



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:35 am GMT

PDB ID : 1L5R
Title : Human liver glycogen phosphorylase a complexed with riboflavin, N-Acetyl-b
eta-D-Glucopyranosylamine and CP-403,700
Authors : Ekstrom, J.L.; Pauly, T.A.; Carty, M.D.; Soeller, W.C.; Culp, J.; Danley,
D.E.; Hoover, D.J.; Treadway, J.L.; Gibbs, E.M.; Fletterick, R.J.; Day, Y.S.N.;
Myszka, D.G.; Rath, V.L.
Deposited on : 2002-03-07
Resolution : 2.10 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

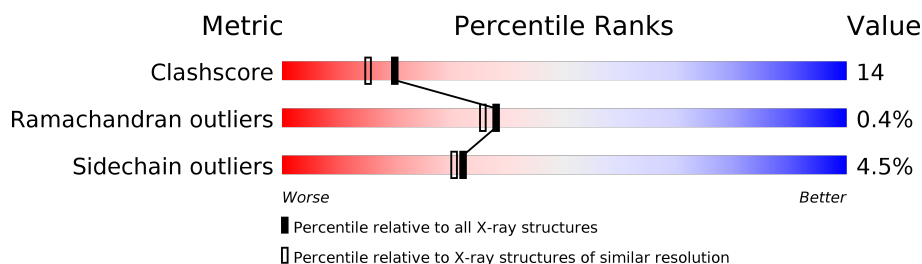
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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))
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	847	 65% 26% • 7%
1	B	847	 65% 27% • 7%

2 Entry composition [i](#)

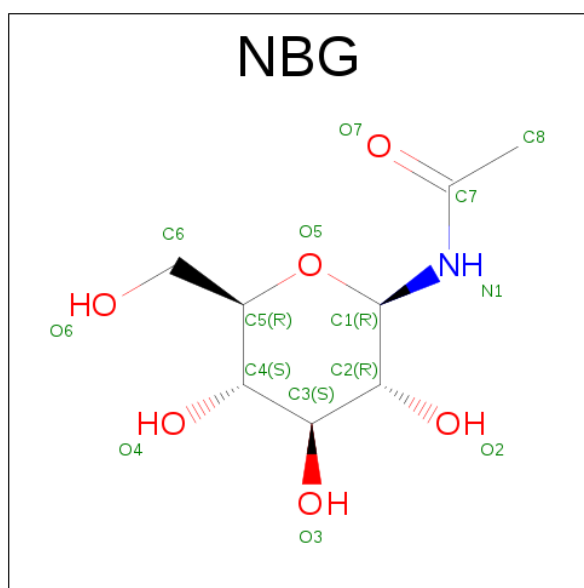
There are 7 unique types of molecules in this entry. The entry contains 13497 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 glycogen phosphorylase, liver form.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	790	Total	C	N	O	S	0	0	0
			6417	4125	1089	1174	29			
1	B	791	Total	C	N	O	S	0	0	0
			6423	4128	1090	1176	29			

- Molecule 2 is SUGAR (1-N-ACETYL-BETA-D-GLUCOSAMINE) (three-letter code: NBG) (formula: $C_8H_{15}NO_6$).



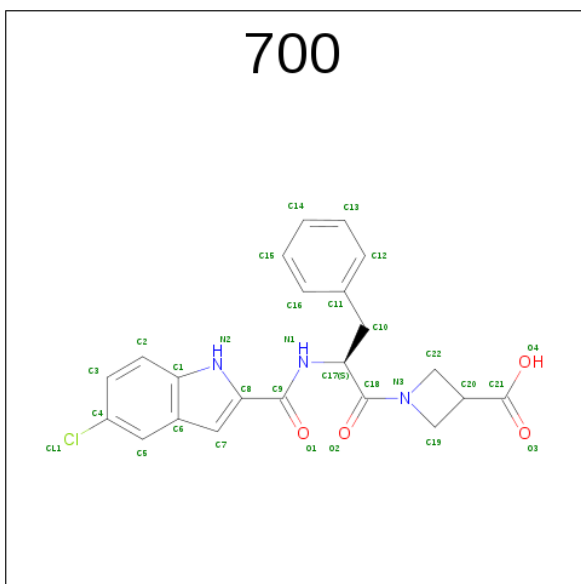
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	8	1	6		

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



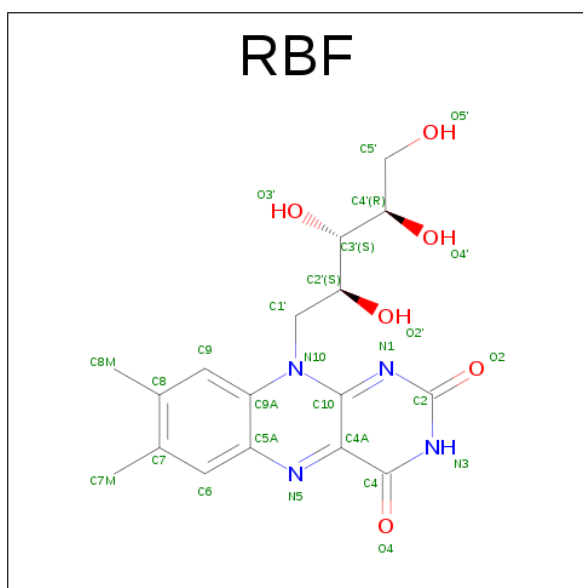
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 4 is [5-CHLORO-1H-INDOL-2-CARBONYL-PHENYLALANINYL]-AZETIDINE-3-CARBOXYLIC ACID (three-letter code: 700) (formula: C₂₂H₂₀ClN₃O₄).



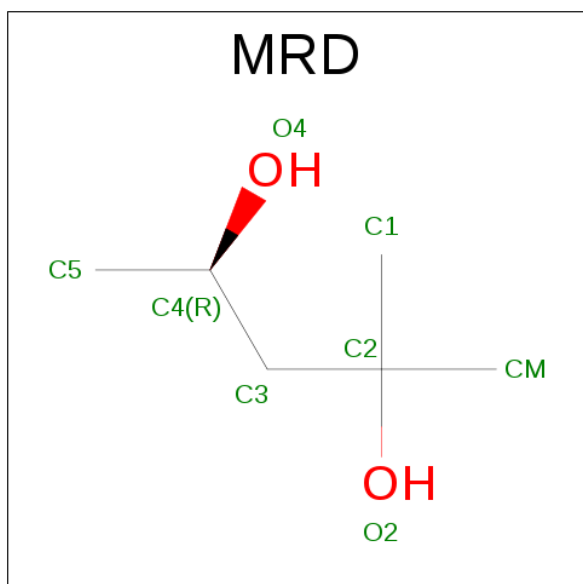
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	0	0
			30	22	1	3	4		

- Molecule 5 is RIBOFLAVIN (three-letter code: RBF) (formula: $C_{17}H_{20}N_4O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			27	17	4	6		

- Molecule 6 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			8	6	2		

- Molecule 7 is water.

