



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:04 PM GMT

PDB ID : 1RWQ  
Title : Human Dipeptidyl peptidase IV in complex with 5-aminomethyl-6-(2,4-dichloro-phenyl)-2-(3,5-dimethoxy-phenyl)-pyrimidin-4-ylamine  
Authors : Hennig, M.; Thoma, R.; Stihle, M.  
Deposited on : 2003-12-17  
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

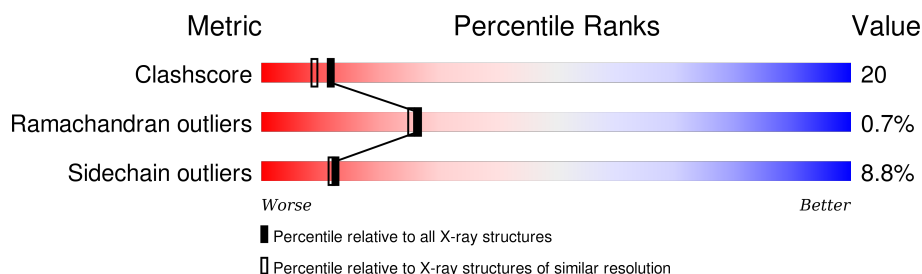
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 Å.



Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	728	 <div>59% 34% 7%</div>
1	B	728	 <div>62% 32% 6%</div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	B	797	X	-	-	-

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 12190 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 Dipeptidyl peptidase IV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	728	Total	C	N	O	S	0	0	0
			5963	3827	982	1128	26			
1	B	728	Total	C	N	O	S	0	0	0
			5963	3827	982	1128	26			

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



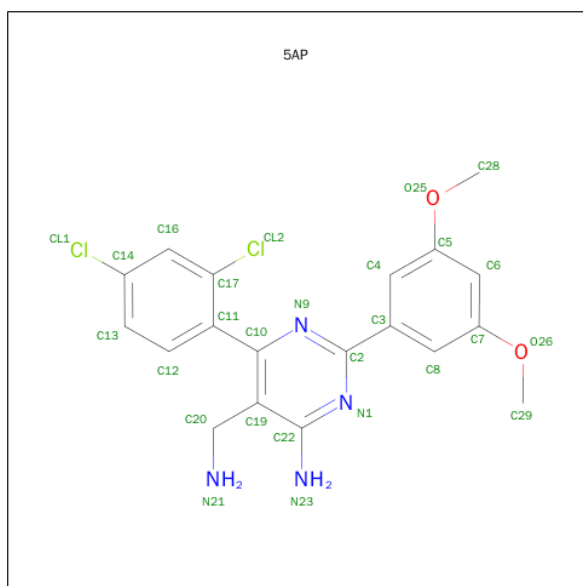
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	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		

- Molecule 3 is 5-(AMINOMETHYL)-6-(2,4-DICHLOROPHENYL)-2-(3,5-DIMETHOXYPHENYL)PYRIMIDIN-4-AMINE (three-letter code: 5AP) (formula: C<sub>19</sub>H<sub>18</sub>Cl<sub>2</sub>N<sub>4</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0
			27	19	2	4	2	0
3	B	1	Total	C	Cl	N	O	0
			27	19	2	4	2	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	47	Total	O	0	0
			47	47		
4	B	51	Total	O	0	0
			51	51		



WORLDWIDE  
**PDB**  
PROTEIN DATA BANK

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.68 Å 69.14 Å 422.56 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.20	Depositor
% Data completeness (in resolution range)	84.3 (15.00-2.20)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
Refinement program	REFMAC 5	Depositor
R, $R_{free}$	0.239 , 0.290	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12190	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5AP, NAG

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	0.99	2/6135 (0.0%)	1.14	30/8344 (0.4%)
1	B	1.03	4/6135 (0.1%)	1.16	32/8344 (0.4%)
All	All	1.01	6/12270 (0.0%)	1.15	62/16688 (0.4%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	124	TRP	CG-CD1	5.87	1.45	1.36
1	B	429	ARG	NE-CZ	5.84	1.40	1.33
1	A	745	SER	CB-OG	-5.64	1.34	1.42
1	A	248	TYR	CD1-CE1	5.59	1.47	1.39
1	B	243	ASP	CB-CG	5.44	1.63	1.51
1	B	719	ILE	CA-CB	-5.33	1.42	1.54

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	413	ASP	CB-CG-OD2	9.51	126.86	118.30
1	A	301	CYS	CA-CB-SG	-9.32	97.23	114.00
1	A	501	ASP	CB-CG-OD2	8.29	125.76	118.30
1	A	729	ASP	CB-CG-OD2	8.19	125.67	118.30
1	B	274	ASP	CB-CG-OD2	8.10	125.59	118.30
1	B	669	ARG	NE-CZ-NH1	8.08	124.34	120.30
1	B	65	ASP	CB-CG-OD2	7.90	125.41	118.30
1	A	669	ARG	NE-CZ-NH1	7.75	124.18	120.30
1	A	678	ASP	CB-CG-OD2	7.72	125.25	118.30
1	B	200	ASP	CB-CG-OD2	7.71	125.24	118.30
1	B	669	ARG	NE-CZ-NH2	-7.56	116.52	120.30
1	A	104	ASP	CB-CG-OD2	7.50	125.05	118.30
