



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:16 AM UTC

PDB ID : 1GC4 / pdb_00001gc4
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

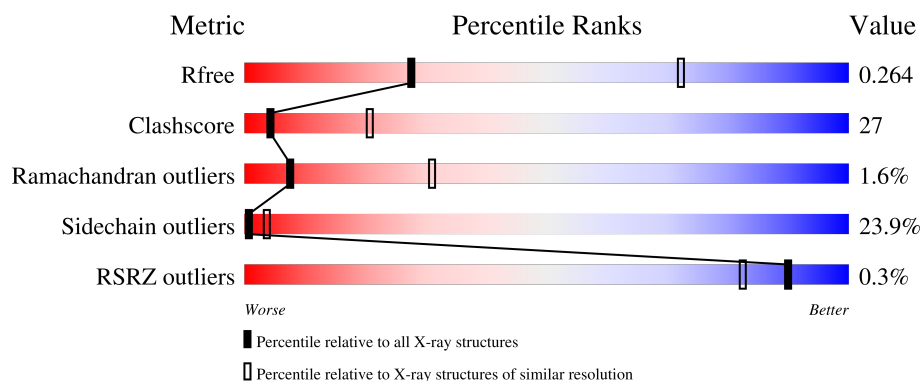
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	385	 40% 38% 18% ..
1	B	385	 40% 38% 19% ..
1	C	385	 39% 39% 19% ..
1	D	385	 39% 39% 18% ..

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	ASP	D	1914	-	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.

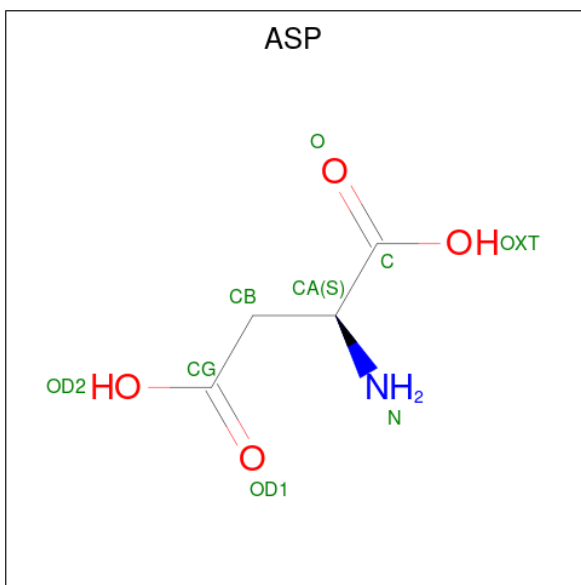
- Molecule 1 is a protein called ASPARTATE AMINOTRANSFERASE.

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:

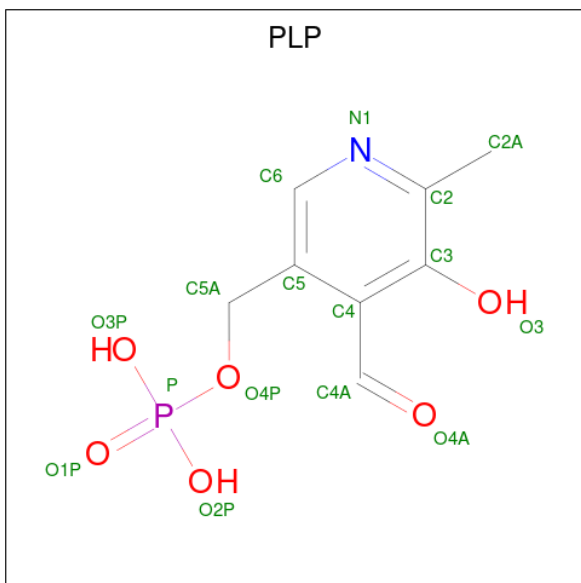
Chain	Residue	Modelled	Actual	Comment	Reference
A	14	ASP	SER	engineered mutation	UNP Q56232
A	16	VAL	THR	engineered mutation	UNP Q56232
A	101	SER	LYS	engineered mutation	UNP Q56232
A	261	ARG	SER	engineered mutation	UNP Q56232
B	514	ASP	SER	engineered mutation	UNP Q56232
B	516	VAL	THR	engineered mutation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

- Molecule 2 is ASPARTIC ACID (CCD ID: 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 (CCD ID: PLP) (formula: $C_8H_{10}NO_6P$).

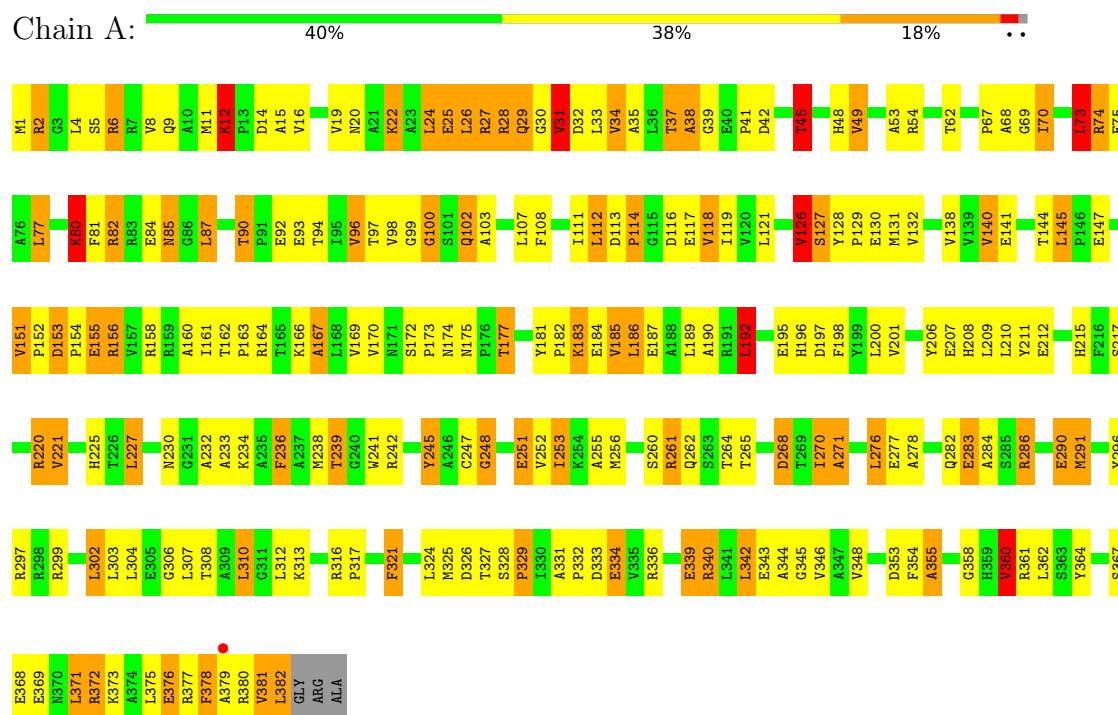


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

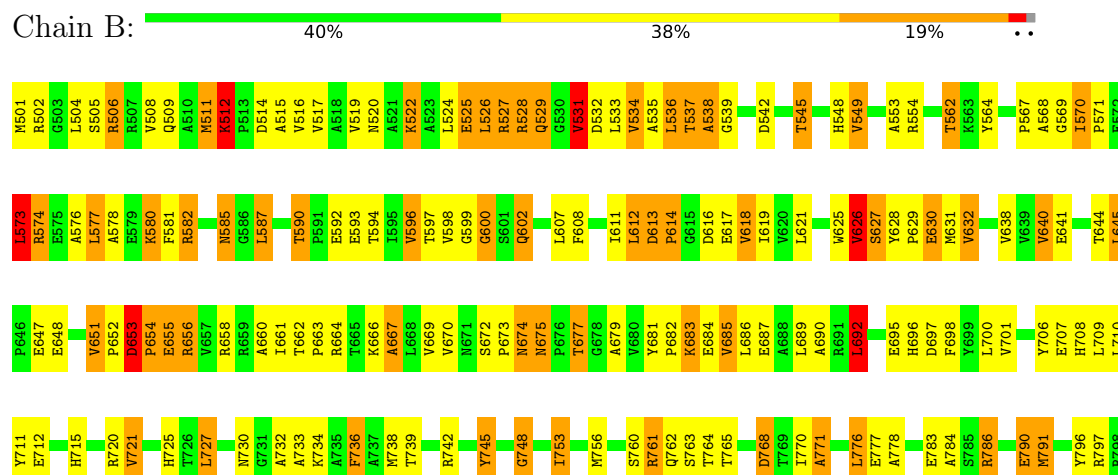
3 Residue-property plots

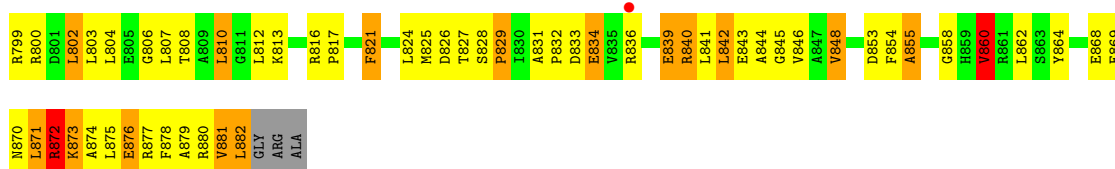
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: ASPARTATE AMINOTRANSFERASE

