



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:21 am GMT

PDB ID : 3CEJ
Title : Human glycogen phosphorylase (tense state) in complex with the allosteric inhibitor AVE2865
Authors : Wendt, K.U.; Dreyer, M.K.; Anderka, O.; Klabunde, T.; Loenze, P.; Defossa, E.; Schmoll, D.
Deposited on : 2008-02-29
Resolution : 3.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

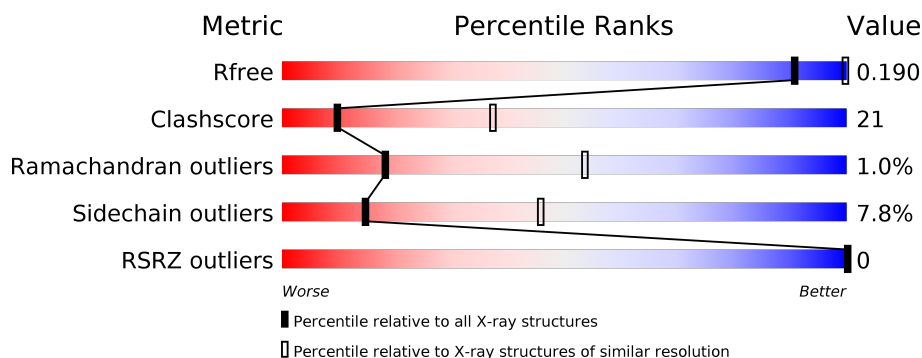
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 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}	100719	1034 (3.36-3.24)
Clashscore	112137	1100 (3.36-3.24)
Ramachandran outliers	110173	1081 (3.36-3.24)
Sidechain outliers	110143	1080 (3.36-3.24)
RSRZ outliers	101464	1039 (3.36-3.24)

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

Mol	Chain	Length	Quality of chain
1	A	809	
1	B	809	

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
3	PLP	A	832	-	-	X	-

2 Entry composition [i](#)

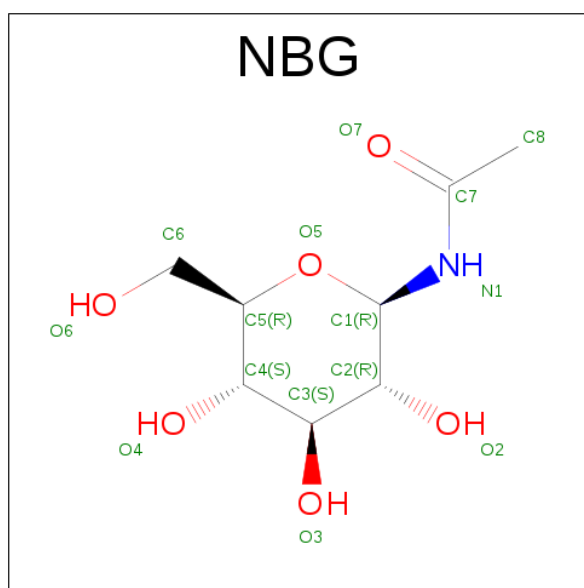
There are 5 unique types of molecules in this entry. The entry contains 13095 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

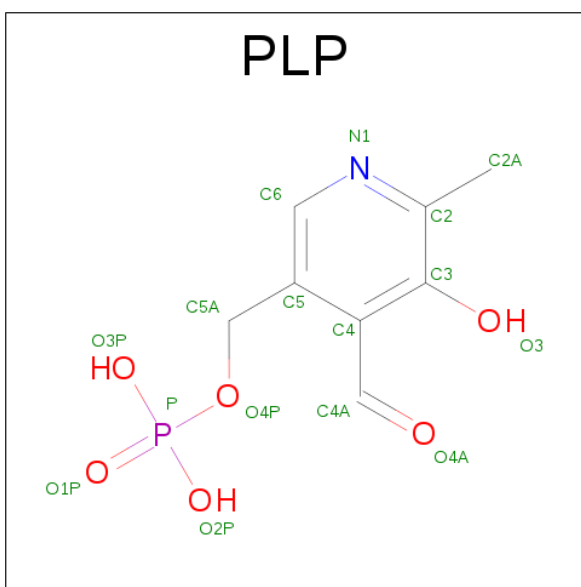
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	790	Total	C	N	O	S	0	0	0
			6415	4123	1088	1175	29			
1	B	790	Total	C	N	O	S	0	0	0
			6415	4123	1088	1175	29			

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



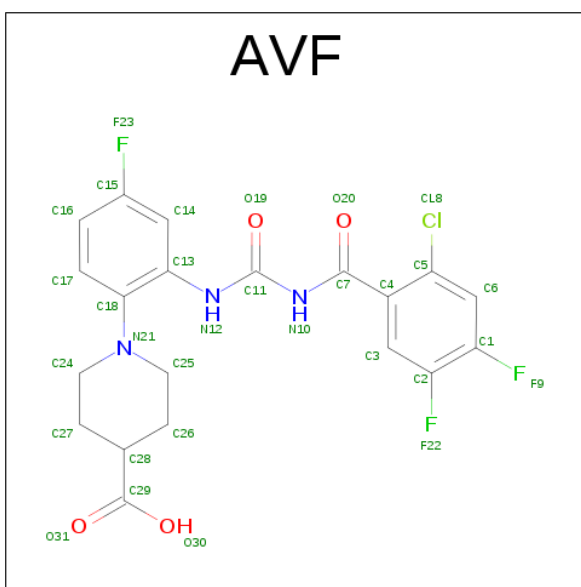
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	8	1	6		
2	B	1	Total	C	N	O	0	0
			15	8	1	6		

- 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
			16	8	1	6	1		
3	B	1	Total	C	N	O	P	0	0
			16	8	1	6	1		

- Molecule 4 is 1-{2-[3-(2-CHLORO-4,5-DIFLUORO-BENZOYL)-UREIDO]-4-FLUORO-PHENYL}-PIPERIDINE-4-CARBOXYLIC ACID (three-letter code: AVF) (formula: C₂₀H₁₇ClF₃N₃O₄).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	Cl	F	N	O	0	0
			31	20	1	3	3	4		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	B	1	Total	C	Cl	F	N	O	0	0
			31	20	1	3	3	4		

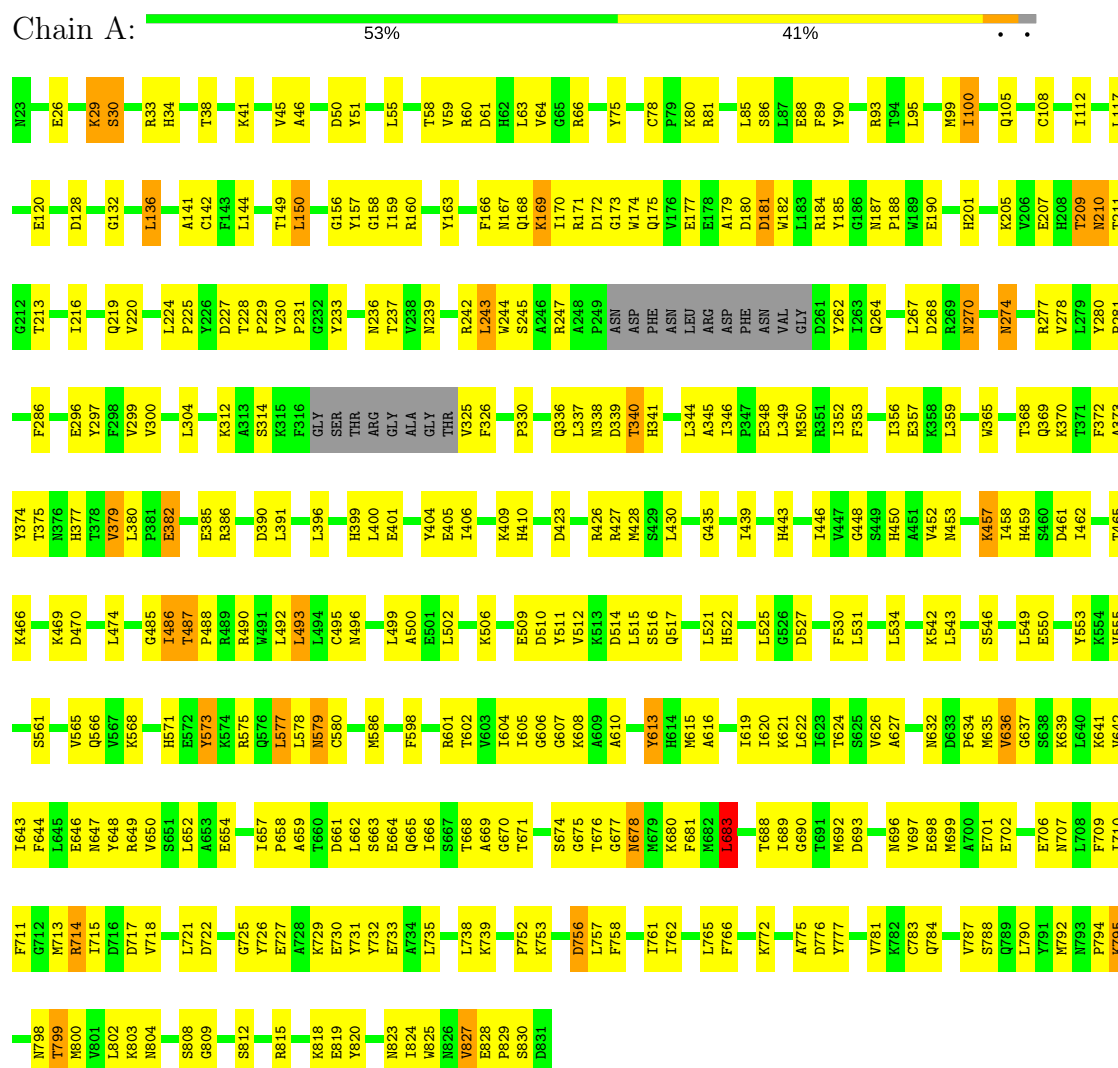
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	63	Total	O	0	0
			63	63		
5	B	78	Total	O	0	0
			78	78		

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.