1	A	65	ASP	CB-CG-OD2	7.48	125.03	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	663	ASP	CB-CG-OD2	7.37	124.93	118.30
1	B	681	ASP	CB-CG-OD2	7.27	124.85	118.30
1	A	739	ASP	CB-CG-OD2	7.20	124.78	118.30
1	A	708	ASP	CB-CG-OD2	7.16	124.74	118.30
1	A	133	ASP	CB-CG-OD2	7.13	124.72	118.30
1	B	230	ASP	CB-CG-OD2	7.11	124.70	118.30
1	B	302	ASP	CB-CG-OD2	6.99	124.59	118.30
1	A	488	ASP	CB-CG-OD2	6.93	124.54	118.30
1	A	110	ASP	CB-CG-OD2	6.90	124.51	118.30
1	B	678	ASP	CB-CG-OD2	6.85	124.46	118.30
1	B	729	ASP	CB-CG-OD2	6.78	124.41	118.30
1	B	243	ASP	CB-CG-OD1	6.70	124.33	118.30
1	A	669	ARG	NE-CZ-NH2	-6.61	117.00	120.30
1	A	520	ASN	N-CA-C	-6.38	93.77	111.00
1	B	60	LEU	CA-CB-CG	6.33	129.85	115.30
1	B	133	ASP	CB-CG-OD2	6.30	123.97	118.30
1	B	488	ASP	CB-CG-OD2	6.29	123.96	118.30
1	B	244	GLU	CB-CA-C	-6.15	98.11	110.40
1	B	556	ASP	CB-CG-OD2	6.14	123.83	118.30
1	B	413	ASP	CB-CG-OD2	6.07	123.76	118.30
1	B	354	VAL	CB-CA-C	-6.04	99.92	111.40
1	A	545	ASP	CB-CG-OD2	6.04	123.73	118.30
1	A	329	ASP	CB-CG-OD2	5.95	123.66	118.30
1	A	230	ASP	CB-CG-OD2	5.87	123.59	118.30
1	B	111	GLY	N-CA-C	5.86	127.76	113.10
1	B	155	VAL	CB-CA-C	-5.78	100.41	111.40
1	B	605	ASP	CB-CG-OD2	5.69	123.42	118.30
1	B	390	ASP	CB-CG-OD2	5.69	123.42	118.30
1	A	515	ASP	CB-CG-OD2	5.67	123.41	118.30
1	B	110	ASP	CB-CG-OD2	5.65	123.39	118.30
1	B	737	ASP	CB-CG-OD2	5.62	123.36	118.30
1	A	605	ASP	CB-CG-OD2	5.52	123.27	118.30
1	A	542	LEU	CB-CG-CD1	-5.50	101.65	111.00
1	B	535	ASP	CB-CG-OD2	5.47	123.23	118.30
1	A	316	LEU	CA-CB-CG	5.47	127.88	115.30
1	A	133	ASP	N-CA-C	-5.43	96.33	111.00
1	A	709	ASP	CB-CG-OD2	5.40	123.16	118.30
1	A	156	THR	OG1-CB-CG2	-5.37	97.65	110.00
1	B	171	ASP	CB-CG-OD2	5.35	123.12	118.30
1	A	47	ASP	CB-CG-OD2	5.34	123.10	118.30
1	B	243	ASP	OD1-CG-OD2	-5.33	113.18	123.30
1	B	328	CYS	CA-CB-SG	-5.32	104.42	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	223	LEU	CB-CG-CD2	-5.25	102.08	111.00
1	A	556	ASP	CB-CG-OD1	5.25	123.02	118.30
1	A	40	ARG	N-CA-C	5.11	124.81	111.00
1	A	415	LEU	CB-CG-CD2	-5.10	102.34	111.00
1	B	492	ARG	CB-CA-C	-5.04	100.31	110.40
1	B	472	CYS	CA-CB-SG	5.02	123.04	114.00
1	A	401	THR	OG1-CB-CG2	-5.00	98.49	110.00

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5963	0	5681	241	0
1	B	5963	0	5683	232	0
2	A	56	0	52	2	0
2	B	56	0	52	8	0
3	A	27	0	18	5	0
3	B	27	0	18	0	0
4	A	47	0	0	4	0
4	B	51	0	0	0	0
All	All	12190	0	11504	473	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 20.

All (473) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:ASN:HD21	2:B:793:NAG:C1	1.45	1.28
1:B:600:THR:CG2	1:B:601:PHE:H	1.59	1.15
1:B:267:LYS:HD2	1:B:286:GLN:HE22	1.06	1.12
1:B:92:ASN:HD22	2:B:797:NAG:C1	1.65	1.08
1:B:600:THR:HG22	1:B:601:PHE:H	1.23	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:GLN:OE1	1:A:669:ARG:HG2	1.61	0.99
1:B:520:ASN:O	1:B:521:GLU:HB2	1.59	0.99
1:B:600:THR:CG2	1:B:601:PHE:N	2.27	0.96
1:B:146:GLU:O	1:B:175:LYS:NZ	2.01	0.93
1:B:163:LYS:HZ3	1:B:273:THR:CG2	1.83	0.92
1:B:150:ASN:HD21	2:B:793:NAG:C2	1.83	0.91
1:A:221:THR:O	1:A:273:THR:HB	1.70	0.90
1:B:221:THR:O	1:B:273:THR:HB	1.71	0.89