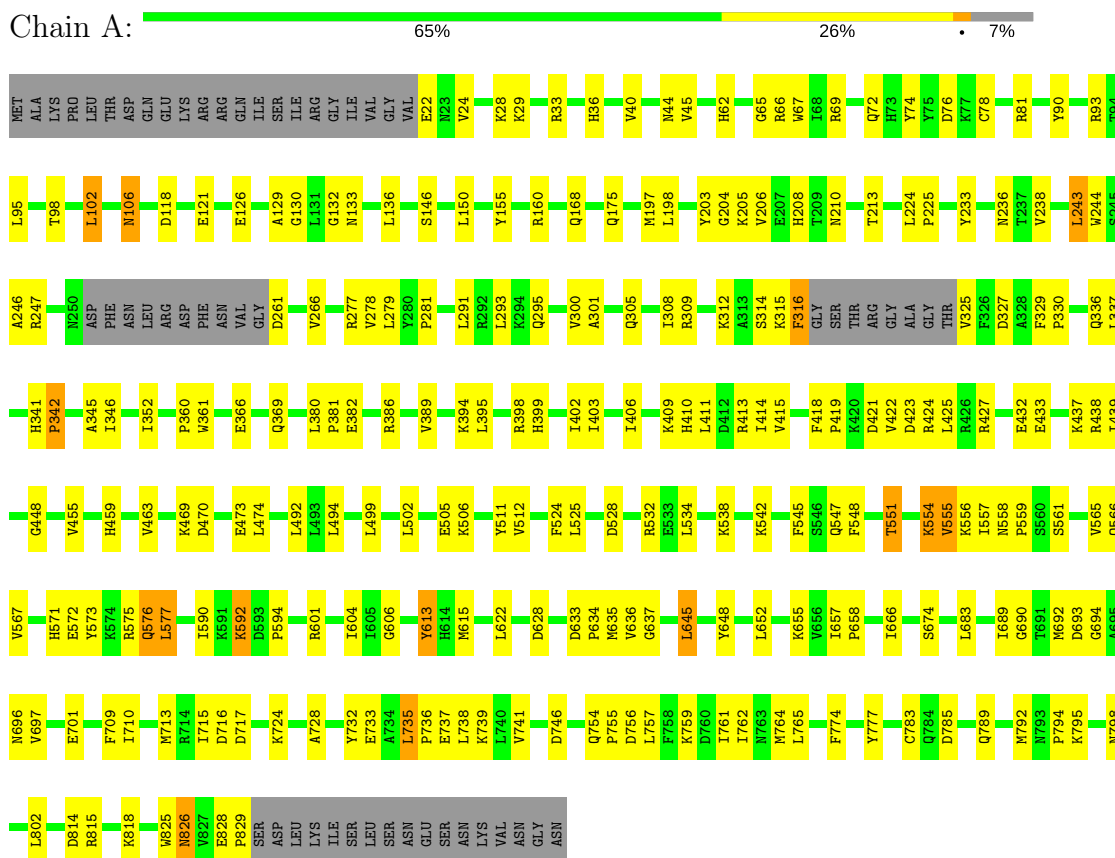
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	307	Total 307	O 307	0	0
7	B	240	Total 240	O 240	0	0

3 Residue-property plots

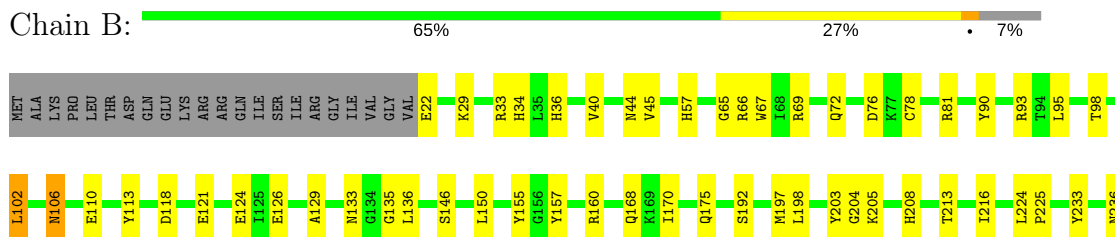
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

Note EDS was not executed.

- Molecule 1: glycogen phosphorylase, liver form



- Molecule 1: glycogen phosphorylase, liver form



T237	V238	F329	P330	C445	V565	H691	D785
L243	V244	Q336	L337	G448	Q566	H692	K786
S245	A246	H341	P342	V455	V567	D693	Q789
R247		A345	I346	H459	H571	A695	M792
N250	ASP	I352	W361	V463	E572	N696	N793
PHE	ASN	E382	Y374	K469	Y573	V697	P794
LEU	ARG	R386	E382	D470	K574	E701	L802
ASP	ASN	V359	K394	E473	Q576	L708	D814
ARG	PHE	H399	I402	L474	L577	F709	R815
ASN	ASN	I403	I406	T487	K592	I710	K818
VAL	GLY	I406	K409	P488	D593		W825
D261		K410	H410	R489	P594		N826
V266		L411	D412	L492	V599		N827
E273		L414	I415	L493	P600		E828
R277		V415	F418	L494	I604		P829
V278		Q305	P419	L499	G606		ASP
P281		R309	K420	L502	Y613		LEU
N282		F311	D421	L505	H614		LYS
D283		A313	V422	E505	M615		ILE
N284		S314	R424	K506	M618		SER
F285		K315	L425	L622	L622		SER
V300		F316	R426	V512	D628		ASN
A301		GLY	R427	K513	D633		GLU
A302		SER	E432	F524	P634		ASN
F303		THR	E433	L525	M635		GLY
L304		ARG	E437	D528	V636		ASN
Q305		ALA	K437	R532	G637		VAL
I308		GLY	I439	R538	L645		ASN
R309		SER		K542	E646		GLY
R310		THR		L543	N647		ASN
F311		ARG		F544	Y648		GLY
K312		GLY		F545	L652		ASN
A313		ALA		S546	K655		ASN
S314		ALA		Q547	V656		ASN
K315		THR		F548	I657		ASN
F316		THR		T551	P658		ASN
GLY		THR		K554	I666		ASN
SER		THR		V555	S674		ASN
THR		THR		K556	L683		ASN
ARG		THR		I557	I689		ASN
GLY		THR		N558	G690		ASN
ALA		THR		S561			ASN
GLY		THR					ASN
THR		THR					ASN
V325		THR					ASN