- Molecule 1: Glycogen phosphorylase, liver form



- Molecule 1: Glycogen phosphorylase, liver form



S768	E702	Y613	S523	V447	K361	P281	H208	M101	N23
M793	F709	H614	F524	G448	S362	E287	T209	Q105	K29
P794	F710	M615	L525	S449	K363	E287	M210	S30	S30
M798	F711	I619	F530	V452	L367	L294	T211	D118	R33
V801	G712	L620	L531	N453	T368	K293	T213	L122	H34
L802	M713	K621	H532	G454	Q369	Q295	D217	I125	L35
K803	R714	V636	E533	V455	K370	V299	T218	E126	H36
N804	D717	S638	L534	K457	Y374	V300	Q219	E127	F37
I805	V718	K639	A535	I458	T378	T303	V220	D128	L39
A806	A719	K538	K538	H459	S382	L304	V221	V40	L40
S813	A720	K542	K542	D461	E382	Q305	K223	L131	K41
D814	L721	L543	L543	I462	E385	D306	L224	G132	D42
R815	D722	N647	Q547	V463	E385	I307	P225	N133	R43
T816	K723	Y648	Q547	K464	K386	I308	L222	G137	N44
I817	K724	R649	K554	T465	K387	R309	P229	R138	V45
I824	E727	V650	K554	F468	V392	R310	V230	G146	A46
E828	A728	S651	S560	K469	L395	S314	P231	F143	R49
P829	K729	L652	F563	D470	L395	K315	G232	L144	D50
S830	E730	A653	D564	E473	R398	F316	N235	D145	F53
D831	Y731	I657	V565	P476	T402	GLY	V238	S146	A54
	E733	A659	Q566	D477	E405	THR	N239	M147	L55
	K739	T660	V567	K478	N407	ARG	L243	T149	A56
	I742	D681	R569	K482	N407	ALA	S245	G151	H57
	D743	L662	Y573	T487	Q408	GLY	N246	Y157	L63
	S751	E664	K574	P488	K409	V325	R247	G158	H67
	P752	Q665	R575	R489	H410	F326	A248	I159	Q71
	K753	T666	Q576	R490	L411	A328	P249	R160	Q72
	Q754	T668	L577	W491	D412	F329	ASN	Y161	H73
	L757	A669	N579	L492	R413	P330	ASP	F166	Y74
	I761	S674	C580	L493	A416	D331	PHE	M167	Y75
	I762	M678	L581	L494	L417	Q332	ASN	Q168	D76
	N763	M679	H582	C495	F418	L337	LEU	K169	K77
	F766	K680	M586	N496	D421	T340	PHE	I170	C78
	F771	F681	Y587	G498	R426	A343	ASN	W174	P79
	K772	M682	K591	L499	R427	L344	VAL	Q175	R81
	A775	L683	D593	A500	M428	A345	GLY	D181	L85
	D776	G685	K596	I503	S429	I346	Y262	L87	S86
	Y777	A686	L597	I507	L430	P347	Q264	R184	L87
	Y780	T687	F598	K506	S436	E348	A265	M187	E88
	V781	T688	F599	I507	K437	L349	V266	P188	F89
	K782	G690	P600	Y511	R438	I352	R269	W189	N91
	C783	R601	R601	V512	L439	F353	N274	R193	G92
	Q784	M692	T602	M441	M41	V354	N275	P194	R93
	K785	D693	V603	L515	L442	D355	S276	M197	T94
	K786	M696	I604	L518	H443	K358	R277	F202	L95
	V787	E698	G606	H522	L444	L359	Y280	Y280	Q96

4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	123.27Å 123.27Å 121.88Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.47 – 3.30 19.47 – 3.30	Depositor EDS
% Data completeness (in resolution range)	81.2 (19.47-3.30) 81.2 (19.47-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 3.29Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.176 , 0.271 0.182 , 0.190	Depositor DCC
R_{free} test set	1243 reflections (5.19%)	DCC
Wilson B-factor (Å ²)	65.4	Xtriage
Anisotropy	0.126	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 23.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.074 for -h,-k,l 0.185 for h,-h-k,-l 0.078 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13095	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% 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: AVF, 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	0.48	1/6559 (0.0%)	0.63	1/8869 (0.0%)
1	B	0.47	0/6559	0.63	0/8869
All	All	0.48	1/13118 (0.0%)	0.63	1/17738 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	108	CYS	CB-SG	-5.59	1.72	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	683	LEU	CA-CB-CG	5.03	126.87	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6415	0	6411	276	0
1	B	6415	0	6409	274	0
2	A	15	0	15	0	0
2	B	15	0	15	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	16	0	8	8	0
3	B	16	0	6	2	0
4	A	31	0	16	3	0
4	B	31	0	16	6	0
5	A	63	0	0	8	0
5	B	78	0	0	11	0
All	All	13095	0	12896	551	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 21.

