	2.35	0.41
1:B:618:VAL:HG21	1:B:632:VAL:HG22	2.02	0.41
1:A:327:THR:CG2	1:A:360:VAL:HB	2.51	0.41
1:B:776:LEU:O	1:B:776:LEU:HD23	2.19	0.41
1:A:162:THR:HB	1:A:163:PRO:CD	2.50	0.41
1:D:1873:LYS:O	1:D:1877:ARG:HG2	2.21	0.41
1:A:345:GLY:HA3	1:A:377:ARG:HH12	1.85	0.41
1:A:92:GLU:CD	1:A:92:GLU:H	2.23	0.41
1:C:1345:GLY:HA3	1:C:1377:ARG:HH12	1.86	0.41
1:D:1854:PHE:O	1:D:1855:ALA:HB3	2.21	0.41
1:A:255:ALA:CB	1:B:504:LEU:HD23	2.50	0.41
1:B:873:LYS:O	1:B:877:ARG:HG2	2.21	0.41
1:B:683:LYS:O	1:B:687:GLU:HB2	2.21	0.41
1:A:166:LYS:HD3	1:B:501:MET:O	2.20	0.41
1:A:270:ILE:N	1:A:270:ILE:HD12	2.36	0.41
1:D:1689:LEU:HD13	1:D:1689:LEU:N	2.35	0.41
1:C:1002:ARG:HG3	1:D:1698:PHE:CA	2.49	0.41
1:D:1673:PRO:HB2	1:D:1706:TYR:HB2	2.03	0.41
1:D:1529:GLN:H	1:D:1529:GLN:HG2	1.72	0.41
1:A:261:ARG:NH2	1:B:517:VAL:HG23	2.35	0.41
1:D:1569:GLY:HA3	1:D:1596:VAL:HG23	2.03	0.41
1:C:1286:ARG:HB3	1:C:1286:ARG:CZ	2.50	0.41
1:D:1512:LYS:HA	1:D:1513:PRO:HD3	1.79	0.41
1:B:570:ILE:HA	1:B:571:PRO:HD3	1.90	0.41
1:C:1153:ASP:HA	1:C:1154:PRO:HD2	1.74	0.41
1:B:804:LEU:HD11	1:B:817:PRO:HD2	2.02	0.41
1:C:1034:VAL:O	1:C:1346:VAL:HA	2.20	0.41
1:C:1048:HIS:O	1:C:1277:GLU:HG2	2.21	0.41
1:D:1618:VAL:HG21	1:D:1632:VAL:HG22	2.02	0.41
1:B:577:LEU:HD23	1:B:594:THR:CG2	2.51	0.41
1:C:1077:LEU:HD23	1:C:1094:THR:CG2	2.51	0.41
1:A:69:GLY:HA3	1:A:96:VAL:HG21	2.02	0.41
1:B:534:VAL:O	1:B:846:VAL:HA	2.20	0.41
1:A:217:SER:O	1:A:220:ARG:HD3	2.21	0.41
1:A:48:HIS:O	1:A:277:GLU:HG2	2.21	0.41
1:A:342:LEU:HD23	1:A:342:LEU:HA	1.84	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1686:LEU:HD12	1:D:1686:LEU:HA	1.76	0.41
1:C:1270:ILE:N	1:C:1270:ILE:HD12	2.36	0.41
1:D:1581:PHE:O	1:D:1587:LEU:HB2	2.21	0.40
1:A:211:TYR:HB3	1:A:297:ARG:NH1	2.35	0.40
1:B:621:LEU:HD13	1:B:652:PRO:HB3	2.02	0.40
1:D:1618:VAL:HG13	1:D:1667:ALA:HB3	2.03	0.40
1:B:662:THR:HB	1:B:663:PRO:CD	2.51	0.40
1:C:1027:ARG:HB3	1:C:1027:ARG:HE	1.69	0.40
1:C:1211:TYR:HB3	1:C:1297:ARG:NH1	2.36	0.40
1:B:581:PHE:O	1:B:587:LEU:HB2	2.20	0.40
1:B:812:LEU:HD11	1:B:882:LEU:HD21	2.04	0.40
1:B:674:ASN:OD1	1:B:675:ASN:N	2.55	0.40
1:C:1261:ARG:NH2	1:D:1517:VAL:HG23	2.36	0.40
1:D:1690:ALA:HA	1:D:1700:LEU:CD1	2.50	0.40
1:B:569:GLY:HA3	1:B:596:VAL:HG21	2.02	0.40
1:D:1569:GLY:HA3	1:D:1596:VAL:HG21	2.03	0.40
1:D:1770:ILE:HD12	1:D:1770:ILE:N	2.36	0.40
1:C:1312:LEU:HD23	1:C:1312:LEU:HA	1.79	0.40
1:A:173:PRO:HB2	1:A:206:TYR:HB2	2.02	0.40
1:B:653:ASP:HA	1:B:654:PRO:HD2	1.74	0.40
1:B:690:ALA:HA	1:B:700:LEU:CD1	2.51	0.40
1:C:1069:GLY:HA3	1:C:1096:VAL:HG21	2.02	0.40
1:B:816:ARG:HG3	1:B:816:ARG:NH1	2.37	0.40
1:A:276:LEU:HD23	1:A:276:LEU:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:528:ARG:O	1:D:1525:GLU:OE1[1_445]	2.19	0.01