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	124.42Å 124.42Å 124.01Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	55.61 – 2.10	Depositor
% Data completeness (in resolution range)	95.5 (55.61-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.247 , 0.283	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13497	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

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: MRD, RBF, 700, NBG, 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	0.44	0/6561	0.65	1/8873 (0.0%)
1	B	0.43	0/6567	0.65	1/8881 (0.0%)
All	All	0.43	0/13128	0.65	2/17754 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	129	ALA	N-CA-C	-5.82	95.29	111.00
1	A	129	ALA	N-CA-C	-5.38	96.47	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6417	0	6412	191	0
1	B	6423	0	6417	183	0
2	A	15	0	15	0	0
3	A	15	0	7	0	0
3	B	15	0	7	0	0
4	A	30	0	18	0	0
5	A	27	0	20	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	8	0	14	0	0
7	A	307	0	0	28	0
7	B	240	0	0	18	0
All	All	13497	0	12910	368	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (368) 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:B:110:GLU:HA	7:B:2505:HOH:O	1.65	0.93
1:B:113:TYR:HB3	7:B:2505:HOH:O	1.69	0.93
1:A:213:THR:HB	7:A:2504:HOH:O	1.70	0.91
1:A:710:ILE:HD13	7:A:2205:HOH:O	1.72	0.89
1:A:798:ASN:HB3	7:A:2061:HOH:O	1.72	0.87
1:A:247:ARG:HD3	7:A:2472:HOH:O	1.76	0.85
1:A:547:GLN:O	1:A:551:THR:HG23	1.76	0.85
1:B:547:GLN:O	1:B:551:THR:HG23	1.77	0.84
1:B:308:ILE:CD1	1:B:352:ILE:HG21	2.10	0.82
1:A:645:LEU:HD13	1:A:652:LEU:HD11	1.61	0.81
1:A:469:LYS:HG3	7:A:2489:HOH:O	1.81	0.79
1:B:645:LEU:HD13	1:B:652:LEU:HD11	1.62	0.79
1:A:645:LEU:CD1	1:A:652:LEU:HD11	2.13	0.79
1:A:308:ILE:CD1	1:A:352:ILE:HG21	2.13	0.78
1:B:645:LEU:CD1	1:B:652:LEU:HD11	2.15	0.76
1:A:278:VAL:HG21	1:B:266:VAL:HG11	1.69	0.74
1:A:279:LEU:HD22	7:A:2498:HOH:O	1.89	0.72
1:A:198:LEU:HD21	1:A:309:ARG:NH2	2.05	0.71
1:A:615:MET:CE	1:A:761:ILE:HG12	2.20	0.71
1:B:615:MET:HE1	1:B:761:ILE:HG12	1.72	0.70
1:B:599:VAL:HB	7:B:2328:HOH:O	1.91	0.70
1:A:205:LYS:HB2	7:A:2292:HOH:O	1.91	0.70
1:B:615:MET:CE	1:B:761:ILE:HG12	2.21	0.69
1:A:279:LEU:CD2	7:A:2498:HOH:O	2.41	0.69
1:B:198:LEU:HD21	1:B:309:ARG:NH2	2.08	0.69
1:A:615:MET:HE1	1:A:761:ILE:HG12	1.73	0.68
1:A:130:GLY:O	7:A:2498:HOH:O	2.11	0.68
1:A:146:SER:O	1:A:150:LEU:HD13	1.92	0.68
1:B:433:GLU:HG2	1:B:437:LYS:HE2	1.76	0.68
1:A:433:GLU:HG2	1:A:437:LYS:HE2	1.76	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:LYS:HG2	1:B:33:ARG:NH2	2.08	0.67
1:A:266:VAL:HG11	1:B:278:VAL:HG21	1.76	0.67
1:A:29:LYS:HG2	1:A:33:ARG:NH2	2.09	0.67
1:B:455:VAL:HG23	1:B:674:SER:HB2	1.76	0.67
1:A:160:ARG:HB2	1:A:243:LEU:HB3	1.77	0.67
1:A:532:ARG:HH11	1:A:532:ARG:HB2	1.60	0.67
1:B:532:ARG:HB2	1:B:532:ARG:HH11	1.58	0.67
1:B:455:VAL:H	1:B:459:HIS:HD2	1.43	0.66
1:A:594:PRO:HG3	1:A:635:MET:SD	2.34	0.66
1:B:146:SER:O	1:B:150:LEU:HD13	1.95	0.66
1:B:81:ARG:NH1	1:B:155:TYR:OH	2.29	0.66
1:A:325:VAL:HG12	1:A:327:ASP:H	1.62	0.65
1:A:534:LEU:HD23	7:A:2061:HOH:O	1.94	0.65
1:B:160:ARG:HB2	1:B:243:LEU:HB3	1.77	0.65
1:B:192:SER:HB3	7:B:2004:HOH:O	1.96	0.65
1:B:415:VAL:HG22	1:B:425:LEU:HD11	1.79	0.65
1:B:594:PRO:HG3	1:B:635:MET:SD	2.37	0.65
1:A:278:VAL:HG21	1:B:266:VAL:CG1	2.26	0.64
1:A:81:ARG:NH1	1:A:155:TYR:OH	2.30	0.64
1:A:415:VAL:HG22	1:A:425:LEU:HD11	1.79	0.64
1:A:409:LYS:O	1:A:413:ARG:HG2	1.97	0.64