1:B:163:LYS:NZ	1:B:273:THR:CG2	2.35	0.89
1:A:735:TYR:OH	1:A:750:HIS:HD2	1.54	0.89
1:B:377:ASN:C	1:B:377:ASN:HD22	1.72	0.89
1:A:726:VAL:HG12	1:A:728:VAL:HG23	1.53	0.89
1:B:267:LYS:HD2	1:B:286:GLN:NE2	1.88	0.88
1:A:745:SER:O	1:A:749:GLN:HG3	1.73	0.88
1:A:614:SER:O	1:A:615:LYS:C	2.11	0.88
1:B:236:ILE:HD12	1:B:712:HIS:CD2	2.09	0.87
1:A:594:ILE:CD1	1:A:601:PHE:HB2	2.04	0.87
1:A:69:LEU:CD1	1:A:107:ILE:HD12	2.06	0.84
1:B:600:THR:HG23	1:B:601:PHE:N	1.93	0.84
1:A:463:LYS:O	1:A:464:GLU:HB2	1.75	0.84
1:A:471:ARG:HG3	1:A:471:ARG:O	1.76	0.84
1:A:73:GLU:N	4:A:912:HOH:O	2.12	0.83
1:A:375:ILE:HG22	1:A:376:SER:O	1.77	0.83
1:B:549:GLY:O	1:B:552:SER:OG	1.96	0.83
1:B:163:LYS:HZ2	1:B:273:THR:HG21	1.45	0.82
1:A:621:ASN:C	1:A:621:ASN:HD22	1.82	0.81
1:B:110:ASP:OD2	1:B:161:GLY:N	2.14	0.81
1:B:657:SER:H	1:B:715:GLN:NE2	1.78	0.81
1:B:653:VAL:HG22	1:B:703:ILE:HD12	1.61	0.81
1:A:487:ASN:O	1:A:489:LYS:N	2.14	0.81
1:B:277:SER:HB3	1:B:280:THR:HB	1.62	0.80
1:B:600:THR:HG23	1:B:601:PHE:H	1.44	0.80
1:A:654:ALA:N	1:A:655:PRO:CD	2.45	0.80
1:B:680:LEU:HD22	1:B:684:ARG:CD	2.12	0.79
1:A:69:LEU:HD13	1:A:107:ILE:HD12	1.65	0.78
1:A:44:THR:HG22	1:A:46:THR:H	1.47	0.78
1:B:163:LYS:NZ	1:B:273:THR:HG21	1.99	0.77
1:A:680:LEU:HD11	1:A:684:ARG:HD3	1.64	0.77
1:A:43:TYR:CD2	1:A:565:THR:HG22	2.20	0.76
1:B:143:ILE:HD13	1:B:179:ASN:HA	1.64	0.76
1:B:403:GLU:H	1:B:420:ASN:HD21	1.32	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:ILE:HD13	1:B:69:LEU:HG	1.68	0.76
1:B:680:LEU:HD22	1:B:684:ARG:HD2	1.66	0.76
1:A:403:GLU:H	1:A:420:ASN:HD21	1.32	0.76
1:B:109:PRO:HD2	1:B:161:GLY:O	1.87	0.75
1:A:104:ASP:OD1	1:A:105:TYR:N	2.19	0.75
1:A:499:ALA:O	1:A:502:LYS:HG3	1.87	0.74
1:B:320:GLN:OE1	1:B:669:ARG:HD3	1.87	0.73
1:B:163:LYS:HZ3	1:B:273:THR:HG22	1.52	0.73
1:A:163:LYS:HZ2	1:A:273:THR:CG2	2.01	0.73
1:A:219:ASN:HB2	1:A:308:GLN:OE1	1.88	0.73
1:A:613:PHE:O	1:A:616:MET:HB2	1.89	0.73
1:B:41:LYS:NZ	1:B:42:THR:O	2.21	0.73
1:B:46:THR:HG23	1:B:50:LYS:HD2	1.71	0.72
1:B:155:VAL:HG12	1:B:156:THR:N	2.05	0.72
1:A:561:LEU:O	4:A:925:HOH:O	2.08	0.71
1:A:392:LYS:HD2	1:A:393:ASP:OD2	1.90	0.71
1:A:430:ASN:OD1	1:A:446:SER:OG	2.09	0.71
1:B:351:THR:HG22	1:B:592:HIS:ND1	2.05	0.70
1:A:726:VAL:HG12	1:A:728:VAL:CG2	2.21	0.70
1:B:110:ASP:CG	1:B:161:GLY:H	1.94	0.70
1:B:377:ASN:ND2	1:B:379:GLU:H	1.90	0.70
1:A:351:THR:OG1	1:A:592:HIS:HD2	1.74	0.70
1:A:562:ASN:O	1:A:565:THR:HB	1.92	0.69
1:B:42:THR:HG23	1:B:570:THR:OG1	1.91	0.69
1:B:236:ILE:HD12	1:B:712:HIS:CG	2.28	0.69
1:A:528:MET:HE3	1:A:530:LEU:HD21	1.74	0.69
1:A:680:LEU:HD11	1:A:684:ARG:CD	2.23	0.69
1:B:735:TYR:OH	1:B:750:HIS:HD2	1.75	0.68
1:A:82:GLU:HB2	1:A:467:TYR:OH	1.94	0.68
1:A:481:THR:OG1	1:A:483:HIS:HE1	1.76	0.68
1:A:105:TYR:HB2	1:A:114:ILE:HD11	1.76	0.67
1:A:736:THR:HG21	1:B:717:ALA:O	1.94	0.67
1:B:347:GLU:OE2	1:B:373:LYS:NZ	2.25	0.67
1:A:693:GLU:O	1:A:696:LYS:HG2	1.94	0.67
1:B:143:ILE:CD1	1:B:145:GLU:O	2.43	0.67
1:A:163:LYS:NZ	1:A:273:THR:CG2	2.57	0.67
1:B:435:GLN:NE2	1:B:441:LYS:HD2	2.09	0.66
1:A:163:LYS:HZ2	1:A:273:THR:HG22	1.58	0.66
1:B:742:ILE:HG22	1:B:742:ILE:O	1.96	0.66
