



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:05 PM UTC

PDB ID : 1EM6 / pdb_00001em6
Title : HUMAN LIVER GLYCOGEN PHOSPHORYLASE A COMPLEXED WITH
GLCNAC AND CP-526,423
Authors : Rath, V.L.; Ammirati, M.; Danley, D.E.; Ekstrom, J.L.; Hynes, T.R.; Olson,
T.V.; Hoover, D.J.
Deposited on : 2000-03-16
Resolution : 2.20 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

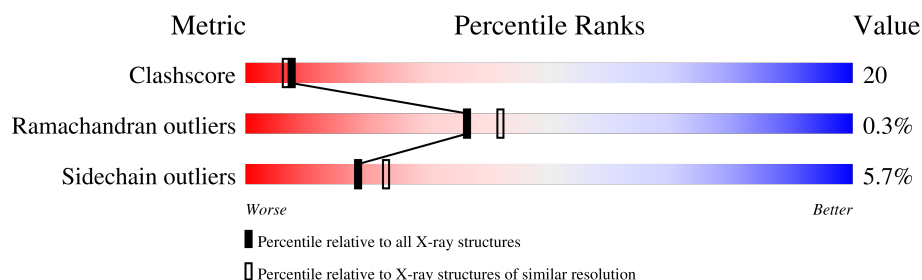
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	847	
1	B	847	

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
5	MPD	B	1902	X	-	-	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 13599 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.

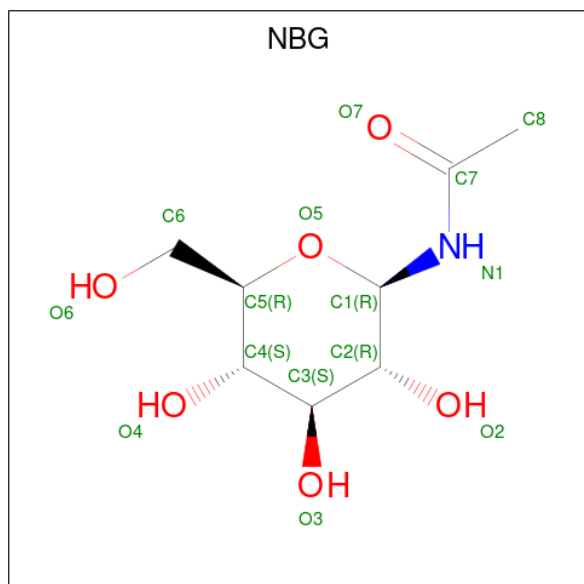
- Molecule 1 is a protein called LIVER GLYCOGEN PHOSPHORYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	787	Total	C	N	O	S	0	0	0
			6380	4097	1082	1172	29			
1	B	787	Total	C	N	O	S	0	0	0
			6380	4097	1082	1172	29			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	569	ARG	SER	SEE REMARK 999	UNP P06737
B	569	ARG	SER	SEE REMARK 999	UNP P06737

- Molecule 2 is N-acetyl-beta-D-glucopyranosylamine (CCD ID: NBG) (formula: $C_8H_{15}NO_6$).



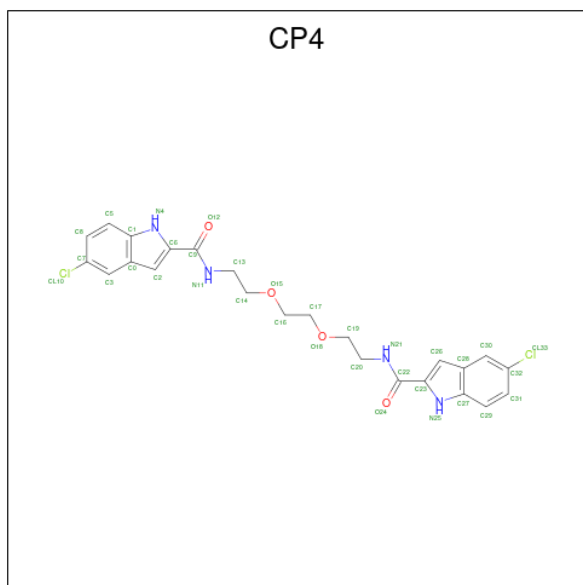
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	8	1	6		

Continued on next page...

Continued from previous page...

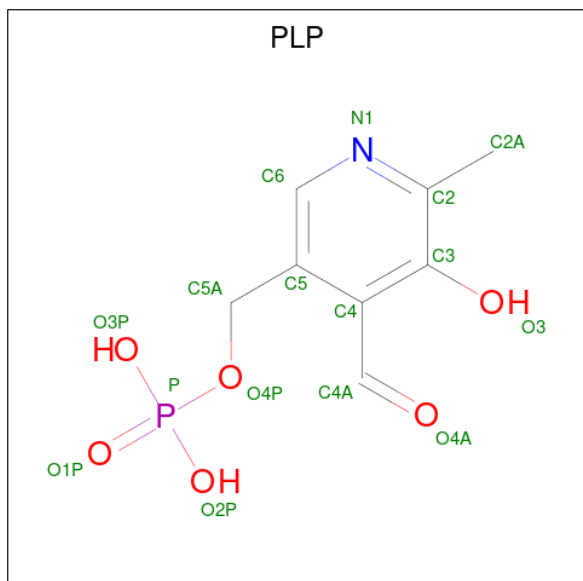
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			15	8	1	6		

- Molecule 3 is BIS[5-CHLORO-1H-INDOL-2-YL-CARBONYL-AMINOETHYL]-ETHYLENE GLYCOL (CCD ID: CP4) (formula: $C_{24}H_{24}Cl_2N_4O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	
			34	24	2	4	4	0

- Molecule 4 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: $C_8H_{10}NO_6P$).



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

- Molecule 5 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



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

- Molecule 6 is water.

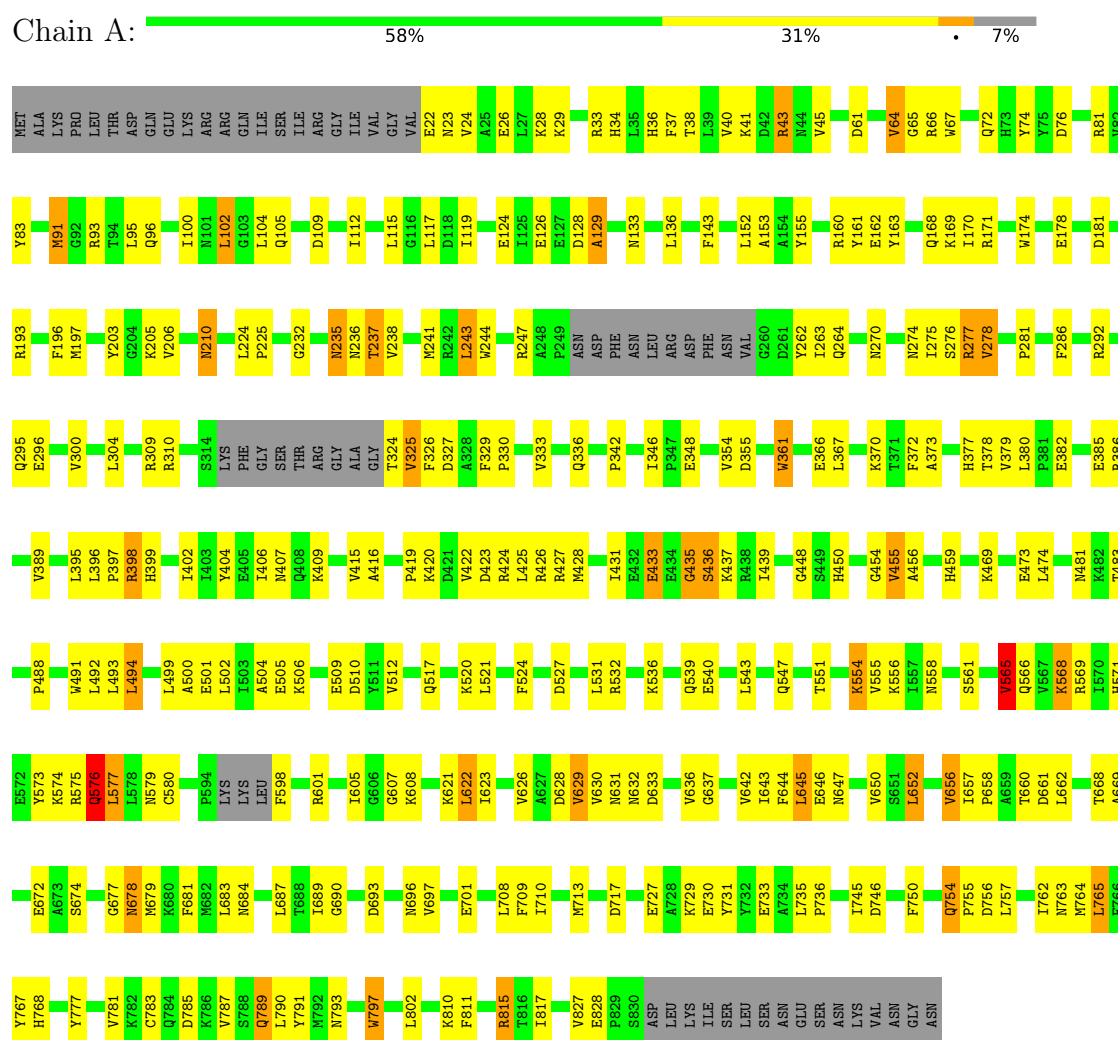
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	379	Total	O	0	0
			379	379		
6	B	358	Total	O	0	0
			358	358		