1:A:455:VAL:H	1:A:459:HIS:HD2	1.43	0.64
1:B:469:LYS:O	1:B:473:GLU:HG3	1.97	0.63
1:A:278:VAL:CG2	1:B:266:VAL:HG11	2.28	0.63
1:B:828:GLU:HG3	1:B:829:PRO:HD2	1.80	0.63
1:A:386:ARG:NH2	1:A:438:ARG:HD2	2.14	0.63
1:A:455:VAL:HG23	1:A:674:SER:HB2	1.81	0.62
1:B:346:ILE:HD13	1:B:448:GLY:HA3	1.80	0.62
1:B:386:ARG:NH2	1:B:438:ARG:HD2	2.15	0.62
1:A:118:ASP:OD1	1:A:121:GLU:HG3	2.00	0.62
1:A:366:GLU:HA	7:A:2453:HOH:O	2.00	0.61
1:B:409:LYS:O	1:B:413:ARG:HG2	1.99	0.61
1:A:764:MET:SD	1:A:765:LEU:HD12	2.41	0.61
1:A:469:LYS:O	1:A:473:GLU:HG3	2.00	0.60
1:B:118:ASP:OD1	1:B:121:GLU:HG3	2.02	0.60
1:B:308:ILE:HD12	1:B:352:ILE:HG21	1.84	0.60
1:A:615:MET:HE3	1:A:615:MET:O	2.01	0.60
1:A:316:PHE:CD2	1:A:316:PHE:N	2.67	0.60
1:A:421:ASP:OD1	1:A:424:ARG:HD2	2.02	0.59
1:B:814:ASP:O	1:B:818:LYS:HG3	2.03	0.59
1:A:93:ARG:HG2	1:A:126:GLU:HG2	1.85	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:ILE:HD13	1:A:448:GLY:HA3	1.85	0.59
1:A:399:HIS:O	1:A:403:ILE:HG13	2.01	0.59
1:B:124:GLU:OE2	7:B:2413:HOH:O	2.16	0.58
1:B:470:ASP:O	1:B:474:LEU:HD13	2.03	0.58
1:B:615:MET:O	1:B:615:MET:HE3	2.02	0.58
1:A:369:GLN:HB2	7:A:2453:HOH:O	2.02	0.58
1:A:423:ASP:O	1:A:427:ARG:HG3	2.03	0.58
1:B:204:GLY:C	1:B:205:LYS:HD2	2.24	0.58
1:B:543:LEU:HB3	7:B:2406:HOH:O	2.04	0.58
1:A:233:TYR:CZ	1:A:512:VAL:HG11	2.39	0.58
1:A:814:ASP:O	1:A:818:LYS:HG3	2.04	0.57
1:B:399:HIS:O	1:B:403:ILE:HG13	2.03	0.57
1:B:386:ARG:HB3	1:B:438:ARG:HD3	1.85	0.57
1:B:422:VAL:HG23	1:B:423:ASP:N	2.19	0.57
1:B:433:GLU:CG	1:B:437:LYS:HE2	2.34	0.57
1:A:386:ARG:HB3	1:A:438:ARG:HD3	1.86	0.57
1:A:433:GLU:CG	1:A:437:LYS:HE2	2.35	0.57
1:B:785:ASP:O	1:B:789:GLN:HG2	2.05	0.57
1:A:266:VAL:CG1	1:B:278:VAL:HG21	2.34	0.56
1:A:325:VAL:HA	7:A:2508:HOH:O	2.04	0.56
1:A:330:PRO:HB2	7:A:2416:HOH:O	2.05	0.56
1:A:735:LEU:HD23	1:A:777:TYR:HD2	1.70	0.56
1:B:592:LYS:O	1:B:594:PRO:HD3	2.06	0.56
1:B:81:ARG:NH2	7:B:2240:HOH:O	2.35	0.56
1:A:470:ASP:O	1:A:474:LEU:HD13	2.05	0.56
1:B:752:PRO:HG2	7:B:2354:HOH:O	2.05	0.56
1:B:753:LYS:HG2	7:B:2354:HOH:O	2.06	0.56
1:A:421:ASP:CG	1:A:424:ARG:HB2	2.26	0.56
1:A:709:PHE:HB3	1:A:783:CYS:SG	2.46	0.56
1:A:266:VAL:HG11	1:B:278:VAL:CG2	2.37	0.56
1:A:204:GLY:C	1:A:205:LYS:HD2	2.27	0.55
1:A:422:VAL:HG23	1:A:423:ASP:N	2.21	0.55
1:B:538:LYS:O	1:B:542:LYS:HG3	2.07	0.55
1:B:421:ASP:CG	1:B:424:ARG:HB2	2.27	0.55
1:B:309:ARG:NH2	7:B:2450:HOH:O	2.33	0.55
1:B:422:VAL:CG2	1:B:423:ASP:N	2.71	0.54
1:A:592:LYS:O	1:A:594:PRO:HD3	2.07	0.54
1:A:785:ASP:O	1:A:789:GLN:HG2	2.08	0.54
1:B:423:ASP:O	1:B:427:ARG:HG3	2.07	0.54
1:A:314:SER:O	1:A:315:LYS:HB3	2.07	0.54
1:B:421:ASP:OD1	1:B:424:ARG:HD2	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:532:ARG:NH1	1:B:532:ARG:HB2	2.22	0.53
1:A:572:GLU:HG3	1:A:613:TYR:OH	2.08	0.53
1:B:118:ASP:HA	7:B:2363:HOH:O	2.07	0.53
1:A:132:GLY:N	7:A:2498:HOH:O	2.42	0.53
1:B:314:SER:O	1:B:315:LYS:HB3	2.07	0.53
1:A:106:ASN:HD22	1:A:106:ASN:N	2.06	0.53
1:A:532:ARG:NH1	1:A:532:ARG:HB2	2.23	0.53
1:A:538:LYS:O	1:A:542:LYS:HG3	2.08	0.53
1:B:106:ASN:N	1:B:106:ASN:HD22	2.07	0.53
1:A:422:VAL:CG2	1:A:423:ASP:N	2.71	0.53
1:B:565:VAL:HG22	1:B:604:ILE:HB	1.91	0.53
1:B:735:LEU:HD23	1:B:777:TYR:HD2	1.73	0.53
1:A:316:PHE:HD2	1:A:316:PHE:N	2.05	0.52
1:A:459:HIS:O	1:A:463:VAL:HG23	2.10	0.52
1:A:206:VAL:HG13	7:A:2504:HOH:O	2.08	0.52
1:B:93:ARG:HG2	1:B:126:GLU:HG2	1.92	0.52
1:B:697:VAL:O	1:B:701:GLU:HG3	2.10	0.52
1:B:709:PHE:HB3	1:B:783:CYS:SG	2.50	0.52