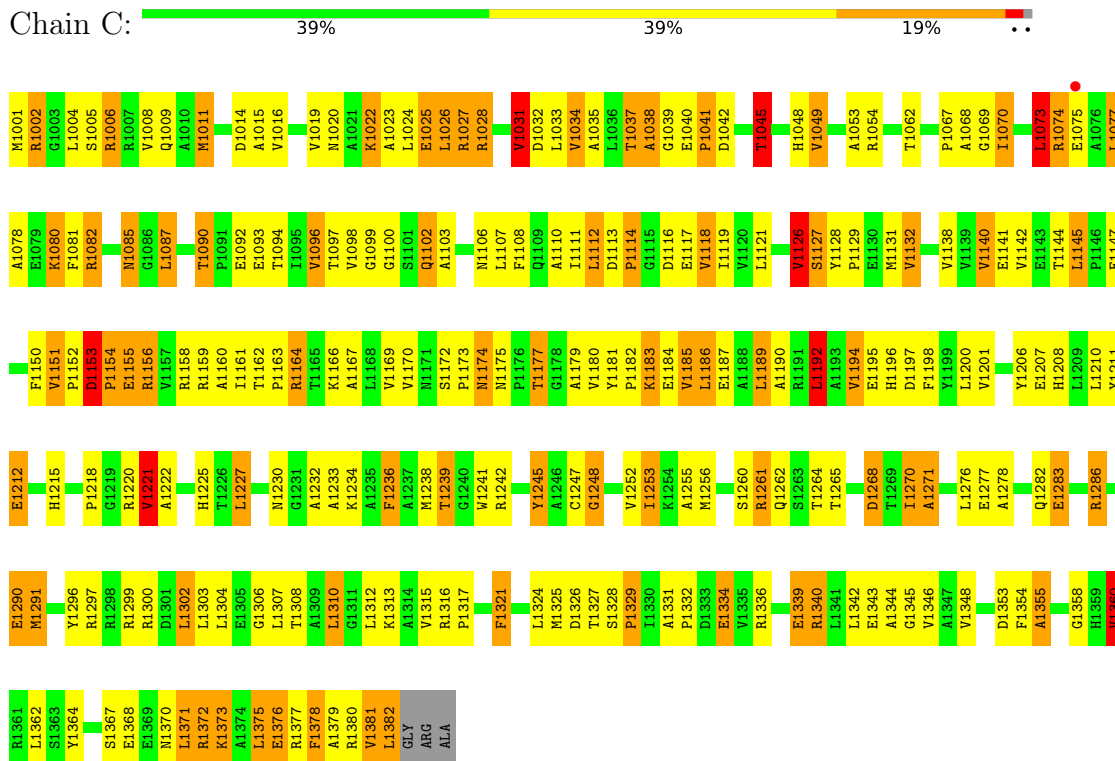


• Molecule 1: ASPARTATE AMINOTRANSFERASE

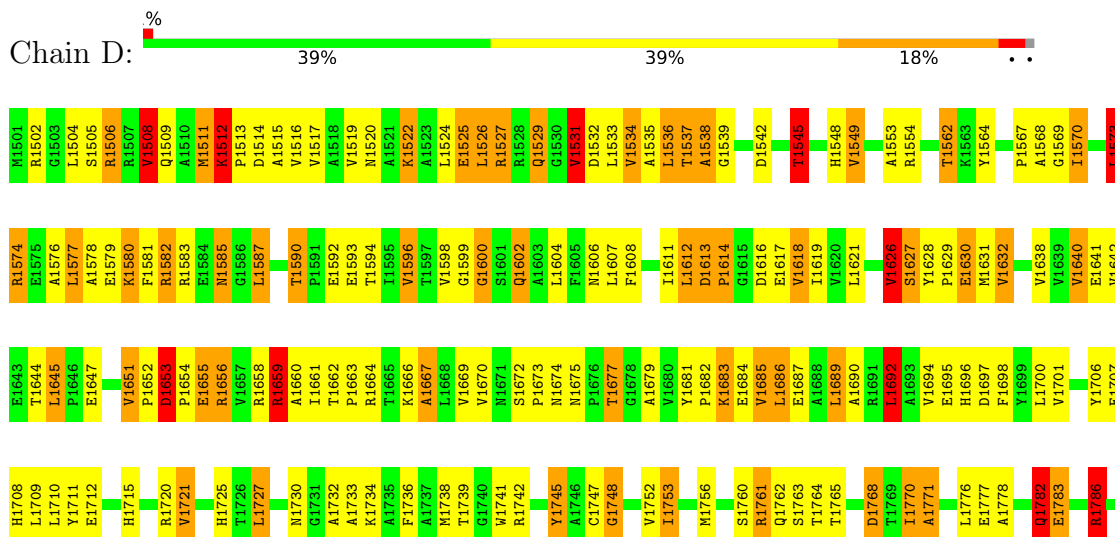


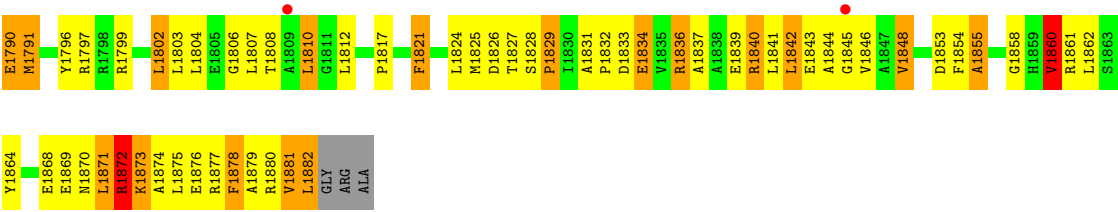


• Molecule 1: ASPARTATE AMINOTRANSFERASE



• 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 8.00 – 3.30	Depositor EDS
% Data completeness (in resolution range)	97.0 (8.00-3.30) 89.9 (8.00-3.30)	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	2263 reflections (9.94%)	wwPDB-VP
Wilson B-factor (Å ²)	43.9	Xtriage
Anisotropy	0.526	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 64.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.050 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.88	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, 0.333 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: 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	0.55	0/3009	1.36	71/4092 (1.7%)
1	B	0.55	0/3009	1.37	75/4092 (1.8%)
1	C	0.53	0/3009	1.35	67/4092 (1.6%)
1	D	0.56	0/3009	1.38	77/4092 (1.9%)
All	All	0.55	0/12036	1.36	290/16368 (1.8%)

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

There are no bond length outliers.