1:B:435:GLN:HE22	1:B:441:LYS:HD2	1.62	0.65
1:A:415:LEU:C	1:A:415:LEU:HD23	2.17	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:415:LEU:HD23	1:B:415:LEU:C	2.16	0.65
1:B:143:ILE:HG13	1:B:143:ILE:O	1.96	0.65
1:A:482:LEU:HD13	1:A:491:LEU:HD12	1.76	0.65
1:B:509:MET:HE3	1:B:510:PRO:HD2	1.77	0.65
1:A:219:ASN:CB	1:A:308:GLN:OE1	2.45	0.65
1:B:75:ASN:OD1	1:B:92:ASN:HB3	1.96	0.64
1:B:107:ILE:HG13	1:B:114:ILE:HG13	1.79	0.64
1:B:107:ILE:CG1	1:B:114:ILE:HD12	2.27	0.64
1:A:499:ALA:O	1:A:502:LYS:CG	2.46	0.64
1:A:123:GLN:HG2	1:A:124:TRP:H	1.63	0.64
1:A:320:GLN:OE1	1:A:669:ARG:CG	2.43	0.64
1:A:72:GLN:O	1:A:73:GLU:HB2	1.97	0.64
1:B:594:ILE:HD11	1:B:602:GLU:H	1.62	0.63
1:A:657:SER:H	1:A:715:GLN:NE2	1.96	0.63
1:A:123:GLN:HG2	1:A:124:TRP:N	2.13	0.63
1:B:332:GLU:HG2	1:B:333:SER:N	2.13	0.63
1:A:596:ARG:NH2	1:A:678:ASP:OD1	2.30	0.62
1:B:651:ILE:HD11	1:B:759:ILE:HD12	1.79	0.62
2:A:793:NAG:H3	2:A:793:NAG:H83	1.79	0.62
1:B:293:MET:O	1:B:298:HIS:HD2	1.82	0.62
1:B:471:ARG:O	1:B:471:ARG:HG2	1.99	0.62
1:A:594:ILE:HD11	1:A:601:PHE:HB2	1.77	0.62
1:B:150:ASN:ND2	2:B:793:NAG:C2	2.58	0.62
1:B:107:ILE:HG12	1:B:114:ILE:HD12	1.80	0.62
1:B:620:ASP:OD1	1:B:620:ASP:O	2.18	0.62
1:B:78:VAL:HG23	1:B:89:PHE:HB2	1.82	0.61
1:B:649:CYS:HB3	1:B:699:GLU:HB2	1.81	0.61
1:B:377:ASN:C	1:B:377:ASN:ND2	2.45	0.61
1:A:180:LEU:HD12	1:A:181:PRO:HD3	1.81	0.61
1:A:417:TYR:CE1	1:A:434:ILE:HD11	2.36	0.61
1:B:120:TYR:OH	1:B:122:LYS:HB2	2.01	0.61
1:B:520:ASN:O	1:B:521:GLU:CB	2.40	0.60
1:A:422:TYR:O	1:A:424:GLY:N	2.34	0.60
1:A:105:TYR:C	1:A:105:TYR:CD1	2.73	0.60
1:A:123:GLN:HG2	1:A:124:TRP:CG	2.37	0.60
1:A:654:ALA:N	1:A:655:PRO:HD2	2.16	0.60
1:A:463:LYS:O	1:A:464:GLU:CB	2.47	0.60
1:B:41:LYS:HE3	1:B:53:TYR:OH	2.02	0.60
1:A:471:ARG:CG	1:A:471:ARG:O	2.48	0.60
1:B:42:THR:CG2	1:B:570:THR:OG1	2.49	0.60
1:A:123:GLN:HG2	1:A:124:TRP:CD1	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:MET:HE2	1:A:324:VAL:HG23	1.84	0.59
1:A:455:GLN:HB2	1:A:475:PRO:HD3	1.84	0.59
1:B:69:LEU:HD23	1:B:78:VAL:HG22	1.85	0.59
1:B:414:TYR:CD1	1:B:433:LYS:HE2	2.38	0.59
1:B:237:GLU:HG2	1:B:253:ARG:HG2	1.83	0.59
1:B:330:TYR:HB2	1:B:337:TRP:CH2	2.37	0.59
1:B:143:ILE:HD11	1:B:145:GLU:O	2.03	0.59
1:A:351:THR:OG1	1:A:592:HIS:CD2	2.55	0.59
1:A:481:THR:OG1	1:A:483:HIS:CE1	2.55	0.59
1:A:293:MET:CE	1:A:324:VAL:HG23	2.33	0.59
1:B:387:PHE:CE2	1:B:394:CYS:HB3	2.38	0.58
1:B:46:THR:HG23	1:B:50:LYS:CD	2.33	0.58
1:A:305:TRP:CZ3	1:A:311:ILE:HG12	2.37	0.58
1:A:69:LEU:HD13	1:A:107:ILE:CD1	2.33	0.58
1:B:177:GLU:HB2	1:B:180:LEU:HD23	1.85	0.58
1:A:105:TYR:O	1:A:105:TYR:CD1	2.57	0.58
1:A:89:PHE:CE2	1:A:107:ILE:HD13	2.38	0.58
1:A:340:LEU:HB3	1:A:343:ARG:HD2	1.86	0.58
1:A:312:SER:O	1:A:313:LEU:HD23	2.04	0.57
1:A:431:LEU:HD22	1:A:432:TYR:N	2.20	0.57
1:B:105:TYR:CD1	1:B:105:TYR:C	2.78	0.57
1:B:651:ILE:HD11	1:B:759:ILE:CD1	2.34	0.57
1:A:272:ASN:C	1:A:272:ASN:OD1	2.42	0.57
1:B:217:SER:HB2	1:B:222:PHE:HB2	1.87	0.57
1:B:277:SER:CB	1:B:280:THR:HB	2.33	0.57
1:B:320:GLN:OE1	1:B:669:ARG:CD	2.53	0.56
1:B:306:ALA:HB3	1:B:310:ARG:HG2	1.85	0.56
1:A:163:LYS:NZ	1:A:273:THR:HG22	2.19	0.56