1:A:329:PHE:HB3	1:A:330:PRO:CD	2.40	0.52
1:B:308:ILE:HD12	1:B:352:ILE:HD13	1.92	0.52
1:A:565:VAL:HG22	1:A:604:ILE:HB	1.91	0.51
1:A:308:ILE:HD12	1:A:352:ILE:HG21	1.91	0.51
1:A:233:TYR:CE2	1:A:512:VAL:HG11	2.46	0.51
1:B:459:HIS:O	1:B:463:VAL:HG23	2.10	0.51
1:B:410:HIS:O	1:B:414:ILE:HD13	2.09	0.51
1:A:208:HIS:ND1	1:A:213:THR:HG22	2.26	0.51
1:A:22:GLU:HB3	1:A:62:HIS:HE1	1.76	0.51
1:A:735:LEU:CD1	1:A:735:LEU:N	2.73	0.51
1:B:208:HIS:ND1	1:B:213:THR:HG22	2.25	0.51
1:B:329:PHE:HB3	1:B:330:PRO:HD3	1.93	0.51
1:B:735:LEU:CD1	1:B:735:LEU:N	2.74	0.51
1:B:246:ALA:O	1:B:247:ARG:HD2	2.11	0.51
1:B:300:VAL:CG1	1:B:345:ALA:HA	2.41	0.50
1:A:410:HIS:O	1:A:414:ILE:HD13	2.10	0.50
1:B:168:GLN:HG3	1:B:175:GLN:HG3	1.92	0.50
1:B:67:TRP:HA	1:B:238:VAL:HB	1.93	0.50
1:A:693:ASP:O	1:A:696:ASN:HB2	2.12	0.50
1:B:66:ARG:HD2	1:B:236:ASN:HA	1.93	0.50
1:B:45:VAL:HG12	1:B:45:VAL:O	2.11	0.50
1:B:693:ASP:O	1:B:696:ASN:HB2	2.10	0.50
1:B:764:MET:SD	1:B:765:LEU:HD12	2.52	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:572:GLU:HG3	1:B:613:TYR:OH	2.11	0.50
1:A:795:LYS:HB2	7:A:2122:HOH:O	2.11	0.50
1:A:411:LEU:O	1:A:415:VAL:HG23	2.12	0.50
1:A:697:VAL:O	1:A:701:GLU:HG3	2.12	0.50
1:A:308:ILE:O	1:A:312:LYS:HG3	2.12	0.49
1:A:66:ARG:HD2	1:A:236:ASN:HA	1.94	0.49
1:B:300:VAL:HG13	1:B:345:ALA:HA	1.94	0.49
1:A:329:PHE:HB3	1:A:330:PRO:HD3	1.93	0.49
1:B:826:ASN:HD22	1:B:826:ASN:C	2.14	0.49
1:B:577:LEU:CD1	1:B:765:LEU:HD11	2.42	0.49
1:A:198:LEU:HD21	1:A:309:ARG:CZ	2.42	0.49
1:B:411:LEU:O	1:B:415:VAL:HG23	2.12	0.49
1:A:66:ARG:CD	1:A:236:ASN:HA	2.42	0.49
1:A:828:GLU:HG3	1:A:829:PRO:HD2	1.94	0.49
1:B:826:ASN:O	1:B:826:ASN:ND2	2.38	0.49
1:A:737:GLU:O	1:A:741:VAL:HG23	2.12	0.49
1:B:737:GLU:O	1:B:741:VAL:HG23	2.12	0.49
1:A:246:ALA:O	1:A:247:ARG:HD2	2.12	0.48
1:A:615:MET:HE2	1:A:761:ILE:HG12	1.93	0.48
1:A:645:LEU:HD11	1:A:652:LEU:HD11	1.90	0.48
1:B:157:TYR:HD2	1:B:303:THR:HG1	1.58	0.48
1:A:369:GLN:NE2	7:A:2453:HOH:O	2.46	0.48
1:A:67:TRP:HA	1:A:238:VAL:HB	1.95	0.48
1:B:66:ARG:CD	1:B:236:ASN:HA	2.43	0.48
1:B:724:LYS:O	1:B:724:LYS:HD3	2.13	0.48
1:A:197:MET:HE2	1:A:224:LEU:HD13	1.95	0.48
1:A:225:PRO:HB3	1:A:244:TRP:CZ3	2.49	0.48
1:A:494:LEU:HD23	1:A:494:LEU:C	2.34	0.48
1:B:198:LEU:HD21	1:B:309:ARG:CZ	2.44	0.48
1:B:652:LEU:HD13	1:B:652:LEU:O	2.14	0.48
1:A:556:LYS:HD3	1:A:557:ILE:N	2.28	0.48
1:A:133:ASN:OD1	1:A:281:PRO:HA	2.14	0.48
1:A:689:ILE:O	1:A:689:ILE:HG23	2.14	0.48
1:A:65:GLY:O	1:A:69:ARG:HG3	2.14	0.48
1:A:45:VAL:O	1:A:45:VAL:HG12	2.14	0.48
1:B:205:LYS:HG3	7:B:2302:HOH:O	2.13	0.47
1:B:689:ILE:HG23	1:B:689:ILE:O	2.14	0.47
1:A:301:ALA:O	1:A:305:GLN:HG3	2.13	0.47
1:A:386:ARG:HA	1:A:439:ILE:O	2.14	0.47
1:A:724:LYS:O	1:A:724:LYS:HD3	2.14	0.47
1:B:329:PHE:HB3	1:B:330:PRO:CD	2.44	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:645:LEU:HD11	1:B:652:LEU:HD11	1.94	0.47
1:B:65:GLY:O	1:B:69:ARG:HG3	2.15	0.47
1:A:545:PHE:O	1:A:548:PHE:HB3	2.14	0.47
1:A:577:LEU:CD1	1:A:765:LEU:HD11	2.44	0.47
1:A:261:ASP:N	7:A:2495:HOH:O	2.47	0.47
1:A:414:ILE:CG2	1:A:425:LEU:HD23	2.45	0.47
1:B:532:ARG:CB	1:B:532:ARG:NH1	2.78	0.47
1:B:655:LYS:O	1:B:658:PRO:HD2	2.15	0.47
1:B:746:ASP:HB2	1:B:762:ILE:HG13	1.97	0.47
1:A:203:TYR:HE2	1:A:394:LYS:HD2	1.80	0.47
1:A:511:TYR:N	7:A:2148:HOH:O	2.47	0.47
1:A:746:ASP:HB2	1:A:762:ILE:HG13	1.97	0.47
1:A:132:GLY:O	7:A:2498:HOH:O	2.20	0.47
1:A:532:ARG:NH1	1:A:532:ARG:CB	2.78	0.47
1:B:506:LYS:HD2	1:B:524:PHE:CE2	2.50	0.47
