



Full wwPDB X-ray Structure Validation Report i

Feb 28, 2014 – 10:10 PM GMT

PDB ID : 1ORW
Title : Crystal Structure of Porcine Dipeptidyl Peptidase IV (CD26) in Complex with a Peptidomimetic Inhibitor
Authors : Engel, M.; Hoffmann, T.; Wagner, L.; Wermann, M.; Heiser, U.; Kiefersauer, R.; Huber, R.; Bode, W.; Demuth, H.U.; Brandstetter, H.
Deposited on : 2003-03-16
Resolution : 2.84 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

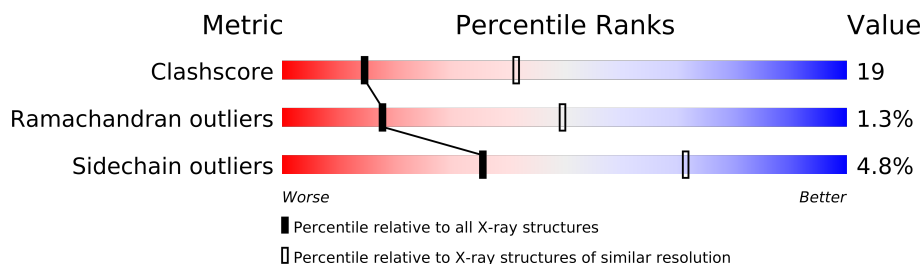
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	FAILED
Percentile statistics	:	21963
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.84 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	79885	2848 (2.88-2.80)
Ramachandran outliers	78287	2786 (2.88-2.80)
Sidechain outliers	78261	2789 (2.88-2.80)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	728	
1	B	728	
1	C	728	
1	D	728	

2 Entry composition i

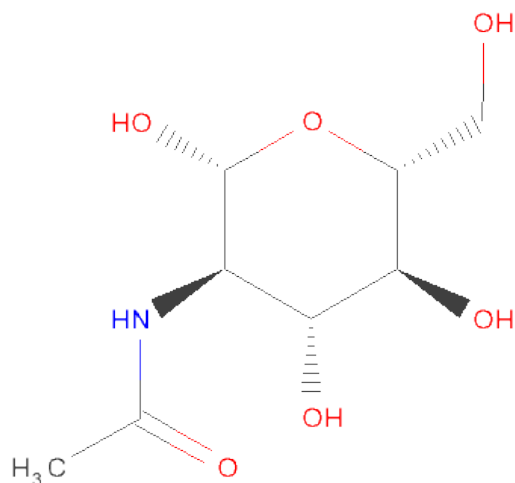
There are 7 unique types of molecules in this entry. The entry contains 25262 atoms, of which 0 are hydrogen and 0 are deuterium.

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 dipeptidyl peptidase IV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	728	Total	C	N	O	S	71	0	0
			5966	3825	986	1132	23			
1	B	728	Total	C	N	O	S	42	0	0
			5966	3825	986	1132	23			
1	C	728	Total	C	N	O	S	62	0	0
			5966	3825	986	1132	23			
1	D	728	Total	C	N	O	S	36	0	0
			5966	3825	986	1132	23			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	3	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	2	Total	C	N	O	0	0
			28	16	2	10		
3	A	2	Total	C	N	O	0	0
			28	16	2	10		
3	B	2	Total	C	N	O	0	0
			28	16	2	10		
3	C	2	Total	C	N	O	0	0
			28	16	2	10		
3	D	2	Total	C	N	O	0	0
			28	16	2	10		
3	D	2	Total	C	N	O	0	0
			28	16	2	10		

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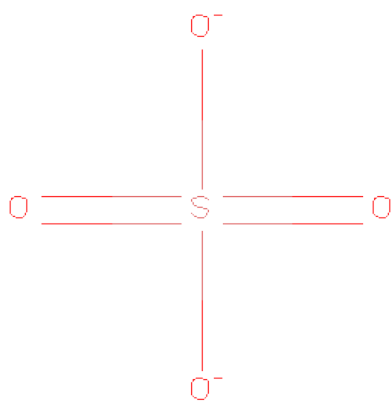
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	D	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is a polymer of unknown type called SUGAR (3-MER).

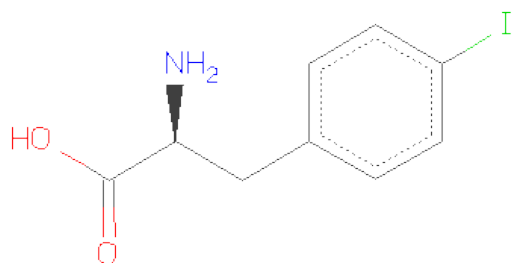
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	3	Total	C	N	O	0	0
			39	22	2	15		
4	D	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 5 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is IODO-PHENYLALANINE (three-letter code: PHI, P2Y) (formula: C₉H₁₀INO₂, C₅H₁₂N₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	2	Total	C	I	N	O	0	0
			19	14	1	3	1		
6	B	2	Total	C	I	N	O	0	0
			19	14	1	3	1		
6	C	2	Total	C	I	N	O	0	0
			19	14	1	3	1		
6	D	2	Total	C	I	N	O	0	0
			19	14	1	3	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	206	Total	O	0	0
			206	206		
7	B	226	Total	O	0	0
			226	226		
7	C	213	Total	O	0	0
			213	213		
7	D	173	Total	O	0	0
			173	173		

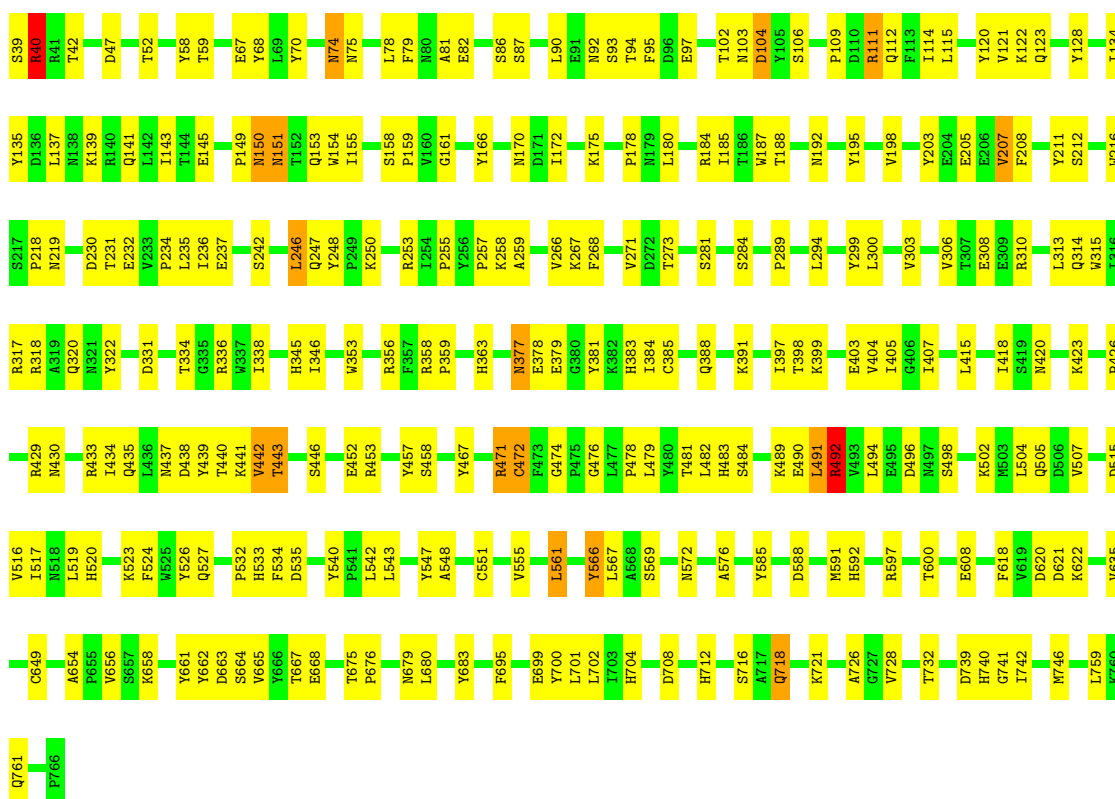
3 Residue-property plots

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

Note EDS failed to run properly.

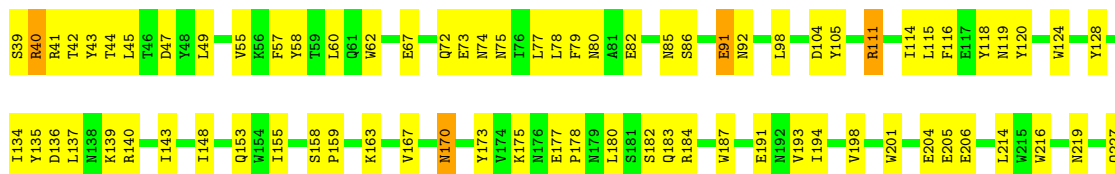
- Molecule 1: dipeptidyl peptidase IV

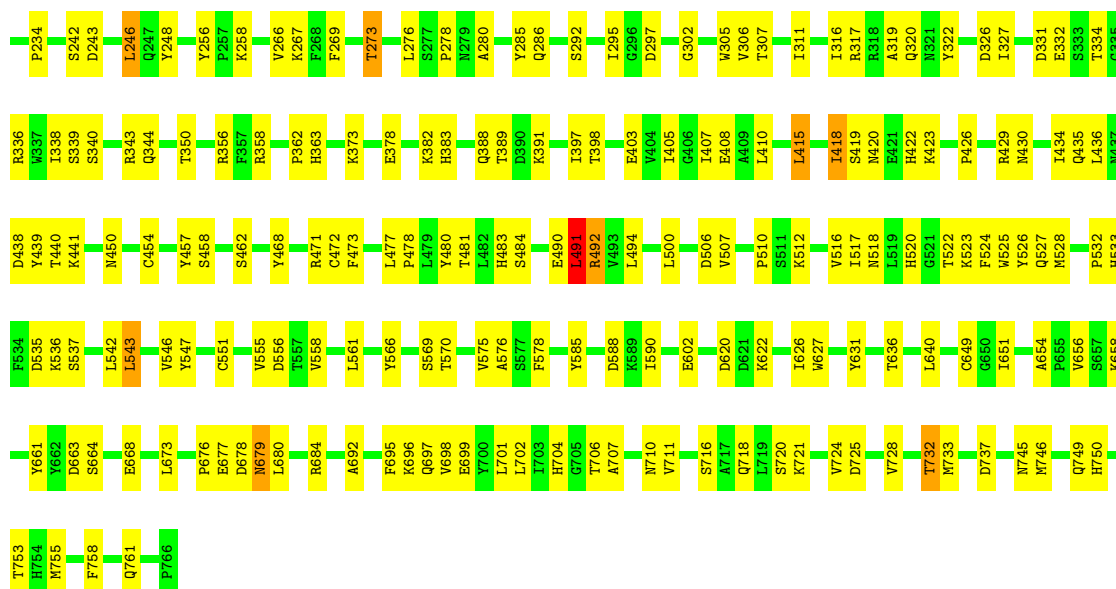
Chain A:



- Molecule 1: dipeptidyl peptidase IV

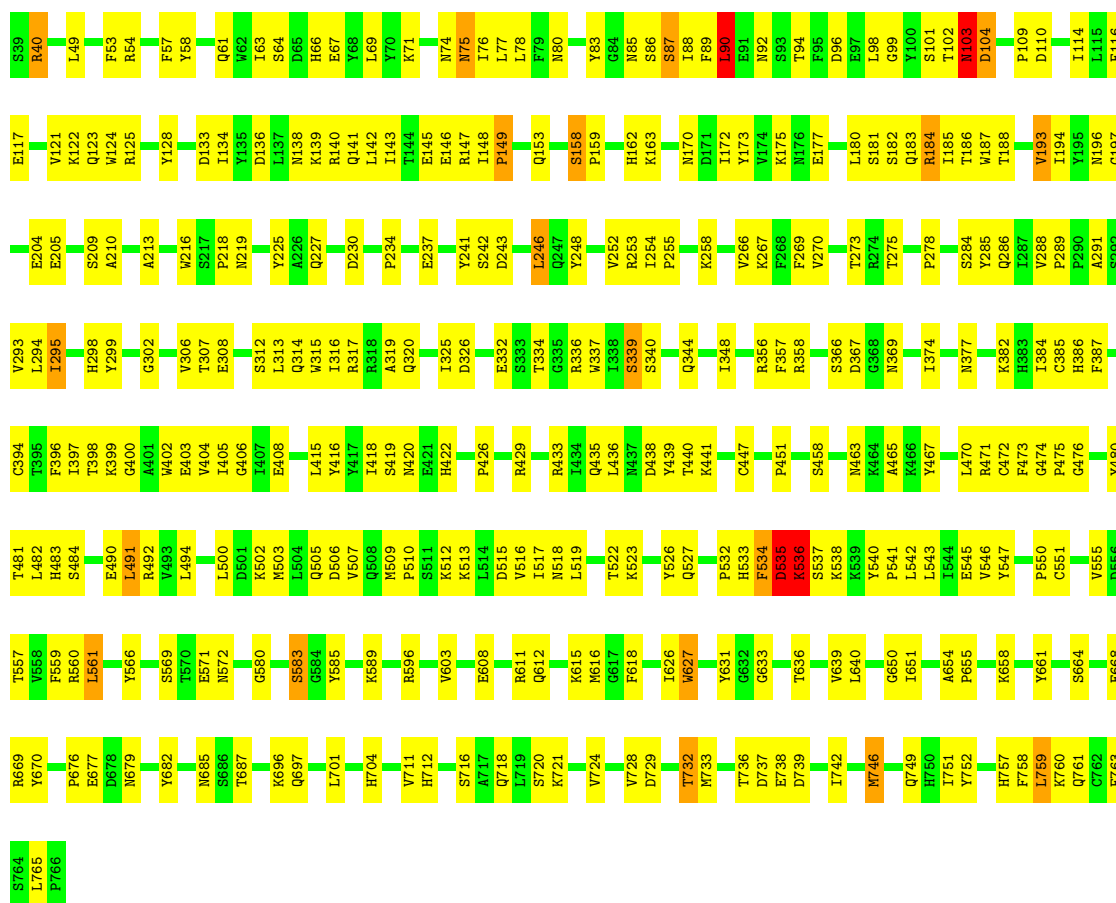
Chain B:





• Molecule 1: dipeptidyl peptidase IV

Chain C:



• Molecule 1: dipeptidyl peptidase IV

Chain D:

Y700	V603	S511	I295	E204	N119	S39
L701	E604	K512	I407	E205	K122	R40
L702	D605	R513	A408	E206	Q123	R41
L703		L514	A409	E207	W124	
H704	E608	D515	L410	F208		L45
	A609	V516	L415			T46
A707	T610	I517	L419	Y211	S127	D47
	R611	N518	S419	S212	Y128	Y48
V711	Q612	G521	N420	W216	D133	L49
H712	F613	T522	A421	S217	I134	R50
F713		K523	H422	P218	S51	S51
Q714	D620	F524	R423	P219	Y135	T52
Q715		R525	G424	N219	D136	F53
S716	T626	Y526	H425	F222		S54
A717	W629	Q527	L434	L223	K139	
Q718	R630	P532	Q435	A224	R140	W62
Q719	G632		L436		Q141	L63
D725		D535	S446	F228	L142	S64
V728		R536	C447		I143	D65
	V635	R537	E448	P234	T144	R66
T732	T636	K538	E457	L235	E145	E67
M733		K539	B453	I236	E146	Y68
W734	L640	Y540	C454			
Y735		P541	Y457	Y241	N150	K71
T736	C649	I544	N463	S242	N151	Q72
D737	G650		K464	D243	T152	E73
E738	A654	A548	K465	E244	Q153	N74
	P655	G549	A466	S245	W154	N75
G741	V656	P550	Y467	L246	I155	L77
I742	S657	C551	B471	Q247	S158	L78
A743	K658	K554	C472	Y248	P159	F79
S744		V555		R253	K163	N80
	Y661		G476	L254	E82	A81
Q749	Y662	L561	L477	P255	Y166	Y83
H750	D663		P478	N263	V167	G84
I751	S664	Y566	L479	P264	N170	N85
	V665	L567	Y480	T265	D171	S86
M755	T667	A668	T481	V266	E177	S87
S756	E668	S569	L482	K267	P178	I88
H757	R669	T570	S487	F268	N179	F89
		E571	L491	F269	L180	L90
	L673	N572	R492	V270		F91
	P674	I573	K502	V271	R184	N92
	T675	S577	N503	T273		L98
	P676	R581	K504	L276	K190	N103
	E677	I590	M505	S284	E191	D104
	D678	M591	L504	Y285	N192	Y105
N679	L680	M595	O505	V288	V193	S106
		N596	B506	T289	I194	V107
		G599	V507	F290	Y195	
		T600	P510	A291	N196	D110
				L294	G197	R111
					V198	I114
					T199	
					Y203	Y118

4 Data and refinement statistics

EDS failed to run properly - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	61.97Å 117.71Å 133.56Å 112.65° 94.81° 91.17°	Depositor
Resolution (Å)	29.79 – 2.84	Depositor
% Data completeness (in resolution range)	96.3 (29.79-2.84)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.12 (at 2.85Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.187 , 0.246	Depositor
Wilson B-factor (Å ²)	30.5	Xtriage
Anisotropy	0.613	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 157559 reflections	Xtriage
Total number of atoms	25262	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PHI, BMA, P2Y, NAG, SO4

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	0.42	0/6141	0.67	1/8353 (0.0%)
1	B	0.42	0/6141	0.67	1/8353 (0.0%)
1	C	0.43	0/6141	0.70	2/8353 (0.0%)
1	D	0.39	0/6141	0.66	1/8353 (0.0%)
All	All	0.42	0/24564	0.68	5/33412 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	104	ASP	N-CA-C	-8.55	87.90	111.00
1	C	103	ASN	N-CA-C	7.38	130.91	111.00
1	B	656	VAL	N-CA-C	-5.32	96.65	111.00
1	A	656	VAL	N-CA-C	-5.18	97.01	111.00
1	D	656	VAL	N-CA-C	-5.09	97.26	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	468	TYR	Sidechain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5966	0	5662	207	0
1	B	5966	0	5662	212	0
1	C	5966	0	5661	264	0
1	D	5966	0	5662	247	0
2	A	56	0	52	1	0
2	B	56	0	52	5	0
2	C	70	0	65	2	0
2	D	28	0	26	1	0
3	A	56	0	50	1	0
3	B	28	0	25	0	0
3	C	28	0	25	0	0
3	D	84	0	75	1	0
4	B	39	0	34	1	0
4	D	39	0	34	2	0
5	A	5	0	0	0	0
5	B	5	0	0	0	0
5	C	5	0	0	0	0
5	D	5	0	0	0	0
6	A	19	0	18	5	0
6	B	19	0	18	7	0
6	C	19	0	18	7	0
6	D	19	0	18	8	0
7	A	206	0	0	10	0
7	B	226	0	0	14	0
7	C	213	0	0	18	0
7	D	173	0	0	5	0
All	All	25262	0	23157	910	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 19.

All (910) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:358:ARG:NH2	6:D:807:PHI:I	2.51	1.13

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:358:ARG:NH2	6:B:803:PHI:I	2.57	1.08
1:A:358:ARG:NH2	6:A:801:PHI:I	2.60	1.05
1:B:358:ARG:NH1	6:B:803:PHI:I	2.65	0.99
1:C:535:ASP:C	1:C:536:LYS:HD3	1.83	0.99
1:C:358:ARG:NH2	6:C:805:PHI:I	2.69	0.95
1:B:358:ARG:CZ	6:B:803:PHI:I	2.84	0.95
1:D:358:ARG:CZ	6:D:807:PHI:I	2.84	0.94
1:A:388:GLN:HB2	1:A:391:LYS:HB2	1.51	0.92
1:D:75:ASN:ND2	1:D:92:ASN:H	1.69	0.90
1:A:40:ARG:HH11	1:A:40:ARG:HB2	1.35	0.90
1:B:134:ILE:HG21	1:B:178:PRO:HB3	1.53	0.90
1:C:77:LEU:HD23	1:C:88:ILE:HA	1.51	0.89
1:C:253:ARG:HH21	1:D:253:ARG:NH2	1.69	0.89
1:C:536:LYS:HG2	1:C:537:SER:H	1.39	0.86
1:A:75:ASN:HB3	1:A:92:ASN:N	1.91	0.86
1:A:492:ARG:HH21	1:A:492:ARG:HB3	1.41	0.83
1:A:237:GLU:HG2	1:A:253:ARG:HG2	1.60	0.83
1:A:492:ARG:HB3	1:A:492:ARG:NH2	1.92	0.82
1:A:540:TYR:HE2	1:A:572:ASN:HD22	1.28	0.82
1:B:184:ARG:NH1	1:B:187:TRP:HA	1.96	0.81
1:C:640:LEU:HD11	1:C:650:GLY:HA3	1.63	0.80
1:B:170:ASN:N	1:B:170:ASN:HD22	1.78	0.80
1:A:358:ARG:CZ	6:A:801:PHI:I	3.00	0.79
1:D:408:GLU:HG2	7:D:1031:HOH:O	1.83	0.79
1:C:481:THR:OG1	1:C:483:HIS:HE1	1.66	0.79
1:D:291:ALA:O	1:D:295:ILE:HG13	1.81	0.79
1:D:654:ALA:HA	1:D:704:HIS:CD2	2.18	0.78
1:C:358:ARG:CZ	6:C:805:PHI:I	3.01	0.78
1:B:704:HIS:HD2	1:B:716:SER:OG	1.67	0.78
1:B:316:ILE:HD11	1:B:320:GLN:HA	1.64	0.78
1:D:288:VAL:HG13	1:D:289:PRO:HD2	1.64	0.78
1:B:388:GLN:HB3	1:B:391:LYS:HB2	1.64	0.77
1:D:75:ASN:HD22	1:D:92:ASN:H	1.34	0.76
1:D:472:CYS:O	1:D:478:PRO:HA	1.87	0.75
1:C:242:SER:HB3	1:C:246:LEU:HD12	1.67	0.75
1:B:75:ASN:ND2	1:B:92:ASN:H	1.85	0.75
1:C:420:ASN:HD22	1:C:426:PRO:HA	1.52	0.75
1:C:40:ARG:HB2	1:C:506:ASP:O	1.88	0.73
1:A:153:GLN:HE22	1:A:170:ASN:ND2	1.87	0.73
1:D:640:LEU:HD11	1:D:650:GLY:HA3	1.71	0.73
1:B:516:VAL:HG13	1:B:524:PHE:O	1.89	0.73
1:C:183:GLN:OE1	1:C:278:PRO:HA	1.88	0.73