5.3 Torsion angles

5.3.1 Protein backbone

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

The Analysed column shows the number of residues for which the backbone conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	380/385 (99%)	329 (87%)	45 (12%)	6 (2%)	12	48
1	B	380/385 (99%)	329 (87%)	46 (12%)	5 (1%)	15	52
1	C	380/385 (99%)	330 (87%)	44 (12%)	6 (2%)	12	48
1	D	380/385 (99%)	329 (87%)	44 (12%)	7 (2%)	11	46
All	All	1520/1540 (99%)	1317 (87%)	179 (12%)	24 (2%)	12	48

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	31	VAL
1	B	531	VAL
1	C	1031	VAL
1	D	1531	VAL
1	D	1626	VAL
1	D	1782	GLN
1	D	1783	GLU
1	A	126	VAL
1	B	626	VAL
1	C	1126	VAL
1	A	183	LYS
1	B	654	PRO
1	B	683	LYS
1	C	1183	LYS
1	D	1654	PRO
1	D	1683	LYS
1	A	154	PRO
1	A	329	PRO
1	B	829	PRO
1	C	1329	PRO
1	C	1154	PRO
1	D	1829	PRO
1	A	41	PRO
1	C	1041	PRO

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	305/306 (100%)	242 (79%)	63 (21%)	1	6
1	B	305/306 (100%)	245 (80%)	60 (20%)	1	7
1	C	305/306 (100%)	241 (79%)	64 (21%)	1	6
1	D	305/306 (100%)	241 (79%)	64 (21%)	1	6
All	All	1220/1224 (100%)	969 (79%)	251 (21%)	1	6