3 Residue-property plots

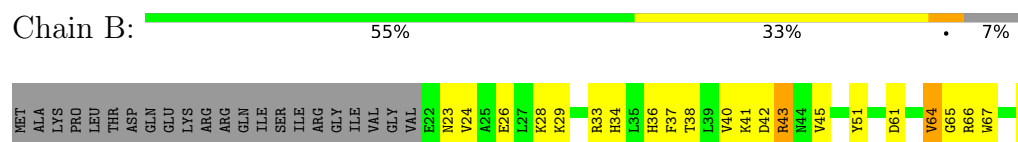
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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: LIVER GLYCOGEN PHOSPHORYLASE



• Molecule 1: LIVER GLYCOGEN PHOSPHORYLASE



R81	V278	I439	K544	D633	I710	W797
V82	L279	E366	F545	V636	F711	R815
Y83	Y280	L387	S546	G637	G712	T816
M91	L183	Q547	S449	V642	M713	L802
G92	R184	H450	F548	V643	D717	K810
R93	R193	G454	T551	I643	A720	R815
T94	F285	V455	K554	F644	K723	T816
L95	F196	A456	V555	E646	K723	I817
Q96	M197	K457	K558	N647	W726	W827
I100	Y203	H459	N558	Y648	E727	E828
M101	Y203	K469	S561	R649	A728	S830
L102	N210	E473	V565	V650	K729	ASP
Q105	T211	Q566	Q567	L652	E730	LEU
N106	K214	R385	K568	V656	Y731	LYS
D109	W215	M481	V567	I657	Y732	LYS
E110	I216	K482	K569	P658	E733	ILE
A111	L224	T483	R569	P658	A734	SER
I112	P225	P488	I570	A659	L735	LEU
L115	G232	H571	E572	T660	P736	SER
G116	G232	L492	Y573	D661	W745	ASN
L117	N235	L493	K574	L662	D746	GLU
D118	N236	L494	R575	T668	F750	SER
I119	T237	A500	Q576	A669	Q754	ASN
E126	V238	A501	L578	G670	L755	LYS
E127	M241	E501	K579	T671	W756	VAL
D128	R242	L502	C580	A672	D756	ASN
A129	L244	E505	F594	A673	L757	GLY
N133	W244	K506	LYS	S674	F758	ASN
L136	R247	I507	LEU	G675	K759	VAL
F143	A248	G508	F598	T676	I762	LYS
M147	P249	D510	F598	G677	N763	LYS
L152	ASN	Y511	R601	N678	M764	VAL
A153	ASP	V512	I605	K680	L765	ASN
Y155	PHE	F329	T605	F681	F766	GLY
ASN	ASN	P330	G606	M682	Y767	ASN
R160	VAL	P419	G607	N684	H768	
Y161	G260	K420	K608	L687	F774	
E162	D261	D421	M615	T688	Y777	
Y163	Y262	V422	I619	G690	W781	
Q168	I263	D423	K621	D693	K782	
K169	Q264	R424	L623	N696	C783	
I170	Q264	L425	V626	V697	D784	
R171	N270	M428	A627	E698	K786	
W174	N274	I431	K628	M699	W787	
S276	I275	E432	D628	A700	S788	
R277	S276	E434	V629	E701	Q789	
		G435	N631	E702	L790	
		K437	N632	L708	Y791	
		R438		F709	W792	
					N793	

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	123.31Å 123.31Å 122.32Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	99.00 – 2.20	Depositor
% Data completeness (in resolution range)	92.7 (99.00-2.20)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.233 , 0.264	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13599	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PLP, MPD, NBG, CP4

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	0.40	0/6522	0.91	24/8822 (0.3%)
1	B	0.40	0/6522	0.91	25/8822 (0.3%)
All	All	0.40	0/13044	0.91	49/17644 (0.3%)

There are no bond length outliers.

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	354	VAL	N-CA-C	7.21	117.30	110.74
1	B	575	ARG	N-CA-C	7.20	121.33	111.39
1	A	575	ARG	N-CA-C	7.19	121.31	111.39
1	B	754	GLN	CA-C-N	7.14	128.76	119.84
1	B	754	GLN	C-N-CA	7.14	128.76	119.84
1	B	91	MET	N-CA-C	7.08	120.04	111.82
1	A	754	GLN	CA-C-N	7.05	128.66	119.84
1	A	754	GLN	C-N-CA	7.05	128.66	119.84
1	B	64	VAL	N-CA-C	7.00	117.51	110.23
1	A	354	VAL	N-CA-C	6.77	116.90	110.74
1	B	684	ASN	N-CA-C	6.73	120.47	112.93
1	A	565	VAL	N-CA-C	6.70	118.44	108.46
1	A	684	ASN	N-CA-C	6.59	120.32	112.93
1	B	576	GLN	N-CA-C	-6.53	105.18	113.01
1	A	64	VAL	N-CA-C	6.51	117.00	110.23
1	B	454	GLY	N-CA-C	-6.49	102.33	112.58
1	A	105	GLN	N-CA-C	6.41	118.80	111.11
1	B	203	TYR	CB-CA-C	-6.30	109.33	116.63
1	A	576	GLN	N-CA-C	-6.28	105.48	113.01
1	A	454	GLY	N-CA-C	-6.26	102.70	112.58
1	B	565	VAL	N-CA-C	6.24	117.76	108.46
1	B	372	PHE	N-CA-C	6.04	119.93	110.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	203	TYR	CB-CA-C	-6.03	109.64	116.63
1	B	129	ALA	N-CA-C	-5.93	97.50	108.24
1	A	277	ARG	N-CA-C	5.91	117.52	111.14
1	A	129	ALA	N-CA-C	-5.91	98.28	108.56
1	A	91	MET	N-CA-C	5.89	119.66	112.23
1	A	372	PHE	N-CA-C	5.73	119.44	110.32
1	B	650	VAL	N-CA-C	5.48	116.11	110.36
1	B	105	GLN	N-CA-C	5.43	117.63	111.11
1	B	162	GLU	N-CA-C	-5.42	105.53	111.82
1	B	333	VAL	N-CA-C	5.40	116.06	108.17
1	A	650	VAL	N-CA-C	5.38	116.01	110.36
1	B	699	MET	N-CA-C	-5.33	105.55	111.36
1	B	677	GLY	N-CA-C	-5.33	106.33	112.73
1	A	232	GLY	N-CA-C	-5.31	105.49	112.82
1	A	491	TRP	N-CA-C	5.27	118.83	112.93
1	A	677	GLY	N-CA-C	-5.26	106.36	113.24
1	A	162	GLU	N-CA-C	-5.22	105.76	111.82
1	B	675	GLY	N-CA-C	-5.21	106.17	112.48
1	B	232	GLY	N-CA-C	-5.20	105.64	112.82
1	B	277	ARG	N-CA-C	5.20	116.75	111.14
1	B	656	VAL	N-CA-C	5.18	115.95	110.72
1	A	333	VAL	N-CA-C	5.18	115.73	108.17
1	A	811	PHE	N-CA-C	5.16	118.71	112.93
1	B	455	VAL	N-CA-C	5.16	117.13	111.77
1	A	455	VAL	N-CA-C	5.12	117.10	111.77
1	A	656	VAL	N-CA-C	5.08	115.86	110.72
1	B	216	ILE	N-CA-C	5.03	116.10	108.96

There are no chirality outliers.

There are no planarity outliers.

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	6380	0	6361	247	2
1	B	6380	0	6361	275	1

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	15	0	15	1	0
2	B	15	0	15	1	0
3	A	34	0	24	0	0
4	A	15	0	7	0	0
4	B	15	0	6	0	0
5	B	8	0	14	0	0
6	A	379	0	0	21	0
6	B	358	0	0	33	1
All	All	13599	0	12803	518	2

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 20.