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:114:ILE:HG23	1:B:135:TYR:HB3	1.71	0.73
1:C:90:LEU:HD13	1:C:90:LEU:O	1.89	0.73
1:D:680:LEU:HD11	1:D:684:ARG:HE	1.53	0.73
1:C:513:LYS:HE2	1:C:515:ASP:HB2	1.72	0.72
1:C:704:HIS:HD2	1:C:716:SER:OG	1.72	0.72
1:C:75:ASN:ND2	1:C:92:ASN:HB2	2.06	0.71
1:B:184:ARG:HH12	1:B:187:TRP:HA	1.54	0.71
1:C:320:GLN:OE1	1:C:669:ARG:HD3	1.91	0.71
1:D:694:ASN:N	1:D:694:ASN:HD22	1.88	0.70
1:C:103:ASN:HA	1:C:117:GLU:O	1.90	0.70
1:D:718:GLN:HE21	1:D:718:GLN:HA	1.56	0.70
1:C:733:MET:HA	1:D:732:THR:CG2	2.22	0.70
1:C:746:MET:HG3	1:D:725:ASP:OD1	1.91	0.70
1:C:159:PRO:HD3	1:C:216:TRP:CB	2.21	0.70
1:C:367:ASP:OD2	1:C:369:ASN:HB2	1.92	0.70
1:C:357:PHE:CD1	6:C:805:PHI:HE2	2.26	0.69
1:B:114:ILE:CG2	1:B:135:TYR:HB3	2.23	0.69
1:A:74:ASN:O	1:A:95:PHE:HE2	1.75	0.69
1:D:177:GLU:HB2	1:D:180:LEU:HD23	1.74	0.69
1:D:193:VAL:HG22	1:D:194:ILE:HG12	1.75	0.69
1:B:408:GLU:HG2	7:B:921:HOH:O	1.90	0.69
1:D:317:ARG:HD2	1:D:322:TYR:HB3	1.75	0.69
1:C:285:TYR:CE1	1:C:336:ARG:HB2	2.28	0.69
1:B:378:GLU:CD	1:B:378:GLU:H	1.96	0.69
1:A:718:GLN:HE22	1:A:721:LYS:NZ	1.91	0.69
1:A:492:ARG:CB	1:A:492:ARG:HH21	2.05	0.68
1:D:190:LYS:HG2	1:D:193:VAL:CG1	2.23	0.68
1:C:253:ARG:HH21	1:D:253:ARG:HH22	1.41	0.68
1:C:732:THR:O	1:D:732:THR:HG22	1.93	0.68
1:B:332:GLU:HG3	7:B:986:HOH:O	1.94	0.68
1:B:356:ARG:HB3	1:B:551:CYS:SG	2.34	0.68
1:B:458:SER:OG	1:B:471:ARG:HB2	1.93	0.68
1:A:718:GLN:HA	1:A:718:GLN:HE21	1.58	0.68
1:D:357:PHE:HB3	6:D:807:PHI:I	2.64	0.68
1:A:242:SER:HB3	1:A:246:LEU:HD12	1.75	0.68
1:D:358:ARG:NE	6:D:807:PHI:I	2.97	0.67
1:A:502:LYS:O	1:A:505:GLN:HG2	1.94	0.67
1:A:453:ARG:NH2	1:A:479:LEU:HB2	2.10	0.67
1:C:175:LYS:HG3	1:C:182:SER:HB3	1.75	0.67
1:B:334:THR:OG1	1:B:336:ARG:HG2	1.94	0.67
1:C:519:LEU:HD22	1:C:608:GLU:OE1	1.94	0.67
1:C:184:ARG:HH11	1:C:187:TRP:HA	1.60	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:67:GLU:HB3	1:A:78:LEU:HD11	1.75	0.67
1:C:704:HIS:HE1	1:C:711:VAL:O	1.77	0.67
1:A:378:GLU:H	1:A:378:GLU:CD	1.97	0.67
1:C:184:ARG:HD3	1:C:186:THR:O	1.95	0.66
1:D:136:ASP:CG	1:D:139:LYS:HG2	2.15	0.66
1:B:438:ASP:OD2	1:B:441:LYS:HE3	1.95	0.66
1:C:134:ILE:HD11	1:C:148:ILE:HD11	1.78	0.66
1:C:475:PRO:HD3	1:C:557:THR:HB	1.78	0.66
1:A:491:LEU:O	1:A:492:ARG:HB3	1.95	0.66
1:D:167:VAL:HG21	1:D:198:VAL:HG13	1.77	0.66
1:B:159:PRO:HD3	1:B:216:TRP:CB	2.26	0.66
1:D:273:THR:HA	1:D:276:LEU:HD22	1.78	0.66
1:C:732:THR:HG22	1:D:732:THR:HG23	1.77	0.65
1:D:696:LYS:HG3	1:D:728:VAL:HG22	1.79	0.65
1:C:733:MET:HA	1:D:732:THR:HG21	1.79	0.65
1:A:433:ARG:NH1	1:A:443:THR:HG21	2.11	0.65
1:C:720:SER:O	1:C:724:VAL:HG23	1.96	0.65
1:D:67:GLU:CD	1:D:111:ARG:HH12	2.00	0.65
1:D:219:ASN:HB2	1:D:308:GLU:CD	2.17	0.65
1:D:320:GLN:OE1	1:D:669:ARG:HD3	1.96	0.65
1:B:651:ILE:HG21	1:B:755:MET:HE2	1.78	0.65
1:B:167:VAL:HG21	1:B:198:VAL:HG13	1.79	0.65
1:A:103:ASN:O	1:A:104:ASP:HB2	1.97	0.64
1:D:532:PRO:HD3	1:D:569:SER:HA	1.79	0.64
1:D:453:ARG:HG3	1:D:476:GLY:HA3	1.80	0.64
1:A:93:SER:C	1:A:95:PHE:H	1.99	0.64
1:C:159:PRO:HD3	1:C:216:TRP:HB3	1.78	0.64
2:C:767(A):NAG:H61	7:C:1112:HOH:O	1.96	0.64
1:B:170:ASN:H	1:B:170:ASN:HD22	1.42	0.64
1:C:400:GLY:HA3	1:C:402:TRP:NE1	2.12	0.64
1:A:75:ASN:ND2	1:A:92:ASN:ND2	2.46	0.64
1:B:72:GLN:HG2	1:B:73:GLU:HG2	1.80	0.64
1:D:114:ILE:HG22	1:D:135:TYR:HB3	1.79	0.64
1:B:67:GLU:HB3	1:B:78:LEU:HD11	1.80	0.64
1:B:316:ILE:CD1	1:B:320:GLN:HA	2.28	0.63
1:A:746:MET:HG3	1:B:725:ASP:HA	1.80	0.63
1:B:481:THR:OG1	1:B:483:HIS:HE1	1.81	0.63
1:D:150:ASN:O	1:D:151:ASN:HB2	1.96	0.63
1:C:357:PHE:HB3	6:C:805:PHI:I	2.69	0.63
1:B:410:LEU:HD13	1:B:415:LEU:CD2	2.28	0.63
1:D:153:GLN:HE22	1:D:170:ASN:ND2	1.97	0.63
1:C:420:ASN:ND2	1:C:426:PRO:HA	2.13	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:153:GLN:HE22	1:C:170:ASN:ND2	1.97	0.62
1:C:358:ARG:NH1	6:C:805:PHI:I	3.03	0.62
1:B:177:GLU:HB2	1:B:180:LEU:HB2	1.81	0.62
1:B:153:GLN:HE22	1:B:170:ASN:ND2	1.97	0.62
1:D:114:ILE:CG2	1:D:135:TYR:HB3	2.29	0.62
1:B:305:TRP:CE2	1:B:311:ILE:HD12	2.35	0.62
1:B:41:ARG:O	1:B:507:VAL:HG23	1.99	0.62
1:C:136:ASP:O	1:C:140:ARG:HA	2.00	0.61
1:D:353:TRP:CZ2	1:D:591:MET:HE3	2.34	0.61
1:C:54:ARG:O	1:C:500:LEU:HD13	2.00	0.61
1:A:75:ASN:HD22	1:A:92:ASN:ND2	1.98	0.61
1:D:299:TYR:HB2	1:D:316:ILE:CG2	2.31	0.61
1:B:631:TYR:H	6:B:804:P2Y:HNA2	1.47	0.61
1:D:377:ASN:HD22	1:D:381:TYR:HB2	1.66	0.61
1:D:536:LYS:O	1:D:537:SER:CB	2.48	0.61
1:A:481:THR:OG1	1:A:483:HIS:HE1	1.84	0.61
1:D:364:PHE:CD2	1:D:371:PHE:HB3	2.36	0.61
1:D:67:GLU:HB3	1:D:78:LEU:HD11	1.82	0.61
1:A:172:ILE:HB	1:A:185:ILE:HB	1.82	0.61
1:D:502:LYS:O	1:D:505:GLN:HG2	2.01	0.60
1:C:80:ASN:HB2	2:C:767(A):NAG:H82	1.81	0.60
1:A:75:ASN:ND2	1:A:92:ASN:HD22	2.00	0.60
1:C:288:VAL:HG11	1:C:294:LEU:HD11	1.82	0.60
1:A:377:ASN:HB3	1:A:379:GLU:H	1.66	0.60
1:B:651:ILE:HG21	1:B:755:MET:CE	2.31	0.60
1:B:746:MET:HG2	7:B:1062:HOH:O	2.02	0.60
1:C:415:LEU:HB2	1:C:436:LEU:HD11	1.84	0.59
1:C:658:LYS:HG3	1:C:687:THR:HG22	1.83	0.59
1:A:317:ARG:HG2	7:A:974:HOH:O	2.02	0.59
1:D:289:PRO:HB3	1:D:315:TRP:CD2	2.37	0.59
1:B:410:LEU:HD13	1:B:415:LEU:HD23	1.83	0.59
1:C:438:ASP:OD2	1:C:441:LYS:HG3	2.01	0.59
1:A:516:VAL:HG13	1:A:524:PHE:O	2.02	0.59
1:A:70:TYR:HB3	1:A:79:PHE:CE2	2.38	0.59
1:A:207:VAL:HG23	1:A:208:PHE:CD1	2.37	0.59
1:D:751:ILE:O	1:D:755:MET:HG3	2.02	0.59
1:B:316:ILE:HD11	1:B:320:GLN:CA	2.33	0.59
1:C:184:ARG:NH1	1:C:187:TRP:HA	2.17	0.59
1:D:504:LEU:HA	1:D:507:VAL:CG1	2.33	0.59
1:D:154:TRP:CE2	1:D:212:SER:HB3	2.38	0.59
1:A:75:ASN:HB3	1:A:92:ASN:H	1.67	0.59
1:C:463:ASN:C	1:C:465:ALA:H	2.06	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:420:ASN:HB2	1:B:426:PRO:HA	1.85	0.59
1:D:205:GLU:OE2	6:D:807:PHI:N	2.36	0.59
1:C:580:GLY:O	1:C:583:SER:OG	2.21	0.59
1:B:340:SER:O	1:B:344:GLN:HG3	2.03	0.59
1:D:236:ILE:HG12	1:D:712:HIS:CE1	2.38	0.59
1:A:299:TYR:CZ	1:A:665:VAL:HG22	2.38	0.59
1:A:58:TYR:CD2	1:A:494:LEU:HB3	2.36	0.59
1:C:253:ARG:NH2	1:D:253:ARG:NH2	2.45	0.58
1:D:242:SER:HB3	1:D:246:LEU:HD12	1.85	0.58
1:A:219:ASN:N	1:A:308:GLU:OE2	2.30	0.58
1:C:696:LYS:HG3	1:C:728:VAL:HG22	1.85	0.58
1:C:125:ARG:NH2	1:C:205:GLU:OE2	2.32	0.58
1:A:159:PRO:HB2	1:A:218:PRO:O	2.04	0.58
1:D:235:LEU:HD23	1:D:255:PRO:HA	1.84	0.58
1:B:80:ASN:HB3	1:B:85:ASN:OD1	2.03	0.58
1:C:173:TYR:CE2	1:C:184:ARG:HG3	2.39	0.58
1:D:536:LYS:O	1:D:537:SER:HB2	2.04	0.58
1:D:133:ASP:HB3	1:D:142:LEU:HD21	1.86	0.58
1:D:415:LEU:HB2	1:D:436:LEU:HD11	1.85	0.58
1:B:170:ASN:ND2	1:B:170:ASN:N	2.51	0.58
1:A:695:PHE:HB2	1:A:728:VAL:HG11	1.86	0.57
1:D:142:LEU:O	1:D:144:THR:HG23	2.04	0.57
1:A:331:ASP:HB2	1:A:338:ILE:HD12	1.87	0.57
1:A:234:PRO:HB2	1:B:248:TYR:CZ	2.38	0.57
1:B:704:HIS:CE1	1:B:711:VAL:O	2.57	0.57
1:C:291:ALA:O	1:C:295:ILE:HG13	2.05	0.57
1:C:313:LEU:HD12	1:C:313:LEU:N	2.19	0.57
1:C:543:LEU:HD22	1:C:759:LEU:HD11	1.85	0.57
1:D:299:TYR:CZ	1:D:665:VAL:HG22	2.39	0.57
1:A:658:LYS:HD3	1:A:661:TYR:CZ	2.40	0.57
1:D:357:PHE:CD1	6:D:807:PHI:HE2	2.40	0.57
1:C:718:GLN:HE21	1:C:718:GLN:HA	1.70	0.57
1:C:306:VAL:HG12	1:C:307:THR:HG23	1.86	0.56
1:B:191:GLU:O	1:B:193:VAL:HG23	2.05	0.56
1:C:458:SER:HG	1:C:473:PHE:HE1	1.53	0.56
1:B:673:LEU:HD12	1:B:673:LEU:N	2.19	0.56
1:C:739:ASP:HB2	7:C:954:HOH:O	2.05	0.56
1:A:93:SER:C	1:A:95:PHE:N	2.57	0.56
1:B:704:HIS:HE1	1:B:711:VAL:O	1.88	0.56
1:A:159:PRO:HD3	1:A:216:TRP:CB	2.35	0.56
1:C:248:TYR:CZ	1:D:234:PRO:HB2	2.41	0.56
1:D:526:TYR:HA	1:D:555:VAL:HG21	1.86	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:522:THR:HB	1:D:524:PHE:CE1	2.39	0.56
1:B:136:ASP:HB2	1:B:143:ILE:HD11	1.88	0.56
1:A:306:VAL:HB	1:A:310:ARG:HG2	1.87	0.56
1:A:597:ARG:O	1:A:597:ARG:HG3	2.05	0.56
1:C:484:SER:HB2	1:C:491:LEU:HD21	1.87	0.56
1:C:76:ILE:HD12	1:C:90:LEU:HD11	1.86	0.56
1:D:299:TYR:HB2	1:D:316:ILE:HG22	1.87	0.56
1:A:236:ILE:HG12	1:A:712:HIS:CE1	2.40	0.56
1:D:203:TYR:HA	1:D:207:VAL:HG13	1.87	0.56
1:B:704:HIS:CD2	1:B:716:SER:OG	2.55	0.56
1:B:415:LEU:HB2	1:B:436:LEU:HD11	1.88	0.56
1:B:39:SER:OG	1:B:40:ARG:N	2.37	0.56
1:C:57:PHE:HA	1:C:480:TYR:CE1	2.40	0.56
1:B:516:VAL:HG11	1:B:523:LYS:HD2	1.88	0.56
1:D:410:LEU:HD13	1:D:415:LEU:HD12	1.87	0.56
1:C:146:GLU:OE1	1:C:181:SER:HA	2.06	0.56
1:D:83:TYR:HB3	1:D:85:ASN:OD1	2.04	0.56
1:A:92:ASN:C	1:A:94:THR:H	2.09	0.56
1:C:64:SER:HB2	7:C:1113:HOH:O	2.06	0.56
1:C:67:GLU:HB3	1:C:78:LEU:HD11	1.88	0.55
1:D:87:SER:HB3	2:D:767(A):NAG:O6	2.06	0.55
1:B:42:THR:HB	1:B:569:SER:OG	2.05	0.55
1:C:299:TYR:HB2	1:C:316:ILE:HG13	1.87	0.55
1:B:60:LEU:C	1:B:60:LEU:HD12	2.26	0.55
1:D:532:PRO:CD	1:D:569:SER:HA	2.36	0.55
1:D:155:ILE:HG13	1:D:166:TYR:HB3	1.89	0.55
1:A:527:GLN:HB3	1:A:555:VAL:HG13	1.87	0.55
1:B:173:TYR:CE2	1:B:184:ARG:HG3	2.42	0.55
1:A:517:ILE:HG23	1:A:526:TYR:CE2	2.42	0.55
1:B:73:GLU:O	1:B:74:ASN:HB2	2.06	0.55
1:D:154:TRP:CD2	1:D:212:SER:HB3	2.42	0.55
1:D:356:ARG:HB3	1:D:551:CYS:SG	2.47	0.55
1:C:763:PHE:HB3	1:C:765:LEU:HG	1.88	0.55
1:A:446:SER:HB2	1:A:457:TYR:CZ	2.41	0.55
1:A:600:THR:HG22	3:A:773(A):NAG:HN2	1.72	0.54
1:C:273:THR:HB	7:C:1034:HOH:O	2.07	0.54
1:C:219:ASN:N	1:C:308:GLU:OE2	2.35	0.54
1:D:402:TRP:CD2	1:D:421:GLU:HB2	2.42	0.54
1:C:491:LEU:H	1:C:491:LEU:CD2	2.20	0.54
1:A:695:PHE:CB	1:A:728:VAL:HG11	2.38	0.54
1:C:502:LYS:O	1:C:505:GLN:HG2	2.08	0.54
1:C:340:SER:O	1:C:344:GLN:HG3	2.07	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:280:ALA:HB2	1:D:285:TYR:HD1	1.72	0.54
4:B:768(A):NAG:H62	4:B:769(B):NAG:H82	1.89	0.54
1:A:81:ALA:HA	1:A:482:LEU:HD21	1.90	0.54
1:D:548:ALA:HB3	1:D:635:VAL:HG21	1.90	0.54
1:C:334:THR:OG1	1:C:336:ARG:HG2	2.08	0.54
1:D:658:LYS:HB3	1:D:661:TYR:CD2	2.42	0.54
1:A:675:THR:C	1:A:680:LEU:HB2	2.28	0.54
1:A:676:PRO:HD3	1:A:680:LEU:HD22	1.90	0.54
1:C:536:LYS:HG2	1:C:537:SER:N	2.18	0.54
1:C:138:ASN:O	1:C:140:ARG:HG3	2.08	0.54
1:B:454:CYS:HB3	1:B:457:TYR:CE1	2.43	0.54
1:C:470:LEU:HD12	1:C:483:HIS:CE1	2.43	0.54
1:D:522:THR:HG22	1:D:523:LYS:N	2.22	0.54
1:D:159:PRO:HD3	1:D:216:TRP:CB	2.37	0.54
1:C:757:HIS:O	1:C:761:GLN:HG2	2.08	0.54
1:C:242:SER:CB	1:C:246:LEU:HD12	2.35	0.54
1:C:535:ASP:O	1:C:536:LYS:HD3	2.08	0.54
1:D:179:ASN:C	1:D:180:LEU:HD22	2.28	0.54
1:B:397:ILE:HG13	1:B:398:THR:HG23	1.89	0.54
1:A:446:SER:HB2	1:A:457:TYR:CE1	2.43	0.54
1:B:183:GLN:HE22	1:B:278:PRO:HA	1.73	0.54
1:C:483:HIS:HA	1:C:491:LEU:HD23	1.90	0.53
1:D:718:GLN:NE2	1:D:718:GLN:HA	2.22	0.53
1:A:67:GLU:CD	1:A:111:ARG:HH12	2.12	0.53
1:C:676:PRO:HG2	1:C:677:GLU:OE2	2.09	0.53
1:B:422:HIS:CD2	1:B:423:LYS:HD3	2.43	0.53
1:A:438:ASP:HB3	1:A:441:LYS:HD2	1.89	0.53
1:D:516:VAL:HG12	1:D:517:ILE:N	2.23	0.53
1:C:219:ASN:H	1:C:308:GLU:CD	2.11	0.53
1:C:633:GLY:HA3	1:C:655:PRO:HB3	1.90	0.53
1:C:704:HIS:CE1	1:C:711:VAL:O	2.60	0.53
1:C:253:ARG:NH2	1:D:253:ARG:HH21	2.06	0.53
1:C:336:ARG:HD2	7:C:1063:HOH:O	2.08	0.53
1:C:527:GLN:HB3	1:C:555:VAL:HG13	1.91	0.53
1:A:139:LYS:O	1:A:141:GLN:HG3	2.09	0.53
1:A:534:PHE:CZ	1:A:618:PHE:HB2	2.43	0.53
1:A:377:ASN:HB2	1:A:381:TYR:H	1.73	0.53
4:D:768(A):NAG:H62	4:D:769(B):NAG:HN2	1.73	0.53
1:C:536:LYS:CG	1:C:537:SER:H	2.13	0.53
1:D:676:PRO:HG2	1:D:677:GLU:OE1	2.07	0.53
1:B:331:ASP:HB2	1:B:338:ILE:CD1	2.38	0.53
1:A:620:ASP:O	1:A:622:LYS:N	2.42	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:362:PRO:HA	1:B:373:LYS:HB2	1.90	0.53
1:C:71:LYS:NZ	1:C:103:ASN:ND2	2.56	0.53
1:D:159:PRO:HD3	1:D:216:TRP:HB3	1.90	0.53
1:A:271:VAL:HG22	1:A:284:SER:HB3	1.89	0.53
1:B:732:THR:HG23	1:B:733:MET:N	2.24	0.53
1:B:484:SER:HB2	1:B:491:LEU:HD21	1.91	0.53
1:B:415:LEU:HB3	1:B:434:ILE:CG2	2.39	0.53
1:C:356:ARG:HD3	1:C:551:CYS:SG	2.49	0.53
1:D:51:SER:O	1:D:54:ARG:HD2	2.09	0.53
1:D:90:LEU:HD12	1:D:140:ARG:NH2	2.24	0.53
1:A:467:TYR:CD1	1:A:484:SER:HA	2.44	0.53
1:D:288:VAL:CG1	1:D:289:PRO:HD2	2.38	0.52
1:D:72:GLN:HE21	1:D:77:LEU:CD1	2.21	0.52
1:C:205:GLU:OE2	6:C:805:PHI:N	2.42	0.52
1:D:377:ASN:HB3	1:D:379:GLU:H	1.74	0.52
1:C:325:ILE:O	1:C:344:GLN:HA	2.09	0.52
1:D:177:GLU:CB	1:D:180:LEU:HD23	2.38	0.52
1:A:726:ALA:HB3	1:A:728:VAL:HG23	1.90	0.52
1:B:491:LEU:HB3	1:B:492:ARG:NH1	2.24	0.52
1:A:300:LEU:HB2	1:A:315:TRP:CZ3	2.44	0.52
1:B:184:ARG:HD3	1:B:187:TRP:CD2	2.44	0.52
1:A:47:ASP:HA	1:A:52:THR:HG23	1.91	0.52
1:A:496:ASP:OD2	1:A:498:SER:HB3	2.09	0.52
1:A:534:PHE:HZ	1:A:618:PHE:HB2	1.75	0.52
1:C:733:MET:HA	1:D:732:THR:HG22	1.89	0.52
1:B:305:TRP:CZ2	1:B:311:ILE:HD12	2.45	0.52
1:A:120:TYR:HE2	1:A:122:LYS:HB2	1.75	0.52
1:A:94:THR:O	1:A:94:THR:HG22	2.10	0.52
1:A:504:LEU:HA	1:A:507:VAL:HG12	1.91	0.52
1:C:736:THR:O	1:C:737:ASP:HB2	2.10	0.52
1:A:718:GLN:HA	1:A:718:GLN:NE2	2.24	0.52
1:D:379:GLU:HG2	1:D:379:GLU:O	2.10	0.52
1:A:114:ILE:HG22	1:A:135:TYR:HB3	1.92	0.52
1:B:696:LYS:HB2	7:B:955:HOH:O	2.09	0.52
1:B:327:ILE:HB	1:B:343:ARG:HB3	1.91	0.52
1:B:658:LYS:HB3	1:B:661:TYR:CD2	2.45	0.52
1:C:77:LEU:CD2	1:C:88:ILE:HG12	2.40	0.52
1:C:658:LYS:HG3	1:C:687:THR:CG2	2.40	0.52