All (290) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	527	ARG	N-CA-C	-11.84	98.10	111.71
1	A	145	LEU	N-CA-C	10.72	125.11	110.31
1	D	1721	VAL	N-CA-C	10.51	120.30	110.74
1	C	1145	LEU	N-CA-C	10.41	124.67	110.31
1	D	1645	LEU	N-CA-C	10.31	124.54	110.31
1	B	645	LEU	N-CA-C	10.19	124.37	110.31
1	A	175	ASN	N-CA-C	-10.02	94.01	109.64
1	C	1175	ASN	N-CA-C	-9.96	94.09	109.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1675	ASN	N-CA-C	-9.87	94.25	109.64
1	B	542	ASP	N-CA-C	-9.53	101.77	113.97
1	D	1542	ASP	N-CA-C	-9.49	101.82	113.97
1	A	42	ASP	N-CA-C	-9.39	101.95	113.97
1	B	590	THR	N-CA-C	-9.37	98.12	110.40
1	A	90	THR	N-CA-C	-9.35	98.15	110.40
1	C	1090	THR	N-CA-C	-9.31	98.20	110.40
1	D	1590	THR	N-CA-C	-9.16	98.40	110.40
1	B	675	ASN	N-CA-C	-9.04	95.54	109.64
1	D	1871	LEU	N-CA-C	-9.04	101.43	111.28
1	C	1042	ASP	N-CA-C	-9.03	102.42	113.97
1	A	371	LEU	N-CA-C	-8.93	101.55	111.28
1	A	31	VAL	N-CA-C	8.74	127.51	109.34
1	B	674	ASN	N-CA-C	8.61	122.94	109.07
1	C	1038	ALA	N-CA-C	8.45	122.41	110.50
1	A	38	ALA	N-CA-C	8.45	122.41	110.50
1	A	127	SER	N-CA-C	8.43	121.69	111.40
1	C	1371	LEU	N-CA-C	-8.43	102.09	111.28
1	B	613	ASP	N-CA-C	-8.42	99.44	110.39
1	D	1538	ALA	N-CA-C	8.42	122.37	110.50
1	C	1113	ASP	N-CA-C	-8.38	99.50	110.39
1	C	1127	SER	N-CA-C	8.35	121.59	111.40
1	B	538	ALA	N-CA-C	8.35	122.27	110.50
1	B	627	SER	N-CA-C	8.32	121.55	111.40
1	B	871	LEU	N-CA-C	-8.31	102.22	111.28
1	D	1613	ASP	N-CA-C	-8.26	99.66	110.39
1	A	113	ASP	N-CA-C	-8.13	99.82	110.39
1	D	1627	SER	N-CA-C	8.04	121.20	111.40
1	B	786	ARG	N-CA-C	-7.96	102.55	111.07
1	A	156	ARG	N-CA-C	-7.87	102.71	111.28
1	D	1562	THR	N-CA-C	7.85	122.17	112.59
1	C	1080	LYS	N-CA-C	-7.83	102.34	111.03
1	B	531	VAL	N-CA-C	7.79	125.54	109.34
1	C	1027	ARG	N-CA-C	-7.74	102.81	111.71
1	D	1531	VAL	N-CA-C	7.74	125.44	109.34
1	D	1580	LYS	N-CA-C	-7.70	102.48	111.03
1	D	1626	VAL	N-CA-C	7.68	125.31	109.34
1	D	1674	ASN	N-CA-C	7.68	121.43	109.07
1	A	2	ARG	N-CA-C	7.59	119.60	110.19
1	A	185	VAL	N-CA-C	-7.53	103.45	110.53
1	A	368	GLU	N-CA-C	-7.50	102.47	111.69
1	A	80	LYS	N-CA-C	-7.49	102.72	111.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	562	THR	N-CA-C	7.47	122.13	112.26
1	D	1502	ARG	N-CA-C	7.41	119.37	110.19
1	C	1062	THR	N-CA-C	7.39	122.02	112.26
1	D	1651	VAL	N-CA-C	-7.39	101.71	108.95
1	A	62	THR	N-CA-C	7.38	122.00	112.26
1	C	1126	VAL	N-CA-C	7.34	124.62	109.34
1	B	585	ASN	N-CA-C	7.32	121.91	113.19
1	B	721	VAL	N-CA-C	7.32	117.40	110.74
1	A	340	ARG	N-CA-C	-7.30	102.92	111.03
1	C	1031	VAL	N-CA-C	7.29	124.50	109.34
1	D	1641	GLU	N-CA-C	7.28	121.11	109.24
1	A	126	VAL	N-CA-C	7.28	124.48	109.34
1	B	580	LYS	N-CA-C	-7.28	102.95	111.03
1	C	1174	ASN	N-CA-C	7.25	120.74	109.07
1	C	1185	VAL	N-CA-C	-7.24	103.73	110.53
1	D	1821	PHE	N-CA-C	7.23	119.64	110.61
1	D	1685	VAL	N-CA-C	-7.22	103.74	110.53
1	B	502	ARG	N-CA-C	7.21	119.14	110.19
1	C	1368	GLU	N-CA-C	-7.21	102.43	112.45
1	B	626	VAL	N-CA-C	7.18	124.28	109.34
1	A	321	PHE	N-CA-C	7.17	119.58	110.61
1	D	1585	ASN	N-CA-C	7.17	121.72	113.19
1	C	1085	ASN	N-CA-C	7.16	121.70	113.19
1	A	192	LEU	N-CA-C	-7.14	103.58	111.36
1	A	141	GLU	N-CA-C	7.12	120.85	109.24
1	C	1221	VAL	N-CA-C	7.11	117.21	110.74
1	C	1141	GLU	N-CA-C	7.08	120.78	109.24
1	D	1508	VAL	N-CA-C	-7.07	104.52	113.22
1	C	1151	VAL	N-CA-C	-7.05	102.04	108.95
1	A	270	ILE	N-CA-C	-7.05	103.91	110.53
1	B	685	VAL	N-CA-C	-7.03	103.92	110.53
1	B	770	ILE	N-CA-C	-7.03	103.92	110.53
1	A	85	ASN	N-CA-C	6.99	121.51	113.19
1	A	27	ARG	N-CA-C	-6.97	103.69	111.71
1	B	656	ARG	N-CA-C	-6.93	103.74	111.71
1	B	641	GLU	N-CA-C	6.92	120.51	109.24
1	C	1270	ILE	N-CA-C	-6.87	104.07	110.53
1	B	821	PHE	N-CA-C	6.84	119.84	110.06
1	B	840	ARG	N-CA-C	-6.83	103.44	111.03
1	B	736	PHE	N-CA-C	6.81	120.90	112.59
1	C	1002	ARG	N-CA-C	6.79	118.61	110.19
1	D	1786	ARG	N-CA-C	-6.73	103.87	111.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	221	VAL	N-CA-C	6.72	116.86	110.74
1	C	1156	ARG	N-CA-C	-6.70	103.98	111.28
1	A	177	THR	N-CA-C	6.67	121.51	113.23
1	A	151	VAL	N-CA-C	-6.61	102.47	108.95
1	D	1770	ILE	N-CA-C	-6.61	104.31	110.53
1	C	1008	VAL	N-CA-C	-6.58	105.12	113.22
1	C	1192	LEU	N-CA-C	-6.58	103.60	111.69
1	C	1355	ALA	N-CA-C	-6.58	104.55	112.58
1	C	1037	THR	N-CA-C	6.57	124.78	110.80
1	C	1035	ALA	N-CA-C	6.56	120.55	107.62
1	C	1177	THR	N-CA-C	6.55	121.35	113.23
1	A	174	ASN	N-CA-C	6.55	120.13	109.59
1	B	508	VAL	N-CA-C	-6.55	105.17	113.22
1	B	692	LEU	N-CA-C	-6.54	104.23	111.36
1	C	1236	PHE	N-CA-C	6.53	120.55	112.59
1	D	1825	MET	N-CA-C	6.53	119.54	107.99
1	B	677	THR	N-CA-C	6.52	121.31	113.23
1	A	35	ALA	N-CA-C	6.52	120.46	107.62
1	C	1073	LEU	N-CA-C	-6.52	104.22	111.71
1	D	1868	GLU	N-CA-C	-6.51	103.68	111.69
1	A	233	ALA	N-CA-C	6.50	121.29	113.23
1	D	1535	ALA	N-CA-C	6.49	120.40	107.62
1	B	733	ALA	N-CA-C	6.46	121.24	113.23
1	C	1233	ALA	N-CA-C	6.44	121.21	113.23
1	C	1286	ARG	N-CA-C	-6.41	104.21	111.07
1	C	1340	ARG	N-CA-C	-6.40	102.98	111.24
1	D	1512	LYS	CA-C-N	6.39	126.76	119.92
1	D	1512	LYS	C-N-CA	6.39	126.76	119.92
1	A	73	LEU	N-CA-C	-6.37	104.38	111.71
1	D	1736	PHE	N-CA-C	6.36	120.34	112.59
1	C	1321	PHE	N-CA-C	6.32	119.10	110.06
1	A	361	ARG	NE-CZ-NH1	-6.30	115.20	121.50
1	A	325	MET	N-CA-C	6.29	120.02	107.62
1	B	537	THR	N-CA-C	6.29	124.21	110.80
1	A	37	THR	N-CA-C	6.27	124.15	110.80
1	B	661	ILE	N-CA-C	6.27	116.52	108.12
1	D	1677	THR	N-CA-C	6.26	120.99	113.23
1	D	1660	ALA	N-CA-C	6.25	120.51	113.01
1	B	860	VAL	N-CA-C	-6.25	99.20	108.45
1	D	1733	ALA	N-CA-C	6.25	120.98	113.23
1	C	1151	VAL	CA-C-N	6.25	126.16	119.85
1	C	1151	VAL	C-N-CA	6.25	126.16	119.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	834	GLU	N-CA-C	-6.24	104.72	112.90
1	C	1334	GLU	N-CA-C	-6.24	104.72	112.90
1	D	1527	ARG	N-CA-C	-6.21	104.56	111.71
1	A	8	VAL	N-CA-C	-6.20	105.59	113.22
1	C	1160	ALA	N-CA-C	6.20	120.45	113.01
1	B	825	MET	N-CA-C	6.20	119.83	107.62
1	C	1325	MET	N-CA-C	6.19	119.81	107.62
1	D	1834	GLU	N-CA-C	-6.19	104.79	112.90
1	D	1840	ARG	N-CA-C	-6.17	103.28	111.24