All (551) 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:A:680:LYS:HZ1	3:A:832:PLP:C4A	1.30	1.42
1:A:680:LYS:NZ	3:A:832:PLP:H4A	0.91	1.23
1:A:64:VAL:HG13	1:B:40:VAL:HG13	1.35	1.08
1:A:713:MET:HB2	1:A:717:ASP:HB2	1.41	1.02
1:B:88:GLU:HG2	1:B:132:GLY:HA2	1.47	0.95
1:B:184:ARG:HH11	1:B:184:ARG:HG3	1.32	0.95
1:A:120:GLU:HG2	5:A:886:HOH:O	1.69	0.93
1:B:168:GLN:HG3	1:B:175:GLN:HG3	1.50	0.92
1:A:675:GLY:HA3	1:A:678:ASN:HD21	1.32	0.91
1:A:680:LYS:HZ2	3:A:832:PLP:H4A	1.09	0.90
1:B:160:ARG:HB2	1:B:243:LEU:HB3	1.50	0.90
1:B:274:ASN:HD22	1:B:277:ARG:HE	1.14	0.90
1:B:34:HIS:CE1	1:B:57:HIS:HB3	2.07	0.90
1:B:410:HIS:HE1	1:B:428:MET:O	1.55	0.90
1:A:575:ARG:NH2	1:A:776:ASP:HB2	1.88	0.89
1:B:455:VAL:H	1:B:459:HIS:HD2	1.20	0.88
1:A:100:ILE:HG13	1:A:105:GLN:OE1	1.75	0.87
1:A:181:ASP:OD2	1:A:184:ARG:HB2	1.74	0.87
1:A:649:ARG:HH11	1:A:649:ARG:HG2	1.40	0.87
1:A:680:LYS:HZ3	3:A:832:PLP:H4A	1.35	0.86
1:B:507:ILE:HG12	1:B:507:ILE:O	1.77	0.84
1:B:599:VAL:HB	5:B:884:HOH:O	1.77	0.83
1:A:274:ASN:ND2	1:A:277:ARG:HE	1.75	0.83
1:B:274:ASN:ND2	1:B:277:ARG:HE	1.74	0.83
1:A:714:ARG:HH11	1:A:714:ARG:CG	1.90	0.83
1:A:550:GLU:HA	5:A:863:HOH:O	1.82	0.79
1:A:713:MET:HB2	1:A:717:ASP:CB	2.12	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:575:ARG:HH22	1:A:776:ASP:HB2	1.48	0.78
1:B:714:ARG:HD2	1:B:714:ARG:N	1.97	0.78
1:B:680:LYS:O	1:B:682:MET:N	2.18	0.77
1:A:777:TYR:O	1:A:781:VAL:HG23	1.84	0.77
1:B:308:ILE:HD13	1:B:352:ILE:HG21	1.66	0.76
1:A:665:GLN:HB2	1:A:696:ASN:HD21	1.50	0.76
1:A:29:LYS:HB3	1:A:33:ARG:HH12	1.52	0.75
1:B:535:ALA:HB2	1:B:798:ASN:HD21	1.52	0.74
1:A:756:ASP:O	1:A:758:PHE:N	2.21	0.74
1:A:75:TYR:HA	1:A:81:ARG:HH22	1.53	0.74
1:B:329:PHE:HB3	1:B:330:PRO:HD3	1.69	0.74
1:B:78:CYS:SG	1:B:314:SER:HB2	2.27	0.74
1:B:55:LEU:HD22	1:B:122:LEU:HD12	1.69	0.73
1:A:30:SER:HB3	1:A:58:THR:HG23	1.69	0.73
1:A:729:LYS:O	1:A:733:GLU:HG2	1.89	0.73
1:B:184:ARG:NH1	1:B:184:ARG:HG3	2.03	0.73
1:B:455:VAL:H	1:B:459:HIS:CD2	2.06	0.73
1:A:515:LEU:C	1:A:517:GLN:H	1.92	0.73
1:B:93:ARG:HB3	1:B:126:GLU:OE1	1.89	0.73
1:A:168:GLN:HB3	1:A:647:ASN:HA	1.69	0.73
1:B:39:LEU:HD12	1:B:50:ASP:OD1	1.89	0.73
1:B:665:GLN:HB2	1:B:696:ASN:HD21	1.54	0.72
1:A:325:VAL:HB	5:A:853:HOH:O	1.91	0.71
1:B:665:GLN:CB	1:B:696:ASN:HD21	2.03	0.71
4:A:833:AVF:H14	4:A:833:AVF:O19	1.89	0.71
1:A:575:ARG:HB3	1:A:578:LEU:HB3	1.73	0.70
1:B:29:LYS:O	1:B:33:ARG:HB2	1.91	0.70
1:A:493:LEU:HD11	1:A:512:VAL:HG11	1.74	0.70
1:B:649:ARG:HH11	1:B:649:ARG:HG2	1.56	0.70
1:B:410:HIS:CE1	1:B:428:MET:O	2.43	0.70
1:A:649:ARG:HG2	1:A:649:ARG:NH1	2.07	0.69
1:A:495:CYS:HB2	1:A:654:GLU:O	1.92	0.69
1:B:657:ILE:HB	1:B:658:PRO:HD3	1.74	0.69
1:B:213:THR:HG21	1:B:398:ARG:NH2	2.08	0.69
1:A:622:LEU:HD23	1:A:626:VAL:HG23	1.75	0.69
1:B:777:TYR:O	1:B:781:VAL:HG23	1.93	0.68
1:B:713:MET:HB2	1:B:717:ASP:HB2	1.74	0.68
1:B:197:MET:HE2	1:B:222:LEU:HB3	1.75	0.68
1:B:554:LYS:O	1:B:554:LYS:HG3	1.94	0.68
1:A:515:LEU:O	1:A:517:GLN:N	2.27	0.67
1:A:675:GLY:HA3	1:A:678:ASN:ND2	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:714:ARG:HH11	1:A:714:ARG:HG3	1.60	0.67
1:B:174:TRP:CE2	1:B:621:LYS:HG3	2.30	0.67
1:A:692:MET:HE2	1:A:710:ILE:HG21	1.77	0.66
1:A:515:LEU:HB3	5:A:842:HOH:O	1.93	0.66
1:B:606:GLY:HA3	1:B:645:LEU:HB2	1.77	0.66
1:B:193:ARG:HB2	1:B:225:PRO:HG2	1.78	0.66
1:B:89:PHE:HD1	5:B:900:HOH:O	1.76	0.66
1:A:613:TYR:HE1	1:A:615:MET:HB3	1.61	0.66
1:B:405:GLU:OE1	1:B:405:GLU:HA	1.93	0.66
1:A:457:LYS:NZ	1:A:701:GLU:OE2	2.27	0.66
1:A:88:GLU:HG2	1:A:132:GLY:HA2	1.77	0.65
1:A:149:THR:HG23	1:A:233:TYR:HB3	1.77	0.65
1:A:330:PRO:HB3	1:A:370:LYS:HB3	1.78	0.65
1:A:732:TYR:CE1	1:A:739:LYS:HG3	2.31	0.65
1:A:230:VAL:HB	1:A:239:ASN:HB2	1.79	0.64
1:B:577:LEU:O	1:B:581:LEU:HG	1.97	0.64
1:B:566:GLN:HE22	1:B:579:ASN:HB2	1.62	0.64
1:A:714:ARG:HH11	1:A:714:ARG:HG2	1.62	0.64
1:B:680:LYS:O	1:B:683:LEU:N	2.29	0.64
1:B:85:LEU:HD21	1:B:300:VAL:HG22	1.78	0.64
1:B:149:THR:HA	1:B:235:ASN:ND2	2.12	0.64
1:A:553:TYR:OH	1:A:646:GLU:HG3	1.98	0.64
1:B:455:VAL:N	1:B:459:HIS:HD2	1.93	0.64
1:B:428:MET:SD	1:B:470:ASP:HB3	2.37	0.63
1:B:754:GLN:HB3	1:B:757:LEU:HB2	1.79	0.63
1:B:72:GLN:HG3	4:B:833:AVF:C16	2.29	0.63
1:A:225:PRO:HB3	1:A:244:TRP:CZ3	2.33	0.63
1:A:262:TYR:OH	1:B:166:PHE:HB3	1.98	0.63
1:A:726:TYR:HE1	1:A:775:ALA:HB2	1.64	0.63
1:B:224:LEU:HD12	1:B:225:PRO:HD2	1.81	0.63
1:A:149:THR:CG2	1:A:233:TYR:HB3	2.28	0.63
1:B:457:LYS:O	1:B:461:ASP:HB2	1.99	0.63
1:A:326:PHE:CE1	1:A:357:GLU:HG3	2.34	0.62
1:A:573:TYR:CD1	1:A:671:THR:HB	2.35	0.62
1:A:142:CYS:SG	1:A:487:THR:HG22	2.40	0.62
1:A:209:THR:OG1	1:A:210:ASN:N	2.27	0.62
1:A:60:ARG:HD3	1:A:188:PRO:O	2.00	0.61
1:B:615:MET:HA	1:B:615:MET:HE3	1.80	0.61
1:B:751:SER:HB2	1:B:754:GLN:O	2.00	0.61
1:B:482:LYS:HE2	1:B:824:ILE:HD12	1.80	0.61
1:B:543:LEU:O	1:B:547:GLN:HG3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:525:LEU:HD21	1:B:803:LYS:HG2	1.81	0.61
1:B:593:ASP:HB3	5:B:894:HOH:O	2.00	0.61
1:A:336:GLN:OE1	1:A:373:ALA:HB3	2.01	0.61
3:B:832:PLP:O4A	3:B:832:PLP:H5A1	2.01	0.61
1:A:515:LEU:HD22	1:A:812:SER:HB2	1.83	0.61
1:B:665:GLN:NE2	1:B:678:ASN:HA	2.15	0.61
1:A:169:LYS:HB3	1:A:171:ARG:HD3	1.83	0.61
1:A:446:ILE:HG12	1:A:452:VAL:HG21	1.82	0.61
1:A:136:LEU:HD12	1:A:377:HIS:CG	2.36	0.61
1:A:174:TRP:CZ2	1:A:621:LYS:HG3	2.36	0.61
1:A:650:VAL:HA	3:A:832:PLP:H2A1	1.83	0.60
1:B:449:SER:O	1:B:478:LYS:HE2	2.01	0.60
1:A:168:GLN:HB3	1:A:647:ASN:CA	2.31	0.60
1:B:496:ASN:HD22	1:B:658:PRO:HB3	1.66	0.60
1:A:278:VAL:HB	1:B:266:VAL:HG11	1.83	0.60
1:A:608:LYS:HE3	1:A:648:TYR:O	2.02	0.60
1:B:410:HIS:HD2	5:B:889:HOH:O	1.83	0.60
1:A:274:ASN:HD22	1:A:277:ARG:HE	1.46	0.60
1:A:29:LYS:CB	1:A:33:ARG:HH12	2.14	0.60
1:A:677:GLY:HA2	1:A:680:LYS:HD2	1.83	0.60
1:A:184:ARG:HD2	1:A:185:TYR:CZ	2.36	0.60
1:A:304:LEU:HD22	1:A:349:LEU:HD13	1.83	0.60
1:A:647:ASN:O	1:A:649:ARG:NH1	2.35	0.60
1:A:136:LEU:HD12	1:A:377:HIS:CD2	2.36	0.60
1:B:174:TRP:CZ2	1:B:621:LYS:HG3	2.36	0.60
1:B:74:TYR:OH	1:B:239:ASN:ND2	2.33	0.60
1:B:662:LEU:HD22	1:B:787:VAL:HG11	1.82	0.60
1:B:567:VAL:HA	1:B:606:GLY:O	2.01	0.59
1:A:731:TYR:O	1:A:735:LEU:HB2	2.02	0.59
1:B:41:LYS:HD2	1:B:46:ALA:HA	1.84	0.59
1:A:615:MET:O	1:A:619:ILE:HG13	2.03	0.59
1:A:80:LYS:HB3	1:A:827:VAL:HG13	1.84	0.59
1:B:499:LEU:HD22	1:B:503:ILE:HD11	1.83	0.59
1:A:243:LEU:HB2	5:A:834:HOH:O	2.01	0.58
1:B:680:LYS:O	1:B:681:PHE:C	2.42	0.58
1:B:138:ARG:HH22	1:B:490:ARG:HH11	1.52	0.58
1:B:714:ARG:H	1:B:714:ARG:HD2	1.69	0.58
1:B:410:HIS:CD2	5:B:889:HOH:O	2.55	0.58
1:B:713:MET:HB2	1:B:717:ASP:CB	2.33	0.58
1:B:542:LYS:HA	1:B:659:ALA:HB1	1.84	0.58
1:B:387:TRP:HD1	1:B:441:MET:HG3	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:506:LYS:HD2	1:B:524:PHE:CE2	2.39	0.58
1:B:668:THR:OG1	1:B:771:PHE:O	2.15	0.58
1:A:665:GLN:CB	1:A:696:ASN:HD21	2.17	0.58
1:A:514:ASP:O	1:A:517:GLN:HG2	2.03	0.57
1:A:29:LYS:HB3	1:A:33:ARG:NH1	2.18	0.57
1:A:500:ALA:O	1:A:511:TYR:OH	2.21	0.57
1:B:649:ARG:HG2	1:B:649:ARG:NH1	2.19	0.57
1:A:160:ARG:HB2	1:A:243:LEU:HB3	1.86	0.57
1:B:565:VAL:HA	1:B:604:ILE:O	2.04	0.57
1:A:493:LEU:HD21	1:A:512:VAL:HG13	1.87	0.57
1:B:729:LYS:O	1:B:733:GLU:HG2	2.04	0.57
1:B:732:TYR:CZ	1:B:739:LYS:HD2	2.40	0.57
1:A:493:LEU:HD21	1:A:512:VAL:CG1	2.35	0.57
1:A:575:ARG:HH22	1:A:776:ASP:CB	2.15	0.56
1:B:430:LEU:HD21	1:B:444:LEU:HA	1.87	0.56
1:B:327:ASP:OD1	1:B:363:LYS:HE2	2.05	0.56
1:B:221:VAL:HG21	1:B:275:ILE:HD12	1.87	0.56
1:A:613:TYR:CE1	1:A:615:MET:HB3	2.41	0.56
1:B:678:ASN:OD1	1:B:679:MET:N	2.39	0.56
1:B:698:GLU:O	1:B:702:GLU:HG2	2.05	0.56
1:B:500:ALA:HA	1:B:511:TYR:OH	2.05	0.56
1:A:401:GLU:O	1:A:405:GLU:HB2	2.05	0.56
1:A:568:LYS:O	1:A:607:GLY:HA3	2.06	0.55
1:B:564:ASP:HB3	1:B:603:VAL:HA	1.88	0.55
1:A:571:HIS:CD2	1:A:613:TYR:HE2	2.24	0.55
1:A:34:HIS:HE1	1:A:61:ASP:OD2	1.89	0.55
1:B:71:GLN:HG3	4:B:833:AVF:CL8	2.44	0.55
1:B:131:LEU:HD22	1:B:161:TYR:HB2	1.87	0.55
1:B:522:HIS:HD2	1:B:525:LEU:HD11	1.71	0.55
1:B:709:PHE:HE2	1:B:786:LYS:HB3	1.69	0.55
1:A:580:CYS:SG	1:A:622:LEU:HD22	2.46	0.55
1:A:605:ILE:O	1:A:644:PHE:HA	2.06	0.55
1:B:496:ASN:OD1	1:B:499:LEU:HB2	2.07	0.55
1:B:579:ASN:ND2	5:B:868:HOH:O	2.39	0.55