1:A:248:TYR:CZ	1:B:234:PRO:HB2	2.44	0.52
1:D:118:TYR:O	1:D:119:ASN:HB2	2.09	0.52
1:A:281:SER:HB2	7:A:1044:HOH:O	2.10	0.52
1:B:397:ILE:HD12	1:B:434:ILE:HD13	1.91	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:88:ILE:HG21	1:D:91:GLU:HG3	1.92	0.51
1:D:354:VAL:CG1	1:D:359:PRO:HB3	2.40	0.51
1:A:205:GLU:OE2	6:A:801:PHI:HB3	2.10	0.51
1:D:75:ASN:HD22	1:D:92:ASN:N	2.04	0.51
1:C:177:GLU:HB2	1:C:180:LEU:HD23	1.92	0.51
1:B:631:TYR:N	6:B:804:P2Y:NA	2.52	0.51
1:B:41:ARG:NH1	1:B:47:ASP:OD1	2.43	0.51
1:C:219:ASN:ND2	7:C:908:HOH:O	2.40	0.51
1:B:148:ILE:HD13	1:B:155:ILE:HD12	1.92	0.51
1:A:516:VAL:HG11	1:A:523:LYS:HB2	1.92	0.51
1:C:534:PHE:O	1:C:535:ASP:C	2.49	0.51
1:B:651:ILE:HD11	1:B:758:PHE:HD2	1.76	0.51
1:B:510:PRO:HD3	1:B:569:SER:HB2	1.93	0.51
1:D:47:ASP:HA	1:D:52:THR:HG23	1.93	0.51
1:B:706:THR:HB	7:B:1038:HOH:O	2.10	0.51
1:B:104:ASP:OD1	1:B:105:TYR:N	2.40	0.51
1:C:83:TYR:HB2	1:C:85:ASN:OD1	2.11	0.51
1:B:175:LYS:HG2	1:B:182:SER:HB3	1.92	0.51
1:A:662:TYR:CE2	6:A:802:P2Y:HD2	2.46	0.51
1:D:139:LYS:O	1:D:141:GLN:HG3	2.11	0.50
1:D:273:THR:CA	1:D:276:LEU:HD22	2.41	0.50
1:D:518:ASN:HA	1:D:522:THR:O	2.11	0.50
1:C:416:TYR:CE2	1:C:433:ARG:HD3	2.46	0.50
1:D:289:PRO:HB3	1:D:315:TRP:CE2	2.46	0.50
1:D:191:GLU:O	1:D:193:VAL:HG12	2.11	0.50
1:B:331:ASP:HB2	1:B:338:ILE:HD12	1.92	0.50
1:B:45:LEU:HD21	1:B:753:THR:HA	1.92	0.50
1:D:271:VAL:HG22	1:D:284:SER:HB3	1.93	0.50
1:A:188:THR:HG21	7:A:1031:HOH:O	2.10	0.50
1:C:158:SER:OG	1:C:163:LYS:HB2	2.11	0.50
1:C:258:LYS:HD2	1:D:247:GLN:HG2	1.93	0.50
1:A:153:GLN:HE22	1:A:170:ASN:HD22	1.55	0.50
1:D:386:HIS:O	1:D:394:CYS:HB2	2.11	0.50
1:B:214:LEU:O	1:B:214:LEU:HD12	2.12	0.50
1:B:602:GLU:OE2	1:B:602:GLU:N	2.45	0.50
1:D:662:TYR:CE2	6:D:808:P2Y:HD2	2.47	0.50
1:B:67:GLU:CD	1:B:111:ARG:HH12	2.15	0.50
1:B:516:VAL:HG12	1:B:517:ILE:N	2.26	0.50
1:B:458:SER:HG	1:B:473:PHE:HE1	1.57	0.50
1:C:403:GLU:OE1	1:C:585:TYR:HA	2.11	0.50
1:C:317:ARG:HG2	7:C:990:HOH:O	2.09	0.50
1:C:721:LYS:HB3	7:C:947:HOH:O	2.11	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:403:GLU:OE1	1:A:585:TYR:HA	2.12	0.50
1:C:386:HIS:O	1:C:394:CYS:HB2	2.10	0.50
1:D:317:ARG:HB3	7:D:1008:HOH:O	2.12	0.50
1:C:463:ASN:C	1:C:465:ALA:N	2.65	0.50
1:C:270:VAL:HG11	1:C:337:TRP:CE2	2.46	0.50
1:D:539:LYS:HB3	1:D:620:ASP:HB2	1.93	0.50
1:C:148:ILE:HG23	1:C:149:PRO:HD2	1.94	0.50
1:C:512:LYS:HE3	1:C:527:GLN:NE2	2.27	0.50
1:A:42:THR:HB	1:A:569:SER:OG	2.12	0.50
1:B:285:TYR:CE1	1:B:336:ARG:HB2	2.47	0.50
1:A:159:PRO:HD3	1:A:216:TRP:HB3	1.93	0.50
1:D:554:LYS:HB3	1:D:577:SER:HB3	1.93	0.50
1:A:732:THR:OG1	1:B:733:MET:HA	2.12	0.49
1:A:235:LEU:HD23	1:A:255:PRO:HA	1.94	0.49
1:D:199:THR:CG2	1:D:208:PHE:HD2	2.25	0.49
1:B:405:ILE:HG13	1:B:429:ARG:HD2	1.92	0.49
1:C:540:TYR:HE2	1:C:572:ASN:HD22	1.61	0.49
1:D:139:LYS:HG3	1:D:141:GLN:HG3	1.94	0.49
1:B:383:HIS:HB3	1:B:398:THR:OG1	2.12	0.49
1:A:741:GLY:O	1:A:742:ILE:C	2.50	0.49
1:C:285:TYR:CE1	1:C:336:ARG:CB	2.95	0.49
1:B:547:TYR:OH	6:B:804:P2Y:NA	2.45	0.49
1:D:403:GLU:O	1:D:419:SER:HB2	2.13	0.49
1:D:224:ALA:HB1	1:D:268:PHE:CZ	2.47	0.49
1:A:591:MET:HE3	1:A:592:HIS:CD2	2.47	0.49
1:B:472:CYS:O	1:B:478:PRO:HA	2.12	0.49
1:C:288:VAL:CG1	1:C:294:LEU:HD11	2.41	0.49
1:D:741:GLY:O	1:D:742:ILE:C	2.51	0.49
1:B:512:LYS:HE3	1:B:527:GLN:NE2	2.28	0.49
1:A:184:ARG:HD3	1:A:187:TRP:CZ3	2.48	0.49
1:D:310:ARG:NE	1:D:329:ASP:OD1	2.37	0.49
1:D:150:ASN:O	1:D:151:ASN:CB	2.61	0.49
1:B:422:HIS:NE2	1:B:423:LYS:HD3	2.27	0.49
1:D:471:ARG:HG2	1:D:471:ARG:HH11	1.78	0.49
1:A:74:ASN:HB3	1:A:92:ASN:HB2	1.94	0.49
1:D:704:HIS:HE1	1:D:711:VAL:O	1.96	0.49
1:A:322:TYR:OH	1:A:346:ILE:HD13	2.11	0.49
1:C:384:ILE:HG13	1:C:404:VAL:HG21	1.95	0.49
1:B:175:LYS:CG	1:B:182:SER:HB3	2.42	0.49
1:B:626:ILE:HG23	1:B:636:THR:HG23	1.93	0.49
1:D:158:SER:OG	1:D:163:LYS:HB2	2.12	0.49
1:D:110:ASP:C	1:D:110:ASP:OD1	2.51	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:418:ILE:HD12	7:A:1059:HOH:O	2.12	0.49
1:D:491:LEU:O	1:D:492:ARG:HB3	2.13	0.49
1:C:332:GLU:HG3	7:C:986:HOH:O	2.11	0.49
1:D:377:ASN:HB2	1:D:381:TYR:H	1.78	0.49
1:B:278:PRO:HG2	2:B:772(A):NAG:C8	2.43	0.49
1:B:269:PHE:CE2	1:B:286:GLN:HG3	2.47	0.49
1:B:526:TYR:HB3	1:B:578:PHE:HD1	1.78	0.49
1:C:738:GLU:HB3	1:C:742:ILE:HA	1.94	0.49
1:C:751:ILE:HG23	1:C:752:TYR:N	2.27	0.49
1:C:535:ASP:CA	1:C:536:LYS:HD3	2.42	0.48
1:D:510:PRO:HD3	1:D:569:SER:HB2	1.94	0.48
1:C:288:VAL:HG13	1:C:289:PRO:HD2	1.94	0.48
1:A:377:ASN:ND2	1:A:383:HIS:CD2	2.81	0.48
1:A:383:HIS:HB3	1:A:398:THR:OG1	2.13	0.48
1:D:354:VAL:HG12	1:D:359:PRO:HB3	1.94	0.48
1:C:484:SER:CB	1:C:491:LEU:HD21	2.43	0.48
1:C:732:THR:HG22	1:D:732:THR:CG2	2.43	0.48
1:C:481:THR:OG1	1:C:483:HIS:CE1	2.57	0.48
1:A:453:ARG:HG3	1:A:476:GLY:HA3	1.94	0.48
1:C:661:TYR:OH	1:C:718:GLN:HG3	2.12	0.48
1:D:241:TYR:O	1:D:242:SER:HB3	2.13	0.48
1:D:550:PRO:O	1:D:551:CYS:HB3	2.14	0.48
1:D:127:SER:HB3	1:D:211:TYR:CD1	2.47	0.48
1:D:244:GLU:HG2	7:D:921:HOH:O	2.13	0.48
1:B:718:GLN:HE22	1:B:721:LYS:NZ	2.11	0.48
1:D:512:LYS:HE3	1:D:527:GLN:CD	2.34	0.48
1:C:491:LEU:O	1:C:492:ARG:HB3	2.13	0.48
1:C:551:CYS:HB3	7:C:907:HOH:O	2.13	0.48
1:D:471:ARG:N	1:D:471:ARG:HD3	2.28	0.48
1:D:377:ASN:HD21	1:D:383:HIS:CD2	2.32	0.48
1:B:278:PRO:HG2	2:B:772(A):NAG:H82	1.95	0.48
1:D:79:PHE:CD1	1:D:86:SER:HB3	2.48	0.48
1:B:306:VAL:HG12	1:B:307:THR:HG23	1.96	0.48
1:D:640:LEU:HD11	1:D:650:GLY:CA	2.42	0.48
1:D:167:VAL:HA	1:D:171:ASP:O	2.14	0.48
1:B:350:THR:HG22	2:B:773(A):NAG:H81	1.94	0.48
1:B:326:ASP:OD1	1:B:339:SER:OG	2.32	0.48
1:C:615:LYS:HG2	1:C:616:MET:N	2.29	0.48
1:B:543:LEU:HD13	1:B:575:VAL:HG13	1.96	0.48
1:C:253:ARG:HH21	1:D:253:ARG:HH21	1.53	0.48
1:D:675:THR:C	1:D:680:LEU:HB2	2.33	0.48
1:B:266:VAL:HG22	1:B:267:LYS:N	2.29	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:712:HIS:HB3	7:C:968:HOH:O	2.13	0.48
1:A:219:ASN:H	1:A:308:GLU:CD	2.15	0.48
1:A:122:LYS:HG2	1:A:123:GLN:N	2.28	0.48
1:B:382:LYS:NZ	1:B:588:ASP:OD1	2.47	0.48
1:D:393:ASN:H	1:D:393:ASN:HD22	1.62	0.48
1:A:388:GLN:CB	1:A:391:LYS:HB2	2.34	0.47
1:C:387:PHE:CD2	1:C:394:CYS:HB3	2.49	0.47
1:B:695:PHE:HB3	1:B:728:VAL:HG11	1.96	0.47
1:C:124:TRP:HB2	1:C:204:GLU:OE2	2.14	0.47
1:A:314:GLN:NE2	1:A:359:PRO:HB2	2.29	0.47
1:C:109:PRO:HG3	1:C:159:PRO:O	2.13	0.47
1:D:518:ASN:HD21	1:D:521:GLY:HA2	1.79	0.47
1:A:418:ILE:CD1	1:A:458:SER:HA	2.44	0.47
1:B:242:SER:HB3	1:B:246:LEU:HD12	1.96	0.47
1:D:502:LYS:HD2	1:D:505:GLN:OE1	2.13	0.47
1:D:310:ARG:HH21	1:D:329:ASP:CG	2.17	0.47
1:C:61:GLN:O	1:C:63:ILE:HG23	2.14	0.47
1:C:63:ILE:O	1:C:63:ILE:HG13	2.14	0.47
1:A:92:ASN:O	1:A:94:THR:N	2.45	0.47
1:C:718:GLN:NE2	1:C:718:GLN:HA	2.30	0.47
1:D:471:ARG:HG2	1:D:471:ARG:NH1	2.29	0.47
1:C:397:ILE:HG13	1:C:398:THR:HG23	1.96	0.47
1:C:405:ILE:HG13	1:C:429:ARG:CD	2.44	0.47
1:C:463:ASN:HD22	1:C:463:ASN:N	2.13	0.47
1:B:158:SER:OG	1:B:163:LYS:HB2	2.15	0.47
1:C:626:ILE:HG23	1:C:636:THR:HG23	1.96	0.47
1:D:71:LYS:HA	1:D:75:ASN:O	2.14	0.47
1:A:40:ARG:HB2	1:A:40:ARG:NH1	2.16	0.47
1:C:89:PHE:O	1:C:90:LEU:HB3	2.14	0.47
1:C:184:ARG:HD2	1:C:187:TRP:CE2	2.50	0.47
1:B:697:GLN:HG3	7:B:955:HOH:O	2.13	0.47
1:D:104:ASP:OD1	1:D:105:TYR:N	2.48	0.47
1:B:75:ASN:HD22	1:B:92:ASN:H	1.57	0.47
1:D:694:ASN:N	1:D:694:ASN:ND2	2.56	0.47
1:A:378:GLU:CD	1:A:378:GLU:N	2.66	0.47
1:C:471:ARG:HG2	1:C:480:TYR:CD2	2.50	0.47
1:C:763:PHE:CB	1:C:765:LEU:HG	2.45	0.47
1:C:314:GLN:HE21	1:C:325:ILE:HD11	1.79	0.47
1:D:664:SER:O	1:D:668:GLU:HB2	2.15	0.47
1:A:154:TRP:CD2	1:A:212:SER:HB2	2.49	0.47
1:C:128:TYR:CD1	1:C:128:TYR:C	2.88	0.47
1:A:363:HIS:CE1	1:A:407:ILE:HB	2.50	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:112:GLN:O	1:A:137:LEU:HB2	2.15	0.47
1:D:680:LEU:O	1:D:684:ARG:HG2	2.15	0.47
1:D:718:GLN:HE21	1:D:718:GLN:CA	2.21	0.47
1:C:248:TYR:CE2	1:D:234:PRO:HB2	2.50	0.47
1:D:82:GLU:H	1:D:491:LEU:HD13	1.80	0.47
1:C:123:GLN:HG2	1:C:124:TRP:CD2	2.50	0.47
1:A:739:ASP:HB2	7:A:1078:HOH:O	2.14	0.47
1:B:273:THR:HA	1:B:276:LEU:HG	1.96	0.47
1:A:175:LYS:NZ	1:A:178:PRO:O	2.43	0.47
1:A:516:VAL:HG12	1:A:517:ILE:N	2.30	0.47
1:D:738:GLU:HB3	1:D:742:ILE:HA	1.97	0.47
1:C:408:GLU:HG2	7:C:943:HOH:O	2.14	0.47
1:D:464:LYS:O	1:D:465:ALA:HB3	2.14	0.47
1:C:732:THR:HG23	1:C:733:MET:N	2.29	0.47
1:A:334:THR:O	1:C:275:THR:HA	2.15	0.47
1:C:86:SER:O	1:C:87:SER:HB3	2.15	0.47
1:C:603:VAL:HG13	1:C:639:VAL:HG23	1.97	0.47
1:C:241:TYR:CD1	1:C:241:TYR:N	2.83	0.47
1:A:457:TYR:HA	1:A:471:ARG:O	2.14	0.46
1:B:317:ARG:HB3	7:B:1023:HOH:O	2.14	0.46
1:C:589:LYS:HB3	7:C:1032:HOH:O	2.15	0.46
1:B:297:ASP:HA	7:B:1026:HOH:O	2.15	0.46
1:B:410:LEU:HD13	1:B:415:LEU:HD22	1.97	0.46
1:D:516:VAL:HG11	1:D:523:LYS:HB2	1.97	0.46
1:A:430:ASN:HB2	7:A:990:HOH:O	2.14	0.46
1:C:234:PRO:HB2	1:D:248:TYR:CZ	2.49	0.46
1:C:170:ASN:HD22	1:C:170:ASN:N	2.13	0.46
1:A:662:TYR:HB3	1:A:667:THR:OG1	2.15	0.46
1:A:397:ILE:HG22	1:A:439:TYR:CE2	2.50	0.46
1:B:118:TYR:CE2	1:B:119:ASN:ND2	2.84	0.46
1:C:237:GLU:HG2	1:C:253:ARG:HG2	1.97	0.46
1:D:180:LEU:HD22	1:D:180:LEU:N	2.30	0.46
1:D:224:ALA:HA	1:D:269:PHE:O	2.14	0.46
1:D:105:TYR:C	1:D:105:TYR:CD1	2.88	0.46
1:B:140:ARG:NH1	1:B:140:ARG:HG2	2.31	0.46
1:D:600:THR:O	1:D:603:VAL:HG13	2.15	0.46
1:B:75:ASN:HD22	1:B:91:GLU:HA	1.80	0.46
1:A:438:ASP:OD1	1:A:440:THR:HB	2.15	0.46
1:D:393:ASN:H	1:D:393:ASN:ND2	2.13	0.46
1:A:109:PRO:HG2	1:A:161:GLY:O	2.15	0.46
1:D:331:ASP:HB2	1:D:338:ILE:HD12	1.98	0.46
1:D:626:ILE:HG23	1:D:636:THR:HG23	1.97	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:489:LYS:N	7:A:962:HOH:O	2.47	0.46
1:C:438:ASP:C	1:C:440:THR:H	2.17	0.46
1:B:327:ILE:HD13	1:B:389:THR:HG23	1.98	0.46
1:D:649:CYS:HB3	1:D:699:GLU:HB2	1.97	0.46
1:C:516:VAL:HG11	1:C:523:LYS:HB2	1.98	0.46
1:B:58:TYR:CD2	1:B:494:LEU:HB3	2.51	0.46
1:B:205:GLU:OE2	6:B:803:PHI:N	2.49	0.46
1:B:319:ALA:O	1:B:320:GLN:HB2	2.15	0.46
1:D:566:TYR:CE2	1:D:567:LEU:HD23	2.51	0.46
1:A:143:ILE:HD12	1:A:143:ILE:N	2.31	0.46
1:C:175:LYS:NZ	1:C:180:LEU:O	2.49	0.46
1:A:458:SER:OG	1:A:471:ARG:HD3	2.16	0.46
1:A:289:PRO:HB3	1:A:315:TRP:CD2	2.51	0.46
1:B:403:GLU:OE1	1:B:585:TYR:HA	2.16	0.46
1:D:480:TYR:N	1:D:480:TYR:CD1	2.83	0.46
1:D:80:ASN:OD1	1:D:83:TYR:HD2	1.98	0.45
1:B:105:TYR:HA	1:B:115:LEU:O	2.15	0.45
1:B:680:LEU:HD11	1:B:684:ARG:HE	1.81	0.45
1:B:98:LEU:HD11	1:B:116:PHE:CD1	2.50	0.45
1:A:472:CYS:O	1:A:478:PRO:HA	2.15	0.45
1:D:454:CYS:HB3	1:D:457:TYR:CZ	2.51	0.45
1:C:559:PHE:CZ	1:C:561:LEU:HD13	2.52	0.45
1:C:535:ASP:O	1:C:536:LYS:HB3	2.16	0.45
1:A:718:GLN:HE22	1:A:721:LYS:HZ2	1.61	0.45
1:A:420:ASN:ND2	1:A:426:PRO:HA	2.31	0.45
1:D:218:PRO:HD3	1:D:305:TRP:HB3	1.97	0.45
1:C:71:LYS:HD2	1:C:103:ASN:ND2	2.32	0.45
1:A:718:GLN:HE21	1:A:718:GLN:CA	2.21	0.45
1:B:79:PHE:CD1	1:B:86:SER:HB2	2.50	0.45
1:A:588:ASP:O	1:A:592:HIS:HB2	2.16	0.45
1:D:62:TRP:CE3	1:D:68:TYR:HB3	2.52	0.45
1:A:704:HIS:HD2	1:A:716:SER:OG	1.99	0.45
1:D:541:PRO:HG2	1:D:573:ILE:HG23	1.97	0.45
1:A:39:SER:O	1:A:40:ARG:NH1	2.49	0.45
1:C:612:GLN:O	1:C:615:LYS:HG2	2.16	0.45
1:C:697:GLN:HA	1:C:697:GLN:HE21	1.81	0.45
1:B:184:ARG:HD3	1:B:187:TRP:CE2	2.52	0.45
1:C:467:TYR:HD1	1:C:484:SER:HA	1.82	0.45
1:B:159:PRO:HD3	1:B:216:TRP:HB3	1.98	0.45
1:B:492:ARG:HD2	7:B:911:HOH:O	2.16	0.45
1:D:486:SER:OG	1:D:487:SER:N	2.50	0.45
1:D:128:TYR:CD1	1:D:128:TYR:C	2.90	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:336:ARG:HH11	1:A:336:ARG:HG3	1.82	0.45
1:D:90:LEU:HD12	1:D:140:ARG:HH22	1.82	0.45
1:C:204:GLU:HA	1:C:210:ALA:O	2.17	0.45
1:A:268:PHE:CE2	1:A:313:LEU:HD21	2.51	0.45
1:B:516:VAL:HG22	1:B:525:TRP:CD2	2.51	0.45
1:D:170:ASN:N	1:D:170:ASN:HD22	2.14	0.45
1:A:482:LEU:O	1:A:490:GLU:O	2.35	0.45
1:D:512:LYS:HE2	1:D:514:LEU:HD11	1.99	0.45
1:A:155:ILE:HG13	1:A:166:TYR:HB3	1.99	0.45
1:D:673:LEU:HD12	1:D:673:LEU:HA	1.84	0.45
1:C:661:TYR:CZ	1:C:718:GLN:HG3	2.51	0.45
1:D:72:GLN:HE21	1:D:77:LEU:HD12	1.81	0.45
1:B:242:SER:OG	1:B:243:ASP:N	2.49	0.45
1:B:258:LYS:HA	1:B:663:ASP:HA	1.99	0.45
1:B:124:TRP:HB2	1:B:204:GLU:OE2	2.16	0.45
1:C:704:HIS:CD2	1:C:716:SER:OG	2.60	0.45
1:A:434:ILE:HA	1:A:442:VAL:HA	1.99	0.45
1:A:433:ARG:HH11	1:A:443:THR:HG21	1.81	0.45
1:D:599:GLY:O	3:D:776(A):NAG:H83	2.16	0.45
1:C:159:PRO:HB2	1:C:218:PRO:O	2.17	0.45
1:D:316:ILE:HD11	1:D:320:GLN:HB3	1.99	0.45
1:B:477:LEU:HD13	1:B:500:LEU:HD23	1.99	0.45
1:C:326:ASP:OD1	1:C:339:SER:OG	2.35	0.45
1:B:302:GLY:HA3	7:B:1080:HOH:O	2.17	0.45
1:C:491:LEU:HD22	1:C:491:LEU:N	2.31	0.44
1:D:704:HIS:CD2	1:D:716:SER:OG	2.69	0.44
1:A:353:TRP:CZ2	1:A:591:MET:HE3	2.52	0.44
1:C:516:VAL:CG1	1:C:523:LYS:HB2	2.47	0.44
1:C:491:LEU:CD2	1:C:491:LEU:N	2.80	0.44
1:B:654:ALA:HA	1:B:704:HIS:CD2	2.53	0.44
1:D:658:LYS:HB3	1:D:661:TYR:CE2	2.53	0.44
1:B:148:ILE:HD13	1:B:155:ILE:CD1	2.47	0.44
1:B:526:TYR:C	1:B:526:TYR:CD1	2.90	0.44
1:C:509:MET:HE3	1:C:510:PRO:HD2	1.99	0.44
1:B:418:ILE:HA	1:B:430:ASN:O	2.16	0.44
1:A:433:ARG:NH2	7:A:992:HOH:O	2.35	0.44