1	D	1669	VAL	N-CA-C	6.16	116.69	107.51
1	B	535	ALA	N-CA-C	6.15	119.74	107.62
1	D	1748	GLY	CA-C-N	6.13	126.46	119.83
1	D	1748	GLY	C-N-CA	6.13	126.46	119.83
1	C	1184	GLU	N-CA-C	6.11	118.91	111.82
1	B	868	GLU	N-CA-C	-6.11	103.25	112.04
1	B	855	ALA	N-CA-C	-6.11	105.13	112.58
1	B	669	VAL	N-CA-C	6.10	116.60	107.51
1	A	151	VAL	CA-C-N	6.09	126.00	119.85
1	A	151	VAL	C-N-CA	6.09	126.00	119.85
1	D	1870	ASN	N-CA-C	6.08	119.16	111.69
1	D	1573	LEU	N-CA-C	-6.08	104.72	111.71
1	B	651	VAL	N-CA-C	-6.07	103.00	108.95
1	C	1161	ILE	N-CA-C	6.06	116.23	108.12
1	A	236	PHE	N-CA-C	6.02	119.93	112.59
1	B	684	GLU	N-CA-C	6.02	118.80	111.82
1	B	573	LEU	N-CA-C	-6.01	104.80	111.71
1	D	1651	VAL	CA-C-N	6.00	125.91	119.85
1	D	1651	VAL	C-N-CA	6.00	125.91	119.85
1	A	160	ALA	N-CA-C	5.98	120.18	113.01
1	A	334	GLU	N-CA-C	-5.98	105.07	112.90
1	D	1855	ALA	N-CA-C	-5.97	105.30	112.58
1	A	45	THR	CA-C-N	5.96	127.30	119.84
1	A	45	THR	C-N-CA	5.96	127.30	119.84
1	A	355	ALA	N-CA-C	-5.96	105.31	112.58
1	A	161	ILE	N-CA-C	5.93	116.07	108.12
1	B	651	VAL	CA-C-N	5.93	125.84	119.85
1	B	651	VAL	C-N-CA	5.93	125.84	119.85
1	A	169	VAL	N-CA-C	5.93	116.34	107.51
1	C	1370	ASN	N-CA-C	5.92	118.98	111.69
1	D	1684	GLU	N-CA-C	5.91	118.67	111.82
1	A	184	GLU	N-CA-C	5.89	118.66	111.82
1	C	1015	ALA	N-CA-C	-5.86	104.97	111.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1169	VAL	N-CA-C	5.86	116.24	107.51
1	D	1545	THR	CA-C-N	5.85	127.15	119.84
1	D	1545	THR	C-N-CA	5.85	127.15	119.84
1	D	1537	THR	N-CA-C	5.85	123.25	110.80
1	B	660	ALA	N-CA-C	5.83	120.23	113.18
1	D	1810	LEU	N-CA-C	-5.82	105.50	113.30
1	C	1153	ASP	CA-C-N	5.80	127.09	119.84
1	C	1153	ASP	C-N-CA	5.80	127.09	119.84
1	D	1661	ILE	N-CA-C	5.79	115.88	108.12
1	A	310	LEU	N-CA-C	-5.78	105.56	113.30
1	B	810	LEU	N-CA-C	-5.77	105.56	113.30
1	B	554	ARG	N-CA-C	-5.74	104.63	111.69
1	A	15	ALA	N-CA-C	-5.74	105.11	111.36
1	D	1860	VAL	N-CA-C	-5.73	99.97	108.45
1	C	1360	VAL	N-CA-C	-5.70	99.58	108.81
1	B	748	GLY	CA-C-N	5.69	125.98	119.83
1	B	748	GLY	C-N-CA	5.69	125.98	119.83
1	D	1554	ARG	N-CA-C	-5.68	104.70	111.69
1	A	201	VAL	N-CA-C	-5.68	100.41	108.58
1	A	153	ASP	CA-C-N	5.66	126.91	119.84
1	A	153	ASP	C-N-CA	5.66	126.91	119.84
1	D	1656	ARG	N-CA-C	-5.65	105.21	111.71
1	B	515	ALA	N-CA-C	-5.63	105.23	111.36
1	A	144	THR	N-CA-C	-5.62	99.26	108.76
1	A	360	VAL	N-CA-C	-5.62	99.71	108.81
1	D	1600	GLY	N-CA-C	-5.60	105.87	113.37
1	D	1576	ALA	N-CA-C	-5.57	105.36	111.82
1	C	1144	THR	N-CA-C	-5.57	99.34	108.76
1	D	1644	THR	N-CA-C	-5.57	98.83	108.69
1	D	1701	VAL	N-CA-C	-5.57	100.56	108.58
1	B	870	ASN	N-CA-C	5.57	118.54	111.69
1	A	195	GLU	N-CA-C	5.51	117.28	111.28
1	B	512	LYS	CA-C-N	5.51	125.48	120.03
1	B	512	LYS	C-N-CA	5.51	125.48	120.03
1	D	1515	ALA	N-CA-C	-5.50	105.36	111.36
1	C	1045	THR	CA-C-N	5.50	126.71	119.84
1	C	1045	THR	C-N-CA	5.50	126.71	119.84
1	B	640	VAL	N-CA-C	-5.48	99.26	107.37
1	B	653	ASP	CA-C-N	5.47	126.68	119.84
1	B	653	ASP	C-N-CA	5.47	126.68	119.84
1	A	12	LYS	CA-C-N	5.47	125.78	119.92
1	A	12	LYS	C-N-CA	5.47	125.78	119.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	545	THR	CA-C-N	5.46	126.67	119.84
1	B	545	THR	C-N-CA	5.46	126.67	119.84
1	C	1310	LEU	N-CA-C	-5.45	106.00	113.30
1	C	1201	VAL	N-CA-C	-5.44	100.75	108.58
1	C	1106	ASN	N-CA-C	-5.42	105.02	111.69
1	D	1695	GLU	N-CA-C	5.42	117.19	111.28
1	A	112	LEU	N-CA-C	5.41	117.46	108.20
1	B	701	VAL	N-CA-C	-5.41	100.78	108.58
1	C	1112	LEU	N-CA-C	5.39	117.53	107.99
1	C	1054	ARG	N-CA-C	-5.37	105.08	111.69
1	C	1378	PHE	N-CA-C	-5.37	105.43	111.28
1	D	1653	ASP	CA-C-N	5.37	126.55	119.84
1	D	1653	ASP	C-N-CA	5.37	126.55	119.84
1	B	644	THR	N-CA-C	-5.37	99.69	108.76
1	D	1667	ALA	N-CA-C	5.36	117.33	109.24
1	A	378	PHE	N-CA-C	-5.36	105.44	111.28
1	B	784	ALA	N-CA-C	5.36	118.98	112.23
1	B	553	ALA	N-CA-C	-5.35	106.25	112.89
1	D	1878	PHE	N-CA-C	-5.33	105.47	111.28
1	A	209	LEU	N-CA-C	-5.33	103.28	110.68
1	C	1248	GLY	CA-C-N	5.33	126.16	119.98
1	C	1248	GLY	C-N-CA	5.33	126.16	119.98
1	D	1708	HIS	N-CA-C	5.33	119.83	113.23
1	B	600	GLY	N-CA-C	-5.32	106.24	113.37
1	B	570	ILE	CA-C-N	5.30	124.97	119.56
1	B	570	ILE	C-N-CA	5.30	124.97	119.56
1	A	140	VAL	N-CA-C	-5.29	99.54	107.37
1	C	1070	ILE	CA-C-N	5.29	124.95	119.56
1	C	1070	ILE	C-N-CA	5.29	124.95	119.56
1	D	1640	VAL	N-CA-C	-5.28	99.55	107.37
1	C	1271	ALA	N-CA-C	5.28	117.78	111.71
1	B	612	LEU	N-CA-C	5.24	117.27	107.99
1	D	1763	SER	N-CA-C	5.24	119.59	112.04
1	B	667	ALA	N-CA-C	5.22	117.12	109.24
1	D	1720	ARG	N-CA-C	-5.21	105.78	111.82
1	D	1570	ILE	CA-C-N	5.21	124.87	119.56
1	D	1570	ILE	C-N-CA	5.21	124.87	119.56
1	B	800	ARG	N-CA-C	-5.20	105.31	110.97
1	A	271	ALA	N-CA-C	5.19	117.68	111.71
1	A	248	GLY	CA-C-N	5.19	126.00	119.98
1	A	248	GLY	C-N-CA	5.19	126.00	119.98
1	D	1553	ALA	N-CA-C	-5.18	106.46	112.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1179	ALA	N-CA-C	5.17	117.71	109.96
1	A	70	ILE	CA-C-N	5.16	124.82	119.56
1	A	70	ILE	C-N-CA	5.16	124.82	119.56
1	D	1612	LEU	N-CA-C	5.16	117.11	107.99
1	A	286	ARG	N-CA-C	-5.15	105.56	111.07
1	B	679	ALA	N-CA-C	5.15	117.69	109.96
1	B	576	ALA	N-CA-C	-5.15	105.85	111.82
1	A	54	ARG	N-CA-C	-5.14	105.37	111.69
1	A	167	ALA	N-CA-C	5.14	117.00	109.24
1	D	1692	LEU	N-CA-C	-5.14	105.37	111.69
1	B	763	SER	N-CA-C	5.13	119.42	112.04
1	C	1053	ALA	N-CA-C	-5.12	106.54	112.89
1	B	841	LEU	N-CA-C	5.12	117.60	111.71
1	D	1837	ALA	N-CA-C	-5.12	105.14	111.33
1	A	53	ALA	N-CA-C	-5.12	106.55	112.89
1	A	208	HIS	N-CA-C	5.11	119.56	113.23
1	D	1679	ALA	N-CA-C	5.11	117.62	109.96
1	B	708	HIS	N-CA-C	5.10	119.56	113.23
1	D	1709	LEU	N-CA-C	-5.10	103.59	110.68
1	C	1208	HIS	N-CA-C	5.10	119.55	113.23
1	D	1771	ALA	N-CA-C	5.10	117.57	111.71
1	A	100	GLY	N-CA-C	-5.09	106.55	113.37
1	C	1140	VAL	N-CA-C	-5.09	99.84	107.37
1	D	1841	LEU	N-CA-C	5.08	117.55	111.71
1	D	1606	ASN	N-CA-C	-5.06	105.46	111.69
1	A	284	ALA	N-CA-C	5.06	118.60	112.23
1	C	1164	ARG	N-CA-C	-5.06	105.42	112.45
1	B	695	GLU	N-CA-C	5.05	116.79	111.28
1	B	709	LEU	N-CA-C	-5.04	103.67	110.68
1	B	771	ALA	N-CA-C	5.03	117.49	111.71