All (518) 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:133:ASN:HD22	1:B:569:ARG:NH2	1.56	1.02
1:B:789:GLN:HE21	1:B:789:GLN:HA	1.24	1.02
1:A:133:ASN:HD22	1:A:569:ARG:NH2	1.60	1.00
1:A:789:GLN:HE21	1:A:789:GLN:HA	1.24	0.98
1:A:133:ASN:HD21	1:A:281:PRO:HA	1.29	0.97
1:B:133:ASN:HD21	1:B:281:PRO:HA	1.30	0.93
1:B:662:LEU:HD12	1:B:787:VAL:HG11	1.52	0.89
1:B:379:VAL:HA	6:B:2254:HOH:O	1.74	0.86
1:A:662:LEU:HD12	1:A:787:VAL:HG11	1.56	0.85
1:A:163:TYR:CE1	1:A:181:ASP:HB3	2.12	0.85
1:B:678:ASN:HD22	1:B:679:MET:H	1.21	0.85
1:A:678:ASN:HD22	1:A:679:MET:H	1.25	0.84
1:B:163:TYR:CE1	1:B:181:ASP:HB3	2.12	0.84
1:B:133:ASN:HD22	1:B:569:ARG:HH22	1.22	0.83
1:A:29:LYS:HE2	1:A:33:ARG:NH1	1.94	0.83
1:A:133:ASN:HD22	1:A:569:ARG:HH22	1.25	0.82
1:B:29:LYS:HE2	1:B:33:ARG:NH1	1.96	0.81
1:B:168:GLN:HE21	1:B:647:ASN:H	1.28	0.81
1:B:378:THR:HG21	6:B:2357:HOH:O	1.80	0.80
1:B:324:THR:HG23	6:B:2486:HOH:O	1.81	0.80
1:B:378:THR:HA	6:B:2008:HOH:O	1.82	0.79
1:A:168:GLN:HE21	1:A:647:ASN:H	1.26	0.79
1:A:274:ASN:HD21	1:B:270:ASN:HD21	1.29	0.78
1:A:660:THR:HG21	1:A:681:PHE:HE2	1.49	0.78
1:B:210:ASN:N	1:B:210:ASN:HD22	1.82	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:547:GLN:O	1:B:551:THR:HG23	1.83	0.78
1:A:547:GLN:O	1:A:551:THR:HG23	1.83	0.77
1:B:662:LEU:HD21	1:B:689:ILE:CG2	2.15	0.76
1:A:797:TRP:HZ3	6:A:2328:HOH:O	1.68	0.76
1:A:555:VAL:HG21	1:A:643:ILE:HD11	1.68	0.75
1:A:109:ASP:HB3	6:A:2581:HOH:O	1.86	0.75
1:A:329:PHE:HB3	1:A:330:PRO:HD3	1.69	0.75
1:A:270:ASN:HD21	1:B:274:ASN:HD21	1.32	0.75
1:B:797:TRP:HZ3	6:B:2580:HOH:O	1.69	0.75
1:B:660:THR:HG21	1:B:681:PHE:HE2	1.52	0.74
1:A:662:LEU:HD21	1:A:689:ILE:CG2	2.17	0.74
1:B:329:PHE:HB3	1:B:330:PRO:HD3	1.69	0.73
1:A:96:GLN:HB3	1:A:494:LEU:HD21	1.69	0.73
1:A:210:ASN:N	1:A:210:ASN:HD22	1.84	0.72
1:B:96:GLN:HB3	1:B:494:LEU:HD21	1.69	0.72
1:B:555:VAL:HG21	1:B:643:ILE:HD11	1.70	0.72
1:B:163:TYR:HE1	1:B:181:ASP:HB3	1.52	0.71
1:B:678:ASN:HD22	1:B:679:MET:N	1.88	0.71
1:B:366:GLU:HG3	1:B:367:LEU:N	2.05	0.71
1:A:366:GLU:HG3	1:A:367:LEU:N	2.04	0.71
1:B:764:MET:HE1	1:B:765:LEU:HD13	1.73	0.70
1:B:629:VAL:HG11	1:B:750:PHE:CD1	2.26	0.70
1:A:566:GLN:HE22	1:A:576:GLN:HA	1.56	0.70
1:A:764:MET:HE1	1:A:765:LEU:HD13	1.74	0.70
1:B:789:GLN:HA	1:B:789:GLN:NE2	2.04	0.70
1:A:629:VAL:HG11	1:A:750:PHE:CD1	2.26	0.70
1:A:163:TYR:HE1	1:A:181:ASP:HB3	1.54	0.69
1:A:756:ASP:HB3	6:A:2336:HOH:O	1.91	0.69
1:A:41:LYS:HD2	1:A:45:VAL:HG23	1.75	0.69
1:A:678:ASN:HD22	1:A:679:MET:N	1.90	0.69
1:A:415:VAL:HG12	1:A:425:LEU:HD11	1.74	0.69
1:A:789:GLN:HA	1:A:789:GLN:NE2	2.04	0.69
1:B:415:VAL:HG12	1:B:425:LEU:HD11	1.75	0.68
1:B:355:ASP:OD2	1:B:398:ARG:HD3	1.93	0.68
1:A:501:GLU:HG2	1:A:505:GLU:OE1	1.94	0.67
1:B:580:CYS:SG	1:B:622:LEU:HD13	2.35	0.67
1:B:662:LEU:HD21	1:B:689:ILE:HG22	1.75	0.67
1:A:262:TYR:CD2	1:A:263:ILE:HD12	2.30	0.67
1:B:501:GLU:HG3	6:B:2529:HOH:O	1.94	0.67
1:B:262:TYR:CD2	1:B:263:ILE:HD12	2.30	0.66
1:B:501:GLU:HG2	1:B:505:GLU:OE1	1.94	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:ILE:HG12	1:B:646:GLU:HG2	1.78	0.66
1:B:810:LYS:O	1:B:815:ARG:HD3	1.95	0.66
1:B:41:LYS:HD2	1:B:45:VAL:HG23	1.76	0.66
1:B:566:GLN:HE22	1:B:576:GLN:HA	1.59	0.66
1:B:759:LYS:HE2	6:B:2111:HOH:O	1.96	0.65
1:A:174:TRP:CE2	1:A:621:LYS:HG3	2.31	0.65
1:A:810:LYS:O	1:A:815:ARG:HD3	1.96	0.65
1:B:509:GLU:O	1:B:512:VAL:HG22	1.96	0.65
1:A:355:ASP:OD2	1:A:398:ARG:HD3	1.95	0.65
1:A:662:LEU:C	1:A:662:LEU:HD23	2.22	0.65
1:B:174:TRP:CE2	1:B:621:LYS:HG3	2.31	0.65
1:A:66:ARG:CD	1:A:236:ASN:HA	2.27	0.65
1:B:678:ASN:ND2	1:B:679:MET:H	1.93	0.65
1:B:66:ARG:CD	1:B:236:ASN:HA	2.27	0.65
1:A:662:LEU:HD21	1:A:689:ILE:HG22	1.77	0.64
1:A:170:ILE:HG12	1:A:646:GLU:HG2	1.77	0.64
1:B:662:LEU:C	1:B:662:LEU:HD23	2.21	0.64
1:B:81:ARG:NH1	1:B:155:TYR:OH	2.31	0.64
1:B:61:ASP:O	1:B:64:VAL:HG22	1.98	0.63
1:A:450:HIS:HD2	6:A:2481:HOH:O	1.81	0.63
1:B:630:VAL:HG21	1:B:642:VAL:HG23	1.81	0.63
1:A:509:GLU:O	1:A:512:VAL:HG22	1.98	0.63
1:B:745:ILE:HG13	1:B:762:ILE:HD11	1.81	0.63
1:A:506:LYS:HD2	1:A:524:PHE:CE2	2.34	0.63
1:B:262:TYR:HD2	1:B:263:ILE:HD12	1.64	0.63
1:B:29:LYS:HE2	1:B:33:ARG:HH11	1.63	0.62
1:B:361:TRP:CZ3	1:B:409:LYS:HD3	2.34	0.62
1:A:170:ILE:O	1:A:171:ARG:HD2	1.99	0.62
1:B:455:VAL:H	1:B:459:HIS:HD2	1.46	0.62
1:A:262:TYR:HD2	1:A:263:ILE:HD12	1.65	0.62
1:B:506:LYS:HD2	1:B:524:PHE:CE2	2.35	0.62
1:A:793:ASN:C	1:A:793:ASN:HD22	2.06	0.62
1:A:29:LYS:HE2	1:A:33:ARG:HH11	1.63	0.61
1:A:745:ILE:HG13	1:A:762:ILE:HD11	1.81	0.61
1:B:571:HIS:H	1:B:576:GLN:NE2	1.98	0.61
1:A:361:TRP:CZ3	1:A:409:LYS:HD3	2.36	0.61
1:A:630:VAL:HG21	1:A:642:VAL:HG23	1.81	0.61
1:A:455:VAL:H	1:A:459:HIS:HD2	1.47	0.61
1:B:170:ILE:O	1:B:171:ARG:HD2	2.00	0.61
1:B:310:ARG:HD3	6:B:2366:HOH:O	2.02	0.60
1:B:469:LYS:O	1:B:473:GLU:HG3	2.01	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:633:ASP:O	1:B:636:VAL:HG22	2.01	0.60
1:B:450:HIS:HE1	6:B:2224:HOH:O	1.84	0.60
1:A:662:LEU:HD21	1:A:689:ILE:HG21	1.83	0.60
1:A:678:ASN:ND2	1:A:679:MET:H	1.97	0.60
1:B:450:HIS:HD2	6:B:2553:HOH:O	1.84	0.60
1:A:61:ASP:O	1:A:64:VAL:HG22	2.01	0.60
1:A:64:VAL:HG23	1:A:65:GLY:N	2.17	0.60
1:A:580:CYS:SG	1:A:622:LEU:HD13	2.42	0.60
1:A:633:ASP:O	1:A:636:VAL:HG22	2.02	0.60
1:A:34:HIS:HD2	1:A:38:THR:OG1	1.83	0.60
1:B:34:HIS:HD2	1:B:38:THR:OG1	1.85	0.60
1:B:793:ASN:C	1:B:793:ASN:HD22	2.08	0.60
1:A:571:HIS:H	1:A:576:GLN:NE2	1.99	0.60
1:A:274:ASN:ND2	1:A:277:ARG:HH21	2.00	0.60
1:A:152:LEU:HD22	1:A:827:VAL:CG1	2.32	0.59
1:A:205:LYS:HG3	6:A:2394:HOH:O	2.02	0.59
1:B:152:LEU:HD22	1:B:827:VAL:CG1	2.33	0.59
1:A:124:GLU:HG2	6:A:2701:HOH:O	2.02	0.59
1:B:727:GLU:HG3	1:B:729:LYS:HG2	1.84	0.59
1:B:662:LEU:HD21	1:B:689:ILE:HG21	1.83	0.59