1:B:673:LEU:CD1	1:B:673:LEU:N	2.79	0.44
1:D:581:ARG:HE	1:D:605:ASP:CG	2.20	0.44
1:D:352:GLY:HA2	1:D:595:ASN:OD1	2.16	0.44
1:A:548:ALA:HB3	1:A:635:VAL:HG21	1.99	0.44
6:D:807:PHI:HA	6:D:808:P2Y:HD3	1.82	0.44
1:B:159:PRO:HD3	1:B:216:TRP:HB2	1.98	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:158:SER:HA	1:A:216:TRP:CD1	2.53	0.44
1:A:658:LYS:HB3	1:A:661:TYR:CD2	2.52	0.44
1:C:471:ARG:HG2	1:C:480:TYR:HD2	1.82	0.44
1:C:541:PRO:HB2	1:C:763:PHE:CE2	2.52	0.44
1:C:302:GLY:HA3	7:C:1050:HOH:O	2.18	0.44
1:A:87:SER:OG	2:A:767(A):NAG:H81	2.17	0.44
1:D:571:GLU:OE1	1:D:571:GLU:HA	2.18	0.44
1:C:293:VAL:HG13	1:C:298:HIS:CB	2.47	0.44
1:A:40:ARG:HH11	1:A:40:ARG:CB	2.18	0.44
1:C:654:ALA:N	1:C:655:PRO:CD	2.81	0.44
1:A:68:TYR:CE1	1:A:79:PHE:HB2	2.52	0.44
1:B:718:GLN:NE2	1:B:718:GLN:HA	2.33	0.44
1:A:654:ALA:HA	1:A:704:HIS:CD2	2.53	0.44
1:A:700:TYR:OH	1:A:702:LEU:HD13	2.18	0.44
1:C:532:PRO:HD3	1:C:569:SER:HA	1.98	0.44
1:A:384:ILE:HG13	1:A:404:VAL:HG21	1.99	0.44
1:A:47:ASP:HA	1:A:52:THR:CG2	2.48	0.44
1:C:114:ILE:HD13	1:C:116:PHE:CZ	2.52	0.44
1:D:397:ILE:HG13	1:D:398:THR:HG23	1.98	0.44
1:A:266:VAL:HG22	1:A:267:LYS:N	2.33	0.44
1:C:319:ALA:O	1:C:320:GLN:HB2	2.18	0.44
1:A:70:TYR:HB3	1:A:79:PHE:HE2	1.81	0.44
1:B:326:ASP:CG	1:B:339:SER:HG	2.20	0.44
1:C:121:VAL:O	1:C:128:TYR:HB2	2.18	0.44
1:C:697:GLN:NE2	1:C:697:GLN:HA	2.32	0.44
1:C:293:VAL:HG13	1:C:298:HIS:HB3	1.98	0.44
1:A:708:ASP:OD2	1:A:740:HIS:HA	2.17	0.44
1:C:538:LYS:O	1:C:618:PHE:HA	2.17	0.44
1:B:128:TYR:CD1	1:B:128:TYR:C	2.90	0.44
1:C:654:ALA:HA	1:C:704:HIS:CD2	2.52	0.44
1:D:273:THR:O	1:D:276:LEU:HB2	2.17	0.44
1:A:433:ARG:O	1:A:442:VAL:HA	2.17	0.44
1:C:110:ASP:OD2	1:C:162:HIS:ND1	2.46	0.44
1:C:266:VAL:HG22	1:C:267:LYS:N	2.33	0.44
1:A:106:SER:HB3	1:A:115:LEU:HB2	1.99	0.44
1:C:77:LEU:HD21	1:C:88:ILE:HG12	1.99	0.44
1:C:759:LEU:HA	1:C:759:LEU:HD23	1.78	0.44
1:A:527:GLN:O	1:A:576:ALA:HA	2.18	0.44
1:D:629:TRP:O	1:D:632:GLY:N	2.51	0.44
1:C:640:LEU:HD11	1:C:650:GLY:CA	2.41	0.43
1:B:718:GLN:HE21	1:B:718:GLN:HA	1.82	0.43
1:A:356:ARG:HD3	1:A:551:CYS:SG	2.58	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:192:ASN:HA	1:A:195:TYR:OH	2.18	0.43
1:C:225:TYR:CE1	1:C:269:PHE:HB2	2.53	0.43
1:B:556:ASP:CG	1:B:558:VAL:HG23	2.38	0.43
1:D:673:LEU:O	1:D:678:ASP:HB3	2.18	0.43
1:C:197:GLY:C	1:C:213:ALA:HB3	2.38	0.43
1:D:423:LYS:O	1:D:424:GLY:C	2.56	0.43
1:D:707:ALA:HB2	1:D:737:ASP:HA	2.01	0.43
1:D:662:TYR:HB3	1:D:667:THR:OG1	2.18	0.43
1:C:533:HIS:O	1:C:535:ASP:N	2.52	0.43
1:C:77:LEU:HD23	1:C:88:ILE:CA	2.37	0.43
1:B:651:ILE:HD11	1:B:758:PHE:CD2	2.54	0.43
1:C:400:GLY:HA3	1:C:402:TRP:HE1	1.81	0.43
1:C:384:ILE:HG21	1:C:397:ILE:HD11	1.99	0.43
1:D:82:GLU:HA	1:D:491:LEU:HD22	2.01	0.43
1:C:615:LYS:CG	1:C:616:MET:N	2.80	0.43
1:B:140:ARG:HG2	1:B:140:ARG:HH11	1.83	0.43
1:A:519:LEU:HD22	1:A:608:GLU:OE2	2.17	0.43
1:A:405:ILE:HG13	1:A:429:ARG:HD2	2.00	0.43
1:A:318:ARG:O	1:A:320:GLN:HG3	2.17	0.43
1:A:502:LYS:HD2	1:A:505:GLN:OE1	2.18	0.43
1:C:175:LYS:CG	1:C:182:SER:HB3	2.45	0.43
1:A:216:TRP:CZ3	1:A:273:THR:HG21	2.53	0.43
1:C:397:ILE:HG22	1:C:439:TYR:CE2	2.53	0.43
1:C:193:VAL:HG12	1:C:194:ILE:HG12	2.01	0.43
1:B:528:MET:HG2	1:B:576:ALA:HB2	2.01	0.43
1:C:518:ASN:HA	1:C:522:THR:O	2.19	0.43
1:A:566:TYR:CE2	1:A:567:LEU:HD23	2.53	0.43
1:A:258:LYS:O	1:A:259:ALA:C	2.55	0.43
1:B:720:SER:O	1:B:724:VAL:HG23	2.19	0.43
1:B:677:GLU:H	1:B:677:GLU:CD	2.22	0.43
1:B:627:TRP:CE3	1:B:755:MET:HE1	2.54	0.43
1:C:139:LYS:HD3	1:C:141:GLN:NE2	2.33	0.43
1:D:133:ASP:HB3	1:D:142:LEU:CD2	2.48	0.43
1:A:154:TRP:CE2	1:A:212:SER:HB2	2.54	0.43
1:B:664:SER:O	1:B:668:GLU:HB2	2.18	0.43
1:D:171:ASP:OD2	1:D:184:ARG:NH1	2.52	0.43
1:D:199:THR:HA	1:D:228:PHE:CE2	2.53	0.43
1:B:49:LEU:HD22	1:B:749:GLN:HA	2.01	0.43
1:D:734:TRP:CD1	1:D:734:TRP:C	2.91	0.43
1:D:612:GLN:HB3	1:D:612:GLN:HE21	1.60	0.43
1:B:136:ASP:CG	1:B:139:LYS:HG2	2.38	0.43
1:D:177:GLU:HA	1:D:178:PRO:HD3	1.89	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:86:SER:C	2:B:767(A):NAG:H81	2.38	0.43
1:A:235:LEU:HD21	1:A:255:PRO:HG3	2.01	0.43
1:C:269:PHE:CE2	1:C:286:GLN:HB2	2.54	0.43
1:C:196:ASN:OD1	1:C:227:GLN:HG3	2.19	0.43
1:B:640:LEU:HB3	1:B:698:VAL:HG21	2.01	0.43
1:A:128:TYR:C	1:A:128:TYR:CD1	2.91	0.43
1:D:190:LYS:HG2	1:D:193:VAL:HG13	1.96	0.43
1:D:535:ASP:O	1:D:536:LYS:C	2.57	0.43
1:D:674:PRO:O	1:D:680:LEU:HD13	2.19	0.43
1:A:453:ARG:CZ	1:A:479:LEU:HB2	2.49	0.43
1:C:312:SER:C	1:C:313:LEU:HD12	2.38	0.43
1:B:490:GLU:O	1:B:491:LEU:C	2.57	0.43
1:D:544:ILE:O	1:D:626:ILE:HA	2.19	0.43
1:A:230:ASP:O	1:A:232:GLU:N	2.52	0.43
1:C:519:LEU:HD22	1:C:608:GLU:CD	2.38	0.42
1:B:85:ASN:ND2	2:B:767(A):NAG:O7	2.52	0.42
1:B:39:SER:O	1:B:40:ARG:O	2.36	0.42
1:C:571:GLU:OE1	1:C:760:LYS:HE3	2.19	0.42
1:D:363:HIS:CD2	1:D:407:ILE:HB	2.53	0.42
6:C:805:PHI:HA	6:C:806:P2Y:HD3	1.90	0.42
1:A:74:ASN:O	1:A:95:PHE:CE2	2.63	0.42
1:D:153:GLN:HE22	1:D:170:ASN:HD21	1.63	0.42
1:D:163:LYS:HE2	7:D:1056:HOH:O	2.19	0.42
1:A:134:ILE:HG21	1:A:178:PRO:HB3	2.00	0.42
1:C:729:ASP:OD2	1:D:757:HIS:HD2	2.01	0.42
1:B:678:ASP:HB3	1:B:679:ASN:H	1.66	0.42
1:A:203:TYR:CD2	1:A:207:VAL:HG21	2.55	0.42
1:D:517:ILE:HG23	1:D:526:TYR:CE2	2.54	0.42
1:C:49:LEU:HB3	1:C:749:GLN:HG2	2.01	0.42
1:C:490:GLU:HG2	1:C:490:GLU:O	2.19	0.42
1:C:143:ILE:HD12	1:C:143:ILE:N	2.34	0.42
1:B:473:PHE:HB3	1:B:558:VAL:HG13	2.00	0.42
1:D:219:ASN:HB2	1:D:308:GLU:CG	2.50	0.42
1:C:313:LEU:N	1:C:313:LEU:CD1	2.82	0.42
1:B:546:VAL:HG11	1:B:626:ILE:HD11	2.02	0.42
1:A:150:ASN:O	1:A:151:ASN:CB	2.67	0.42
1:C:374:ILE:CD1	1:C:406:GLY:HA2	2.50	0.42
1:C:133:ASP:HA	7:C:1042:HOH:O	2.20	0.42
1:D:123:GLN:HG2	1:D:124:TRP:CD2	2.54	0.42
1:C:517:ILE:HG23	1:C:526:TYR:CD2	2.54	0.42
1:C:560:ARG:HD2	7:C:914:HOH:O	2.19	0.42
1:D:703:ILE:HG12	1:D:733:MET:HB3	2.01	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:463:ASN:ND2	1:C:463:ASN:N	2.67	0.42
1:B:80:ASN:OD1	1:B:82:GLU:HB2	2.20	0.42
1:D:522:THR:CG2	1:D:523:LYS:N	2.82	0.42
1:D:515:ASP:HB3	1:D:526:TYR:CZ	2.54	0.42
1:A:620:ASP:C	1:A:620:ASP:OD1	2.58	0.42
1:B:227:GLN:O	1:B:266:VAL:HA	2.19	0.42
1:C:679:ASN:HD21	1:C:682:TYR:HB2	1.84	0.42
1:A:257:PRO:O	1:A:663:ASP:HA	2.19	0.42
1:C:545:GLU:HG3	1:C:627:TRP:NE1	2.34	0.42
1:C:534:PHE:O	1:C:535:ASP:O	2.37	0.42
1:B:143:ILE:N	1:B:143:ILE:HD12	2.35	0.42
1:C:66:HIS:CD2	1:C:67:GLU:HG3	2.55	0.42
1:D:199:THR:CG2	1:D:208:PHE:CD2	3.03	0.42
1:C:142:LEU:C	1:C:142:LEU:HD23	2.40	0.42
1:C:53:PHE:CZ	1:C:507:VAL:HG11	2.55	0.42
1:A:435:GLN:NE2	1:A:441:LYS:HD3	2.34	0.42
1:D:549:GLY:HA2	1:D:631:TYR:CD1	2.54	0.42
1:D:75:ASN:ND2	1:D:92:ASN:N	2.53	0.42
1:A:435:GLN:OE1	1:A:437:ASN:OD1	2.38	0.42
1:A:532:PRO:O	1:A:533:HIS:C	2.58	0.42
1:C:435:GLN:HG2	7:C:1051:HOH:O	2.19	0.42
1:B:120:TYR:C	1:B:120:TYR:CD2	2.92	0.42
1:B:516:VAL:HG11	1:B:523:LYS:HB2	2.02	0.42
1:A:515:ASP:HB3	1:A:526:TYR:CE2	2.55	0.42
1:A:59:THR:O	1:A:70:TYR:HD1	2.03	0.42
1:D:415:LEU:O	1:D:434:ILE:HG22	2.20	0.42
1:C:122:LYS:HG2	1:C:123:GLN:N	2.34	0.42
1:A:161:GLY:HA3	7:A:1030:HOH:O	2.20	0.42
1:C:651:ILE:HD11	1:C:758:PHE:CD2	2.55	0.42
1:D:317:ARG:O	1:D:318:ARG:C	2.57	0.42
1:A:474:GLY:HA2	1:A:476:GLY:O	2.20	0.42
1:D:695:PHE:HB3	1:D:728:VAL:HG11	2.02	0.42
1:B:41:ARG:HG2	1:B:42:THR:O	2.20	0.42
1:A:438:ASP:C	1:A:440:THR:H	2.23	0.42
1:B:137:LEU:O	1:B:140:ARG:NH1	2.53	0.42
1:B:518:ASN:HA	1:B:522:THR:O	2.20	0.42
1:A:452:GLU:OE1	1:A:452:GLU:HA	2.19	0.42
1:A:759:LEU:HA	1:A:759:LEU:HD23	1.86	0.42
1:B:219:ASN:ND2	7:B:1066:HOH:O	2.47	0.42
1:A:74:ASN:HD22	1:A:74:ASN:HA	1.62	0.41
1:C:356:ARG:HB3	1:C:551:CYS:SG	2.60	0.41
1:A:184:ARG:HD3	1:A:187:TRP:CE3	2.55	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:241:TYR:CE2	1:D:714:GLN:HA	2.54	0.41
1:D:446:SER:HB2	1:D:457:TYR:CE1	2.54	0.41
1:C:209:SER:HA	7:C:1007:HOH:O	2.18	0.41
1:B:62:TRP:CG	1:B:462:SER:HA	2.55	0.41
1:B:524:PHE:CE2	1:B:590:ILE:HD12	2.56	0.41
1:B:193:VAL:HG12	1:B:194:ILE:HG12	2.01	0.41
1:D:423:LYS:O	1:D:425:MET:N	2.53	0.41
1:C:96:ASP:O	1:C:98:LEU:HG	2.19	0.41
1:B:206:GLU:HB3	7:B:1039:HOH:O	2.18	0.41
1:C:536:LYS:CG	1:C:537:SER:N	2.82	0.41
1:C:463:ASN:O	1:C:465:ALA:N	2.52	0.41
1:C:58:TYR:CD1	1:C:494:LEU:HD13	2.56	0.41
1:D:266:VAL:HG22	1:D:267:LYS:N	2.36	0.41
1:C:664:SER:O	1:C:668:GLU:HB2	2.19	0.41
1:C:420:ASN:HD22	1:C:426:PRO:CA	2.26	0.41
4:D:769(B):NAG:H82	4:D:769(B):NAG:O3	2.20	0.41
1:A:732:THR:O	1:B:732:THR:HG22	2.20	0.41
1:D:512:LYS:HE3	1:D:527:GLN:NE2	2.35	0.41
1:B:692:ALA:O	1:B:728:VAL:HG21	2.21	0.41
1:C:63:ILE:HG21	1:C:69:LEU:CD1	2.50	0.41
1:A:439:TYR:N	1:A:439:TYR:CD1	2.87	0.41
1:B:676:PRO:HG2	1:B:677:GLU:OE2	2.20	0.41
1:A:535:ASP:C	1:A:535:ASP:OD2	2.57	0.41
1:C:237:GLU:HA	1:C:252:VAL:O	2.19	0.41
1:C:242:SER:OG	1:C:243:ASP:N	2.52	0.41
1:B:327:ILE:CD1	1:B:389:THR:HG23	2.49	0.41
1:B:363:HIS:CD2	1:B:407:ILE:HB	2.55	0.41
1:C:377:ASN:HA	1:C:396:PHE:CZ	2.55	0.41
1:C:422:HIS:CE1	1:C:447:CYS:HB3	2.56	0.41
1:C:550:PRO:HD2	1:C:631:TYR:CE2	2.55	0.41
1:C:172:ILE:HB	1:C:185:ILE:HB	2.02	0.41
1:C:474:GLY:HA2	1:C:476:GLY:O	2.21	0.41
1:D:65:ASP:O	1:D:467:TYR:HD2	2.03	0.41
1:D:45:LEU:O	1:D:49:LEU:HG	2.21	0.41
1:A:198:VAL:HA	1:A:211:TYR:O	2.21	0.41
1:D:98:LEU:HD22	1:D:142:LEU:HD11	2.02	0.41
1:D:47:ASP:HA	1:D:52:THR:CG2	2.51	0.41
1:A:429:ARG:HH11	1:A:429:ARG:HG3	1.85	0.41
1:D:64:SER:C	1:D:463:ASN:HB2	2.41	0.41
1:A:92:ASN:C	1:A:94:THR:N	2.73	0.41
1:D:170:ASN:O	1:D:196:ASN:HB2	2.21	0.41
1:B:44:THR:O	1:B:47:ASP:HB2	2.20	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:280:ALA:HB2	1:D:285:TYR:CD1	2.55	0.41
1:B:49:LEU:HB3	1:B:749:GLN:HG2	2.03	0.41
1:D:145:GLU:O	1:D:146:GLU:HB2	2.21	0.41
1:A:561:LEU:HD12	1:A:561:LEU:HA	1.81	0.41
1:A:153:GLN:HB3	1:A:211:TYR:CE2	2.55	0.41
1:D:143:ILE:HD13	1:D:178:PRO:HB2	2.02	0.41
1:B:44:THR:HB	7:B:1059:HOH:O	2.21	0.41
1:A:74:ASN:HB3	1:A:92:ASN:CB	2.51	0.41
1:C:101:SER:O	1:C:102:THR:CG2	2.69	0.41
1:C:102:THR:HB	1:C:103:ASN:H	1.51	0.41
1:D:67:GLU:OE2	1:D:111:ARG:NH1	2.54	0.41
1:D:320:GLN:N	7:D:918:HOH:O	2.54	0.41
1:B:44:THR:OG1	1:B:47:ASP:OD2	2.37	0.41
1:D:712:HIS:CD2	1:D:712:HIS:N	2.88	0.41
1:B:492:ARG:NE	7:B:911:HOH:O	2.53	0.41
1:C:551:CYS:O	1:C:551:CYS:SG	2.78	0.41
1:D:72:GLN:HE21	1:D:77:LEU:HD11	1.86	0.41
1:B:527:GLN:HB3	1:B:555:VAL:HG13	2.03	0.41
1:D:49:LEU:HB3	1:D:749:GLN:HG2	2.02	0.41
1:B:649:CYS:HB3	1:B:699:GLU:HB2	2.01	0.41
1:A:664:SER:O	1:A:668:GLU:HB2	2.20	0.41
1:D:263:ASN:HB3	1:D:264:PRO:HD2	2.02	0.41
1:B:57:PHE:HA	1:B:480:TYR:CE1	2.56	0.41
1:D:222:PHE:HE2	1:D:308:GLU:O	2.03	0.41
1:C:136:ASP:CG	1:C:139:LYS:HG2	2.42	0.41
1:A:59:THR:O	1:A:70:TYR:CD1	2.74	0.41
1:A:268:PHE:CE1	1:A:303:VAL:HG21	2.56	0.41
1:A:534:PHE:CE1	1:A:540:TYR:CE1	3.08	0.40
1:C:658:LYS:HB3	1:C:661:TYR:CD2	2.55	0.40
1:D:743:ALA:O	1:D:744:SER:C	2.58	0.40
1:D:675:THR:HB	1:D:676:PRO:HD2	2.03	0.40
1:A:505:GLN:HB3	1:A:505:GLN:HE21	1.66	0.40
1:C:289:PRO:HB3	1:C:315:TRP:CD2	2.56	0.40
1:D:524:PHE:CE2	1:D:590:ILE:HD12	2.57	0.40
1:D:122:LYS:HA	1:D:128:TYR:CB	2.51	0.40
1:B:55:VAL:HG22	1:B:500:LEU:HD22	2.03	0.40
1:A:151:ASN:ND2	7:A:1011:HOH:O	2.54	0.40
1:B:532:PRO:O	1:B:533:HIS:C	2.60	0.40
1:D:610:THR:HA	1:D:613:PHE:HD2	1.87	0.40
1:C:546:VAL:HG22	1:C:547:TYR:N	2.36	0.40
1:C:535:ASP:O	1:C:536:LYS:CB	2.70	0.40
1:A:489:LYS:HG3	1:A:491:LEU:H	1.87	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:438:ASP:C	1:B:440:THR:H	2.25	0.40
1:A:79:PHE:CD1	1:A:86:SER:HB3	2.56	0.40
1:D:703:ILE:HG21	1:D:751:ILE:CD1	2.51	0.40
1:A:114:ILE:CG2	1:A:135:TYR:HB3	2.50	0.40
1:A:547:TYR:OH	6:A:802:P2Y:NA	2.54	0.40
1:C:382:LYS:H	1:C:403:GLU:HG2	1.86	0.40
1:B:118:TYR:CD2	1:B:119:ASN:ND2	2.90	0.40
1:B:620:ASP:OD1	1:B:622:LYS:HB2	2.21	0.40
1:B:43:TYR:O	1:B:570:THR:OG1	2.34	0.40
1:B:322:TYR:CD1	1:B:322:TYR:C	2.94	0.40
1:B:143:ILE:HG21	1:B:178:PRO:O	2.21	0.40
1:B:72:GLN:NE2	1:B:77:LEU:HD11	2.37	0.40
1:C:294:LEU:O	1:C:295:ILE:C	2.59	0.40
1:D:735:TYR:OH	1:D:751:ILE:HA	2.21	0.40
1:B:491:LEU:H	1:B:491:LEU:CD2	2.34	0.40
1:B:707:ALA:HB2	1:B:737:ASP:HA	2.02	0.40
1:C:254:ILE:HA	1:C:255:PRO:HD3	1.95	0.40
1:A:345:HIS:N	1:A:345:HIS:ND1	2.70	0.40
1:D:74:ASN:O	1:D:92:ASN:HB3	2.22	0.40
1:C:71:LYS:HD2	1:C:103:ASN:HD21	1.86	0.40
1:B:746:MET:O	1:B:750:HIS:HB2	2.22	0.40
1:A:135:TYR:CD1	1:A:141:GLN:O	2.75	0.40
1:B:491:LEU:H	1:B:491:LEU:HD23	1.87	0.40
1:B:405:ILE:HG12	1:B:419:SER:HA	2.04	0.40
1:C:596:ARG:N	1:C:670:TYR:O	2.46	0.40
1:B:201:TRP:CZ2	1:B:710:ASN:HA	2.56	0.40
1:A:649:CYS:HB3	1:A:699:GLU:HB2	2.04	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	726/728 (100%)	656 (90%)	58 (8%)	12 (2%)	14 40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	726/728 (100%)	670 (92%)	50 (7%)	6 (1%)	27	64
1	C	726/728 (100%)	652 (90%)	59 (8%)	15 (2%)	11	32
1	D	726/728 (100%)	656 (90%)	64 (9%)	6 (1%)	27	64
All	All	2904/2912 (100%)	2634 (91%)	231 (8%)	39 (1%)	18	49