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
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	174	0
1	B	2948	0	2962	165	1
1	C	2948	0	2962	184	0
1	D	2948	0	2962	166	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	642	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 27.

All (642) 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:HG3	1:C:1372:ARG:HH11	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1074:ARG:HH11	1:C:1074:ARG:HG2	1.51	0.75
1:C:1340:ARG:NH2	1:C:1381:VAL:HG22	2.02	0.75
1:B:574:ARG:HG2	1:B:574:ARG:HH11	1.50	0.75
1:D:1607:LEU:HD13	1:D:1727:LEU:HD22	1.67	0.75
1:D:1574:ARG:HG2	1:D:1574:ARG:HH11	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:HG3	1:D:1582:ARG:HH11	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:HG3	1:B:797:ARG:HH11	1.53	0.73
1:D:1797:ARG:HG3	1:D:1797:ARG:HH11	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:B:786:ARG:O	1:B:790:GLU:HG2	1.90	0.71
1:D:1833:ASP:OD1	1:D:1836:ARG:HD3	1.90	0.71
1:C:1297:ARG:HG3	1:C:1297:ARG:HH11	1.55	0.71
1:C:1291:MET:SD	1:C:1291:MET:C	2.74	0.70
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:791:MET:SD	1:B:791:MET:C	2.75	0.69
1:A:2:ARG:HG3	1:B:698:PHE:HA	1.75	0.68
1:A:25:GLU:O	1:A:29:GLN:HG2	1.93	0.68
1:B:653:ASP:CB	1:B:656:ARG:HH21	2.06	0.68
1:B:828:SER:HB3	1:B:829:PRO:HD3	1.74	0.68
1:A:291:MET:SD	1:A:291:MET:C	2.77	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:D:1791:MET:SD	1:D:1791:MET:C	2.78	0.66
1:A:316:ARG:HG3	1:A:316:ARG:HH11	1.61	0.66
1:D:1768:ASP:HB3	1:D:1771:ALA:HB3	1.77	0.66
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: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:B:799:ARG:HB3	1:B:871:LEU:HD11	1.81	0.63
1:A:190:ALA:HA	1:A:200:LEU:HD12	1.80	0.63
1:B:574:ARG:HG2	1:B:574:ARG:NH1	2.13	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:HG3	1:C:1316:ARG:HH11	1.64	0.62
1:C:1268:ASP:HB3	1:C:1271:ALA:HB3	1.79	0.62
1:D:1690:ALA:HA	1:D:1700:LEU:HD12	1.81	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:1117:GLU:HG2	1:C:1138:VAL:CG2	2.30	0.61
1:C:1218:PRO:O	1:C:1221:VAL:HG13	2.00	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:A:98:VAL:HB	1:A:102:GLN:HG3	1.82	0.61
1:A:155:GLU:OE2	1:A:155:GLU:HA	2.01	0.61
1:B:598:VAL:HB	1:B:602:GLN:HG3	1.81	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
1:A:345:GLY:HA3	1:A:377:ARG:NH1	2.16	0.60
1:D:1839:GLU:O	1:D:1843:GLU:HG2	2.02	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:OE2	1:C:1155:GLU:HA	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:A:6:ARG:HG3	1:B:613:ASP:OD1	2.02	0.59
1:A:117:GLU:HG2	1:A:138:VAL:CG2	2.32	0.59
1:B:504:LEU:HD12	1:B:504:LEU:H	1.67	0.59
1:B:617:GLU:HG2	1:B:638:VAL:CG2	2.32	0.59
1:D:1687:GLU:HG3	1:D:1721:VAL:HG21	1.84	0.59
1:A:107:LEU:HD21	1:A:227:LEU:HD13	1.83	0.59
1:B:687:GLU:HG3	1:B:721:VAL:HG21	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:C:1099:GLY:HA3	1:C:1242:ARG:NH2	2.18	0.58
1:D:1786:ARG:O	1:D:1790:GLU:HG2	2.03	0.58
1:C:1067:PRO:HA	1:C:1265:THR:O	2.04	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:LEU:HB3	1:A:94:THR:CG2	2.34	0.58
1:A:177:THR:HG22	1:A:324:LEU:HD12	1.85	0.58
1:D:1567:PRO:HA	1:D:1765:THR:O	2.03	0.58
1:B:675:ASN:ND2	2:B:914:ASP:O	2.37	0.58
1:C:1025:GLU:HA	1:C:1028:ARG:HG2	1.86	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:HG2	1:D:1574:ARG:NH1	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
1:A:128:TYR:HB2	1:A:129:PRO:HD3	1.86	0.57
1:C:1004:LEU:HD12	1:C:1004:LEU:H	1.69	0.57
1:D:1582:ARG:HG3	1:D:1582:ARG:NH1	2.18	0.57
1:D:1599:GLY:HA3	1:D:1742:ARG:NH2	2.19	0.57
1:A:261:ARG:O	1:A:261:ARG:HD3	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:C:1177:THR:HG22	1:C:1324:LEU:HD12	1.85	0.57
1:D:1504:LEU:HD12	1:D:1504:LEU:H	1.70	0.57
1:D:1592:GLU:O	1:D:1753:ILE:HG21	2.05	0.57
1:C:1261:ARG:HD3	1:C:1261:ARG:C	2.30	0.56
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:B:592:GLU:O	1:B:753:ILE:HG21	2.05	0.56
1:B:761:ARG:HD3	1:B:761:ARG:C	2.31	0.56
1:B:568:ALA:O	1:B:596:VAL:HG23	2.06	0.56
1:D:1525:GLU:HG2	1:D:1526:LEU:N	2.20	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:833:ASP:OD2	1:B:836:ARG:HB3	2.07	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:D:1536:LEU:HD12	1:D:1848:VAL:HG13	1.88	0.55
1:D:1585:ASN:CB	1:D:1587:LEU:HD22	2.36	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:C:1372:ARG:HH11	1:C:1372:ARG:CG	2.14	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
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:1092:GLU:O	1:C:1253:ILE:HG21	2.08	0.54
1:C:1331:ALA:HB1	1:C:1332:PRO:HD2	1.89	0.54
1:C:1372:ARG:HG3	1:C:1372:ARG:NH1	2.11	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:A:107:LEU:O	1:A:111:ILE:HG12	2.07	0.54
1:C:1158:ARG:HH21	1:C:1196:HIS:CE1	2.26	0.54
1:A:261:ARG:HD3	1:A:261:ARG:C	2.33	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:A:333:ASP:OD2	1:A:336:ARG:HB3	2.09	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:C:1158:ARG:HB2	1:C:1192:LEU:HD11	1.90	0.53
1:D:1831:ALA:HB1	1:D:1832:PRO:HD2	1.90	0.53
1:A:69:GLY:HA3	1:A:96:VAL:CG2	2.39	0.53
1:B:536:LEU:HD12	1:B:848:VAL:HG13	1.89	0.53
1:B:658:ARG:HB2	1:B:692:LEU:HD11	1.90	0.53
1:C:1185:VAL:O	1:C:1189:LEU:HD22	2.08	0.53
1:C:1286:ARG:O	1:C:1290:GLU:HG2	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:LEU:CB	1:A:94:THR:HG21	2.38	0.53
1:A:331:ALA:HB1	1:A:332:PRO:HD2	1.90	0.53
1:B:585:ASN:CB	1:B:587:LEU:HD22	2.38	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:1069:GLY:HA3	1:C:1096:VAL:CG2	2.40	0.52
1:C:1102:GLN:HG3	1:D:1764:THR:HG22	1.91	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:D:1872:ARG:HA	1:D:1875:LEU:HD12	1.91	0.52
1:B:569:GLY:HA3	1:B:596:VAL:CG2	2.39	0.52
1:B:607:LEU:O	1:B:611:ILE:HG12	2.10	0.52
1:B:839:GLU:O	1:B:843:GLU:HG3	2.10	0.52
1:D:1786:ARG:HD3	1:D:1790:GLU:CD	2.34	0.52
1:A:339:GLU:O	1:A:343:GLU:HG3	2.09	0.52
1:B:816:ARG:HH11	1:B:816:ARG:HG3	1.74	0.52
1:C:1093:GLU:HB3	1:C:1248:GLY:O	2.10	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: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: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:1577:LEU:CB	1:D:1594:THR:HG21	2.40	0.51
1:D:1834:GLU:HG3	1:D:1858:GLY:H	1.76	0.51
1:A:172:SER:HA	1:A:173:PRO:C	2.35	0.51
1:A:262:GLN:HG3	1:B:511:MET:CE	2.40	0.51
1:A:108:PHE:O	1:A:112:LEU:HB2	2.11	0.50
1:A:255:ALA:HB2	1:B:504:LEU:HD23	1.92	0.50
1:A:264:THR:O	1:A:265:THR:HB	2.11	0.50
1:C:1027:ARG:HA	1:C:1031:VAL:O	2.11	0.50
1:C:1172:SER:HA	1:C:1173:PRO:C	2.36	0.50
1:B:526:LEU:C	1:B:528:ARG:N	2.66	0.50
1:D:1607:LEU:O	1:D:1611:ILE:HG12	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1253:ILE:HD12	1:C:1256:MET:HE3	1.94	0.50
1:C:1297:ARG:HG3	1:C:1297:ARG:NH1	2.26	0.50
1:C:1316:ARG:HG3	1:C:1316:ARG:NH1	2.27	0.50
1:D:1653:ASP:N	1:D:1656:ARG:HH21	2.09	0.50
1:A:114:PRO:HD2	1:B:506:ARG:HH21	1.77	0.50
1:B:593:GLU:HB3	1:B:748:GLY:O	2.12	0.50
1:D:1681:TYR:N	1:D:1681:TYR:CD2	2.80	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:HG3	1:A:316:ARG:NH1	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:D:1672:SER:HA	1:D:1673:PRO:C	2.37	0.49
1:C:1085:ASN:HB2	1:C:1087:LEU:HD22	1.94	0.49
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:B:681:TYR:N	1:B:681:TYR:CD2	2.79	0.49
1:C:1339:GLU:O	1:C:1343:GLU:HG3	2.12	0.49
1:A:182:PRO:HG2	1:A:185:VAL:CG2	2.39	0.49