1:B:647:ASN:O	1:B:649:ARG:NH1	2.40	0.55
1:A:34:HIS:HD2	1:A:38:THR:OG1	1.89	0.55
1:A:93:ARG:O	1:A:490:ARG:NH2	2.39	0.55
1:B:158:GLY:O	1:B:243:LEU:HA	2.07	0.55
1:A:542:LYS:HA	1:A:659:ALA:HB1	1.88	0.54
1:B:538:LYS:HZ2	1:B:660:THR:H	1.53	0.54
1:A:41:LYS:HD3	1:A:45:VAL:HG23	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:515:LEU:C	1:A:517:GLN:N	2.60	0.54
1:A:531:LEU:HD22	1:A:798:ASN:HB3	1.89	0.54
1:A:542:LYS:NZ	1:A:561:SER:O	2.36	0.54
1:A:669:ALA:HB3	1:A:718:VAL:HG21	1.90	0.54
1:A:336:GLN:HB2	1:A:825:TRP:HE1	1.73	0.54
1:A:709:PHE:HZ	1:A:790:LEU:HD22	1.72	0.54
1:A:515:LEU:CD2	1:A:812:SER:HB2	2.37	0.54
1:A:280:TYR:CE1	1:B:263:ILE:HG13	2.42	0.54
1:B:535:ALA:HB2	1:B:798:ASN:ND2	2.22	0.54
1:B:34:HIS:HD2	1:B:38:THR:OG1	1.90	0.54
1:B:597:LEU:O	1:B:597:LEU:HG	2.07	0.54
1:B:170:ILE:HG12	1:B:646:GLU:HG2	1.90	0.54
1:B:465:THR:O	1:B:469:LYS:HB2	2.08	0.54
1:A:300:VAL:HG13	1:A:345:ALA:HA	1.89	0.54
1:B:714:ARG:HG2	1:B:714:ARG:HH11	1.73	0.53
1:B:128:ASP:OD2	1:B:651:SER:HB3	2.09	0.53
1:A:485:GLY:O	1:A:486:ILE:HG23	2.08	0.53
1:A:465:THR:O	1:A:469:LYS:HB2	2.08	0.53
1:A:698:GLU:O	1:A:702:GLU:HG2	2.07	0.53
1:B:739:LYS:HG3	1:B:743:ASP:OD2	2.08	0.53
4:A:833:AVF:C14	4:A:833:AVF:O19	2.57	0.53
1:B:248:ALA:HB3	1:B:269:ARG:CZ	2.39	0.53
1:B:76:ASP:O	1:B:315:LYS:HE2	2.07	0.53
1:B:330:PRO:HB3	1:B:370:LYS:HB3	1.91	0.53
1:B:369:GLN:HA	1:B:448:GLY:O	2.09	0.53
1:B:709:PHE:CE2	1:B:786:LYS:HB3	2.44	0.53
1:B:354:VAL:O	1:B:358:LYS:HA	2.08	0.53
1:B:815:ARG:C	1:B:815:ARG:HD2	2.29	0.53
1:A:792:MET:O	1:A:794:PRO:HD3	2.09	0.53
1:B:507:ILE:O	1:B:507:ILE:CG1	2.54	0.53
1:B:184:ARG:CG	1:B:184:ARG:HH11	2.15	0.53
1:B:813:SER:O	1:B:817:ILE:HG12	2.09	0.52
1:A:339:ASP:CG	1:A:340:THR:H	2.12	0.52
1:B:615:MET:HE1	1:B:761:ILE:HG12	1.91	0.52
1:B:502:LEU:HD11	1:B:533:GLU:HB3	1.91	0.52
1:B:144:LEU:HD13	1:B:230:VAL:HG21	1.92	0.52
1:B:538:LYS:NZ	1:B:660:THR:H	2.08	0.52
1:A:172:ASP:O	1:A:174:TRP:CD1	2.62	0.52
1:A:627:ALA:HA	1:A:642:VAL:HB	1.92	0.52
1:B:96:GLN:HE21	1:B:105:GLN:HE22	1.57	0.52
1:B:89:PHE:HB3	1:B:91:MET:HG2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:ILE:HG13	1:B:299:VAL:HB	1.92	0.51
1:A:346:ILE:HD13	1:A:448:GLY:HA3	1.92	0.51
1:A:297:TYR:HB2	1:A:396:LEU:HD11	1.92	0.51
1:A:41:LYS:HD2	1:A:46:ALA:HA	1.91	0.51
1:A:527:ASP:OD1	1:A:530:PHE:HB2	2.10	0.51
1:A:159:ILE:HG13	1:A:299:VAL:HB	1.92	0.51
1:A:488:PRO:O	1:A:492:LEU:HB3	2.11	0.51
1:A:664:GLU:O	1:A:665:GLN:NE2	2.43	0.51
1:A:99:MET:HB3	1:A:105:GLN:HA	1.92	0.51
1:B:409:LYS:O	1:B:412:ASP:HB2	2.09	0.51
1:B:53:PHE:HE1	1:B:188:PRO:HD3	1.75	0.51
1:B:601:ARG:NH2	1:B:788:SER:OG	2.41	0.51
1:A:267:LEU:HD13	1:B:274:ASN:OD1	2.11	0.51
1:A:496:ASN:OD1	1:A:499:LEU:HB2	2.10	0.51
1:A:521:LEU:HB3	1:A:802:LEU:HD11	1.93	0.51
1:A:738:LEU:HB2	1:A:777:TYR:CE2	2.46	0.51
1:A:158:GLY:O	1:A:243:LEU:HA	2.11	0.50
1:A:577:LEU:HD13	1:A:765:LEU:HD21	1.93	0.50
1:A:809:GLY:HA3	5:A:840:HOH:O	2.11	0.50
1:A:459:HIS:HA	1:A:462:ILE:HD12	1.93	0.50
1:A:636:VAL:CG2	1:A:637:GLY:N	2.74	0.50
1:B:413:ARG:HA	1:B:413:ARG:NE	2.26	0.50
1:B:566:GLN:NE2	1:B:579:ASN:HB2	2.26	0.50
1:A:546:SER:HA	1:A:549:LEU:HD12	1.94	0.50
1:A:662:LEU:HD22	1:A:787:VAL:HG11	1.94	0.50
1:B:49:ARG:HA	1:B:125:ILE:HG21	1.93	0.50
1:A:46:ALA:HB3	1:A:51:TYR:CZ	2.47	0.50
1:B:374:TYR:CD2	1:B:452:VAL:HG13	2.46	0.50
1:B:593:ASP:CB	5:B:894:HOH:O	2.59	0.50
1:B:208:HIS:ND1	1:B:213:THR:HB	2.27	0.49
1:A:181:ASP:OD2	1:A:184:ARG:CB	2.55	0.49
1:A:721:LEU:O	1:A:725:GLY:N	2.45	0.49
1:B:67:TRP:CH2	1:B:229:PRO:HD3	2.47	0.49
1:A:669:ALA:HB1	1:A:715:ILE:HA	1.94	0.49
1:A:565:VAL:HG22	1:A:604:ILE:HB	1.94	0.49
1:B:95:LEU:O	1:B:99:MET:HG3	2.13	0.49
1:A:182:TRP:CZ3	1:A:187:ASN:ND2	2.81	0.49
1:B:149:THR:C	1:B:151:GLY:H	2.14	0.49
1:B:525:LEU:HD23	1:B:802:LEU:HD23	1.95	0.49
1:B:600:PRO:HA	1:B:639:LYS:O	2.13	0.49
1:B:71:GLN:CG	4:B:833:AVF:CL8	2.98	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:554:LYS:CG	1:B:554:LYS:O	2.60	0.49
1:B:511:TYR:O	1:B:515:LEU:HA	2.13	0.49
1:B:530:PHE:HE2	1:B:802:LEU:HD13	1.77	0.49
1:A:86:SER:HB3	1:A:89:PHE:CE1	2.47	0.49
1:A:150:LEU:HD21	1:A:818:LYS:HG3	1.93	0.49
1:A:624:THR:O	1:A:627:ALA:HB3	2.12	0.49
1:A:632:ASN:O	1:A:634:PRO:HD3	2.12	0.48
1:A:157:TYR:HE2	1:A:244:TRP:CZ2	2.32	0.48
1:A:423:ASP:O	1:A:427:ARG:HB2	2.13	0.48
1:A:690:GLY:O	1:A:710:ILE:HA	2.13	0.48
1:A:680:LYS:HZ1	3:A:832:PLP:H4A	0.68	0.48
1:A:689:ILE:HG12	1:A:711:PHE:CE2	2.49	0.48
1:A:396:LEU:HB3	1:A:399:HIS:ND1	2.29	0.48
1:B:146:SER:HB2	1:B:817:ILE:HG13	1.95	0.48
1:B:170:ILE:HA	1:B:174:TRP:O	2.14	0.48
1:B:231:PRO:HA	1:B:238:VAL:HG22	1.96	0.48
1:B:679:MET:O	1:B:680:LYS:O	2.31	0.48
1:B:721:LEU:HA	1:B:724:LYS:HB3	1.96	0.48
1:B:87:LEU:HD22	1:B:299:VAL:HG11	1.95	0.48
1:A:602:THR:HG23	1:A:641:LYS:HB2	1.96	0.48
1:B:346:ILE:CD1	1:B:445:CYS:HA	2.44	0.48
1:A:286:PHE:CD1	1:A:385:GLU:HA	2.49	0.48
1:A:225:PRO:HB3	1:A:244:TRP:CE3	2.49	0.48
1:B:669:ALA:HB3	1:B:718:VAL:HG21	1.96	0.48
1:B:75:TYR:HA	1:B:81:ARG:NH2	2.28	0.48
1:B:304:LEU:HD11	1:B:345:ALA:HB1	1.96	0.48
1:B:522:HIS:HB2	5:B:913:HOH:O	2.13	0.48
1:A:380:LEU:HB3	1:A:382:GLU:OE2	2.14	0.47
1:B:446:ILE:HD11	1:B:468:PHE:CE2	2.49	0.47
1:B:428:MET:CG	1:B:470:ASP:HB3	2.43	0.47
1:B:762:ILE:O	1:B:766:PHE:HD1	1.96	0.47
1:A:168:GLN:HG3	1:A:175:GLN:HG3	1.96	0.47
1:B:455:VAL:HG23	1:B:674:SER:HB3	1.97	0.47
1:B:181:ASP:OD2	1:B:184:ARG:NH1	2.48	0.47
1:A:190:GLU:HA	1:A:227:ASP:O	2.14	0.47
1:A:522:HIS:O	1:A:525:LEU:HG	2.13	0.47
1:A:799:THR:O	1:A:803:LYS:HG3	2.15	0.47
1:B:293:LEU:HB2	1:B:387:TRP:CZ3	2.49	0.47
1:B:538:LYS:NZ	1:B:658:PRO:O	2.47	0.47
1:A:174:TRP:CE2	1:A:621:LYS:HG3	2.49	0.47
1:A:692:MET:HG3	1:A:697:VAL:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:GLY:HA3	1:B:358:LYS:HE2	1.96	0.47
1:B:573:TYR:HA	1:B:771:PHE:CG	2.49	0.47
1:B:30:SER:O	1:B:34:HIS:HB2	2.15	0.47
4:B:833:AVF:H14	4:B:833:AVF:O19	2.13	0.47
1:B:340:THR:O	1:B:343:ALA:N	2.48	0.47
1:B:463:VAL:HG13	1:B:468:PHE:HD1	1.80	0.47
1:B:575:ARG:NH2	1:B:776:ASP:HB2	2.30	0.47
1:B:88:GLU:CD	1:B:133:ASN:H	2.17	0.47
1:A:372:PHE:O	1:A:450:HIS:HD2	1.97	0.47
1:A:772:LYS:HB3	1:A:775:ALA:HB3	1.97	0.47
1:B:213:THR:HG23	1:B:355:ASP:OD2	2.15	0.47
1:B:443:HIS:HA	1:B:446:ILE:HD12	1.97	0.47
1:B:742:ILE:HG23	1:B:762:ILE:HD12	1.97	0.47
1:B:518:LEU:O	1:B:806:ALA:HA	2.14	0.47
1:B:665:GLN:HB3	1:B:696:ASN:HD21	1.77	0.47
1:A:180:ASP:O	1:A:182:TRP:N	2.42	0.46
1:A:296:GLU:HB2	1:A:344:LEU:HD12	1.98	0.46
1:A:542:LYS:NZ	1:A:661:ASP:OD2	2.41	0.46
1:A:800:MET:O	1:A:804:ASN:ND2	2.48	0.46
1:B:651:SER:O	1:B:654:GLU:HB2	2.16	0.46
3:B:832:PLP:O4A	3:B:832:PLP:C5A	2.63	0.46
1:A:555:VAL:HG13	1:A:641:LYS:HD2	1.97	0.46
1:B:586:MET:SD	1:B:601:ARG:HD2	2.55	0.46
1:A:410:HIS:HE1	1:A:428:MET:O	1.98	0.46
1:B:711:PHE:CE1	1:B:780:TYR:HB2	2.50	0.46
1:A:157:TYR:HD2	1:A:244:TRP:HE1	1.63	0.46
1:A:676:THR:OG1	3:A:832:PLP:O4A	2.31	0.46
1:B:42:ASP:OD2	1:B:44:ASN:HB2	2.15	0.46
4:B:833:AVF:HN12	4:B:833:AVF:H24A	1.80	0.46
1:A:229:PRO:O	1:A:231:PRO:HD3	2.15	0.46
1:A:341:HIS:HD2	1:A:385:GLU:OE1	1.98	0.46
1:B:781:VAL:O	1:B:784:GLN:HB2	2.16	0.46
1:A:173:GLY:O	1:A:621:LYS:HA	2.15	0.46
1:A:693:ASP:O	1:A:696:ASN:HB2	2.16	0.46
1:B:55:LEU:CD2	1:B:122:LEU:HD12	2.43	0.46
1:B:436:SER:O	1:B:438:ARG:HG3	2.15	0.46
1:A:66:ARG:HD2	1:A:236:ASN:HA	1.97	0.46
1:A:502:LEU:HD11	1:A:534:LEU:HA	1.96	0.46
1:B:161:TYR:HE1	1:B:295:GLN:NE2	2.14	0.46
1:B:308:ILE:CD1	1:B:352:ILE:HG21	2.41	0.46
1:B:578:LEU:O	1:B:579:ASN:C	2.53	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:645:LEU:HA	1:B:645:LEU:HD23	1.79	0.46
1:B:685:GLY:HA2	1:B:801:VAL:HG13	1.97	0.46
1:A:201:HIS:HA	1:A:219:GLN:O	2.16	0.46
1:A:26:GLU:HA	1:A:29:LYS:HG3	1.96	0.46
1:B:430:LEU:HD21	1:B:444:LEU:CA	2.45	0.46
1:A:714:ARG:HG2	1:A:714:ARG:NH1	2.31	0.46
1:B:280:TYR:HA	1:B:281:PRO:HD3	1.79	0.46
1:B:340:THR:OG1	1:B:385:GLU:HG3	2.16	0.46
1:A:555:VAL:HG11	1:A:643:ILE:HD11	1.98	0.45
1:A:78:CYS:SG	1:A:314:SER:HB2	2.56	0.45
1:B:587:TYR:O	1:B:591:LYS:HG2	2.16	0.45
1:A:170:ILE:HG12	1:A:646:GLU:HG2	1.98	0.45
1:A:795:LYS:O	1:A:799:THR:OG1	2.33	0.45
1:B:531:LEU:HD22	1:B:798:ASN:HB3	1.97	0.45