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	B	40	ARG
1	C	103	ASN
1	C	534	PHE
1	C	535	ASP
1	C	536	LYS
1	A	97	GLU
1	A	231	THR
1	A	621	ASP
1	B	273	THR
1	B	491	LEU
1	C	40	ARG
1	C	74	ASN
1	C	104	ASP
1	D	537	SER
1	A	82	GLU
1	A	104	ASP
1	B	292	SER
1	B	439	TYR
1	C	87	SER
1	D	151	ASN
1	A	149	PRO
1	A	377	ASN
1	A	492	ARG
1	C	94	THR
1	C	451	PRO
1	A	102	THR
1	A	121	VAL
1	A	151	ASN
1	B	295	ILE
1	C	90	LEU
1	C	149	PRO
1	D	320	GLN

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Mol	Chain	Res	Type
1	C	295	ILE
1	D	193	VAL
1	D	680	LEU
1	D	143	ILE
1	C	99	GLY
1	C	193	VAL

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	652/652 (100%)	620 (95%)	32 (5%)	35	70
1	B	652/652 (100%)	626 (96%)	26 (4%)	42	78
1	C	652/652 (100%)	618 (95%)	34 (5%)	32	68
1	D	652/652 (100%)	620 (95%)	32 (5%)	35	70
All	All	2608/2608 (100%)	2484 (95%)	124 (5%)	35	71