1:B:133:ASN:ND2	1:B:569:ARG:HH22	1.95	0.59
1:A:81:ARG:NH1	1:A:155:TYR:OH	2.36	0.59
1:A:469:LYS:O	1:A:473:GLU:HG3	2.02	0.58
1:B:377:HIS:HD2	2:B:1861:NBG:O6	1.86	0.58
1:A:286:PHE:CD1	1:A:385:GLU:HG3	2.38	0.58
1:A:657:ILE:HB	1:A:658:PRO:HD3	1.85	0.58
1:B:657:ILE:HB	1:B:658:PRO:HD3	1.84	0.58
1:A:152:LEU:HD22	1:A:827:VAL:HG12	1.85	0.58
1:A:66:ARG:HD3	1:A:236:ASN:HA	1.84	0.58
1:A:629:VAL:HG11	1:A:750:PHE:HD1	1.67	0.58
1:A:133:ASN:ND2	1:A:569:ARG:HH22	1.98	0.57
1:A:304:LEU:HD12	1:A:348:GLU:CG	2.34	0.57
1:B:64:VAL:HG23	1:B:65:GLY:N	2.18	0.57
1:A:727:GLU:HG3	1:A:729:LYS:HG2	1.86	0.57
1:A:689:ILE:HG23	1:A:689:ILE:O	2.05	0.57
1:A:693:ASP:O	1:A:696:ASN:HB2	2.05	0.57
1:B:66:ARG:HD3	1:B:236:ASN:HA	1.86	0.57
1:A:34:HIS:HE1	1:A:61:ASP:OD2	1.87	0.57
1:B:93:ARG:HG2	1:B:126:GLU:HG2	1.87	0.56
1:B:286:PHE:CD1	1:B:385:GLU:HG3	2.40	0.56
1:A:170:ILE:C	1:A:171:ARG:HD2	2.31	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:LEU:HD22	1:B:827:VAL:HG12	1.87	0.56
1:B:274:ASN:ND2	1:B:277:ARG:HH21	2.02	0.56
1:A:790:LEU:HG	1:A:797:TRP:CD1	2.41	0.56
1:B:693:ASP:O	1:B:696:ASN:HB2	2.05	0.56
1:B:656:VAL:O	1:B:660:THR:HG23	2.06	0.56
1:B:629:VAL:HG11	1:B:750:PHE:HD1	1.67	0.56
1:B:235:ASN:CG	1:B:237:THR:HG23	2.31	0.56
1:A:235:ASN:CG	1:A:237:THR:HG23	2.31	0.56
1:B:26:GLU:O	1:B:29:LYS:HG2	2.06	0.56
1:A:93:ARG:HG2	1:A:126:GLU:HG2	1.88	0.56
1:A:169:LYS:HE2	1:A:178:GLU:OE2	2.06	0.55
1:A:423:ASP:O	1:A:427:ARG:HB2	2.06	0.55
1:A:292:ARG:O	1:A:296:GLU:HG3	2.05	0.55
1:B:629:VAL:HG11	1:B:750:PHE:CE1	2.42	0.55
1:A:168:GLN:NE2	1:A:647:ASN:H	2.02	0.55
1:B:790:LEU:HG	1:B:797:TRP:CD1	2.41	0.55
1:B:292:ARG:O	1:B:296:GLU:HG3	2.06	0.55
1:B:160:ARG:HB2	1:B:243:LEU:HB3	1.89	0.55
1:B:423:ASP:O	1:B:427:ARG:HB2	2.05	0.55
1:A:29:LYS:HD3	6:A:2662:HOH:O	2.06	0.55
1:A:493:LEU:HD21	1:A:512:VAL:HG12	1.87	0.55
1:A:324:THR:HA	1:A:327:ASP:OD2	2.07	0.55
1:B:324:THR:HA	1:B:327:ASP:OD2	2.07	0.55
1:B:493:LEU:HD21	1:B:512:VAL:HG12	1.88	0.55
1:A:26:GLU:O	1:A:29:LYS:HG2	2.07	0.54
1:A:395:LEU:HB3	1:A:396:LEU:HD22	1.89	0.54
1:A:274:ASN:HD22	1:A:277:ARG:HE	1.54	0.54
1:A:629:VAL:HG11	1:A:750:PHE:CE1	2.42	0.54
1:A:630:VAL:HG21	1:A:642:VAL:CG2	2.38	0.54
1:B:169:LYS:HE2	1:B:178:GLU:OE2	2.08	0.54
1:B:630:VAL:HG21	1:B:642:VAL:CG2	2.37	0.54
1:B:34:HIS:HE1	1:B:61:ASP:OD2	1.90	0.54
1:B:184:ARG:NH2	6:B:2327:HOH:O	2.39	0.54
1:B:571:HIS:H	1:B:576:GLN:HE22	1.56	0.54
1:B:649:ARG:HB2	6:B:2534:HOH:O	2.06	0.54
1:A:678:ASN:ND2	1:A:679:MET:N	2.55	0.54
1:B:395:LEU:HB3	1:B:396:LEU:HD22	1.89	0.54
1:A:415:VAL:HG13	1:A:425:LEU:HD21	1.90	0.54
1:B:170:ILE:C	1:B:171:ARG:HD2	2.32	0.54
1:A:237:THR:HB	6:A:2677:HOH:O	2.07	0.54
1:B:211:THR:HB	6:B:2598:HOH:O	2.06	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:304:LEU:HD12	1:B:348:GLU:CG	2.37	0.54
1:B:759:LYS:HE3	6:B:2657:HOH:O	2.08	0.54
1:A:377:HIS:HD2	2:A:861:NBG:O6	1.92	0.53
1:B:36:HIS:HD2	6:B:2279:HOH:O	1.92	0.53
1:B:274:ASN:HD22	1:B:277:ARG:HE	1.54	0.53
1:B:28:LYS:NZ	6:B:2595:HOH:O	2.42	0.53
1:B:689:ILE:O	1:B:689:ILE:HG23	2.09	0.53
1:B:435:GLY:O	1:B:436:SER:HB2	2.08	0.53
1:B:558:ASN:HB3	1:B:561:SER:HB3	1.90	0.53
1:B:571:HIS:HB2	6:B:2260:HOH:O	2.06	0.53
1:A:554:LYS:HE2	1:A:554:LYS:O	2.09	0.53
1:B:554:LYS:HE2	1:B:554:LYS:O	2.09	0.53
1:B:790:LEU:HG	1:B:797:TRP:HD1	1.74	0.53
1:B:573:TYR:HE1	1:B:672:GLU:HG2	1.74	0.53
1:A:571:HIS:H	1:A:576:GLN:HE22	1.56	0.53
1:B:527:ASP:O	1:B:531:LEU:HD23	2.08	0.53
1:B:380:LEU:H	1:B:380:LEU:HD22	1.73	0.53
1:A:435:GLY:O	1:A:436:SER:HB2	2.08	0.52
1:B:415:VAL:HG13	1:B:425:LEU:HD21	1.90	0.52
1:B:521:LEU:HB3	1:B:802:LEU:HD11	1.91	0.52
1:B:216:ILE:HA	6:B:2337:HOH:O	2.09	0.52
1:B:309:ARG:NH1	6:B:2239:HOH:O	2.42	0.52
1:A:492:LEU:CD1	1:A:493:LEU:HD23	2.40	0.52
1:A:573:TYR:HE1	1:A:672:GLU:HG2	1.73	0.52
1:B:678:ASN:ND2	1:B:679:MET:N	2.53	0.52
1:A:558:ASN:HB3	1:A:561:SER:HB3	1.91	0.52
1:A:777:TYR:O	1:A:781:VAL:HG23	2.09	0.52
1:B:661:ASP:HB3	1:B:797:TRP:CH2	2.44	0.52
1:A:656:VAL:O	1:A:660:THR:HG23	2.10	0.52
1:B:162:GLU:HG3	6:B:2126:HOH:O	2.08	0.52
1:A:29:LYS:HG3	1:A:33:ARG:NH1	2.25	0.52
1:A:72:GLN:HE21	1:A:76:ASP:CG	2.18	0.52
1:A:304:LEU:HD12	1:A:348:GLU:HG3	1.92	0.52
1:B:605:ILE:O	1:B:644:PHE:HA	2.10	0.52
1:A:136:LEU:HD23	1:A:136:LEU:C	2.35	0.51
1:A:420:LYS:N	1:A:420:LYS:HD2	2.25	0.51
1:A:790:LEU:HG	1:A:797:TRP:HD1	1.74	0.51
1:B:605:ILE:HG21	1:B:623:ILE:HD13	1.91	0.51
1:A:160:ARG:HB2	1:A:243:LEU:HB3	1.91	0.51
1:B:133:ASN:ND2	1:B:569:ARG:NH2	2.41	0.51
1:B:777:TYR:O	1:B:781:VAL:HG23	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:678:ASN:HD22	1:A:678:ASN:N	2.08	0.51
1:A:687:LEU:HD12	1:A:797:TRP:CE2	2.46	0.51
1:B:380:LEU:HB3	1:B:382:GLU:OE1	2.10	0.51
1:B:168:GLN:NE2	1:B:647:ASN:H	2.03	0.51
1:B:29:LYS:HG3	1:B:33:ARG:NH1	2.26	0.51
1:B:492:LEU:CD1	1:B:493:LEU:HD23	2.40	0.51
1:A:521:LEU:HB3	1:A:802:LEU:HD11	1.92	0.51
1:A:527:ASP:O	1:A:531:LEU:HD23	2.11	0.51
1:A:24:VAL:O	1:A:28:LYS:HG3	2.11	0.51
1:B:72:GLN:HE21	1:B:76:ASP:CG	2.19	0.50
1:A:419:PRO:HB2	1:A:420:LYS:HD2	1.93	0.50
1:A:543:LEU:O	1:A:547:GLN:HG3	2.11	0.50
1:B:106:ASN:HB3	6:B:2323:HOH:O	2.11	0.50
1:B:420:LYS:HD2	1:B:420:LYS:N	2.27	0.50
1:A:380:LEU:HD22	1:A:380:LEU:H	1.76	0.50
1:A:661:ASP:HB3	1:A:797:TRP:CH2	2.47	0.50
1:B:419:PRO:HB2	1:B:420:LYS:HD2	1.92	0.50
1:A:109:ASP:OD1	1:A:119:ILE:HD13	2.12	0.50
1:A:210:ASN:N	1:A:210:ASN:ND2	2.54	0.50
1:A:433:GLU:HB3	1:A:437:LYS:HD2	1.93	0.50
1:A:789:GLN:HE21	1:A:789:GLN:CA	2.04	0.50
1:B:380:LEU:HD22	1:B:380:LEU:N	2.27	0.50
1:A:296:GLU:OE2	1:A:385:GLU:OE1	2.29	0.49
1:B:678:ASN:HD22	1:B:678:ASN:N	2.09	0.49
1:A:488:PRO:O	1:A:492:LEU:HB3	2.11	0.49
1:A:661:ASP:O	1:A:797:TRP:HH2	1.95	0.49
1:A:678:ASN:ND2	1:A:679:MET:HG3	2.27	0.49