1:B:565:VAL:HG22	1:B:604:ILE:HB	1.98	0.45
1:A:264:GLN:NE2	1:A:268:ASP:OD1	2.49	0.45
1:A:586:MET:SD	1:A:601:ARG:HD2	2.56	0.45
1:A:820:TYR:CD1	1:A:824:ILE:HD12	2.51	0.45
1:A:663:SER:HB2	1:A:681:PHE:HB3	1.99	0.45
1:B:681:PHE:HB3	1:B:686:ALA:HB3	1.99	0.45
1:B:596:LYS:HG3	1:B:597:LEU:N	2.31	0.45
1:A:549:LEU:HD22	1:A:643:ILE:HG21	1.99	0.45
1:B:511:TYR:CD2	1:B:518:LEU:HD21	2.51	0.45
1:B:691:THR:C	1:B:693:ASP:H	2.20	0.45
1:A:177:GLU:N	1:A:177:GLU:OE1	2.50	0.45
1:A:156:GLY:O	1:A:242:ARG:N	2.46	0.45
1:A:566:GLN:HB2	1:A:664:GLU:HB2	1.98	0.45
1:A:157:TYR:HE2	1:A:244:TRP:HZ2	1.65	0.45
1:A:375:THR:HG23	1:A:453:ASN:HD21	1.82	0.44
1:A:663:SER:HB3	1:A:688:THR:HA	1.99	0.44
4:A:833:AVF:H24A	4:A:833:AVF:HN12	1.81	0.44
1:B:613:TYR:CE1	1:B:615:MET:HB3	2.52	0.44
1:A:458:ILE:HG23	1:A:459:HIS:H	1.81	0.44
1:A:410:HIS:CE1	1:A:428:MET:O	2.71	0.44
1:A:579:ASN:C	1:A:579:ASN:HD22	2.21	0.44
1:B:261:ASP:HB3	1:B:264:GLN:HB3	2.00	0.44
1:B:491:TRP:HA	1:B:495:CYS:SG	2.58	0.44
1:A:386:ARG:HA	1:A:439:ILE:O	2.17	0.44
1:A:575:ARG:HD3	1:A:666:ILE:O	2.18	0.44
1:B:325:VAL:HB	1:B:326:PHE:H	1.63	0.44
1:B:349:LEU:O	1:B:353:PHE:N	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:463:VAL:O	1:B:468:PHE:HB2	2.17	0.44
1:B:575:ARG:HD3	1:B:666:ILE:O	2.18	0.44
1:A:616:ALA:O	1:A:620:ILE:HG13	2.17	0.44
1:A:727:GLU:O	1:A:730:GLU:HG2	2.17	0.44
1:B:482:LYS:HE2	1:B:824:ILE:CD1	2.48	0.44
1:B:804:ASN:H	1:B:804:ASN:HD22	1.64	0.44
1:A:349:LEU:HG	1:A:353:PHE:CE1	2.53	0.44
1:A:325:VAL:HB	1:A:326:PHE:H	1.59	0.44
1:A:604:ILE:HA	1:A:643:ILE:O	2.17	0.44
1:B:407:ASN:HB2	1:B:430:LEU:HB2	2.00	0.44
1:B:464:LYS:NZ	1:B:476:PRO:O	2.50	0.44
1:B:772:LYS:HB3	1:B:775:ALA:HB3	2.00	0.44
1:A:400:LEU:HA	1:A:400:LEU:HD12	1.87	0.43
1:A:657:ILE:HB	1:A:658:PRO:HD3	1.99	0.43
1:A:669:ALA:HB3	1:A:718:VAL:CG2	2.47	0.43
1:A:699:MET:HB3	1:A:699:MET:HE2	1.63	0.43
1:B:34:HIS:CD2	1:B:38:THR:OG1	2.69	0.43
1:B:582:HIS:CD2	1:B:784:GLN:HG3	2.52	0.43
1:B:679:MET:O	1:B:680:LYS:C	2.55	0.43
1:A:493:LEU:HD21	1:A:512:VAL:CG2	2.48	0.43
1:A:550:GLU:HG2	1:A:555:VAL:O	2.18	0.43
1:A:577:LEU:CD1	1:A:765:LEU:HD21	2.48	0.43
1:A:819:GLU:O	1:A:823:ASN:ND2	2.51	0.43
1:B:374:TYR:CG	1:B:445:CYS:HB3	2.53	0.43
1:B:492:LEU:HD12	1:B:492:LEU:HA	1.78	0.43
1:A:379:VAL:O	1:A:380:LEU:C	2.57	0.43
1:A:55:LEU:O	1:A:59:VAL:HG23	2.18	0.43
1:B:575:ARG:C	1:B:577:LEU:N	2.71	0.43
1:B:724:LYS:HE2	5:B:911:HOH:O	2.18	0.43
1:A:163:TYR:CD2	1:A:179:ALA:HB1	2.53	0.43
1:A:348:GLU:O	1:A:352:ILE:HG13	2.18	0.43
1:A:714:ARG:NH1	1:A:714:ARG:CG	2.61	0.43
1:B:80:LYS:HG3	1:B:332:GLN:C	2.39	0.43
1:B:487:THR:HG23	1:B:490:ARG:HB3	2.00	0.43
1:B:506:LYS:HG3	1:B:530:PHE:CD1	2.54	0.43
1:A:300:VAL:CG1	1:A:345:ALA:HA	2.48	0.43
1:A:369:GLN:O	1:A:450:HIS:HB3	2.19	0.43
1:A:711:PHE:HB3	1:A:783:CYS:SG	2.59	0.43
1:A:666:ILE:HG22	1:A:711:PHE:HZ	1.84	0.43
1:B:143:PHE:O	1:B:147:MET:HG3	2.19	0.43
1:B:187:ASN:HA	1:B:188:PRO:HD2	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:418:PHE:HB3	1:B:421:ASP:HB2	2.01	0.43
1:B:652:LEU:O	1:B:652:LEU:HD22	2.19	0.43
1:A:207:GLU:HB2	1:A:216:ILE:HG12	2.01	0.43
1:B:150:LEU:O	1:B:829:PRO:HB3	2.18	0.43
1:B:615:MET:O	1:B:619:ILE:HG13	2.19	0.43
1:A:714:ARG:NH1	5:A:891:HOH:O	2.51	0.43
1:B:363:LYS:O	1:B:367:LEU:HG	2.19	0.43
4:B:833:AVF:H24A	4:B:833:AVF:O20	2.19	0.43
1:B:428:MET:HG2	1:B:470:ASP:HB3	2.00	0.43
1:B:563:PHE:HD2	1:B:659:ALA:O	2.02	0.43
1:B:714:ARG:HH11	1:B:714:ARG:CG	2.32	0.43
1:B:615:MET:CE	1:B:761:ILE:HG12	2.48	0.43
1:B:80:LYS:HE3	1:B:330:PRO:O	2.19	0.43
1:A:141:ALA:O	1:A:144:LEU:HB2	2.19	0.42
1:A:312:LYS:HB3	1:A:312:LYS:HE2	1.84	0.42
1:B:575:ARG:HB3	1:B:578:LEU:CB	2.49	0.42
1:A:187:ASN:HB3	1:A:190:GLU:HG2	2.01	0.42
1:A:356:ILE:HG22	1:A:357:GLU:OE1	2.19	0.42
1:B:131:LEU:CD2	1:B:161:TYR:HB2	2.49	0.42
1:B:360:PRO:O	1:B:361:TRP:C	2.58	0.42
1:B:582:HIS:CE1	1:B:586:MET:SD	3.12	0.42
1:B:683:LEU:O	1:B:683:LEU:HD22	2.19	0.42
1:B:693:ASP:O	1:B:696:ASN:HB2	2.19	0.42
1:B:85:LEU:HD13	1:B:303:THR:HG21	2.02	0.42
1:A:400:LEU:HG	1:A:404:TYR:CE2	2.54	0.42
1:A:85:LEU:HD21	1:A:300:VAL:HG22	2.01	0.42
1:B:392:VAL:HG21	1:B:439:ILE:HD12	2.00	0.42
1:B:538:LYS:HG3	1:B:542:LYS:HD2	2.00	0.42
1:B:720:ALA:O	1:B:724:LYS:N	2.49	0.42
1:A:112:ILE:HG23	1:A:117:LEU:HB2	2.02	0.42
1:A:185:TYR:CD2	1:B:194:PRO:HB3	2.53	0.42
1:A:280:TYR:HA	1:A:281:PRO:HD3	1.77	0.42
1:A:427:ARG:NE	1:A:470:ASP:OD1	2.52	0.42
1:B:387:TRP:CD1	1:B:441:MET:HG3	2.52	0.42
1:B:202:PHE:CD1	1:B:395:LEU:HD11	2.54	0.42
1:B:567:VAL:HB	1:B:648:TYR:CE1	2.55	0.42
1:B:188:PRO:HG2	1:B:189:TRP:CD1	2.55	0.42
1:B:303:THR:O	1:B:307:ILE:HG13	2.20	0.42
1:A:374:TYR:O	1:A:452:VAL:HA	2.19	0.42
1:A:663:SER:HB2	1:A:681:PHE:CB	2.49	0.42
1:A:330:PRO:HG2	1:A:370:LYS:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:506:LYS:HG3	1:A:530:PHE:HE1	1.85	0.42
1:A:663:SER:OG	1:A:665:GLN:NE2	2.53	0.42
1:A:665:GLN:HG3	1:A:678:ASN:HB3	2.02	0.42
1:A:714:ARG:N	1:A:714:ARG:CD	2.82	0.42
1:A:670:GLY:HA3	1:A:715:ILE:HD13	2.02	0.42
1:A:368:THR:HG23	1:A:372:PHE:CD1	2.54	0.42
1:A:604:ILE:HG23	1:A:643:ILE:HB	2.01	0.42
1:A:683:LEU:HD22	1:A:683:LEU:O	2.19	0.42
1:A:706:GLU:HG2	1:A:707:ASN:N	2.35	0.42
1:B:246:ALA:N	1:B:276:SER:OG	2.53	0.42
1:A:170:ILE:CG1	1:A:646:GLU:HG2	2.50	0.41
1:A:668:THR:HB	1:A:671:THR:HG21	2.01	0.41
1:A:689:ILE:HD13	1:A:784:GLN:NE2	2.35	0.41
1:A:812:SER:HB3	5:A:842:HOH:O	2.20	0.41
1:A:64:VAL:HG11	1:B:36:HIS:O	2.20	0.41
1:B:582:HIS:HB2	1:B:780:TYR:HE2	1.85	0.41
1:A:405:GLU:OE2	1:A:409:LYS:HE3	2.19	0.41
1:A:598:PHE:HB3	1:A:639:LYS:HE3	2.03	0.41
1:A:732:TYR:CZ	1:A:739:LYS:HG3	2.55	0.41
1:A:270:ASN:O	1:A:274:ASN:ND2	2.53	0.41
1:B:167:ASN:HD22	1:B:167:ASN:HA	1.65	0.41
1:B:413:ARG:O	1:B:416:ALA:HB3	2.20	0.41
1:B:530:PHE:HE2	1:B:802:LEU:CD1	2.33	0.41
1:B:133:ASN:O	1:B:569:ARG:HD3	2.20	0.41
1:B:157:TYR:HH	1:B:310:ARG:HH22	1.65	0.41
1:B:213:THR:CG2	1:B:398:ARG:NH2	2.81	0.41
1:A:729:LYS:H	1:A:729:LYS:HG3	1.61	0.41
1:B:662:LEU:HD11	1:B:689:ILE:HB	2.03	0.41
1:A:168:GLN:HE21	1:A:175:GLN:HG3	1.86	0.41
1:A:666:ILE:HG22	1:A:711:PHE:CZ	2.55	0.41
1:A:762:ILE:HG23	1:A:766:PHE:CD1	2.55	0.41
1:A:828:GLU:HA	1:A:829:PRO:HD3	1.83	0.41
1:B:88:GLU:HB3	1:B:137:GLY:HA2	2.03	0.41
1:B:688:THR:N	5:B:849:HOH:O	2.53	0.41
1:B:729:LYS:C	1:B:731:TYR:H	2.23	0.41
1:A:493:LEU:HD21	1:A:512:VAL:HG22	2.03	0.41
1:B:361:TRP:CH2	1:B:402:ILE:HG23	2.56	0.41
1:B:733:GLU:H	1:B:733:GLU:HG2	1.69	0.41
1:B:525:LEU:CD2	1:B:803:LYS:HG2	2.50	0.41
1:A:224:LEU:HD12	1:A:225:PRO:HD2	2.02	0.41
1:A:649:ARG:CG	1:A:649:ARG:HH11	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:815:ARG:HD2	1:A:815:ARG:C	2.41	0.41
1:B:664:GLU:OE1	1:B:780:TYR:OH	2.24	0.41
1:B:793:ASN:O	1:B:794:PRO:C	2.58	0.41
1:A:365:TRP:CZ3	1:A:406:ILE:HG12	2.56	0.41
1:B:187:ASN:ND2	5:B:864:HOH:O	2.53	0.41
1:A:144:LEU:HA	1:A:144:LEU:HD23	1.87	0.41
1:A:357:GLU:CB	1:A:359:LEU:HG	2.51	0.41
1:A:338:ASN:OD1	1:A:377:HIS:NE2	2.54	0.41
1:A:470:ASP:O	1:A:474:LEU:HD13	2.21	0.41
1:B:67:TRP:O	1:B:71:GLN:HG2	2.21	0.41
1:B:329:PHE:HB3	1:B:330:PRO:CD	2.47	0.41
1:B:67:TRP:CZ3	1:B:229:PRO:HD3	2.56	0.41
1:B:709:PHE:HB3	1:B:783:CYS:SG	2.60	0.41
1:A:346:ILE:HA	1:A:372:PHE:CE1	2.56	0.40
1:A:606:GLY:HA2	1:A:644:PHE:CE1	2.56	0.40
1:A:680:LYS:HZ3	3:A:832:PLP:C4A	2.07	0.40
1:A:350:MET:SD	1:A:365:TRP:HA	2.61	0.40
1:B:577:LEU:O	1:B:580:CYS:HB3	2.22	0.40
1:A:166:PHE:O	1:A:608:LYS:NZ	2.43	0.40
1:A:41:LYS:HE3	1:A:50:ASP:OD2	2.21	0.40
1:A:458:ILE:O	1:A:461:ASP:HB3	2.21	0.40
1:A:610:ALA:HB3	1:A:613:TYR:HB2	2.03	0.40
1:B:345:ALA:HA	1:B:348:GLU:HB3	2.02	0.40
1:A:368:THR:HG23	1:A:372:PHE:HD1	1.86	0.40
1:A:499:LEU:HD23	1:A:499:LEU:HA	1.88	0.40
1:B:493:LEU:HD21	1:B:512:VAL:CG2	2.51	0.40
1:B:692:MET:HB3	1:B:714:ARG:HG3	2.03	0.40
1:A:428:MET:CE	1:A:474:LEU:HD22	2.51	0.40
1:A:430:LEU:CD2	1:A:443:HIS:HB3	2.51	0.40
1:B:101:ASN:HB3	1:B:232:GLY:O	2.21	0.40
1:B:665:GLN:HB2	1:B:696:ASN:ND2	2.27	0.40
1:B:751:SER:O	1:B:752:PRO:C	2.59	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	784/809 (97%)	659 (84%)	118 (15%)	7 (1%)	20	55
1	B	784/809 (97%)	693 (88%)	83 (11%)	8 (1%)	18	53
All	All	1568/1618 (97%)	1352 (86%)	201 (13%)	15 (1%)	18	53