1:A:424:ARG:HH22	1:A:474:LEU:CD1	2.28	0.46
1:A:738:LEU:HB2	1:A:777:TYR:CE2	2.49	0.46
1:A:293:LEU:HG	1:A:395:LEU:HD23	1.96	0.46
1:A:571:HIS:H	1:A:576:GLN:NE2	2.12	0.46
1:B:301:ALA:O	1:B:305:GLN:HG3	2.15	0.46
1:A:506:LYS:HD2	1:A:524:PHE:CE2	2.50	0.46
1:A:402:ILE:O	1:A:406:ILE:HG13	2.15	0.46
1:A:576:GLN:NE2	1:A:576:GLN:H	2.13	0.46
1:B:732:TYR:CE1	1:B:739:LYS:HA	2.51	0.46
1:A:398:ARG:O	1:A:402:ILE:HG13	2.16	0.46
1:A:592:LYS:HE2	1:A:592:LYS:O	2.15	0.46
1:A:633:ASP:O	1:A:636:VAL:HG22	2.15	0.46
1:B:225:PRO:HB3	1:B:244:TRP:CZ3	2.51	0.46
1:A:732:TYR:CE1	1:A:739:LYS:HA	2.51	0.46
1:A:826:ASN:O	1:A:826:ASN:ND2	2.39	0.46
1:B:754:GLN:HB3	1:B:757:LEU:HB2	1.96	0.46
1:B:402:ILE:O	1:B:406:ILE:HG13	2.16	0.46
1:B:566:GLN:HA	7:B:2012:HOH:O	2.15	0.46
1:A:575:ARG:HD3	1:A:666:ILE:O	2.15	0.46
1:B:576:GLN:H	1:B:576:GLN:NE2	2.13	0.46
1:B:693:ASP:O	1:B:694:GLY:C	2.54	0.46
1:A:136:LEU:C	1:A:136:LEU:HD23	2.36	0.46
1:A:657:ILE:HB	1:A:658:PRO:HD3	1.98	0.45
1:A:826:ASN:C	1:A:826:ASN:HD22	2.19	0.45
1:B:432:GLU:O	1:B:437:LYS:HA	2.17	0.45
1:B:738:LEU:HB2	1:B:777:TYR:CE2	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:715:ILE:HG23	1:A:716:ASP:N	2.30	0.45
1:B:133:ASN:OD1	1:B:281:PRO:HA	2.16	0.45
1:B:216:ILE:HB	7:B:2168:HOH:O	2.16	0.45
1:B:648:TYR:HD1	1:B:652:LEU:HD12	1.81	0.45
1:B:728:ALA:HB1	1:B:774:PHE:CD1	2.51	0.45
1:B:633:ASP:O	1:B:636:VAL:HG22	2.16	0.45
1:A:754:GLN:HB3	1:A:757:LEU:HB2	1.97	0.45
1:B:414:ILE:CG2	1:B:425:LEU:HD23	2.45	0.45
1:B:433:GLU:HG3	1:B:437:LYS:HG2	1.99	0.45
1:B:715:ILE:HG23	1:B:716:ASP:N	2.31	0.45
1:B:72:GLN:HE21	1:B:76:ASP:CG	2.19	0.45
1:A:693:ASP:O	1:A:694:GLY:C	2.54	0.45
1:A:692:MET:HG3	1:A:697:VAL:HG22	1.98	0.45
1:B:592:LYS:O	1:B:592:LYS:HE2	2.15	0.45
1:B:636:VAL:HG23	1:B:637:GLY:N	2.32	0.45
1:A:389:VAL:HG22	1:A:437:LYS:O	2.16	0.45
1:A:168:GLN:HG3	1:A:175:GLN:HG3	1.99	0.45
1:B:545:PHE:O	1:B:548:PHE:HB3	2.16	0.45
1:B:81:ARG:HD3	1:B:155:TYR:HE2	1.82	0.45
1:A:648:TYR:HD1	1:A:652:LEU:HD12	1.82	0.45
1:A:525:LEU:HD23	1:A:802:LEU:HD23	1.99	0.45
1:B:571:HIS:H	1:B:576:GLN:NE2	2.15	0.45
1:A:732:TYR:CD1	1:A:739:LYS:HA	2.52	0.45
1:B:308:ILE:HD13	1:B:352:ILE:HG21	1.92	0.45
1:B:438:ARG:HB3	1:B:438:ARG:HE	1.60	0.45
1:A:380:LEU:HA	1:A:381:PRO:HD3	1.82	0.44
1:A:592:LYS:C	1:A:592:LYS:HE2	2.38	0.44
1:B:81:ARG:HD3	1:B:155:TYR:CE2	2.52	0.44
1:B:315:LYS:HG3	1:B:315:LYS:O	2.17	0.44
1:B:592:LYS:C	1:B:592:LYS:HE2	2.38	0.44
1:B:341:HIS:HB2	1:B:342:PRO:HD3	1.99	0.44
1:A:316:PHE:HD2	1:A:316:PHE:H	1.64	0.44
1:B:732:TYR:CD1	1:B:739:LYS:HA	2.52	0.44
1:B:615:MET:HE2	1:B:761:ILE:HG12	1.96	0.44
1:A:415:VAL:HG22	1:A:425:LEU:CD1	2.48	0.44
1:A:728:ALA:HB1	1:A:774:PHE:CD1	2.52	0.44
1:B:308:ILE:O	1:B:312:LYS:HG3	2.17	0.44
1:B:106:ASN:HB3	7:B:2216:HOH:O	2.17	0.44
1:B:556:LYS:HD3	1:B:557:ILE:N	2.32	0.44
1:B:487:THR:HA	1:B:488:PRO:HD3	1.88	0.44
1:A:336:GLN:OE1	1:A:825:TRP:NE1	2.45	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:558:ASN:HB3	1:A:561:SER:HB3	2.00	0.43
1:B:98:THR:O	1:B:102:LEU:HB2	2.18	0.43
1:B:424:ARG:HH22	1:B:474:LEU:CD1	2.30	0.43
1:A:341:HIS:HB2	1:A:342:PRO:HD3	1.99	0.43
1:A:308:ILE:HD12	1:A:352:ILE:HD13	2.00	0.43
1:A:555:VAL:HG12	1:A:556:LYS:N	2.33	0.43
1:A:81:ARG:HD3	1:A:155:TYR:CE2	2.53	0.43
1:B:567:VAL:HA	1:B:606:GLY:O	2.18	0.43
1:B:575:ARG:HD3	1:B:666:ILE:O	2.18	0.43
1:B:36:HIS:O	1:B:40:VAL:HA	2.19	0.43
1:B:386:ARG:HA	1:B:439:ILE:O	2.17	0.43
1:A:438:ARG:HE	1:A:438:ARG:HB3	1.62	0.43