All (251) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ARG
1	A	12	LYS
1	A	14	ASP
1	A	16	VAL
1	A	22	LYS
1	A	25	GLU
1	A	26	LEU
1	A	28	ARG
1	A	29	GLN
1	A	32	ASP
1	A	45	THR
1	A	73	LEU
1	A	74	ARG
1	A	75	GLU
1	A	77	LEU
1	A	80	LYS
1	A	87	LEU
1	A	90	THR
1	A	96	VAL
1	A	102	GLN
1	A	114	PRO
1	A	116	ASP
1	A	124	TYR
1	A	126	VAL
1	A	147	GLU
1	A	153	ASP
1	A	155	GLU
1	A	158	ARG
1	A	164	ARG
1	A	170	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	186	LEU
1	A	189	LEU
1	A	197	ASP
1	A	207	GLU
1	A	227	LEU
1	A	230	ASN
1	A	239	THR
1	A	245	TYR
1	A	251	GLU
1	A	261	ARG
1	A	268	ASP
1	A	276	LEU
1	A	283	GLU
1	A	290	GLU
1	A	291	MET
1	A	302	LEU
1	A	303	LEU
1	A	307	LEU
1	A	308	THR
1	A	321	PHE
1	A	326	ASP
1	A	339	GLU
1	A	342	LEU
1	A	348	VAL
1	A	360	VAL
1	A	362	LEU
1	A	367	SER
1	A	369	GLU
1	A	372	ARG
1	A	376	GLU
1	A	380	ARG
1	A	381	VAL
1	A	382	LEU
1	B	506	ARG
1	B	514	ASP
1	B	516	VAL
1	B	522	LYS
1	B	524	LEU
1	B	525	GLU
1	B	526	LEU
1	B	529	GLN
1	B	532	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	536	LEU
1	B	545	THR
1	B	573	LEU
1	B	574	ARG
1	B	577	LEU
1	B	580	LYS
1	B	582	ARG
1	B	587	LEU
1	B	590	THR
1	B	596	VAL
1	B	602	GLN
1	B	614	PRO
1	B	616	ASP
1	B	624	TYR
1	B	626	VAL
1	B	647	GLU
1	B	653	ASP
1	B	655	GLU
1	B	658	ARG
1	B	664	ARG
1	B	670	VAL
1	B	686	LEU
1	B	689	LEU
1	B	697	ASP
1	B	707	GLU
1	B	727	LEU
1	B	730	ASN
1	B	739	THR
1	B	745	TYR
1	B	761	ARG
1	B	768	ASP
1	B	776	LEU
1	B	783	GLU
1	B	790	GLU
1	B	791	MET
1	B	802	LEU
1	B	803	LEU
1	B	807	LEU
1	B	808	THR
1	B	821	PHE
1	B	826	ASP
1	B	839	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	842	LEU
1	B	848	VAL
1	B	860	VAL
1	B	862	LEU
1	B	869	GLU
1	B	876	GLU
1	B	880	ARG
1	B	881	VAL
1	B	882	LEU
1	C	1001	MET
1	C	1006	ARG
1	C	1014	ASP
1	C	1016	VAL
1	C	1022	LYS
1	C	1025	GLU
1	C	1026	LEU
1	C	1028	ARG
1	C	1032	ASP
1	C	1045	THR
1	C	1073	LEU
1	C	1074	ARG
1	C	1075	GLU
1	C	1077	LEU
1	C	1080	LYS
1	C	1082	ARG
1	C	1087	LEU
1	C	1090	THR
1	C	1096	VAL
1	C	1102	GLN
1	C	1114	PRO
1	C	1116	ASP
1	C	1124	TYR
1	C	1126	VAL
1	C	1147	GLU
1	C	1153	ASP
1	C	1155	GLU
1	C	1158	ARG
1	C	1164	ARG
1	C	1170	VAL
1	C	1186	LEU
1	C	1189	LEU
1	C	1194	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	1197	ASP
1	C	1207	GLU
1	C	1227	LEU
1	C	1230	ASN
1	C	1239	THR
1	C	1245	TYR
1	C	1261	ARG
1	C	1268	ASP
1	C	1276	LEU
1	C	1283	GLU
1	C	1290	GLU
1	C	1291	MET
1	C	1302	LEU
1	C	1303	LEU
1	C	1307	LEU
1	C	1308	THR
1	C	1321	PHE
1	C	1326	ASP
1	C	1336	ARG
1	C	1339	GLU
1	C	1342	LEU
1	C	1348	VAL
1	C	1360	VAL
1	C	1362	LEU
1	C	1367	SER
1	C	1372	ARG
1	C	1375	LEU
1	C	1376	GLU
1	C	1380	ARG
1	C	1381	VAL
1	C	1382	LEU
1	D	1506	ARG
1	D	1512	LYS
1	D	1514	ASP
1	D	1516	VAL
1	D	1522	LYS
1	D	1524	LEU
1	D	1525	GLU
1	D	1526	LEU
1	D	1528	ARG
1	D	1529	GLN
1	D	1532	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	1536	LEU
1	D	1545	THR
1	D	1573	LEU
1	D	1574	ARG
1	D	1577	LEU
1	D	1580	LYS
1	D	1582	ARG
1	D	1587	LEU
1	D	1590	THR
1	D	1596	VAL
1	D	1602	GLN
1	D	1614	PRO
1	D	1616	ASP
1	D	1624	TYR
1	D	1626	VAL
1	D	1630	GLU
1	D	1647	GLU
1	D	1653	ASP
1	D	1655	GLU
1	D	1658	ARG
1	D	1659	ARG
1	D	1664	ARG
1	D	1670	VAL
1	D	1686	LEU
1	D	1689	LEU
1	D	1697	ASP
1	D	1707	GLU
1	D	1720	ARG
1	D	1727	LEU
1	D	1730	ASN
1	D	1739	THR
1	D	1745	TYR
1	D	1761	ARG
1	D	1768	ASP
1	D	1776	LEU
1	D	1786	ARG
1	D	1790	GLU
1	D	1791	MET
1	D	1802	LEU
1	D	1803	LEU
1	D	1807	LEU
1	D	1808	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	1821	PHE
1	D	1826	ASP
1	D	1842	LEU
1	D	1848	VAL
1	D	1860	VAL
1	D	1862	LEU
1	D	1869	GLU
1	D	1872	ARG
1	D	1880	ARG
1	D	1881	VAL
1	D	1882	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	29	GLN
1	A	59	GLN
1	A	171	ASN
1	A	196	HIS
1	B	520	ASN
1	B	529	GLN
1	B	559	GLN
1	B	671	ASN
1	B	696	HIS
1	C	1020	ASN
1	C	1059	GLN
1	C	1171	ASN
1	C	1174	ASN
1	C	1196	HIS
1	D	1520	ASN
1	D	1529	GLN
1	D	1559	GLN
1	D	1671	ASN
1	D	1696	HIS