1:A:763:ASN:HB2	6:A:2649:HOH:O	2.11	0.49
1:B:284:ASN:ND2	6:B:2008:HOH:O	2.44	0.49
1:A:431:ILE:N	1:A:431:ILE:HD12	2.27	0.49
1:A:793:ASN:C	1:A:793:ASN:ND2	2.70	0.49
1:B:433:GLU:HB3	1:B:437:LYS:HD2	1.94	0.49
1:B:543:LEU:O	1:B:547:GLN:HG3	2.13	0.49
1:A:566:GLN:NE2	1:A:576:GLN:HA	2.26	0.49
1:A:626:VAL:O	1:A:630:VAL:HG13	2.13	0.49
1:B:687:LEU:HD12	1:B:797:TRP:CE2	2.48	0.49
1:A:133:ASN:ND2	1:A:281:PRO:HA	2.13	0.49
1:B:346:ILE:HD13	1:B:448:GLY:HA3	1.94	0.49
1:B:488:PRO:O	1:B:492:LEU:HB3	2.12	0.49
1:B:67:TRP:HA	1:B:238:VAL:HB	1.95	0.49
1:A:64:VAL:HG23	1:A:65:GLY:H	1.76	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:VAL:HG21	1:B:37:PHE:CD1	2.47	0.49
1:A:23:ASN:HD21	1:A:26:GLU:HG2	1.77	0.49
1:A:380:LEU:HB3	1:A:382:GLU:OE1	2.12	0.49
1:A:579:ASN:C	1:A:579:ASN:HD22	2.20	0.49
1:A:605:ILE:HG21	1:A:623:ILE:HD13	1.93	0.49
1:B:304:LEU:HD12	1:B:348:GLU:HG3	1.95	0.49
1:B:399:HIS:HD2	6:B:2009:HOH:O	1.96	0.49
1:B:136:LEU:C	1:B:136:LEU:HD23	2.38	0.48
1:B:275:ILE:O	1:B:295:GLN:HG2	2.13	0.48
1:B:431:ILE:N	1:B:431:ILE:HD12	2.28	0.48
1:A:235:ASN:O	1:A:236:ASN:HB2	2.12	0.48
1:A:67:TRP:HA	1:A:238:VAL:HB	1.96	0.48
1:A:630:VAL:O	1:A:636:VAL:HG21	2.13	0.48
1:B:571:HIS:CD2	6:B:2260:HOH:O	2.65	0.48
1:B:23:ASN:HD21	1:B:26:GLU:HG2	1.78	0.48
1:A:29:LYS:HE2	1:A:33:ARG:HH12	1.74	0.48
1:B:483:THR:O	1:B:815:ARG:NH2	2.41	0.48
1:B:579:ASN:C	1:B:579:ASN:HD22	2.19	0.48
1:B:630:VAL:O	1:B:636:VAL:HG21	2.13	0.48
1:B:767:TYR:HB2	1:B:768:HIS:CE1	2.49	0.48
1:A:22:GLU:HG3	6:A:2290:HOH:O	2.13	0.48
1:A:504:ALA:HB1	6:A:2617:HOH:O	2.14	0.48
1:B:24:VAL:O	1:B:28:LYS:HG3	2.14	0.48
1:B:109:ASP:OD1	1:B:119:ILE:HD13	2.14	0.48
1:A:566:GLN:HA	6:A:2231:HOH:O	2.12	0.48
1:A:91:MET:HB2	1:A:129:ALA:HB3	1.95	0.48
1:A:380:LEU:HD22	1:A:380:LEU:N	2.29	0.48
1:A:767:TYR:HB2	1:A:768:HIS:CE1	2.49	0.48
1:B:286:PHE:CE1	1:B:385:GLU:HG3	2.49	0.48
1:A:286:PHE:CE1	1:A:385:GLU:HG3	2.49	0.47
1:B:455:VAL:HG23	1:B:674:SER:HB2	1.95	0.47
1:A:450:HIS:HE1	6:A:2171:HOH:O	1.96	0.47
1:A:709:PHE:HB3	1:A:783:CYS:SG	2.54	0.47
1:B:64:VAL:HG23	1:B:65:GLY:H	1.78	0.47
1:B:235:ASN:O	1:B:236:ASN:HB2	2.13	0.47
1:B:661:ASP:O	1:B:797:TRP:HH2	1.96	0.47
1:B:678:ASN:ND2	1:B:679:MET:HG3	2.29	0.47
1:A:389:VAL:HG11	1:A:404:TYR:OH	2.15	0.47
1:B:171:ARG:HG2	1:B:171:ARG:HH11	1.79	0.47
1:B:216:ILE:HB	6:B:2373:HOH:O	2.15	0.47
1:B:626:VAL:O	1:B:630:VAL:HG13	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:754:GLN:NE2	1:A:757:LEU:HD13	2.30	0.47
1:B:197:MET:HE2	1:B:224:LEU:HD13	1.96	0.47
1:A:174:TRP:CD2	1:A:621:LYS:HG3	2.50	0.47
1:A:605:ILE:O	1:A:644:PHE:HA	2.14	0.47
1:A:662:LEU:C	1:A:662:LEU:CD2	2.88	0.47
1:B:66:ARG:HD2	1:B:236:ASN:HA	1.97	0.47
1:B:424:ARG:HD2	1:B:428:MET:SD	2.54	0.47
1:B:754:GLN:NE2	1:B:757:LEU:HD13	2.30	0.47
1:A:561:SER:HB2	1:A:601:ARG:HA	1.96	0.47
1:A:197:MET:HE2	1:A:224:LEU:HD13	1.96	0.47
1:A:628:ASP:O	1:A:632:ASN:ND2	2.48	0.47
1:B:389:VAL:HG11	1:B:404:TYR:OH	2.15	0.47
1:B:455:VAL:H	1:B:459:HIS:CD2	2.31	0.47
1:A:764:MET:C	1:A:764:MET:SD	2.99	0.46
1:B:517:GLN:OE1	1:B:520:LYS:HE3	2.15	0.46
1:A:630:VAL:HG23	1:A:631:ASN:N	2.30	0.46
1:B:235:ASN:ND2	1:B:237:THR:H	2.13	0.46
1:B:241:MET:HE3	1:B:243:LEU:HD22	1.97	0.46
1:A:791:TYR:HA	1:A:797:TRP:CD1	2.51	0.46
1:B:507:ILE:HG13	6:B:2377:HOH:O	2.14	0.46
1:B:697:VAL:O	1:B:701:GLU:HG3	2.15	0.46
1:A:83:TYR:HE1	1:A:310:ARG:HH21	1.62	0.46
1:B:91:MET:HB2	1:B:129:ALA:HB3	1.96	0.46
1:B:561:SER:HB2	1:B:601:ARG:HA	1.96	0.46
1:A:569:ARG:O	1:A:574:LYS:HD2	2.16	0.46
1:A:785:ASP:O	1:A:789:GLN:HG2	2.16	0.46
1:B:110:GLU:HB2	6:B:2222:HOH:O	2.14	0.46
1:A:697:VAL:O	1:A:701:GLU:HG3	2.16	0.46
1:A:37:PHE:CD1	1:B:64:VAL:HG21	2.51	0.46
1:A:746:ASP:OD2	1:A:762:ILE:HG21	2.16	0.46
1:B:791:TYR:HA	1:B:797:TRP:CD1	2.51	0.46
1:B:566:GLN:NE2	1:B:576:GLN:HA	2.28	0.45
1:A:424:ARG:HD2	1:A:428:MET:SD	2.56	0.45
1:B:422:VAL:HG23	1:B:423:ASP:N	2.31	0.45
1:A:483:THR:O	1:A:815:ARG:NH2	2.46	0.45
1:B:527:ASP:O	1:B:531:LEU:CD2	2.65	0.45
1:B:630:VAL:HG23	1:B:631:ASN:N	2.30	0.45
1:B:662:LEU:C	1:B:662:LEU:CD2	2.87	0.45
1:A:193:ARG:HB2	1:A:225:PRO:HG2	1.99	0.45
1:A:336:GLN:OE1	1:A:373:ALA:HB3	2.16	0.45
1:A:492:LEU:HD13	1:A:500:ALA:HB2	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:HIS:HD2	6:A:2119:HOH:O	2.00	0.45
1:A:536:LYS:O	1:A:540:GLU:HG3	2.17	0.45
1:B:296:GLU:OE2	1:B:385:GLU:OE1	2.35	0.45
1:B:569:ARG:O	1:B:574:LYS:HD2	2.16	0.45
1:B:709:PHE:HB3	1:B:783:CYS:SG	2.57	0.45
1:A:133:ASN:ND2	1:A:569:ARG:NH2	2.45	0.45
1:A:235:ASN:ND2	1:A:237:THR:H	2.15	0.45
1:A:435:GLY:O	1:A:436:SER:CB	2.64	0.45
1:B:174:TRP:CD2	1:B:621:LYS:HG3	2.52	0.45
1:B:210:ASN:N	1:B:210:ASN:ND2	2.52	0.45
1:B:764:MET:CE	1:B:765:LEU:HD13	2.46	0.45
1:B:402:ILE:O	1:B:406:ILE:HG13	2.17	0.45
1:B:827:VAL:CG1	1:B:828:GLU:N	2.79	0.45
1:A:133:ASN:HD21	1:A:281:PRO:CA	2.16	0.44
1:A:422:VAL:HG23	1:A:423:ASP:N	2.31	0.44
1:A:455:VAL:HG23	1:A:674:SER:HB2	1.99	0.44
1:A:645:LEU:HD22	1:A:652:LEU:HD11	2.00	0.44
1:B:628:ASP:O	1:B:632:ASN:ND2	2.51	0.44
1:A:196:PHE:HD1	1:A:309:ARG:HH11	1.66	0.44
1:A:636:VAL:HG23	1:A:637:GLY:N	2.32	0.44
1:B:330:PRO:HB3	1:B:370:LYS:HB3	1.99	0.44
1:B:396:LEU:HB3	1:B:399:HIS:CD2	2.53	0.44
1:B:678:ASN:ND2	1:B:678:ASN:N	2.66	0.44
1:A:402:ILE:O	1:A:406:ILE:HG13	2.18	0.44
1:B:143:PHE:CG	1:B:817:ILE:HD11	2.53	0.44
1:B:336:GLN:OE1	1:B:373:ALA:HB3	2.17	0.44
1:B:690:GLY:O	1:B:710:ILE:HA	2.18	0.44
1:A:143:PHE:CG	1:A:817:ILE:HD11	2.52	0.44
1:B:112:ILE:HG23	1:B:117:LEU:HB2	1.99	0.44
1:B:793:ASN:C	1:B:793:ASN:ND2	2.72	0.44
1:A:275:ILE:O	1:A:295:GLN:HG2	2.17	0.44
1:B:668:THR:O	1:B:669:ALA:C	2.61	0.44
1:A:325:VAL:HG23	1:A:326:PHE:CD1	2.52	0.44
1:A:678:ASN:ND2	1:A:678:ASN:N	2.66	0.44
1:A:713:MET:HB3	1:A:717:ASP:HB2	2.00	0.44