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	757	LEU
1	A	181	ASP
1	A	435	GLY
1	A	516	SER
1	A	830	SER
1	B	76	ASP
1	B	681	PHE
1	B	730	GLU
1	A	674	SER
1	B	314	SER
1	B	680	LYS
1	A	752	PRO
1	B	568	LYS
1	B	593	ASP
1	B	498	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	692/706 (98%)	634 (92%)	58 (8%)	13	43
1	B	692/706 (98%)	642 (93%)	50 (7%)	17	50
All	All	1384/1412 (98%)	1276 (92%)	108 (8%)	15	46

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LYS
1	A	30	SER
1	A	63	LEU
1	A	90	TYR
1	A	95	LEU
1	A	100	ILE
1	A	128	ASP
1	A	136	LEU
1	A	150	LEU
1	A	167	ASN
1	A	169	LYS
1	A	205	LYS
1	A	209	THR
1	A	210	ASN
1	A	211	THR
1	A	213	THR
1	A	220	VAL
1	A	228	THR
1	A	237	THR
1	A	243	LEU
1	A	245	SER
1	A	247	ARG
1	A	270	ASN
1	A	274	ASN
1	A	337	LEU
1	A	340	THR
1	A	379	VAL
1	A	382	GLU
1	A	390	ASP
1	A	391	LEU
1	A	426	ARG
1	A	457	LYS
1	A	466	LYS
1	A	486	ILE
1	A	487	THR
1	A	493	LEU
1	A	509	GLU
1	A	510	ASP
1	A	543	LEU
1	A	573	TYR
1	A	577	LEU
1	A	579	ASN