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	A	74	ASN
1	A	90	LEU
1	A	111	ARG
1	A	145	GLU
1	A	150	ASN
1	A	180	LEU
1	A	207	VAL
1	A	246	LEU
1	A	247	GLN
1	A	250	LYS
1	A	294	LEU
1	A	385	CYS
1	A	399	LYS
1	A	415	LEU
1	A	423	LYS

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Mol	Chain	Res	Type
1	A	442	VAL
1	A	443	THR
1	A	471	ARG
1	A	472	CYS
1	A	491	LEU
1	A	492	ARG
1	A	520	HIS
1	A	542	LEU
1	A	543	LEU
1	A	561	LEU
1	A	566	TYR
1	A	679	ASN
1	A	683	TYR
1	A	701	LEU
1	A	718	GLN
1	A	761	GLN
1	B	91	GLU
1	B	111	ARG
1	B	170	ASN
1	B	246	LEU
1	B	256	TYR
1	B	415	LEU
1	B	418	ILE
1	B	435	GLN
1	B	450	ASN
1	B	491	LEU
1	B	492	ARG
1	B	506	ASP
1	B	520	HIS
1	B	535	ASP
1	B	536	LYS
1	B	537	SER
1	B	542	LEU
1	B	543	LEU
1	B	561	LEU
1	B	566	TYR
1	B	679	ASN
1	B	701	LEU
1	B	702	LEU
1	B	732	THR
1	B	745	ASN
1	B	761	GLN

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Mol	Chain	Res	Type
1	C	75	ASN
1	C	90	LEU
1	C	145	GLU
1	C	147	ARG
1	C	158	SER
1	C	184	ARG
1	C	188	THR
1	C	230	ASP
1	C	246	LEU
1	C	284	SER
1	C	339	SER
1	C	348	ILE
1	C	366	SER
1	C	385	CYS
1	C	399	LYS
1	C	418	ILE
1	C	419	SER
1	C	472	CYS
1	C	482	LEU
1	C	491	LEU
1	C	503	MET
1	C	535	ASP
1	C	536	LYS
1	C	542	LEU
1	C	561	LEU
1	C	566	TYR
1	C	583	SER
1	C	611	ARG
1	C	627	TRP
1	C	685	ASN
1	C	701	LEU
1	C	732	THR
1	C	746	MET
1	C	759	LEU
1	D	41	ARG
1	D	103	ASN
1	D	107	VAL
1	D	111	ARG
1	D	142	LEU
1	D	184	ARG
1	D	193	VAL
1	D	246	LEU