1:B:43:ARG:NH2	1:B:115:LEU:HB3	2.32	0.44
1:B:569:ARG:HD2	1:B:608:LYS:O	2.17	0.44
1:A:112:ILE:HG23	1:A:117:LEU:HB2	1.99	0.44
1:B:43:ARG:HD2	1:B:51:TYR:HH	1.83	0.44
1:A:171:ARG:HG2	1:A:171:ARG:HH11	1.83	0.43
1:A:274:ASN:ND2	1:A:277:ARG:HE	2.15	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:LEU:HB3	1:A:399:HIS:CD2	2.53	0.43
1:B:196:PHE:HD1	1:B:309:ARG:HH11	1.66	0.43
1:B:510:ASP:HB2	6:B:2665:HOH:O	2.17	0.43
1:A:735:LEU:HA	1:A:736:PRO:HD2	1.87	0.43
1:B:143:PHE:O	1:B:147:MET:HG3	2.18	0.43
1:B:235:ASN:C	1:B:235:ASN:HD22	2.26	0.43
1:B:435:GLY:O	1:B:436:SER:CB	2.66	0.43
1:A:23:ASN:HD21	1:A:26:GLU:CG	2.31	0.43
1:A:827:VAL:CG1	1:A:828:GLU:N	2.81	0.43
1:B:492:LEU:HD13	1:B:500:ALA:HB2	1.99	0.43
1:B:565:VAL:HG11	1:B:660:THR:HG22	1.99	0.43
1:B:764:MET:SD	1:B:764:MET:C	3.02	0.43
1:A:455:VAL:H	1:A:459:HIS:CD2	2.32	0.43
1:A:527:ASP:O	1:A:531:LEU:CD2	2.66	0.43
1:A:568:LYS:O	1:A:607:GLY:HA3	2.17	0.43
1:B:492:LEU:HD12	1:B:493:LEU:HD23	2.00	0.43
1:A:43:ARG:NH2	1:A:115:LEU:HB3	2.34	0.43
1:B:29:LYS:HE2	1:B:33:ARG:HH12	1.77	0.43
1:B:83:TYR:HE1	1:B:310:ARG:HH21	1.64	0.43
1:B:380:LEU:HB3	1:B:382:GLU:CD	2.44	0.43
1:B:746:ASP:OD2	1:B:762:ILE:HG21	2.18	0.43
1:A:36:HIS:HD2	6:A:2604:HOH:O	2.00	0.43
1:A:74:TYR:CZ	1:A:153:ALA:HA	2.53	0.43
1:A:668:THR:O	1:A:669:ALA:C	2.62	0.43
1:B:235:ASN:ND2	1:B:237:THR:HG23	2.34	0.43
1:B:662:LEU:CD2	1:B:689:ILE:HG22	2.47	0.43
1:A:346:ILE:HD13	1:A:448:GLY:HA3	2.00	0.43
1:A:510:ASP:HB2	6:A:2379:HOH:O	2.19	0.43
1:B:274:ASN:ND2	1:B:277:ARG:HE	2.14	0.43
1:B:713:MET:HB3	1:B:717:ASP:HB2	2.00	0.43
1:A:598:PHE:HE1	6:A:2544:HOH:O	2.00	0.43
1:B:235:ASN:ND2	1:B:235:ASN:C	2.77	0.43
1:A:577:LEU:HB2	6:A:2145:HOH:O	2.19	0.43
1:A:386:ARG:HA	1:A:439:ILE:O	2.19	0.42
1:B:163:TYR:HB2	1:B:278:VAL:HG13	2.01	0.42
1:B:568:LYS:O	1:B:607:GLY:HA3	2.19	0.42
1:A:102:LEU:O	1:A:104:LEU:HD13	2.19	0.42
1:B:636:VAL:HG23	1:B:637:GLY:N	2.33	0.42
1:B:726:TYR:OH	1:B:774:PHE:HB2	2.19	0.42
1:A:492:LEU:HD12	1:A:493:LEU:HD23	2.01	0.42
1:A:569:ARG:HD2	1:A:608:LYS:O	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:536:LYS:O	1:B:540:GLU:HG3	2.19	0.42
1:A:241:MET:HE3	1:A:243:LEU:HD22	2.02	0.42
1:A:731:TYR:HB3	1:A:735:LEU:HD12	2.00	0.42
1:B:74:TYR:CZ	1:B:153:ALA:HA	2.54	0.42
1:B:698:GLU:O	1:B:702:GLU:HG2	2.19	0.42
1:B:494:LEU:HD13	1:B:494:LEU:C	2.44	0.42
1:B:735:LEU:HA	1:B:736:PRO:HD2	1.87	0.42
1:A:163:TYR:HB2	1:A:278:VAL:HG13	2.00	0.42
1:B:43:ARG:HD2	1:B:51:TYR:OH	2.20	0.42
1:B:626:VAL:O	1:B:629:VAL:HG13	2.19	0.42
1:B:672:GLU:O	1:B:673:ALA:C	2.62	0.42
1:B:731:TYR:HB3	1:B:735:LEU:HD12	2.02	0.42
1:B:790:LEU:C	1:B:797:TRP:HD1	2.27	0.42
1:B:630:VAL:CG2	1:B:631:ASN:N	2.83	0.42
1:B:100:ILE:HD12	1:B:494:LEU:HD23	2.02	0.42
1:B:619:ILE:O	1:B:623:ILE:HG13	2.20	0.42
1:B:754:GLN:N	1:B:755:PRO:HD3	2.33	0.42
1:A:690:GLY:O	1:A:710:ILE:HA	2.19	0.42
1:B:133:ASN:HD21	1:B:281:PRO:CA	2.16	0.42
1:B:182:TRP:H	1:B:182:TRP:CD1	2.37	0.42
1:A:456:ALA:C	1:A:481:ASN:ND2	2.78	0.41
1:A:494:LEU:C	1:A:494:LEU:HD13	2.45	0.41
1:B:300:VAL:HG13	1:B:345:ALA:HA	2.02	0.41
1:B:415:VAL:HG23	1:B:416:ALA:N	2.35	0.41
1:A:100:ILE:HD12	1:A:494:LEU:CD2	2.50	0.41
1:A:428:MET:HE1	1:A:474:LEU:HD12	2.01	0.41
1:B:379:VAL:HG21	1:B:670:GLY:O	2.20	0.41
1:B:407:ASN:ND2	1:B:431:ILE:HD13	2.35	0.41
1:A:225:PRO:HD3	1:A:244:TRP:CZ3	2.56	0.41
1:B:225:PRO:HD3	1:B:244:TRP:CZ3	2.55	0.41
1:B:720:ALA:O	1:B:723:LYS:HB3	2.21	0.41
1:A:754:GLN:N	1:A:755:PRO:HD3	2.35	0.41
1:A:206:VAL:HG23	1:A:397:PRO:HB2	2.02	0.41
1:A:235:ASN:ND2	1:A:237:THR:HG23	2.36	0.41
1:A:378:THR:HA	6:A:2334:HOH:O	2.19	0.41
1:A:517:GLN:OE1	1:A:520:LYS:HE3	2.21	0.41
1:A:574:LYS:NZ	1:A:672:GLU:OE2	2.53	0.41
1:B:304:LEU:O	1:B:308:ILE:HG12	2.20	0.41
1:B:574:LYS:NZ	1:B:672:GLU:OE2	2.53	0.41
1:B:712:GLY:HA2	6:B:2606:HOH:O	2.20	0.41
1:A:565:VAL:HG11	1:A:660:THR:HG22	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:THR:HB	6:B:2143:HOH:O	2.19	0.41
1:B:339:ASP:O	1:B:342:PRO:HD2	2.21	0.41
1:B:395:LEU:O	1:B:396:LEU:HD13	2.21	0.41
1:B:396:LEU:HD22	1:B:396:LEU:N	2.36	0.41
1:B:456:ALA:C	1:B:481:ASN:ND2	2.79	0.41
1:B:492:LEU:HD13	1:B:492:LEU:C	2.46	0.41
1:A:395:LEU:O	1:A:396:LEU:HD13	2.21	0.41
1:A:415:VAL:HG23	1:A:416:ALA:N	2.34	0.41
1:B:174:TRP:CZ2	1:B:621:LYS:HG3	2.56	0.41
1:B:325:VAL:HG23	1:B:326:PHE:CD1	2.56	0.41
1:B:386:ARG:HA	1:B:439:ILE:O	2.20	0.41
1:B:542:LYS:NZ	6:B:2703:HOH:O	2.53	0.41
1:A:36:HIS:O	1:A:40:VAL:HA	2.21	0.41
1:A:235:ASN:ND2	1:A:235:ASN:C	2.79	0.41
1:A:407:ASN:ND2	1:A:431:ILE:HD13	2.36	0.41
1:A:630:VAL:CG2	1:A:631:ASN:N	2.83	0.41
1:B:42:ASP:HB2	6:B:2717:HOH:O	2.21	0.41
1:B:193:ARG:HB2	1:B:225:PRO:HG2	2.02	0.41
1:B:545:PHE:O	1:B:548:PHE:HB3	2.20	0.41
1:B:785:ASP:O	1:B:789:GLN:HG2	2.20	0.41
1:A:66:ARG:HD2	1:A:236:ASN:HA	2.00	0.41
1:A:355:ASP:HA	6:A:2399:HOH:O	2.19	0.41
1:A:556:LYS:C	1:A:556:LYS:HD3	2.46	0.41
1:A:626:VAL:O	1:A:629:VAL:HG13	2.21	0.41
1:B:100:ILE:HD12	1:B:494:LEU:CD2	2.50	0.41
1:B:410:HIS:O	1:B:414:ILE:HD13	2.21	0.41
1:B:615:MET:O	1:B:619:ILE:HG13	2.21	0.41
1:A:423:ASP:OD2	1:A:426:ARG:NE	2.47	0.40
1:A:790:LEU:C	1:A:797:TRP:HD1	2.28	0.40
1:B:197:MET:HE3	1:B:197:MET:HB2	1.95	0.40
1:A:330:PRO:HB3	1:A:370:LYS:HB3	2.03	0.40
1:A:380:LEU:HB3	1:A:382:GLU:CD	2.46	0.40
1:A:415:VAL:CG1	1:A:425:LEU:HD11	2.48	0.40
1:B:214:LYS:HA	6:B:2706:HOH:O	2.21	0.40
1:A:197:MET:HE3	1:A:197:MET:HB2	1.93	0.40
1:B:36:HIS:O	1:B:40:VAL:HA	2.22	0.40
1:B:415:VAL:CG1	1:B:425:LEU:HD11	2.48	0.40
1:A:109:ASP:CB	6:A:2581:HOH:O	2.57	0.40
1:A:161:TYR:HA	1:A:276:SER:O	2.22	0.40
1:B:280:TYR:OH	1:B:291:LEU:HB3	2.22	0.40
1:B:458:ILE:HG23	1:B:459:HIS:N	2.36	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:687:LEU:HD23	1:B:687:LEU:HA	1.92	0.40