1:B:135:GLY:HA3	7:B:2008:HOH:O	2.18	0.43
1:B:615:MET:CE	1:B:618:MET:HB2	2.48	0.43
1:A:566:GLN:HA	7:A:2057:HOH:O	2.18	0.43
1:B:389:VAL:HG22	1:B:437:LYS:O	2.17	0.43
1:B:415:VAL:HG22	1:B:425:LEU:CD1	2.47	0.43
1:B:555:VAL:HG12	1:B:556:LYS:N	2.33	0.43
1:A:432:GLU:O	1:A:437:LYS:HA	2.19	0.43
1:A:756:ASP:O	1:A:759:LYS:HB2	2.18	0.43
1:B:756:ASP:O	1:B:759:LYS:HB2	2.18	0.43
1:A:198:LEU:CD2	1:A:309:ARG:NH2	2.78	0.43
1:B:311:PHE:CE1	1:B:329:PHE:HA	2.54	0.43
1:B:708:LEU:HG	7:B:2209:HOH:O	2.18	0.43
1:A:636:VAL:HG23	1:A:637:GLY:N	2.33	0.43
1:B:336:GLN:OE1	1:B:825:TRP:NE1	2.47	0.43
1:B:170:ILE:HG12	1:B:646:GLU:HB3	2.01	0.43
1:B:792:MET:O	1:B:794:PRO:HD3	2.18	0.43
1:B:828:GLU:CG	1:B:829:PRO:HD2	2.47	0.43
1:A:567:VAL:HA	1:A:606:GLY:O	2.19	0.42
1:B:197:MET:HE2	1:B:224:LEU:HD13	2.01	0.42
1:B:374:TYR:CG	1:B:445:CYS:HB3	2.54	0.42
1:A:24:VAL:O	1:A:28:LYS:HG3	2.18	0.42
1:B:754:GLN:N	1:B:755:PRO:HD3	2.34	0.42
1:A:360:PRO:HB2	7:A:2441:HOH:O	2.19	0.42
1:A:382:GLU:H	1:A:382:GLU:CD	2.23	0.42
1:A:792:MET:O	1:A:794:PRO:HD3	2.19	0.42
1:B:325:VAL:HA	7:B:2535:HOH:O	2.19	0.42
1:A:818:LYS:HD3	7:A:2547:HOH:O	2.20	0.42
1:A:761:ILE:O	1:A:765:LEU:HD13	2.20	0.42
1:A:74:TYR:HB3	1:A:81:ARG:NH1	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:558:ASN:HB3	1:B:561:SER:HB3	2.01	0.42
1:A:713:MET:HB3	1:A:717:ASP:HB2	2.01	0.42
1:A:735:LEU:HD23	1:A:777:TYR:CD2	2.52	0.42
1:A:210:ASN:ND2	7:A:2270:HOH:O	2.53	0.42
1:A:36:HIS:O	1:A:40:VAL:HA	2.19	0.42
1:A:554:LYS:O	1:A:555:VAL:O	2.38	0.42
1:A:735:LEU:N	1:A:735:LEU:HD12	2.35	0.42
1:B:233:TYR:CD2	1:B:513:LYS:HE3	2.55	0.42
1:B:382:GLU:CD	1:B:382:GLU:H	2.22	0.42
1:B:713:MET:HB3	1:B:717:ASP:HB2	2.02	0.42
1:A:557:ILE:O	1:A:559:PRO:HD3	2.20	0.42
1:A:690:GLY:O	1:A:710:ILE:HA	2.20	0.42
1:A:72:GLN:HE21	1:A:76:ASP:CG	2.23	0.42
1:A:98:THR:O	1:A:102:LEU:HB2	2.18	0.41
1:B:657:ILE:HB	1:B:658:PRO:HD3	2.02	0.41
1:A:300:VAL:HG13	1:A:345:ALA:HA	2.02	0.41
1:A:735:LEU:HA	1:A:736:PRO:HD2	1.86	0.41
1:B:761:ILE:O	1:B:765:LEU:HD13	2.19	0.41
1:A:433:GLU:HG3	1:A:437:LYS:HG2	2.01	0.41
1:B:136:LEU:HD23	1:B:136:LEU:C	2.40	0.41
1:B:283:ASP:O	1:B:284:ASN:HB2	2.20	0.41
1:A:590:ILE:HA	7:A:2392:HOH:O	2.21	0.41
1:A:81:ARG:HD3	1:A:155:TYR:HE2	1.86	0.41
1:B:22:GLU:OE1	1:B:22:GLU:HA	2.20	0.41
1:A:315:LYS:O	1:A:316:PHE:C	2.58	0.41
1:A:754:GLN:N	1:A:755:PRO:HD3	2.36	0.41
1:B:735:LEU:HD23	1:B:777:TYR:CD2	2.54	0.41
1:A:315:LYS:O	1:A:315:LYS:HG3	2.21	0.41
1:B:786:LYS:HB3	1:B:786:LYS:HE2	1.72	0.41
1:A:633:ASP:HA	1:A:634:PRO:HD3	1.91	0.41
1:B:494:LEU:HD23	1:B:494:LEU:C	2.40	0.41
1:B:525:LEU:HD23	1:B:802:LEU:HD23	2.03	0.41
1:B:233:TYR:CZ	1:B:512:VAL:HG11	2.56	0.41
1:B:636:VAL:CG2	1:B:637:GLY:N	2.84	0.41
1:A:300:VAL:CG1	1:A:345:ALA:HA	2.51	0.41
1:B:246:ALA:O	1:B:273:GLU:HG2	2.21	0.41
1:A:281:PRO:HD2	7:A:2410:HOH:O	2.20	0.40
1:A:291:LEU:O	1:A:295:GLN:HG3	2.21	0.40
1:A:601:ARG:HG3	7:A:2212:HOH:O	2.21	0.40
1:B:203:TYR:HE2	1:B:394:LYS:HD2	1.86	0.40
1:B:561:SER:HA	1:B:600:PRO:HG2	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:769:ASP:C	1:B:769:ASP:OD1	2.58	0.40
1:A:418:PHE:N	1:A:419:PRO:HD3	2.36	0.40
1:A:655:LYS:O	1:A:658:PRO:HD2	2.21	0.40
1:B:282:ASN:HB3	1:B:285:PHE:HB3	2.04	0.40
1:B:555:VAL:CG1	1:B:556:LYS:N	2.84	0.40
1:B:34:HIS:CE1	1:B:57:HIS:HB3	2.56	0.40
1:B:692:MET:HG3	1:B:697:VAL:HG22	2.03	0.40
1:B:197:MET:HB2	1:B:197:MET:HE2	1.83	0.40
1:B:418:PHE:N	1:B:419:PRO:HD3	2.36	0.40
1:B:690:GLY:O	1:B:710:ILE:HA	2.21	0.40