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 ⓘ

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	PLP	A	413	2	15,15,16	1.98	4 (26%)	21,22,23	2.22	4 (19%)
2	ASP	A	414	3	2,8,8	0.16	0	0,10,10	0.00	-
3	PLP	B	913	2	15,15,16	2.39	6 (40%)	21,22,23	2.09	6 (28%)
2	ASP	B	914	3	2,8,8	0.46	0	0,10,10	0.00	-
3	PLP	C	1413	2	15,15,16	1.70	4 (26%)	21,22,23	2.32	7 (33%)
2	ASP	C	1414	3	2,8,8	0.70	0	0,10,10	0.00	-
3	PLP	D	1913	2	15,15,16	2.76	5 (33%)	21,22,23	2.08	7 (33%)
2	ASP	D	1914	3	2,8,8	0.78	0	0,10,10	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	A	413	2	-	0/6/6/8	0/1/1/1
2	ASP	A	414	3	-	0/2/8/8	0/0/0/0
3	PLP	B	913	2	-	0/6/6/8	0/1/1/1
2	ASP	B	914	3	-	0/2/8/8	0/0/0/0
3	PLP	C	1413	2	-	0/6/6/8	0/1/1/1
2	ASP	C	1414	3	-	0/2/8/8	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PLP	D	1913	2	-	0/6/6/8	0/1/1/1
2	ASP	D	1914	3	-	0/2/8/8	0/0/0/0

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1913	PLP	C4A-C4	-8.45	1.34	1.51
3	A	413	PLP	C4A-C4	-5.27	1.40	1.51
3	B	913	PLP	O3-C3	-3.91	1.27	1.37
3	C	1413	PLP	P-O3P	-3.03	1.43	1.54
3	D	1913	PLP	C3-C2	-2.98	1.38	1.40
3	C	1413	PLP	C5-C4	-2.94	1.37	1.40
3	A	413	PLP	C3-C4	-2.70	1.33	1.40
3	A	413	PLP	O3-C3	-2.64	1.30	1.37
3	B	913	PLP	P-O3P	-2.37	1.46	1.54
3	D	1913	PLP	P-O3P	-2.03	1.47	1.54
3	A	413	PLP	P-O3P	-2.01	1.47	1.54
3	D	1913	PLP	C2A-C2	2.09	1.54	1.50
3	C	1413	PLP	P-O2P	2.20	1.62	1.54
3	B	913	PLP	C6-N1	2.56	1.39	1.34
3	B	913	PLP	C6-C5	2.75	1.43	1.37
3	C	1413	PLP	C5A-C5	2.91	1.59	1.50
3	D	1913	PLP	C5-C4	3.26	1.44	1.40
3	B	913	PLP	P-O2P	3.47	1.67	1.54
3	B	913	PLP	C5-C4	5.61	1.47	1.40