All (2) 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:A:505:GLU:OE1	1:B:312:LYS:NZ[2_555]	2.03	0.17
1:A:210:ASN:OD1	6:B:2026:HOH:O[2_665]	2.16	0.04

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	779/847 (92%)	737 (95%)	39 (5%)	3 (0%)	30	34
1	B	779/847 (92%)	733 (94%)	44 (6%)	2 (0%)	36	42
All	All	1558/1694 (92%)	1470 (94%)	83 (5%)	5 (0%)	36	42

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	436	SER
1	B	436	SER
1	A	435	GLY
1	B	435	GLY
1	A	342	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	688/740 (93%)	648 (94%)	40 (6%)	18	22
1	B	688/740 (93%)	649 (94%)	39 (6%)	18	23
All	All	1376/1480 (93%)	1297 (94%)	79 (6%)	18	23

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	ARG
1	A	95	LEU
1	A	102	LEU
1	A	128	ASP
1	A	210	ASN
1	A	235	ASN
1	A	237	THR
1	A	243	LEU
1	A	247	ARG
1	A	264	GLN
1	A	278	VAL
1	A	300	VAL
1	A	325	VAL
1	A	361	TRP
1	A	379	VAL
1	A	398	ARG
1	A	433	GLU
1	A	494	LEU
1	A	499	LEU
1	A	502	LEU
1	A	532	ARG
1	A	539	GLN
1	A	554	LYS
1	A	565	VAL
1	A	568	LYS
1	A	576	GLN
1	A	577	LEU
1	A	622	LEU
1	A	629	VAL
1	A	645	LEU
1	A	652	LEU
1	A	678	ASN
1	A	683	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	708	LEU
1	A	730	GLU
1	A	733	GLU
1	A	765	LEU
1	A	789	GLN
1	A	797	TRP
1	A	815	ARG
1	B	43	ARG
1	B	95	LEU
1	B	102	LEU
1	B	128	ASP
1	B	210	ASN
1	B	235	ASN
1	B	237	THR
1	B	243	LEU
1	B	247	ARG
1	B	264	GLN
1	B	278	VAL
1	B	325	VAL
1	B	361	TRP
1	B	379	VAL
1	B	398	ARG
1	B	433	GLU
1	B	494	LEU
1	B	499	LEU
1	B	502	LEU
1	B	532	ARG
1	B	539	GLN
1	B	554	LYS
1	B	565	VAL
1	B	568	LYS
1	B	576	GLN
1	B	577	LEU
1	B	622	LEU
1	B	629	VAL
1	B	645	LEU
1	B	652	LEU
1	B	678	ASN
1	B	683	LEU
1	B	708	LEU
1	B	730	GLU
1	B	733	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	765	LEU
1	B	789	GLN
1	B	797	TRP
1	B	815	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	HIS
1	A	36	HIS
1	A	72	GLN
1	A	133	ASN
1	A	167	ASN
1	A	168	GLN
1	A	210	ASN
1	A	235	ASN
1	A	239	ASN
1	A	264	GLN
1	A	274	ASN
1	A	284	ASN
1	A	369	GLN
1	A	377	HIS
1	A	399	HIS
1	A	450	HIS
1	A	459	HIS
1	A	481	ASN
1	A	484	ASN
1	A	541	ASN
1	A	547	GLN
1	A	566	GLN
1	A	576	GLN
1	A	579	ASN
1	A	678	ASN
1	A	754	GLN
1	A	789	GLN
1	A	793	ASN
1	A	822	GLN
1	A	823	ASN
1	A	826	ASN
1	B	34	HIS
1	B	36	HIS
1	B	72	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	133	ASN
1	B	167	ASN
1	B	168	GLN
1	B	210	ASN
1	B	219	GLN
1	B	235	ASN
1	B	239	ASN
1	B	264	GLN
1	B	274	ASN
1	B	284	ASN
1	B	369	GLN
1	B	377	HIS
1	B	399	HIS
1	B	450	HIS
1	B	459	HIS
1	B	481	ASN
1	B	484	ASN
1	B	541	ASN
1	B	547	GLN
1	B	566	GLN
1	B	576	GLN
1	B	579	ASN
1	B	632	ASN
1	B	678	ASN
1	B	754	GLN
1	B	789	GLN
1	B	793	ASN
1	B	822	GLN
1	B	823	ASN
1	B	826	ASN