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Mol	Chain	Res	Type
1	D	253	ARG
1	D	276	LEU
1	D	294	LEU
1	D	348	ILE
1	D	358	ARG
1	D	393	ASN
1	D	399	LYS
1	D	423	LYS
1	D	448	GLU
1	D	471	ARG
1	D	482	LEU
1	D	507	VAL
1	D	536	LYS
1	D	561	LEU
1	D	566	TYR
1	D	581	ARG
1	D	603	VAL
1	D	608	GLU
1	D	673	LEU
1	D	679	ASN
1	D	694	ASN
1	D	701	LEU
1	D	702	LEU
1	D	732	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (110) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	GLN
1	A	74	ASN
1	A	75	ASN
1	A	119	ASN
1	A	123	GLN
1	A	138	ASN
1	A	141	GLN
1	A	151	ASN
1	A	169	ASN
1	A	170	ASN
1	A	176	ASN
1	A	183	GLN
1	A	192	ASN
1	A	247	GLN

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Mol	Chain	Res	Type
1	A	314	GLN
1	A	377	ASN
1	A	435	GLN
1	A	463	ASN
1	A	469	GLN
1	A	483	HIS
1	A	505	GLN
1	A	572	ASN
1	A	612	GLN
1	A	679	ASN
1	A	694	ASN
1	A	697	GLN
1	A	704	HIS
1	A	718	GLN
1	A	745	ASN
1	B	72	GLN
1	B	75	ASN
1	B	112	GLN
1	B	119	ASN
1	B	170	ASN
1	B	176	ASN
1	B	183	GLN
1	B	192	ASN
1	B	219	ASN
1	B	227	GLN
1	B	247	GLN
1	B	345	HIS
1	B	369	ASN
1	B	435	GLN
1	B	455	GLN
1	B	463	ASN
1	B	483	HIS
1	B	505	GLN
1	B	572	ASN
1	B	586	GLN
1	B	595	ASN
1	B	606	GLN
1	B	612	GLN
1	B	679	ASN
1	B	694	ASN
1	B	704	HIS
1	B	718	GLN

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Mol	Chain	Res	Type
1	B	731	GLN
1	B	749	GLN
1	B	761	GLN
1	C	72	GLN
1	C	75	ASN
1	C	103	ASN
1	C	141	GLN
1	C	170	ASN
1	C	176	ASN
1	C	192	ASN
1	C	227	GLN
1	C	247	GLN
1	C	314	GLN
1	C	369	ASN
1	C	430	ASN
1	C	435	GLN
1	C	463	ASN
1	C	483	HIS
1	C	505	GLN
1	C	572	ASN
1	C	595	ASN
1	C	606	GLN
1	C	612	GLN
1	C	679	ASN
1	C	694	ASN
1	C	697	GLN
1	C	704	HIS
1	C	718	GLN
1	C	745	ASN
1	C	761	GLN
1	D	72	GLN
1	D	75	ASN
1	D	123	GLN
1	D	138	ASN
1	D	141	GLN
1	D	169	ASN
1	D	170	ASN
1	D	176	ASN
1	D	183	GLN
1	D	192	ASN
1	D	227	GLN
1	D	247	GLN

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Mol	Chain	Res	Type
1	D	377	ASN
1	D	393	ASN
1	D	463	ASN
1	D	483	HIS
1	D	572	ASN
1	D	606	GLN
1	D	612	GLN
1	D	679	ASN
1	D	694	ASN
1	D	704	HIS
1	D	718	GLN
1	D	757	HIS

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

20 carbohydrates are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	A	769(A)	1,3	12,14,15	0.48	0	15,19,21	0.60	0
3	NAG	A	770(B)	3	12,14,15	0.46	0	15,19,21	0.83	0
3	NAG	A	773(A)	1,3	12,14,15	0.45	0	15,19,21	0.87	0
3	NAG	A	774(B)	3	12,14,15	0.45	0	15,19,21	0.71	0
4	NAG	B	768(A)	1,4	12,14,15	0.48	0	15,19,21	0.94	0
4	NAG	B	769(B)	4	12,14,15	0.56	0	15,19,21	0.83	0
4	BMA	B	770(C)	4	10,11,12	0.40	0	11,15,17	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	B	774(A)	1,3	12,14,15	0.41	0	15,19,21	1.02	0
3	NAG	B	775(B)	3	12,14,15	0.44	0	15,19,21	0.89	1 (6%)
3	NAG	C	772(A)	1,3	12,14,15	0.42	0	15,19,21	0.80	1 (6%)
3	NAG	C	773(B)	3	12,14,15	0.40	0	15,19,21	0.93	1 (6%)
4	NAG	D	768(A)	1,4	12,14,15	0.44	0	15,19,21	0.83	0
4	NAG	D	769(B)	4	12,14,15	0.53	0	15,19,21	0.49	0
4	BMA	D	770(C)	4	10,11,12	0.52	0	11,15,17	0.57	0
3	NAG	D	771(A)	1,3	12,14,15	0.53	0	15,19,21	0.67	0
3	NAG	D	772(B)	3	12,14,15	0.46	0	15,19,21	0.69	0
3	NAG	D	774(A)	1,3	12,14,15	0.56	0	15,19,21	1.15	1 (6%)
3	NAG	D	775(B)	3	12,14,15	0.47	0	15,19,21	0.73	1 (6%)
3	NAG	D	776(A)	1,3	12,14,15	0.52	0	15,19,21	0.73	0
3	NAG	D	777(B)	3	12,14,15	0.39	0	15,19,21	0.95	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	769(A)	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	770(B)	3	-	0/6/23/26	0/1/1/1
3	NAG	A	773(A)	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	774(B)	3	-	0/6/23/26	0/1/1/1
4	NAG	B	768(A)	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	769(B)	4	-	0/6/23/26	0/1/1/1
4	BMA	B	770(C)	4	-	0/2/19/22	0/1/1/1
3	NAG	B	774(A)	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	775(B)	3	-	0/6/23/26	0/1/1/1
3	NAG	C	772(A)	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	773(B)	3	-	0/6/23/26	0/1/1/1
4	NAG	D	768(A)	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	769(B)	4	-	1/6/23/26	0/1/1/1
4	BMA	D	770(C)	4	-	0/2/19/22	0/1/1/1
3	NAG	D	771(A)	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	772(B)	3	-	0/6/23/26	0/1/1/1
3	NAG	D	774(A)	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	775(B)	3	-	0/6/23/26	0/1/1/1
3	NAG	D	776(A)	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	777(B)	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	774(A)	NAG	C3-C4-C5	-2.24	106.20	110.20
3	B	775(B)	NAG	C3-C2-N2	-2.24	108.35	111.76
3	C	773(B)	NAG	C3-C2-N2	-2.23	108.37	111.76
3	D	775(B)	NAG	C2-N2-C7	-2.09	119.59	123.09
3	D	777(B)	NAG	C6-C5-C4	-2.07	108.00	113.00
3	C	772(A)	NAG	C3-C2-N2	-2.07	108.62	111.76

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	769(B)	NAG	C3-C2-N2-C7

There are no ring outliers.

5.6 Ligand geometry

27 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	NAG	A	767(A)	1	12,14,15	0.45	0	15,19,21	0.63	0
2	NAG	A	768(A)	1	12,14,15	0.42	0	15,19,21	0.84	0
2	NAG	A	771(A)	1	12,14,15	0.42	0	15,19,21	0.70	0
2	NAG	A	772(A)	1	12,14,15	0.45	0	15,19,21	0.84	1 (6%)
6	PHI	A	801	6	12,12,13	5.38	2 (16%)	13,15,17	0.69	1 (7%)
6	P2Y	A	802	1,6	7,7,7	1.76	1 (14%)	8,8,8	1.58	1 (12%)
5	SO4	A	900	-	4,4,4	0.65	0	6,6,6	0.59	0
2	NAG	B	767(A)	1	12,14,15	0.44	0	15,19,21	0.71	0
2	NAG	B	771(A)	1	12,14,15	0.48	0	15,19,21	0.69	0
2	NAG	B	772(A)	1	12,14,15	0.61	0	15,19,21	0.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	B	773(A)	1	12,14,15	0.40	0	15,19,21	0.84	1 (6%)
6	PHI	B	803	6	12,12,13	5.16	2 (16%)	13,15,17	0.83	1 (7%)
6	P2Y	B	804	1,6	7,7,7	2.20	1 (14%)	8,8,8	1.32	2 (25%)
5	SO4	B	901	-	4,4,4	0.54	0	6,6,6	0.66	0
2	NAG	C	767(A)	1	12,14,15	0.46	0	15,19,21	0.98	1 (6%)
2	NAG	C	768(A)	1	12,14,15	0.45	0	15,19,21	0.70	0
2	NAG	C	769(A)	1	12,14,15	0.44	0	15,19,21	0.68	0
2	NAG	C	770(A)	1	12,14,15	0.60	0	15,19,21	0.48	0
2	NAG	C	771(A)	1	12,14,15	0.56	0	15,19,21	1.12	0
6	PHI	C	805	6	12,12,13	5.44	2 (16%)	13,15,17	0.34	0
6	P2Y	C	806	1,6	7,7,7	1.71	1 (14%)	8,8,8	1.31	1 (12%)
5	SO4	C	902	-	4,4,4	0.48	0	6,6,6	0.70	0
2	NAG	D	767(A)	1	12,14,15	0.46	0	15,19,21	0.72	0
2	NAG	D	773(A)	1	12,14,15	0.54	0	15,19,21	0.81	0
6	PHI	D	807	6	12,12,13	5.50	1 (8%)	13,15,17	1.07	1 (7%)
6	P2Y	D	808	1,6	7,7,7	2.01	1 (14%)	8,8,8	1.51	1 (12%)
5	SO4	D	903	-	4,4,4	0.63	0	6,6,6	0.66	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	767(A)	1	-	0/6/23/26	0/1/1/1
2	NAG	A	768(A)	1	-	2/6/23/26	0/1/1/1
2	NAG	A	771(A)	1	-	0/6/23/26	0/1/1/1
2	NAG	A	772(A)	1	-	0/6/23/26	0/1/1/1
6	PHI	A	801	6	-	0/4/6/8	0/1/1/1
6	P2Y	A	802	1,6	-	0/2/9/9	0/1/1/1
5	SO4	A	900	-	-	0/0/0/0	0/0/0/0
2	NAG	B	767(A)	1	-	0/6/23/26	0/1/1/1
2	NAG	B	771(A)	1	-	0/6/23/26	0/1/1/1
2	NAG	B	772(A)	1	-	0/6/23/26	0/1/1/1
2	NAG	B	773(A)	1	-	0/6/23/26	0/1/1/1
6	PHI	B	803	6	-	0/4/6/8	0/1/1/1
6	P2Y	B	804	1,6	-	0/2/9/9	0/1/1/1
5	SO4	B	901	-	-	0/0/0/0	0/0/0/0
2	NAG	C	767(A)	1	-	0/6/23/26	0/1/1/1
2	NAG	C	768(A)	1	-	1/6/23/26	0/1/1/1
2	NAG	C	769(A)	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	770(A)	1	-	0/6/23/26	0/1/1/1
2	NAG	C	771(A)	1	-	0/6/23/26	0/1/1/1
6	PHI	C	805	6	-	0/4/6/8	0/1/1/1
6	P2Y	C	806	1,6	-	0/2/9/9	0/1/1/1
5	SO4	C	902	-	-	0/0/0/0	0/0/0/0
2	NAG	D	767(A)	1	-	0/6/23/26	0/1/1/1
2	NAG	D	773(A)	1	-	1/6/23/26	0/1/1/1
6	PHI	D	807	6	-	0/4/6/8	0/1/1/1
6	P2Y	D	808	1,6	-	0/2/9/9	0/1/1/1
5	SO4	D	903	-	-	0/0/0/0	0/0/0/0

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	807	PHI	O-C	18.82	1.24	1.11
6	C	805	PHI	O-C	18.56	1.24	1.11
6	A	801	PHI	O-C	18.28	1.24	1.11
6	B	803	PHI	O-C	17.68	1.23	1.11
6	B	804	P2Y	C-NA	-5.53	1.32	1.47
6	D	808	P2Y	C-NA	-5.06	1.34	1.47
6	A	802	P2Y	C-NA	-4.57	1.35	1.47
6	C	806	P2Y	C-NA	-4.27	1.36	1.47
6	A	801	PHI	CA-C	2.93	1.53	1.48
6	C	805	PHI	CA-C	2.59	1.53	1.48
6	B	803	PHI	CA-C	2.47	1.52	1.48

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	803	PHI	C-CA-N	2.89	116.72	113.83
6	D	807	PHI	C-CA-N	2.63	116.46	113.83
2	B	773(A)	NAG	C2-N2-C7	-2.61	118.71	123.09
6	D	808	P2Y	CA-C-NA	2.52	122.22	112.67
6	B	804	P2Y	CD-N-CA	2.39	111.12	106.43
6	C	806	P2Y	CA-C-NA	2.34	121.55	112.67
6	A	802	P2Y	CA-C-NA	2.33	121.51	112.67
2	C	767(A)	NAG	C3-C2-N2	-2.30	108.26	111.76
6	A	801	PHI	C-CA-N	-2.29	111.55	113.83
6	B	804	P2Y	CA-C-NA	2.29	121.34	112.67
2	A	772(A)	NAG	C3-C2-N2	-2.10	108.56	111.76

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	768(A)	NAG	C8-C7-N2-C2
2	A	768(A)	NAG	O7-C7-N2-C2
2	D	773(A)	NAG	O7-C7-N2-C2
2	C	768(A)	NAG	O7-C7-N2-C2

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS failed to run properly - this section will therefore be empty.

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

EDS failed to run properly - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS failed to run properly - this section will therefore be empty.

6.4 Ligands ⓘ

EDS failed to run properly - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS failed to run properly - this section will therefore be empty.