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Mol	Chain	Res	Type
1	A	613	TYR
1	A	635	MET
1	A	636	VAL
1	A	652	LEU
1	A	678	ASN
1	A	683	LEU
1	A	714	ARG
1	A	722	ASP
1	A	753	LYS
1	A	756	ASP
1	A	761	ILE
1	A	788	SER
1	A	795	LYS
1	A	799	THR
1	A	808	SER
1	A	827	VAL
1	B	34	HIS
1	B	63	LEU
1	B	90	TYR
1	B	100	ILE
1	B	118	ASP
1	B	128	ASP
1	B	169	LYS
1	B	184	ARG
1	B	210	ASN
1	B	211	THR
1	B	213	THR
1	B	217	ASP
1	B	219	GLN
1	B	245	SER
1	B	274	ASN
1	B	287	GLU
1	B	300	VAL
1	B	305	GLN
1	B	337	LEU
1	B	353	PHE
1	B	363	LYS
1	B	378	THR
1	B	382	GLU
1	B	386	ARG
1	B	405	GLU
1	B	426	ARG

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Mol	Chain	Res	Type
1	B	453	ASN
1	B	473	GLU
1	B	489	ARG
1	B	502	LEU
1	B	507	ILE
1	B	560	SER
1	B	568	LYS
1	B	573	TYR
1	B	577	LEU
1	B	579	ASN
1	B	597	LEU
1	B	613	TYR
1	B	636	VAL
1	B	638	SER
1	B	652	LEU
1	B	674	SER
1	B	683	LEU
1	B	714	ARG
1	B	722	ASP
1	B	727	GLU
1	B	733	GLU
1	B	751	SER
1	B	763	ASN
1	B	828	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	34	HIS
1	A	62	HIS
1	A	167	ASN
1	A	270	ASN
1	A	274	ASN
1	A	284	ASN
1	A	369	GLN
1	A	376	ASN
1	A	410	HIS
1	A	450	HIS
1	A	453	ASN
1	A	459	HIS
1	A	481	ASN