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 [i](#)

There are no oligosaccharides 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	MPD	B	1902	-	7,7,7	0.74	0	9,10,10	0.71	0
2	NBG	B	1861	-	15,15,15	1.54	3 (20%)	21,21,21	1.23	2 (9%)
4	PLP	A	860	1	15,15,16	1.61	2 (13%)	21,22,23	1.28	3 (14%)
3	CP4	A	862	-	37,37,37	2.03	14 (37%)	50,50,50	2.00	12 (24%)
4	PLP	B	1860	1	15,15,16	1.99	2 (13%)	21,22,23	1.39	2 (9%)
2	NBG	A	861	-	15,15,15	1.48	3 (20%)	21,21,21	1.08	1 (4%)

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	MPD	B	1902	-	1/1/2/2	2/5/5/5	-
2	NBG	B	1861	-	-	0/6/26/26	0/1/1/1
4	PLP	A	860	1	-	1/6/6/8	0/1/1/1
3	CP4	A	862	-	-	2/21/21/21	0/4/4/4
4	PLP	B	1860	1	-	0/6/6/8	0/1/1/1
2	NBG	A	861	-	-	0/6/26/26	0/1/1/1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1860	PLP	C4A-C4	-6.16	1.39	1.51
3	A	862	CP4	C6-N4	-4.65	1.31	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	860	PLP	C4A-C4	-4.41	1.42	1.51
3	A	862	CP4	C23-N25	-4.21	1.32	1.38
2	A	861	NBG	C2-C1	4.01	1.57	1.53
3	A	862	CP4	C8-C5	3.30	1.44	1.38
3	A	862	CP4	C31-C32	3.27	1.44	1.38
2	B	1861	NBG	C1-N1	3.21	1.47	1.43
3	A	862	CP4	C30-C32	3.15	1.43	1.38
2	B	1861	NBG	C2-C1	3.15	1.56	1.53
3	A	862	CP4	C3-C7	3.11	1.43	1.38
3	A	862	CP4	C8-C7	3.06	1.43	1.38
3	A	862	CP4	C31-C29	2.99	1.43	1.38
3	A	862	CP4	C9-N11	2.51	1.37	1.33
3	A	862	CP4	C0-C2	2.36	1.51	1.44
3	A	862	CP4	C28-C26	2.34	1.51	1.44
2	A	861	NBG	C3-C2	2.31	1.58	1.52
4	B	1860	PLP	C5A-C5	2.26	1.56	1.50
2	A	861	NBG	C1-N1	2.19	1.46	1.43
3	A	862	CP4	C1-N4	-2.16	1.34	1.38
2	B	1861	NBG	C3-C2	2.14	1.57	1.52
3	A	862	CP4	C29-C27	2.12	1.43	1.39
3	A	862	CP4	C5-C1	2.10	1.43	1.39
4	A	860	PLP	P-O3P	-2.04	1.47	1.54

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	862	CP4	C3-C0-C1	5.15	122.31	119.13
3	A	862	CP4	C1-C0-C2	-5.10	102.62	106.80
3	A	862	CP4	C27-C28-C26	-4.80	102.87	106.80
3	A	862	CP4	C30-C28-C27	4.66	122.01	119.13
3	A	862	CP4	O24-C22-C23	-3.80	116.20	121.09
2	A	861	NBG	C5-O5-C1	3.63	117.52	112.47
3	A	862	CP4	C23-C22-N21	3.63	121.79	116.80
3	A	862	CP4	O12-C9-C6	-3.63	116.42	121.09
2	B	1861	NBG	C5-O5-C1	3.53	117.38	112.47
3	A	862	CP4	C6-C9-N11	3.10	121.07	116.80
4	B	1860	PLP	O4P-C5A-C5	-3.00	103.74	109.36
3	A	862	CP4	C1-N4-C6	2.97	112.20	109.01
3	A	862	CP4	C27-N25-C23	2.71	111.92	109.01
4	A	860	PLP	O2P-P-O4P	-2.48	100.19	106.67
3	A	862	CP4	C28-C30-C32	-2.46	117.44	120.40
3	A	862	CP4	C0-C3-C7	-2.44	117.47	120.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	860	PLP	O3P-P-O2P	2.39	116.75	107.80
4	A	860	PLP	O4P-C5A-C5	-2.31	105.02	109.36
2	B	1861	NBG	C3-C2-C1	2.24	113.15	109.86
4	B	1860	PLP	O3P-P-O4P	-2.12	101.14	106.67

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	B	1902	MPD	C4

All (5) torsion outliers are listed below:

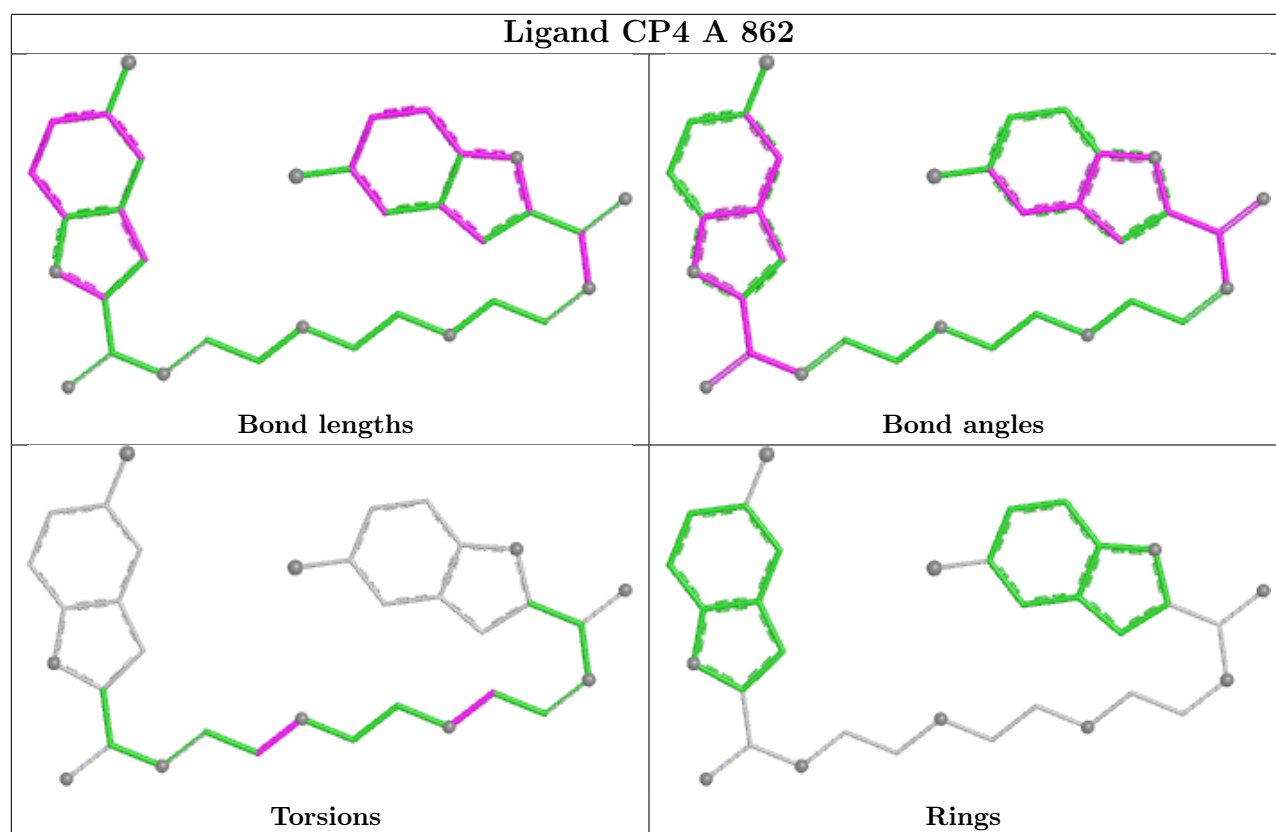
Mol	Chain	Res	Type	Atoms
5	B	1902	MPD	C2-C3-C4-O4
5	B	1902	MPD	C2-C3-C4-C5
4	A	860	PLP	C4-C5-C5A-O4P
3	A	862	CP4	C20-C19-O18-C17
3	A	862	CP4	C13-C14-O15-C16

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1861	NBG	1	0
2	A	861	NBG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.