1:B:645:LEU:HD12	1:B:656:ARG:NH1	2.27	0.49
1:B:834:GLU:HG3	1:B:858:GLY:H	1.78	0.49
1:D:1536:LEU:HD12	1:D:1848:VAL:CG1	2.43	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:C:1155:GLU:OE2	1:C:1158:ARG:HD2	2.13	0.48
1:C:1264:THR:O	1:C:1265:THR:HB	2.13	0.48
1:D:1582:ARG:HA	1:D:1587:LEU:O	2.13	0.48
1:D:1761:ARG:HD3	1:D:1761:ARG:C	2.36	0.48
1:A:155:GLU:OE2	1:A:158:ARG:HD2	2.14	0.48
1:D:1627:SER:HB3	1:D:1631:MET:HE3	1.96	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:A:241:TRP:HE1	1:B:562:THR:HB	1.78	0.48
1:B:876:GLU:O	1:B:879:ALA:HB3	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1082:ARG:HA	1:C:1087:LEU:O	2.13	0.48
1:D:1653:ASP:HB3	1:D:1656:ARG:CZ	2.42	0.48
1:D:1761:ARG:HD3	1:D:1761:ARG:O	2.14	0.48
1:B:672:SER:HA	1:B:673:PRO:C	2.39	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:HG3	1:D:1797:ARG:NH1	2.24	0.48
1:D:1876:GLU:O	1:D:1879:ALA:HB3	2.13	0.48
1:B:812:LEU:HD21	1:B:882:LEU:HD21	1.96	0.48
1:D:1585:ASN:HB2	1:D:1587:LEU:HD22	1.96	0.48
1:D:1519:VAL:HG12	1:D:1537:THR:HG21	1.96	0.48
1:A:181:TYR:N	1:A:181:TYR:CD2	2.82	0.47
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:127:SER:HB3	1:A:131:MET:HE3	1.95	0.47
1:B:512:LYS:N	1:B:630:GLU:OE2	2.47	0.47
1:B:600:GLY:H	3:B:913:PLP:P	2.37	0.47
1:D:1764:THR:O	1:D:1765:THR:HB	2.14	0.47
1:A:26:LEU:C	1:A:31:VAL:HB	2.38	0.47
1:C:1180:VAL:O	1:C:1180:VAL:HG13	2.13	0.47
1:A:19:VAL:HG12	1:A:37:THR:HG21	1.96	0.47
1:A:33:LEU:HD12	1:A:33:LEU:O	2.14	0.47
1:A:93:GLU:HB3	1:A:248:GLY:O	2.14	0.47
1:C:1232:ALA:HB2	1:C:1245:TYR:HE2	1.80	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:2:ARG:HG3	1:B:698:PHE:CA	2.44	0.47
1:A:5:SER:O	1:A:9:GLN:HB2	2.15	0.47
1:A:232:ALA:HB2	1:A:245:TYR:HE2	1.80	0.47
1:B:536:LEU:HD21	1:B:874:ALA:CB	2.45	0.47
1:C:1221:VAL:HG22	1:C:1222:ALA:N	2.28	0.47
1:C:1262:GLN:HG3	1:D:1511:MET:HE2	1.97	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:B:533:LEU:HD12	1:B:533:LEU:O	2.15	0.47
1:C:1114:PRO:HD2	1:D:1506:ARG:HH21	1.80	0.47
1:D:1617:GLU:HG2	1:D:1638:VAL:HG22	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1834:GLU:HG3	1:D:1858:GLY:N	2.30	0.47
1:A:210:LEU:HD13	1:A:215:HIS:HB2	1.97	0.46
1:D:1711:TYR:OH	1:D:1796:TYR:HB3	2.15	0.46
1:B:536:LEU:HD11	1:B:846:VAL:CG1	2.44	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:A:242:ARG:NH1	1:B:564:TYR:HE1	2.14	0.46
1:C:1077:LEU:HD23	1:C:1094:THR:HG22	1.96	0.46
1:C:1334:GLU:HG3	1:C:1358:GLY:N	2.31	0.46
1:D:1529:GLN:O	1:D:1531:VAL:HG23	2.15	0.46
1:D:1533:LEU:HD12	1:D:1533:LEU:O	2.15	0.46
1:D:1842:LEU:HD23	1:D:1842:LEU:HA	1.84	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:B:682:PRO:HG2	1:B:685:VAL:CG2	2.39	0.46
1:B:753:ILE:HD12	1:B:756:MET:HE3	1.98	0.46
1:C:1019:VAL:HG12	1:C:1037:THR:HG21	1.98	0.46
1:C:1372:ARG:CG	1:C:1372:ARG:NH1	2.77	0.46
1:D:1710:LEU:HD13	1:D:1715:HIS:HB2	1.96	0.46
1:D:1753:ILE:HD12	1:D:1756:MET:HE3	1.97	0.46
1:A:77:LEU:HD21	1:A:245:TYR:HB3	1.98	0.46
1:B:519:VAL:HG12	1:B:537:THR:HG21	1.98	0.46
1:B:655:GLU:OE2	1:B:655:GLU:HA	2.14	0.46
1:B:844:ALA:HB2	1:B:881:VAL:CG2	2.45	0.46
1:D:1577:LEU:HD23	1:D:1594:THR:HG22	1.98	0.46
1:A:252:VAL:O	1:A:256:MET:HG3	2.16	0.46
1:A:262:GLN:HG3	1:B:511:MET:HE2	1.97	0.46
1:B:529:GLN:O	1:B:531:VAL:HG23	2.15	0.46
1:C:1100:GLY:N	3:C:1413:PLP:O3P	2.48	0.46
1:C:1117:GLU:HG2	1:C:1138:VAL:HG22	1.96	0.46
1:C:1210:LEU:HD13	1:C:1215:HIS:HB2	1.97	0.46
1:C:1127:SER:HB3	1:C:1131:MET:HE3	1.98	0.46
1:A:28:ARG:HH11	1:A:28:ARG:CG	2.29	0.46
1:A:241:TRP:NE1	1:B:562:THR:HB	2.31	0.46
1:B:600:GLY:N	3:B:913:PLP:O3P	2.49	0.46
1:C:1025:GLU:HG2	1:C:1026:LEU:N	2.31	0.46
1:C:1049:VAL:HG21	1:C:1278:ALA:HB2	1.97	0.46
1:C:1334:GLU:CG	1:C:1358:GLY:H	2.29	0.46
1:D:1539:GLY:O	1:D:1734:LYS:NZ	2.49	0.46
1:A:92:GLU:CD	1:A:92:GLU:H	2.23	0.46
1:B:710:LEU:HD13	1:B:715:HIS:HB2	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1344:ALA:HB2	1:C:1381:VAL:CG2	2.46	0.46
1:A:25:GLU:HG2	1:A:26:LEU:N	2.31	0.46
1:A:70:ILE:HG13	1:A:73:LEU:H	1.81	0.46
1:A:85:ASN:HB3	1:A:87:LEU:HD22	1.97	0.46
1:B:627:SER:HB3	1:B:631:MET:HE3	1.96	0.46
1:D:1505:SER:O	1:D:1509:GLN:HB2	2.16	0.46
1:D:1655:GLU:O	1:D:1659:ARG:HB2	2.15	0.46
1:D:1844:ALA:HB2	1:D:1881:VAL:CG2	2.46	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:A:39:GLY:O	1:A:234:LYS:NZ	2.50	0.45
1:B:585:ASN:HB2	1:B:587:LEU:HD22	1.96	0.45
1:B:732:ALA:HB2	1:B:745:TYR:HE2	1.80	0.45
1:B:842:LEU:HD23	1:B:842:LEU:HA	1.81	0.45
1:D:1645:LEU:HD12	1:D:1656:ARG:NH1	2.30	0.45
1:D:1732:ALA:HB2	1:D:1745:TYR:HE2	1.80	0.45
1:A:117:GLU:HG2	1:A:138:VAL:HG22	1.97	0.45
1:A:166:LYS:O	1:A:198:PHE:HB2	2.16	0.45
1:A:312:LEU:HD23	1:A:312:LEU:HA	1.80	0.45
1:B:539:GLY:O	1:B:734:LYS:NZ	2.48	0.45
1:D:1549:VAL:HG21	1:D:1778:ALA:HB2	1.97	0.45
1:B:536:LEU:HD12	1:B:848:VAL:CG1	2.46	0.45
1:B:653:ASP:N	1:B:656:ARG:HH21	2.13	0.45
1:C:1070:ILE:HG13	1:C:1073:LEU:H	1.80	0.45
1:C:1085:ASN:HB3	1:C:1087:LEU:HD22	1.99	0.45
1:C:1150:PHE:CE1	1:C:1315:VAL:HG21	2.51	0.45
1:D:1577:LEU:HD21	1:D:1745:TYR:HB3	1.99	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:B:626:VAL:HG22	1:B:853:ASP:HB3	1.99	0.45
1:C:1005:SER:O	1:C:1009:GLN:HB2	2.17	0.45
1:C:1049:VAL:CG2	1:C:1278:ALA:HB2	2.46	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:1344:ALA:HB2	1:C:1381:VAL:HG21	1.98	0.45
1:B:618:VAL:HG13	1:B:667:ALA:HB3	1.99	0.45
1:D:1802:LEU:HD22	1:D:1802:LEU:O	2.17	0.45
1:A:19:VAL:CG1	1:A:37:THR:HG21	2.46	0.45
1:A:45:THR:HG21	1:A:241:TRP:NE1	2.29	0.45
1:A:344:ALA:HB2	1:A:381:VAL:HG21	1.99	0.45
1:D:1626:VAL:HG22	1:D:1853:ASP: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:1152:PRO:HD3	1:C:1181:TYR:CZ	2.52	0.45
1:C:1312:LEU:HD21	1:C:1382:LEU:HD21	1.98	0.45
1:D:1782:GLN:O	1:D:1783:GLU:C	2.59	0.45
1:B:834:GLU:HG3	1:B:858:GLY:N	2.32	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:C:1001:MET:CG	1:C:1002:ARG:N	2.80	0.44
1:B:549:VAL:HG21	1:B:778:ALA:HB2	1.97	0.44
1:D:1804:LEU:HD11	1:D:1817:PRO:HD2	2.00	0.44
1:A:49:VAL:HG21	1:A:278:ALA:HB2	2.00	0.44
1:A:334:GLU:HG3	1:A:358:GLY:N	2.32	0.44
1:A:82:ARG:HA	1:A:87:LEU:O	2.18	0.44
1:A:100:GLY:N	3:A:413:PLP:O3P	2.49	0.44
1:A:232:ALA:HB2	1:A:245:TYR:CE2	2.53	0.44
1:A:302:LEU:HD22	1:A:302:LEU:O	2.16	0.44
1:B:732:ALA:O	1:B:738:MET:HB2	2.18	0.44
1:C:1093:GLU:O	1:C:1247:CYS:HB2	2.18	0.44
1:C:1121:LEU:HD13	1:C:1152:PRO:HB3	2.00	0.44
1:C:1126:VAL:HG22	1:C:1353:ASP:HB3	1.98	0.44
1:C:1166:LYS:O	1:C:1198:PHE:HB2	2.18	0.44
1:C:1264:THR:HG22	1:D:1602:GLN:HG3	1.99	0.44
1:A:93:GLU:O	1:A:247:CYS:HB2	2.17	0.44
1:A:286:ARG:HB3	1:A:286:ARG:CZ	2.47	0.44
1:B:582:ARG:HA	1:B:587:LEU:O	2.18	0.44
1:A:198:PHE:O	1:A:225:HIS:HB3	2.18	0.44
1:A:372:ARG:HA	1:A:375:LEU:HD12	1.98	0.44
1:B:666:LYS:O	1:B:698:PHE:HB2	2.17	0.44
1:B:732:ALA:HB2	1:B:745:TYR:CE2	2.52	0.44
1:B:834:GLU:CG	1:B:858:GLY:H	2.31	0.44
1:B:844:ALA:HB2	1:B:881:VAL:HG21	1.99	0.44
1:C:1194:VAL:HG12	1:C:1195:GLU:N	2.32	0.44
1:C:1236:PHE:O	1:C:1238:MET:HG3	2.18	0.44
1:A:118:VAL:HG13	1:A:167:ALA:HB3	2.00	0.44
1:B:577:LEU:HD21	1:B:745:TYR:HB3	2.00	0.44
1:C:1151:VAL:HG23	1:C:1152:PRO:HD2	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:A:34:VAL:O	1:A:346:VAL:HA	2.18	0.44
1:A:77:LEU:HD23	1:A:94:THR:HG22	1.98	0.44
1:A:256:MET:O	1:A:260:SER:HB2	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:520:ASN:HD21	1:B:538:ALA:HB2	1.83	0.44
1:C:1173:PRO:HB2	1:C:1206:TYR:HB2	2.00	0.44
1:C:1252:VAL:O	1:C:1256:MET:HG3	2.18	0.44