1:B:657:SER:H	1:B:715:GLN:HE21	1.51	0.56
1:B:223:LEU:C	1:B:223:LEU:HD22	2.26	0.56
1:B:46:THR:CG2	1:B:50:LYS:CD	2.83	0.56
1:B:518:ILE:HA	1:B:522:THR:O	2.06	0.56
1:B:620:ASP:OD1	1:B:620:ASP:C	2.44	0.56
1:A:331:ASP:OD2	1:A:334:SER:HB3	2.06	0.56
1:A:69:LEU:HD11	1:A:107:ILE:HD12	1.88	0.56
1:B:75:ASN:OD1	1:B:92:ASN:CB	2.54	0.55
1:A:594:ILE:HG23	1:A:594:ILE:O	2.05	0.55
1:B:143:ILE:HD12	1:B:145:GLU:O	2.04	0.55
1:A:735:TYR:OH	1:A:750:HIS:CD2	2.46	0.55
1:B:46:THR:CG2	1:B:50:LYS:HD2	2.36	0.55
1:A:300:LEU:C	1:A:300:LEU:CD2	2.75	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:PRO:HD2	1:A:161:GLY:O	2.07	0.55
1:A:234:PRO:HB2	1:B:248:TYR:CZ	2.41	0.55
1:A:611:ARG:O	1:A:612:GLN:C	2.44	0.55
1:A:629:TRP:O	1:A:632:GLY:N	2.41	0.54
1:A:43:TYR:CD2	1:A:565:THR:CG2	2.90	0.54
1:A:123:GLN:CG	1:A:124:TRP:N	2.69	0.54
1:B:63:ILE:HD13	1:B:69:LEU:CG	2.35	0.54
1:A:158:SER:OG	1:A:163:LYS:HB2	2.07	0.54
1:B:155:VAL:CG1	1:B:156:THR:N	2.71	0.54
1:B:69:LEU:CD2	1:B:78:VAL:HG22	2.38	0.54
1:B:545:ASP:OD1	1:B:545:ASP:C	2.46	0.54
1:B:600:THR:HG22	1:B:601:PHE:N	2.05	0.54
1:A:327:ILE:HB	1:A:343:ARG:HG3	1.89	0.54
1:A:751:ILE:O	1:A:755:MET:HG3	2.07	0.54
1:A:680:LEU:CD1	1:A:684:ARG:CD	2.86	0.53
1:A:680:LEU:CD1	1:A:684:ARG:HD3	2.36	0.53
1:A:479:LEU:HD13	1:A:481:THR:HG23	1.89	0.53
1:B:741:GLY:O	1:B:742:ILE:C	2.47	0.53
1:A:377:ASN:C	1:A:377:ASN:HD22	2.11	0.53
1:A:414:TYR:CE2	1:A:435:GLN:HG3	2.44	0.53
1:B:63:ILE:CD1	1:B:69:LEU:CD1	2.86	0.53
1:A:431:LEU:HD13	1:A:445:LEU:HB2	1.91	0.53
1:A:208:PHE:HZ	1:A:300:LEU:HD13	1.73	0.53
1:A:381:TYR:CZ	1:A:401:THR:HG23	2.43	0.53
1:B:482:LEU:HB2	1:B:494:LEU:HD11	1.90	0.53
1:A:272:ASN:OD1	1:A:274:ASP:N	2.35	0.53
1:B:471:ARG:O	1:B:471:ARG:CG	2.56	0.53
1:A:626:ILE:O	1:A:650:GLY:HA2	2.09	0.53
1:A:357:PHE:HD1	1:A:669:ARG:HH21	1.56	0.52
1:A:621:ASN:ND2	1:A:621:ASN:C	2.54	0.52
1:B:680:LEU:CD2	1:B:684:ARG:NE	2.72	0.52
1:B:45:LEU:HG	1:B:49:LEU:HD22	1.91	0.52
1:B:46:THR:HG22	1:B:50:LYS:HD3	1.91	0.52
1:B:120:TYR:CD1	1:B:120:TYR:C	2.83	0.52
1:B:693:GLU:O	1:B:696:LYS:HG2	2.09	0.52
1:B:92:ASN:HD21	2:B:797:NAG:C1	2.18	0.52
1:A:89:PHE:HE2	1:A:107:ILE:HD13	1.75	0.52
1:B:107:ILE:CG1	1:B:114:ILE:CD1	2.87	0.52
1:A:540:TYR:CD1	1:A:540:TYR:N	2.75	0.52
1:A:540:TYR:HB3	1:A:541:PRO:HD2	1.92	0.52
1:A:654:ALA:N	1:A:655:PRO:HD3	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:666:TYR:CZ	3:A:900:5AP:H13	2.44	0.52
1:B:562:ASN:HD22	1:B:562:ASN:C	2.14	0.52
1:A:357:PHE:HB2	1:A:358:ARG:NH1	2.25	0.51
1:A:422:TYR:C	1:A:424:GLY:N	2.64	0.51
1:A:571:GLU:HB2	1:A:573:ILE:HD12	1.92	0.51
1:A:431:LEU:HD13	1:A:445:LEU:HD12	1.91	0.51
1:A:519:LEU:C	1:A:520:ASN:O	2.48	0.51
1:A:356:ARG:NH2	1:A:403:GLU:OE1	2.43	0.51
1:A:533:HIS:O	1:A:534:PHE:C	2.48	0.51
1:B:377:ASN:ND2	1:B:378:GLU:N	2.59	0.51
1:A:48:TYR:CD2	1:A:49:LEU:HD13	2.45	0.51
1:B:236:ILE:HG12	1:B:237:GLU:N	2.26	0.51
1:B:293:MET:O	1:B:298:HIS:CD2	2.64	0.51
1:B:46:THR:CG2	1:B:50:LYS:HD3	2.41	0.51
1:B:651:ILE:CD1	1:B:759:ILE:CD1	2.89	0.51
1:B:651:ILE:CD1	1:B:759:ILE:HD11	2.41	0.51
1:B:614:SER:OG	1:B:624:ILE:HD11	2.11	0.51