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	913	PLP	C3-C4-C5	-5.09	113.22	118.78
3	C	1413	PLP	C4A-C4-C5	-3.81	116.91	120.88
3	D	1913	PLP	C3-C4-C5	-2.71	115.82	118.78
3	D	1913	PLP	C2A-C2-C3	-2.17	118.42	121.04
3	C	1413	PLP	O3P-P-O4P	-2.07	100.60	106.56
3	D	1913	PLP	C5-C6-N1	-2.05	120.31	123.86
3	D	1913	PLP	C4A-C4-C3	2.08	124.12	120.36
3	B	913	PLP	C6-C5-C4	2.13	119.96	118.15
3	C	1413	PLP	C4A-C4-C3	2.26	124.45	120.36
3	C	1413	PLP	C6-C5-C4	2.42	120.20	118.15
3	B	913	PLP	O3P-P-O1P	2.48	118.55	110.58
3	A	413	PLP	O3P-P-O1P	2.49	118.59	110.58
3	A	413	PLP	C6-C5-C4	2.55	120.31	118.15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1913	PLP	C6-C5-C4	2.62	120.37	118.15
3	C	1413	PLP	O3P-P-O1P	2.63	119.06	110.58
3	A	413	PLP	O3-C3-C2	2.67	122.30	117.66
3	C	1413	PLP	O2P-P-O4P	2.96	115.08	106.56
3	B	913	PLP	O4P-C5A-C5	2.98	113.91	108.99
3	D	1913	PLP	O3P-P-O1P	3.40	121.52	110.58
3	B	913	PLP	C4-C3-C2	3.89	126.68	120.05
3	B	913	PLP	C4A-C4-C5	4.82	125.90	120.88
3	D	1913	PLP	O4P-C5A-C5	6.59	119.88	108.99
3	C	1413	PLP	O4P-C5A-C5	7.59	121.55	108.99
3	A	413	PLP	O4P-C5A-C5	7.96	122.15	108.99

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	413	PLP	1	0
3	B	913	PLP	2	0
2	B	914	ASP	3	0
3	C	1413	PLP	1	0
3	D	1913	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	382/385 (99%)	-0.36	2 (0%) 91 90	2, 13, 35, 52	0
1	B	382/385 (99%)	-0.45	0 100 100	2, 12, 35, 57	0
1	C	382/385 (99%)	-0.31	3 (0%) 87 84	2, 14, 38, 52	0
1	D	382/385 (99%)	-0.33	1 (0%) 94 94	2, 13, 35, 55	0
All	All	1528/1540 (99%)	-0.36	6 (0%) 93 92	2, 13, 36, 57	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1381	VAL	3.0
1	C	1382	LEU	2.5
1	D	1528	ARG	2.5
1	C	1379	ALA	2.4
1	A	23	ALA	2.2
1	A	344	ALA	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 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. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	ASP	B	914	9/9	0.84	0.29	3.76	15,22,26,27	0
2	ASP	C	1414	9/9	0.87	0.21	3.17	17,24,29,29	0
2	ASP	A	414	9/9	0.86	0.28	3.14	2,7,24,29	0
2	ASP	D	1914	9/9	0.90	0.25	1.74	18,30,36,39	0
3	PLP	C	1413	15/16	0.96	0.15	0.01	2,6,10,11	0
3	PLP	B	913	15/16	0.95	0.16	-0.25	2,5,11,14	0
3	PLP	A	413	15/16	0.97	0.15	-0.60	3,8,13,17	0
3	PLP	D	1913	15/16	0.97	0.14	-0.68	6,13,21,22	0

6.5 Other polymers ⓘ

There are no such residues in this entry.