There are no symmetry-related clashes.

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	784/847 (93%)	742 (95%)	39 (5%)	3 (0%)	38	35
1	B	785/847 (93%)	742 (94%)	39 (5%)	4 (0%)	32	28
All	All	1569/1694 (93%)	1484 (95%)	78 (5%)	7 (0%)	38	35

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	555	VAL
1	B	555	VAL
1	A	554	LYS
1	B	554	LYS
1	A	342	PRO
1	B	342	PRO
1	B	694	GLY

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	692/740 (94%)	662 (96%)	30 (4%)	33	32
1	B	693/740 (94%)	661 (95%)	32 (5%)	31	29
All	All	1385/1480 (94%)	1323 (96%)	62 (4%)	32	30

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	78	CYS
1	A	90	TYR
1	A	95	LEU
1	A	102	LEU
1	A	106	ASN
1	A	243	LEU
1	A	277	ARG
1	A	316	PHE
1	A	337	LEU
1	A	361	TRP
1	A	492	LEU
1	A	499	LEU
1	A	502	LEU
1	A	505	GLU
1	A	528	ASP
1	A	551	THR
1	A	573	TYR
1	A	576	GLN
1	A	577	LEU
1	A	592	LYS
1	A	613	TYR
1	A	622	LEU
1	A	628	ASP
1	A	645	LEU
1	A	683	LEU
1	A	733	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	735	LEU
1	A	815	ARG
1	A	826	ASN
1	B	44	ASN
1	B	78	CYS
1	B	90	TYR
1	B	95	LEU
1	B	102	LEU
1	B	106	ASN
1	B	243	LEU
1	B	277	ARG
1	B	281	PRO
1	B	325	VAL
1	B	337	LEU
1	B	361	TRP
1	B	489	ARG
1	B	492	LEU
1	B	499	LEU
1	B	502	LEU
1	B	505	GLU
1	B	528	ASP
1	B	551	THR
1	B	573	TYR
1	B	576	GLN
1	B	577	LEU
1	B	592	LYS
1	B	613	TYR
1	B	622	LEU
1	B	628	ASP
1	B	645	LEU
1	B	683	LEU
1	B	733	GLU
1	B	735	LEU
1	B	815	ARG
1	B	826	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	HIS
1	A	72	GLN
1	A	97	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	106	ASN
1	A	250	ASN
1	A	369	GLN
1	A	459	HIS
1	A	576	GLN
1	B	96	GLN
1	B	105	GLN
1	B	106	ASN
1	B	250	ASN
1	B	369	GLN
1	B	459	HIS
1	B	576	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

6 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	$\# Z > 2$
5	RBF	A	859	-	27,29,29	2.26	11 (40%)	32,43,43	2.92	11 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PLP	A	860	1	15,15,16	2.09	2 (13%)	20,22,23	1.32	3 (15%)
2	NBG	A	861	-	15,15,15	1.32	3 (20%)	21,21,21	1.23	2 (9%)
4	700	A	862	-	24,33,33	1.87	8 (33%)	33,47,47	1.51	5 (15%)
3	PLP	B	860	1	15,15,16	2.19	2 (13%)	20,22,23	0.89	0
6	MRD	B	902	-	7,7,7	0.67	0	9,10,10	0.67	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
5	RBF	A	859	-	-	0/12/14/14	0/3/3/3
3	PLP	A	860	1	-	0/6/6/8	0/1/1/1
2	NBG	A	861	-	-	0/5/26/26	0/1/1/1
4	700	A	862	-	-	0/15/32/32	0/4/4/4
3	PLP	B	860	1	-	0/6/6/8	0/1/1/1
6	MRD	B	902	-	-	0/5/5/5	0/0/0/0

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	860	PLP	C4A-C4	-5.63	1.40	1.51
3	A	860	PLP	C4A-C4	-5.18	1.41	1.51
3	B	860	PLP	C3-C2	-5.03	1.37	1.40
5	A	859	RBF	C4A-N5	-2.34	1.30	1.33
5	A	859	RBF	C4'-C3'	-2.03	1.49	1.53
5	A	859	RBF	C10-N1	2.04	1.36	1.33
2	A	861	NBG	C3-C2	2.08	1.57	1.52
5	A	859	RBF	C5'-C4'	2.30	1.58	1.52
2	A	861	NBG	C1-N1	2.31	1.46	1.43
4	A	862	700	C12-C11	2.41	1.43	1.38
4	A	862	700	C15-C14	2.43	1.43	1.38
4	A	862	700	C13-C12	2.53	1.43	1.38
5	A	859	RBF	C9A-N10	2.69	1.42	1.38
5	A	859	RBF	C8-C7	2.72	1.47	1.41
2	A	861	NBG	C2-C1	2.72	1.55	1.52
4	A	862	700	C16-C11	2.75	1.44	1.38
4	A	862	700	C7-C6	2.94	1.52	1.41
4	A	862	700	C2-C3	2.96	1.42	1.36
5	A	859	RBF	C8M-C8	2.97	1.56	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	862	700	C3-C4	3.09	1.44	1.38
3	A	860	PLP	C5A-C5	3.23	1.59	1.50
5	A	859	RBF	C4-N3	3.52	1.39	1.33
5	A	859	RBF	C5A-N5	3.71	1.41	1.35
4	A	862	700	C5-C4	3.94	1.44	1.36
5	A	859	RBF	C1'-N10	4.83	1.53	1.48
5	A	859	RBF	C4-C4A	5.74	1.52	1.41

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	859	RBF	C4A-C10-N10	-6.49	116.02	120.52
5	A	859	RBF	O5'-C5'-C4'	-5.70	98.52	111.11
5	A	859	RBF	C4-C4A-C10	-5.58	115.45	119.96
4	A	862	700	C7-C6-C1	-4.40	102.44	106.27
5	A	859	RBF	C5A-C9A-N10	-4.03	114.67	117.66
3	A	860	PLP	O3P-P-O4P	-2.86	99.13	106.73
5	A	859	RBF	O4'-C4'-C5'	-2.56	103.29	109.21
4	A	862	700	C4-C5-C6	-2.48	117.49	119.18
5	A	859	RBF	C1'-N10-C10	-2.33	116.11	118.50
5	A	859	RBF	C4A-C4-N3	-2.32	120.19	123.48
4	A	862	700	C3-C2-C1	-2.28	118.05	120.84
2	A	861	NBG	C2-C1-N1	-2.20	108.72	111.30
3	A	860	PLP	C2A-C2-C3	2.13	123.51	120.96
5	A	859	RBF	C1'-N10-C9A	2.53	120.67	118.35
3	A	860	PLP	O3P-P-O2P	2.67	118.38	107.61
4	A	862	700	C8-C9-N1	3.51	122.36	115.20
4	A	862	700	C8-N2-C1	3.70	112.10	104.47
2	A	861	NBG	C5-O5-C1	3.91	117.92	112.53
5	A	859	RBF	C10-C4A-N5	4.45	125.71	120.59
5	A	859	RBF	O4'-C4'-C3'	4.86	121.16	109.09
5	A	859	RBF	C4-N3-C2	7.85	122.03	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.