1:B:463:LYS:O	1:B:464:GLU:HB2	2.11	0.51
1:B:215:TRP:CH2	1:B:303:VAL:HG21	2.46	0.51
1:B:596:ARG:C	1:B:597:ARG:HG3	2.31	0.51
1:B:680:LEU:HD21	1:B:684:ARG:NE	2.26	0.50
1:A:105:TYR:HA	1:A:115:LEU:O	2.12	0.50
1:B:651:ILE:HD12	1:B:759:ILE:HD11	1.93	0.50
1:B:387:PHE:CD2	1:B:394:CYS:HB3	2.46	0.50
1:B:125:ARG:HD2	1:B:126:HIS:CE1	2.47	0.50
1:B:432:TYR:CE2	1:B:444:CYS:HB2	2.47	0.50
1:B:429:ARG:HG3	1:B:456:TYR:CE2	2.47	0.50
1:B:267:LYS:CD	1:B:286:GLN:HE22	1.99	0.50
1:A:543:LEU:HD22	1:A:543:LEU:C	2.32	0.50
1:B:377:ASN:ND2	1:B:379:GLU:N	2.57	0.50
1:A:377:ASN:ND2	1:A:379:GLU:H	2.10	0.50
1:B:758:PHE:O	1:B:758:PHE:CD2	2.65	0.50
1:A:612:GLN:O	1:A:613:PHE:C	2.49	0.50
1:A:621:ASN:HD22	1:A:622:LYS:N	2.09	0.50
1:B:227:GLN:O	1:B:266:VAL:HA	2.11	0.50
1:B:236:ILE:HD12	1:B:712:HIS:NE2	2.25	0.50
1:A:221:THR:O	1:A:273:THR:CB	2.54	0.50
1:B:108:SER:OG	1:B:113:PHE:HB2	2.12	0.50
1:A:422:TYR:C	1:A:424:GLY:H	2.16	0.49
1:B:63:ILE:HD13	1:B:69:LEU:CD1	2.42	0.49
1:B:459:VAL:HG22	1:B:460:SER:N	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:383:HIS:HD2	1:B:398:THR:CB	2.23	0.49
1:A:329:ASP:O	1:A:337:TRP:HA	2.12	0.49
1:A:98:PHE:CE2	1:A:100:HIS:HB2	2.47	0.49
1:A:198:ILE:HA	1:A:211:TYR:O	2.13	0.49
1:B:377:ASN:HD22	1:B:378:GLU:N	2.09	0.49
1:A:458:SER:OG	1:A:471:ARG:CG	2.61	0.49
1:A:42:THR:HG23	1:A:570:THR:OG1	2.13	0.49
1:B:736:THR:O	1:B:737:ASP:HB2	2.12	0.49
1:B:428:GLY:O	1:B:429:ARG:HG2	2.12	0.49
1:B:236:ILE:HD12	1:B:712:HIS:CE1	2.48	0.49
1:B:422:TYR:CE2	1:B:423:LYS:HE3	2.48	0.48
1:A:614:SER:O	1:A:616:MET:N	2.45	0.48
1:A:334:SER:OG	1:A:336:ARG:HG3	2.13	0.48
1:A:739:ASP:OD1	1:A:739:ASP:C	2.51	0.48
1:B:75:ASN:OD1	1:B:92:ASN:CG	2.52	0.48
1:B:386:TYR:HB2	1:B:397:ILE:CD1	2.43	0.48
1:B:402:TRP:CD1	1:B:421:GLU:HG3	2.48	0.48
1:A:167:VAL:HG11	1:A:198:ILE:HG12	1.96	0.48
1:A:296:GLY:O	1:A:298:HIS:HD2	1.97	0.48
1:A:173:TYR:OH	1:A:184:ARG:HD2	2.14	0.48
1:B:122:LYS:HG2	1:B:123:GLN:N	2.29	0.48
1:B:162:HIS:O	1:B:162:HIS:CD2	2.67	0.48
1:A:420:ASN:C	1:A:420:ASN:HD22	2.15	0.48
1:A:594:ILE:HD13	1:A:601:PHE:HB2	1.93	0.47
1:B:522:THR:HG22	1:B:523:LYS:N	2.28	0.47
1:A:327:ILE:HD13	1:A:389:ILE:HD13	1.97	0.47
1:A:622:LYS:O	1:A:648:LYS:HD2	2.15	0.47
1:A:487:ASN:O	1:A:488:ASP:C	2.53	0.47
1:B:429:ARG:HG3	1:B:456:TYR:CZ	2.50	0.47
1:A:57:LEU:HD22	1:A:480:TYR:OH	2.14	0.47
1:B:636:THR:O	1:B:640:LEU:HG	2.14	0.47
1:B:415:LEU:HD23	1:B:416:TYR:N	2.29	0.47
1:B:507:VAL:HG23	1:B:508:GLN:N	2.29	0.47
1:A:431:LEU:CD2	1:A:432:TYR:N	2.78	0.47
1:A:456:TYR:HB2	1:A:557:THR:OG1	2.15	0.47
1:A:169:ASN:O	1:A:170:ASN:HB2	2.14	0.47
1:A:540:TYR:O	1:A:619:VAL:HA	2.14	0.47
1:A:314:GLN:HG3	1:A:325:MET:HG3	1.96	0.47
1:B:91:GLU:OE1	1:B:94:THR:OG1	2.31	0.47
1:B:110:ASP:HB2	1:B:161:GLY:HA2	1.97	0.47
1:A:500:LEU:HA	1:A:503:MET:CE	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:GLU:HG3	1:B:132:TYR:CE1	2.50	0.47
1:A:680:LEU:HD11	1:A:684:ARG:NE	2.30	0.46
1:A:331:ASP:C	1:A:331:ASP:OD1	2.53	0.46
1:A:708:ASP:HA	1:A:739:ASP:HA	1.97	0.46
1:B:71:LYS:HB3	1:B:71:LYS:HZ2	1.79	0.46
1:B:429:ARG:CZ	1:B:456:TYR:OH	2.63	0.46
1:A:230:ASP:OD1	1:A:264:PRO:HB3	2.15	0.46