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Mol	Chain	Res	Type
1	A	566	GLN
1	A	579	ASN
1	A	696	ASN
1	A	822	GLN
1	B	34	HIS
1	B	96	GLN
1	B	167	ASN
1	B	239	ASN
1	B	270	ASN
1	B	274	ASN
1	B	305	GLN
1	B	332	GLN
1	B	341	HIS
1	B	410	HIS
1	B	459	HIS
1	B	481	ASN
1	B	522	HIS
1	B	541	ASN
1	B	547	GLN
1	B	566	GLN
1	B	579	ASN
1	B	798	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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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
2	NBG	A	1	-	15,15,15	0.53	0	21,21,21	0.79	0
3	PLP	A	832	1	16,16,16	1.19	1 (6%)	22,23,23	1.04	2 (9%)
4	AVF	A	833	-	30,33,33	1.23	4 (13%)	44,47,47	1.66	6 (13%)
2	NBG	B	2	-	15,15,15	0.75	1 (6%)	21,21,21	1.48	4 (19%)
3	PLP	B	832	1	16,16,16	2.65	5 (31%)	22,23,23	1.46	4 (18%)
4	AVF	B	833	-	30,33,33	1.27	4 (13%)	44,47,47	1.69	9 (20%)

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	NBG	A	1	-	-	0/5/26/26	0/1/1/1
3	PLP	A	832	1	-	0/8/8/8	0/1/1/1
4	AVF	A	833	-	-	0/16/30/30	0/3/3/3
2	NBG	B	2	-	-	0/5/26/26	0/1/1/1
3	PLP	B	832	1	-	0/8/8/8	0/1/1/1
4	AVF	B	833	-	-	0/16/30/30	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	832	PLP	C3-C2	-8.27	1.35	1.40
3	B	832	PLP	C4-C5	-3.84	1.37	1.42
4	A	833	AVF	C13-N12	-3.35	1.35	1.41
4	B	833	AVF	C11-N10	-3.11	1.32	1.39
3	B	832	PLP	C4-C3	-3.06	1.35	1.40
4	B	833	AVF	C13-N12	-2.89	1.36	1.41
4	B	833	AVF	C18-N21	-2.62	1.35	1.41
4	B	833	AVF	C7-N10	-2.54	1.33	1.37
4	A	833	AVF	C11-N10	-2.45	1.34	1.39
4	A	833	AVF	C7-N10	-2.35	1.33	1.37
3	B	832	PLP	P-O3P	-2.23	1.45	1.54
4	A	833	AVF	C18-N21	-2.09	1.36	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	832	PLP	P-O2P	-2.06	1.46	1.54
2	B	2	NBG	C1-N1	2.04	1.45	1.43
3	A	832	PLP	C2-N1	2.20	1.38	1.33

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	833	AVF	C17-C18-N21	-5.33	113.91	122.28
4	A	833	AVF	C7-N10-C11	-5.12	122.95	128.13
4	B	833	AVF	C7-N10-C11	-4.35	123.72	128.13
4	A	833	AVF	C17-C18-N21	-4.35	115.45	122.28
3	B	832	PLP	O4A-C4A-C4	-3.44	117.17	125.08
4	A	833	AVF	C16-C15-C14	-3.25	119.03	123.29
3	B	832	PLP	C2A-C2-C3	-2.91	117.50	120.96
4	B	833	AVF	C25-N21-C18	-2.51	110.52	116.33
3	A	832	PLP	C5-C6-N1	-2.24	120.07	123.87
4	B	833	AVF	C6-C5-C4	-2.23	120.03	121.59
3	A	832	PLP	O4A-C4A-C4	-2.21	120.00	125.08
4	B	833	AVF	C16-C15-C14	-2.14	120.49	123.29
4	B	833	AVF	C14-C13-C18	-2.12	117.58	119.57
4	A	833	AVF	C18-C13-N12	2.23	122.78	118.68
4	B	833	AVF	C13-C14-C15	2.33	121.37	117.75
2	B	2	NBG	O5-C1-C2	2.34	112.24	109.84
3	B	832	PLP	C2A-C2-N1	2.39	122.66	117.89
3	B	832	PLP	O4P-P-O1P	2.50	113.48	106.47
2	B	2	NBG	O5-C5-C6	2.69	112.86	106.41
4	A	833	AVF	C13-C14-C15	2.87	122.20	117.75
4	B	833	AVF	C5-C6-C1	2.93	120.44	118.59
4	A	833	AVF	C13-C18-N21	3.12	126.11	120.17
4	B	833	AVF	C13-C18-N21	3.13	126.14	120.17
2	B	2	NBG	C4-C3-C2	3.15	116.39	110.84
2	B	2	NBG	C3-C2-C1	3.69	115.31	109.93

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	832	PLP	8	0
4	A	833	AVF	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	832	PLP	2	0
4	B	833	AVF	6	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	790/809 (97%)	-0.28	0 100 100	41, 56, 79, 86	0
1	B	790/809 (97%)	-0.32	0 100 100	38, 52, 68, 75	0
All	All	1580/1618 (97%)	-0.30	0 100 100	38, 54, 76, 86	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	NBG	B	2	15/15	0.93	0.23	1.06	57,58,60,61	0
4	AVF	B	833	31/31	0.96	0.23	0.75	51,53,56,56	0
3	PLP	A	832	16/16	0.94	0.23	0.39	43,46,49,49	0
3	PLP	B	832	16/16	0.97	0.19	0.35	42,45,47,47	0
2	NBG	A	1	15/15	0.96	0.22	0.04	52,53,55,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	AVF	A	833	31/31	0.97	0.20	-0.06	52,55,56,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.