1:D:1666:LYS:O	1:D:1698:PHE:HB2	2.18	0.44
1:D:1683:LYS:O	1:D:1687:GLU:HB2	2.18	0.44
1:C:1028:ARG:HH11	1:C:1028:ARG:CG	2.31	0.43
1:D:1520:ASN:HD21	1:D:1538:ALA:HB2	1.83	0.43
1:D:1549:VAL:CG2	1:D:1778:ALA:HB2	2.48	0.43
1:D:1834:GLU:CG	1:D:1858:GLY:H	2.30	0.43
1:A:2:ARG:CZ	1:B:725:HIS:CD2	3.01	0.43
1:B:651:VAL:HG23	1:B:652:PRO:HD2	1.99	0.43
1:B:658:ARG:HH21	1:B:696:HIS:HE1	1.65	0.43
1:B:736:PHE:O	1:B:738:MET:HG3	2.18	0.43
1:A:12:LYS:HB2	1:A:130:GLU:OE2	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:B:607:LEU:HD13	1:B:727:LEU:CD2	2.40	0.43
1:B:756:MET:O	1:B:760:SER:HB2	2.18	0.43
1:B:827:THR:CG2	1:B:860:VAL:HB	2.48	0.43
1:C:1190:ALA:HB3	1:C:1221:VAL:HG21	2.01	0.43
1:C:1256:MET:O	1:C:1260:SER:HB2	2.18	0.43
1:D:1844:ALA:HB2	1:D:1881:VAL:HG21	2.00	0.43
1:A:49:VAL:CG2	1:A:278:ALA:HB2	2.47	0.43
1:A:121:LEU:HD13	1:A:152:PRO:HB3	2.01	0.43
1:A:324:LEU:HD23	1:A:324:LEU:HA	1.77	0.43
1:B:549:VAL:CG2	1:B:778:ALA:HB2	2.48	0.43
1:C:1232:ALA:HB2	1:C:1245:TYR:CE2	2.52	0.43
1:C:1262:GLN:HG3	1:D:1511:MET:HE1	2.00	0.43
1:D:1526:LEU:O	1:D:1531:VAL:HB	2.19	0.43
1:D:1536:LEU:HD11	1:D:1846:VAL:CG1	2.49	0.43
1:D:1600:GLY:H	3:D:1913:PLP:P	2.41	0.43
1:B:570:ILE:HG13	1:B:573:LEU:H	1.82	0.43
1:D:1593:GLU:O	1:D:1747:CYS:HB2	2.19	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: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:B:854:PHE:O	1:B:855:ALA:HB3	2.18	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1732:ALA:HB2	1:D:1745:TYR:CE2	2.53	0.43
1:D:1732:ALA:O	1:D:1738:MET:HB2	2.19	0.43
1:C:1290:GLU:HG2	1:C:1290:GLU:H	1.51	0.43
1:C:1302:LEU:HD22	1:C:1302:LEU:O	2.19	0.43
1:A:45:THR:HG22	1:B:562:THR:OG1	2.18	0.43
1:B:548:HIS:O	1:B:777:GLU:HG2	2.19	0.43
1:B:802:LEU:HD22	1:B:802:LEU:O	2.18	0.43
1:C:1026:LEU:C	1:C:1028:ARG:N	2.76	0.43
1:C:1118:VAL:HG21	1:C:1132:VAL:HG22	2.01	0.43
1:C:1232:ALA:O	1:C:1238:MET:HB2	2.19	0.43
1:C:1327:THR:CG2	1:C:1360:VAL:HB	2.49	0.43
1:A:20:ASN:HD21	1:A:38:ALA:HB2	1.84	0.42
1:A:24:LEU:O	1:A:27:ARG:HB2	2.19	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: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:D:1827:THR:CG2	1:D:1860:VAL:HB	2.49	0.42
1:A:354:PHE:O	1:A:355:ALA:HB3	2.18	0.42
1:B:648:GLU:OE2	1:B:656:ARG:NH2	2.53	0.42
1:A:211:TYR:OH	1:A:296:TYR:HB3	2.20	0.42
1:A:217:SER:HB2	1:A:220:ARG:HD2	2.02	0.42
1:B:845:GLY:HA3	1:B:877:ARG:HH12	1.84	0.42
1:A:81:PHE:O	1:A:87:LEU:HB2	2.19	0.42
1:A:282:GLN:O	1:A:283:GLU:C	2.62	0.42
1:B:698:PHE:O	1:B:725:HIS:HB3	2.19	0.42
1:C:1145:LEU:CD1	1:C:1156:ARG:NH1	2.78	0.42
1:C:1180:VAL:O	1:C:1180:VAL:CG1	2.67	0.42
1:C:1190:ALA:HA	1:C:1200:LEU:CD1	2.49	0.42
1:D:1548:HIS:O	1:D:1777:GLU:HG2	2.20	0.42
1:D:1651:VAL:HG23	1:D:1652:PRO:HD2	2.01	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:80:LYS:HZ3	1:A:84:GLU:HB2	1.84	0.42
1:A:126:VAL:HG22	1:A:353:ASP:HB3	2.01	0.42
1:C:1020:ASN:HD21	1:C:1038:ALA:HB2	1.84	0.42
1:D:1662:THR:HB	1:D:1663:PRO:CD	2.50	0.42
1:A:186:LEU:HD12	1:A:186:LEU:HA	1.80	0.42
1:A:251:GLU:CD	1:B:504:LEU:HD11	2.42	0.42
1:C:1040:GLU:HA	1:C:1041:PRO:HD3	1.95	0.42
1:C:1336:ARG:HD2	1:C:1336:ARG:HA	1.73	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:PRO:HD3	1:A:181:TYR:CZ	2.54	0.42
1:A:28:ARG:HG2	1:A:28:ARG:HH11	1.85	0.42
1:A:183:LYS:O	1:A:187:GLU:HB2	2.19	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:C:1077:LEU:HD21	1:C:1245:TYR:HB3	2.01	0.42
1:C:1121:LEU:HA	1:C:1142:VAL:O	2.20	0.42
1:C:1186:LEU:HD12	1:C:1186:LEU:HA	1.79	0.42
1:D:1534:VAL:O	1:D:1846:VAL:HA	2.20	0.42
1:D:1845:GLY:HA3	1:D:1877:ARG:HH12	1.85	0.42
1:C:1081:PHE:O	1:C:1087:LEU:HB2	2.19	0.42
1:C:1118:VAL:HG13	1:C:1167:ALA:HB3	2.02	0.42
1:C:1198:PHE:O	1:C:1225:HIS:HB3	2.20	0.42
1:D:1536:LEU:HD21	1:D:1874:ALA:CB	2.50	0.42
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: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:C:1162:THR:HB	1:C:1163:PRO:CD	2.50	0.41
1:D:1604:LEU:O	1:D:1608:PHE:CD1	2.73	0.41
1:D:1621:LEU:HA	1:D:1642:VAL:O	2.20	0.41
1:D:1690:ALA:O	1:D:1694:VAL:HG23	2.20	0.41
1:C:1045:THR:HG22	1:D:1562:THR:OG1	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:C:1110:ALA:HA	1:D:1508:VAL:HG11	2.02	0.41
1:C:1373:LYS:O	1:C:1377:ARG:HG2	2.20	0.41
1:A:327:THR:CG2	1:A:360:VAL:HB	2.51	0.41
1:B:618:VAL:HG21	1:B:632:VAL:HG22	2.02	0.41
1:B:625:TRP:NE1	2:B:914:ASP:HB3	2.35	0.41
1:B:776:LEU:HD23	1:B:776:LEU:O	2.19	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:A:131:MET:HE2	1:B:762:GLN:O	2.19	0.41
1:A:162:THR:HB	1:A:163:PRO:CD	2.50	0.41
1:A:345:GLY:HA3	1:A:377:ARG:HH12	1.85	0.41
1:C:1011:MET:HE3	1:C:1011:MET:HB3	1.85	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:D:1873:LYS:O	1:D:1877:ARG:HG2	2.21	0.41
1:A:26:LEU:C	1:A:28:ARG:N	2.78	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:LYS:HD3	1:B:501:MET:O	2.20	0.41
1:A:255:ALA:CB	1:B:504:LEU:HD23	2.50	0.41
1:A:270:ILE:N	1:A:270:ILE:HD12	2.36	0.41
1:B:683:LYS:O	1:B:687:GLU:HB2	2.21	0.41
1:B:873:LYS:O	1:B:877:ARG:HG2	2.21	0.41
1:C:1131:MET:HE2	1:D:1762:GLN:O	2.20	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:1689:LEU:HD13	1:D:1689:LEU:N	2.35	0.41
1:A:261:ARG:NH2	1:B:517:VAL:HG23	2.35	0.41
1:A:327:THR:O	1:A:328:SER:C	2.63	0.41
1:B:570:ILE:HA	1:B:571:PRO:HD3	1.90	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:C:1153:ASP:HA	1:C:1154:PRO:HD2	1.74	0.41
1:C:1282:GLN:O	1:C:1283:GLU:C	2.63	0.41
1:C:1286:ARG:CZ	1:C:1286:ARG:HB3	2.50	0.41
1:D:1512:LYS:HA	1:D:1513:PRO:HD3	1.79	0.41
1:D:1529:GLN:HG2	1:D:1529:GLN:H	1.72	0.41
1:D:1569:GLY:HA3	1:D:1596:VAL:HG23	2.03	0.41
1:D:1618:VAL:HG21	1:D:1632:VAL:HG22	2.02	0.41
1:A:48:HIS:O	1:A:277:GLU:HG2	2.21	0.41
1:A:69:GLY:HA3	1:A:96:VAL:HG21	2.02	0.41
1:A:217:SER:O	1:A:220:ARG:HD3	2.21	0.41
1:A:342:LEU:HD23	1:A:342:LEU:HA	1.84	0.41
1:B:534:VAL:O	1:B:846:VAL:HA	2.20	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:C:1270:ILE:HD12	1:C:1270:ILE:N	2.36	0.41
1:D:1686:LEU:HD12	1:D:1686:LEU:HA	1.76	0.41
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:B:662:THR:HB	1:B:663:PRO:CD	2.51	0.40
1:C:1022:LYS:O	1:C:1023:ALA:C	2.64	0.40
1:D:1581:PHE:O	1:D:1587:LEU:HB2	2.21	0.40
1:D:1618:VAL:HG13	1:D:1667:ALA:HB3	2.03	0.40
1:B:581:PHE:O	1:B:587:LEU:HB2	2.20	0.40
1:B:674:ASN:OD1	1:B:675:ASN:N	2.55	0.40
1:B:812:LEU:HD11	1:B:882:LEU:HD21	2.04	0.40
1:C:1027:ARG:HE	1:C:1027:ARG:HB3	1.69	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1211:TYR:HB3	1:C:1297:ARG:NH1	2.36	0.40
1:C:1261:ARG:NH2	1:D:1517:VAL:HG23	2.36	0.40
1:B:569:GLY:HA3	1:B:596:VAL:HG21	2.02	0.40
1:C:1212:GLU:CD	1:C:1300:ARG:HH12	2.29	0.40
1:D:1569:GLY:HA3	1:D:1596:VAL:HG21	2.03	0.40
1:D:1690:ALA:HA	1:D:1700:LEU:CD1	2.50	0.40
1:D:1770:ILE:HD12	1:D:1770:ILE:N	2.36	0.40
1:D:1827:THR:O	1:D:1828:SER:C	2.64	0.40
1:A:173:PRO:HB2	1:A:206:TYR:HB2	2.02	0.40
1:C:1312:LEU:HA	1:C:1312:LEU:HD23	1.79	0.40
1:A:276:LEU:HD23	1:A:276:LEU:O	2.21	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:B:761:ARG:C	1:B:761:ARG:CD	2.95	0.40
1:B:816:ARG:HG3	1:B:816:ARG:NH1	2.37	0.40
1:C:1069:GLY:HA3	1:C:1096:VAL:HG21	2.02	0.40
1:C:1327:THR:O	1:C:1328:SER:C	2.63	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 [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	380/385 (99%)	329 (87%)	45 (12%)	6 (2%)	7	31
1	B	380/385 (99%)	329 (87%)	46 (12%)	5 (1%)	9	35
1	C	380/385 (99%)	330 (87%)	44 (12%)	6 (2%)	7	31