1:A:71:LYS:HA	1:A:75:ASN:O	2.16	0.46
1:A:703:ILE:HA	1:A:733:MET:O	2.15	0.46
1:B:115:LEU:HD11	1:B:155:VAL:HG11	1.97	0.46
1:B:563:TRP:HH2	1:B:759:ILE:HD13	1.80	0.46
1:A:417:TYR:O	1:A:431:LEU:HD23	2.16	0.46
1:B:658:ARG:NH2	1:B:660:GLU:OE1	2.49	0.46
1:B:327:ILE:HG21	1:B:343:ARG:HD3	1.97	0.46
1:B:626:ILE:O	1:B:626:ILE:HG23	2.15	0.46
2:B:793:NAG:H82	2:B:793:NAG:C1	2.46	0.46
1:B:196:ASN:OD1	1:B:227:GLN:HG3	2.15	0.46
1:A:763:PHE:O	1:A:765:LEU:HG	2.16	0.46
1:A:271:VAL:CG1	1:A:272:ASN:N	2.77	0.46
1:B:715:GLN:HB3	1:B:715:GLN:HE21	1.55	0.46
1:A:57:LEU:CD2	1:A:480:TYR:OH	2.64	0.46
1:A:558:VAL:HG12	1:A:559:PHE:N	2.30	0.46
1:B:43:TYR:HB3	1:B:569:SER:HB3	1.99	0.46
1:B:624:ILE:HG22	1:B:647:PHE:CD2	2.50	0.46
1:B:163:LYS:NZ	1:B:273:THR:HG22	2.20	0.45
1:A:431:LEU:C	1:A:431:LEU:HD22	2.36	0.45
1:A:205:GLU:OE2	3:A:900:5AP:N21	2.49	0.45
1:A:366:LEU:HD23	1:A:366:LEU:HA	1.69	0.45
1:B:680:LEU:CD2	1:B:684:ARG:CD	2.90	0.45
1:A:300:LEU:C	1:A:300:LEU:HD22	2.36	0.45
1:A:235:LEU:HD23	1:A:255:PRO:HA	1.98	0.45
1:B:107:ILE:O	1:B:108:SER:C	2.53	0.45
1:A:327:ILE:HD13	1:A:389:ILE:CD1	2.47	0.45
1:A:567:LEU:HD22	1:A:573:ILE:HD13	1.97	0.45
1:A:558:VAL:CG1	1:A:559:PHE:N	2.79	0.45
1:A:69:LEU:HD23	1:A:69:LEU:HA	1.72	0.45
1:B:51:ASN:OD1	1:B:54:ARG:HG2	2.17	0.45
1:B:604:GLU:O	1:B:607:ILE:HB	2.16	0.45
3:A:900:5AP:H283	4:A:940:HOH:O	2.17	0.45
1:B:207:VAL:HG12	1:B:208:PHE:CD1	2.51	0.45
1:B:146:GLU:OE1	1:B:181:PRO:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:543:LEU:CD2	1:A:543:LEU:C	2.85	0.45
1:A:765:LEU:HA	1:A:766:PRO:HD3	1.82	0.45
1:A:44:THR:HG22	1:A:45:LEU:N	2.32	0.45
1:B:107:ILE:HG13	1:B:114:ILE:CD1	2.47	0.45
1:B:107:ILE:O	1:B:108:SER:O	2.34	0.45
1:A:406:GLY:O	1:A:417:TYR:HB2	2.17	0.45
1:A:571:GLU:HA	1:A:571:GLU:OE1	2.17	0.45
1:A:146:GLU:HG3	1:A:180:LEU:C	2.38	0.44
1:B:403:GLU:H	1:B:420:ASN:ND2	2.08	0.44
1:B:403:GLU:OE1	1:B:585:TYR:HA	2.17	0.44
1:B:599:GLY:N	1:B:602:GLU:OE2	2.35	0.44
1:B:594:ILE:HD11	1:B:602:GLU:N	2.30	0.44
1:A:562:ASN:O	1:A:565:THR:N	2.50	0.44
1:B:379:GLU:N	1:B:379:GLU:CD	2.71	0.44
1:A:666:TYR:OH	3:A:900:5AP:H13	2.18	0.44
1:A:196:ASN:OD1	1:A:227:GLN:HG3	2.17	0.44
1:B:580:GLY:C	1:B:581:ARG:O	2.52	0.44
1:B:420:ASN:C	1:B:420:ASN:HD22	2.20	0.44
1:A:371:PHE:CE1	1:A:387:PHE:HB2	2.53	0.44
1:A:581:ARG:HB2	1:A:605:ASP:OD2	2.18	0.44
1:B:107:ILE:HG13	1:B:114:ILE:CG1	2.45	0.44
1:B:462:SER:O	1:B:463:LYS:C	2.55	0.44
1:A:195:TYR:O	1:A:227:GLN:HA	2.18	0.44
1:A:403:GLU:H	1:A:420:ASN:ND2	2.08	0.43
1:B:156:THR:HG22	1:B:157:TRP:O	2.18	0.43
1:A:446:SER:O	1:A:447:CYS:C	2.55	0.43
1:B:594:ILE:O	1:B:595:ASN:C	2.54	0.43
1:A:116:LEU:O	1:A:132:TYR:HA	2.17	0.43
1:A:326:ASP:OD1	1:A:344:GLN:HG2	2.18	0.43
1:B:82:GLU:OE1	1:B:467:TYR:OH	2.23	0.43
1:A:219:ASN:HB3	1:A:221:THR:OG1	2.18	0.43
1:A:331:ASP:CG	1:A:334:SER:HB3	2.39	0.43
1:B:619:VAL:O	1:B:619:VAL:HG22	2.17	0.43
1:B:510:PRO:HD3	1:B:569:SER:HB2	2.00	0.43
1:A:414:TYR:HE2	1:A:435:GLN:HG3	1.84	0.43
1:B:405:ILE:HD13	1:B:429:ARG:HD3	2.00	0.43
1:A:320:GLN:CD	1:A:669:ARG:HG2	2.34	0.43
1:B:299:TYR:CZ	1:B:665:VAL:HG22	2.54	0.43
1:A:224:ALA:HA	1:A:270:VAL:HA	2.00	0.43