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	380/385 (99%)	329 (87%)	44 (12%)	7 (2%)	6	29
All	All	1520/1540 (99%)	1317 (87%)	179 (12%)	24 (2%)	7	31

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%)	231 (76%)	74 (24%)	1	3
1	B	305/306 (100%)	231 (76%)	74 (24%)	1	3
1	C	305/306 (100%)	232 (76%)	73 (24%)	1	4
1	D	305/306 (100%)	233 (76%)	72 (24%)	1	4
All	All	1220/1224 (100%)	927 (76%)	293 (24%)	1	3

All (293) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ARG
1	A	11	MET
1	A	12	LYS
1	A	14	ASP
1	A	16	VAL
1	A	22	LYS
1	A	24	LEU
1	A	25	GLU
1	A	26	LEU
1	A	28	ARG
1	A	29	GLN
1	A	32	ASP
1	A	34	VAL
1	A	45	THR
1	A	49	VAL
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	97	THR
1	A	102	GLN
1	A	114	PRO
1	A	116	ASP
1	A	118	VAL
1	A	126	VAL
1	A	132	VAL
1	A	147	GLU
1	A	153	ASP
1	A	155	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	164	ARG
1	A	170	VAL
1	A	186	LEU
1	A	189	LEU
1	A	192	LEU
1	A	197	ASP
1	A	207	GLU
1	A	212	GLU
1	A	220	ARG
1	A	227	LEU
1	A	230	ASN
1	A	239	THR
1	A	245	TYR
1	A	251	GLU
1	A	253	ILE
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	313	LYS
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	373	LYS
1	A	376	GLU
1	A	380	ARG
1	A	381	VAL
1	A	382	LEU
1	B	506	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	511	MET
1	B	512	LYS
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	531	VAL
1	B	532	ASP
1	B	534	VAL
1	B	536	LEU
1	B	545	THR
1	B	549	VAL
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	597	THR
1	B	602	GLN
1	B	614	PRO
1	B	616	ASP
1	B	618	VAL
1	B	626	VAL
1	B	630	GLU
1	B	632	VAL
1	B	647	GLU
1	B	653	ASP
1	B	655	GLU
1	B	664	ARG
1	B	670	VAL
1	B	686	LEU
1	B	689	LEU
1	B	692	LEU
1	B	697	ASP
1	B	707	GLU
1	B	712	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	720	ARG
1	B	727	LEU
1	B	730	ASN
1	B	739	THR
1	B	745	TYR
1	B	753	ILE
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	813	LYS
1	B	821	PHE
1	B	826	ASP
1	B	839	GLU
1	B	842	LEU
1	B	848	VAL
1	B	860	VAL
1	B	862	LEU
1	B	869	GLU
1	B	872	ARG
1	B	873	LYS
1	B	876	GLU
1	B	880	ARG
1	B	881	VAL
1	B	882	LEU
1	C	1006	ARG
1	C	1011	MET
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	1034	VAL
1	C	1045	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	1049	VAL
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	1097	THR
1	C	1102	GLN
1	C	1114	PRO
1	C	1116	ASP
1	C	1118	VAL
1	C	1126	VAL
1	C	1132	VAL
1	C	1147	GLU
1	C	1153	ASP
1	C	1155	GLU
1	C	1164	ARG
1	C	1170	VAL
1	C	1186	LEU
1	C	1189	LEU
1	C	1192	LEU
1	C	1194	VAL
1	C	1197	ASP
1	C	1207	GLU
1	C	1212	GLU
1	C	1220	ARG
1	C	1221	VAL
1	C	1227	LEU
1	C	1230	ASN
1	C	1239	THR
1	C	1245	TYR
1	C	1253	ILE
1	C	1261	ARG
1	C	1268	ASP
1	C	1276	LEU
1	C	1283	GLU
1	C	1290	GLU
1	C	1291	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	1302	LEU
1	C	1303	LEU
1	C	1307	LEU
1	C	1308	THR
1	C	1313	LYS
1	C	1321	PHE
1	C	1326	ASP
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	1373	LYS
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	1508	VAL
1	D	1511	MET
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	1529	GLN
1	D	1531	VAL
1	D	1532	ASP
1	D	1534	VAL
1	D	1536	LEU
1	D	1545	THR
1	D	1549	VAL
1	D	1573	LEU
1	D	1574	ARG
1	D	1577	LEU
1	D	1580	LYS
1	D	1582	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	1618	VAL
1	D	1626	VAL
1	D	1630	GLU
1	D	1632	VAL
1	D	1647	GLU
1	D	1653	ASP
1	D	1655	GLU
1	D	1659	ARG
1	D	1664	ARG
1	D	1670	VAL
1	D	1686	LEU
1	D	1689	LEU
1	D	1692	LEU
1	D	1697	ASP
1	D	1707	GLU
1	D	1712	GLU
1	D	1727	LEU
1	D	1730	ASN
1	D	1739	THR
1	D	1745	TYR
1	D	1753	ILE
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
1	D	1821	PHE
1	D	1826	ASP
1	D	1836	ARG
1	D	1842	LEU
1	D	1848	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	1860	VAL
1	D	1862	LEU
1	D	1869	GLU
1	D	1872	ARG
1	D	1873	LYS
1	D	1880	ARG
1	D	1881	VAL
1	D	1882	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	59	GLN
1	A	196	HIS
1	B	520	ASN
1	B	559	GLN
1	B	671	ASN
1	B	696	HIS
1	C	1020	ASN
1	C	1059	GLN
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 oligosaccharides 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$
2	ASP	C	1414	3	7,8,8	1.66	1 (14%)	6,10,10	0.97	0
2	ASP	D	1914	3	7,8,8	2.16	3 (42%)	6,10,10	1.73	2 (33%)
3	PLP	A	413	2	15,15,16	2.10	3 (20%)	21,22,23	2.02	4 (19%)
3	PLP	B	913	2	15,15,16	2.47	6 (40%)	21,22,23	2.06	5 (23%)
2	ASP	A	414	3	7,8,8	2.16	3 (42%)	6,10,10	1.27	1 (16%)
3	PLP	D	1913	2	15,15,16	2.80	4 (26%)	21,22,23	1.92	7 (33%)
3	PLP	C	1413	2	15,15,16	1.76	5 (33%)	21,22,23	2.20	7 (33%)
2	ASP	B	914	3	7,8,8	2.14	2 (28%)	6,10,10	1.01	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ASP	C	1414	3	-	4/8/8/8	-
2	ASP	D	1914	3	-	7/8/8/8	-
3	PLP	A	413	2	-	0/6/6/8	0/1/1/1
3	PLP	B	913	2	-	4/6/6/8	0/1/1/1
2	ASP	A	414	3	-	3/8/8/8	-
3	PLP	D	1913	2	-	2/6/6/8	0/1/1/1
3	PLP	C	1413	2	-	0/6/6/8	0/1/1/1
2	ASP	B	914	3	-	3/8/8/8	-

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1913	PLP	C4A-C4	-8.62	1.34	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	913	PLP	C5-C4	5.76	1.47	1.40
3	A	413	PLP	C4A-C4	-5.37	1.40	1.51
2	B	914	ASP	O-C	4.61	1.35	1.22
2	A	414	ASP	CB-CG	4.00	1.61	1.51
3	B	913	PLP	O3-C3	-3.94	1.27	1.36
2	D	1914	ASP	CB-CG	3.80	1.61	1.51
3	A	413	PLP	C3-C4	-3.61	1.33	1.40
2	C	1414	ASP	OXT-C	-3.45	1.19	1.30
3	D	1913	PLP	C5-C4	3.35	1.44	1.40
3	B	913	PLP	P-O2P	3.33	1.67	1.54
3	C	1413	PLP	C5A-C5	3.21	1.59	1.50
3	B	913	PLP	C6-C5	3.03	1.43	1.37
3	C	1413	PLP	C5-C4	-3.03	1.37	1.40
3	C	1413	PLP	P-O3P	-2.95	1.43	1.54
2	B	914	ASP	CB-CG	-2.81	1.43	1.51
3	B	913	PLP	C6-N1	2.72	1.39	1.34
3	A	413	PLP	O3-C3	-2.64	1.30	1.36
3	D	1913	PLP	C2A-C2	2.61	1.54	1.50
2	A	414	ASP	OD2-CG	-2.55	1.22	1.30
2	A	414	ASP	OD1-CG	2.44	1.30	1.22
2	D	1914	ASP	CB-CA	2.41	1.63	1.53
2	D	1914	ASP	O-C	2.39	1.29	1.22
3	B	913	PLP	P-O3P	-2.32	1.46	1.54
3	D	1913	PLP	C3-C2	-2.18	1.38	1.41
3	C	1413	PLP	C3-C4	-2.15	1.36	1.40
3	C	1413	PLP	P-O2P	2.10	1.62	1.54

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	413	PLP	O4P-C5A-C5	6.83	122.15	109.36
3	C	1413	PLP	O4P-C5A-C5	6.50	121.55	109.36
3	D	1913	PLP	O4P-C5A-C5	5.62	119.88	109.36
3	B	913	PLP	C4A-C4-C5	4.81	125.90	120.94
3	B	913	PLP	C4-C3-C2	4.55	126.68	119.89
3	B	913	PLP	C3-C4-C5	-4.47	113.22	118.59
3	C	1413	PLP	C4A-C4-C5	-3.91	116.91	120.94
3	C	1413	PLP	O2P-P-O4P	3.22	115.08	106.67
2	D	1914	ASP	CB-CA-N	-3.03	99.17	112.42
3	D	1913	PLP	C6-C5-C4	2.77	120.37	118.10
3	D	1913	PLP	O3P-P-O1P	2.74	121.52	110.83
3	A	413	PLP	C6-C5-C4	2.69	120.31	118.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1914	ASP	OXT-C-O	2.59	129.96	124.08
3	C	1413	PLP	C6-C5-C4	2.56	120.20	118.10
3	B	913	PLP	O4P-C5A-C5	2.43	113.91	109.36
2	A	414	ASP	OXT-C-O	2.36	129.43	124.08
3	C	1413	PLP	C4A-C4-C3	2.35	124.45	120.52
3	C	1413	PLP	O3P-P-O4P	-2.33	100.60	106.67
3	D	1913	PLP	C3-C4-C5	-2.31	115.82	118.59
3	A	413	PLP	O3-C3-C2	2.27	122.30	117.58
3	B	913	PLP	C6-C5-C4	2.27	119.96	118.10
3	D	1913	PLP	C5-C6-N1	-2.17	120.31	123.83
3	D	1913	PLP	C4A-C4-C3	2.15	124.12	120.52
3	C	1413	PLP	O3P-P-O1P	2.11	119.06	110.83
3	A	413	PLP	C5-C6-N1	-2.10	120.41	123.83
3	D	1913	PLP	C2A-C2-C3	-2.03	118.42	120.80

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	414	ASP	O-C-CA-N
2	A	414	ASP	C-CA-CB-CG
2	D	1914	ASP	O-C-CA-N
2	D	1914	ASP	C-CA-CB-CG
3	B	913	PLP	C5A-O4P-P-O1P
3	B	913	PLP	C5A-O4P-P-O2P
3	B	913	PLP	C5A-O4P-P-O3P
3	D	1913	PLP	C4-C5-C5A-O4P
2	A	414	ASP	OXT-C-CA-N
2	D	1914	ASP	OXT-C-CA-N
2	C	1414	ASP	CA-CB-CG-OD1
2	C	1414	ASP	CA-CB-CG-OD2
2	D	1914	ASP	CA-CB-CG-OD1
2	D	1914	ASP	O-C-CA-CB
2	D	1914	ASP	CA-CB-CG-OD2
3	D	1913	PLP	C6-C5-C5A-O4P
2	B	914	ASP	C-CA-CB-CG
2	C	1414	ASP	C-CA-CB-CG
2	B	914	ASP	CA-CB-CG-OD2
2	D	1914	ASP	OXT-C-CA-CB
2	B	914	ASP	CA-CB-CG-OD1
3	B	913	PLP	C6-C5-C5A-O4P
2	C	1414	ASP	OXT-C-CA-N

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
3	D	1913	PLP	1	0
3	C	1413	PLP	1	0
2	B	914	ASP	3	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%)	-0.29	1 (0%) 90 82	2, 12, 35, 52	0
1	B	382/385 (99%)	-0.40	1 (0%) 90 82	2, 12, 35, 57	0
1	C	382/385 (99%)	-0.36	1 (0%) 90 82	2, 14, 38, 52	0
1	D	382/385 (99%)	-0.16	2 (0%) 87 76	2, 13, 35, 55	0
All	All	1528/1540 (99%)	-0.30	5 (0%) 90 82	2, 13, 36, 57	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1845	GLY	2.5
1	A	379	ALA	2.4
1	D	1809	ALA	2.3
1	B	836	ARG	2.2
1	C	1075	GLU	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ASP	A	414	9/9	0.79	0.14	2,7,24,29	0
2	ASP	B	914	9/9	0.81	0.15	15,22,26,27	0
2	ASP	D	1914	9/9	0.85	0.13	18,30,36,39	0
2	ASP	C	1414	9/9	0.87	0.13	17,24,29,29	0
3	PLP	B	913	15/16	0.95	0.08	2,5,11,14	0
3	PLP	C	1413	15/16	0.95	0.09	2,6,10,11	0
3	PLP	D	1913	15/16	0.96	0.07	6,13,21,22	0
3	PLP	A	413	15/16	0.97	0.07	3,8,13,17	0

6.5 Other polymers [i](#)

There are no such residues in this entry.