1:B:562:ASN:HD21	1:B:564:ALA:HB3	1.84	0.43
1:B:613:PHE:O	1:B:616:MET:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:436:LEU:HD23	1:B:436:LEU:N	2.31	0.43
1:B:107:ILE:CG1	1:B:114:ILE:HG13	2.47	0.43
1:B:90:LEU:HD11	1:B:95:PHE:HE2	1.83	0.43
1:A:431:LEU:CD2	1:A:431:LEU:C	2.85	0.43
1:A:180:LEU:HD12	1:A:180:LEU:HA	1.69	0.43
1:A:44:THR:CG2	1:A:45:LEU:N	2.82	0.43
1:A:327:ILE:CD1	1:A:389:ILE:HD13	2.48	0.43
1:A:349:SER:HB3	1:A:352:GLY:O	2.18	0.43
1:A:653:VAL:C	1:A:655:PRO:HD3	2.39	0.43
1:B:236:ILE:CD1	1:B:712:HIS:CG	3.00	0.42
1:B:563:TRP:CH2	1:B:759:ILE:HD13	2.54	0.42
1:B:94:THR:O	1:B:95:PHE:HB2	2.19	0.42
1:B:364:PHE:HE2	1:B:389:ILE:HD11	1.84	0.42
1:B:158:SER:OG	1:B:163:LYS:HB2	2.19	0.42
1:B:309:GLU:HB3	1:B:330:TYR:HB3	2.01	0.42
1:A:630:SER:O	1:A:631:TYR:C	2.56	0.42
1:A:408:GLU:O	1:A:409:ALA:HB2	2.19	0.42
1:B:150:ASN:ND2	2:B:793:NAG:N2	2.67	0.42
1:A:357:PHE:HD1	1:A:669:ARG:NH2	2.16	0.42
1:A:333:SER:OG	1:A:334:SER:N	2.53	0.42
1:A:281:ASN:ND2	2:A:795:NAG:C7	2.82	0.42
1:A:269:PHE:CD1	1:A:269:PHE:N	2.86	0.42
1:A:702:LEU:O	1:A:732:ALA:HA	2.19	0.42
1:A:662:TYR:OH	3:A:900:5AP:N21	2.53	0.42
1:B:64:SER:OG	1:B:66:HIS:CD2	2.73	0.42
1:A:756:SER:O	1:A:760:LYS:HG3	2.20	0.42
1:A:519:LEU:HA	1:A:519:LEU:HD23	1.75	0.42
1:B:544:LEU:HD12	1:B:576:ALA:O	2.19	0.42
1:B:362:PRO:O	1:B:362:PRO:HG2	2.19	0.42
1:A:141:GLN:HG2	1:A:142:LEU:O	2.19	0.42
1:A:340:LEU:HA	1:A:340:LEU:HD12	1.87	0.42
1:B:223:LEU:HD23	1:B:223:LEU:HA	1.51	0.42
1:B:383:HIS:HD2	1:B:398:THR:HB	1.84	0.42
1:B:340:LEU:O	1:B:341:VAL:C	2.58	0.42
1:A:40:ARG:HD3	1:A:40:ARG:HA	1.38	0.42
1:A:594:ILE:HD12	1:A:594:ILE:HA	1.62	0.42
1:A:387:PHE:CE2	1:A:394:CYS:HB3	2.55	0.42
1:B:299:TYR:CE1	1:B:665:VAL:HG22	2.55	0.42
1:B:105:TYR:CE1	1:B:107:ILE:HD12	2.55	0.42
1:A:596:ARG:HA	1:A:670:TYR:O	2.20	0.42
1:A:417:TYR:HE1	1:A:434:ILE:HD11	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:596:ARG:HA	1:B:670:TYR:O	2.19	0.42
1:A:741:GLY:O	1:A:742:ILE:C	2.58	0.42
1:A:664:SER:O	1:A:668:GLU:HB2	2.19	0.42
1:B:195:TYR:CD1	1:B:195:TYR:N	2.88	0.42
1:A:522:THR:HG22	1:A:523:LYS:N	2.34	0.42
1:B:206:GLU:OE2	1:B:663:ASP:OD2	2.38	0.42
1:B:325:MET:HE1	1:B:371:PHE:CZ	2.54	0.42
1:B:191:GLU:O	1:B:193:ILE:HG13	2.19	0.42
1:B:734:TRP:CD1	1:B:734:TRP:C	2.93	0.42
1:A:458:SER:OG	1:A:471:ARG:HG2	2.19	0.41
1:B:327:ILE:CG2	1:B:343:ARG:HD3	2.50	0.41
1:B:619:VAL:CG2	1:B:619:VAL:O	2.67	0.41
1:A:509:MET:HA	1:A:510:PRO:HD3	1.97	0.41
1:B:596:ARG:O	1:B:597:ARG:HG3	2.20	0.41
1:A:135:TYR:HD1	1:A:142:LEU:HD23	1.85	0.41
1:A:49:LEU:HG	1:A:749:GLN:HA	2.01	0.41
1:A:41:LYS:HG2	1:A:42:THR:N	2.32	0.41
1:A:42:THR:CG2	1:A:570:THR:OG1	2.68	0.41
1:B:72:GLN:O	1:B:73:GLU:C	2.58	0.41
1:A:433:LYS:HB3	1:A:443:THR:HB	2.02	0.41
1:A:397:ILE:HG22	1:A:439:TYR:CE2	2.55	0.41
1:A:304:THR:O	1:A:305:TRP:C	2.59	0.41
1:B:219:ASN:N	1:B:308:GLN:OE1	2.54	0.41
1:B:78:VAL:O	2:B:794:NAG:H81	2.19	0.41
1:B:375:ILE:HD13	1:B:387:PHE:HZ	1.86	0.41
1:A:153:GLN:OE1	1:A:169:ASN:N	2.53	0.41
1:A:470:LEU:HD12	1:A:483:HIS:CE1	2.55	0.41
1:B:430:ASN:OD1	1:B:446:SER:OG	2.38	0.41
1:A:50:LYS:O	1:A:51:ASN:HB2	2.20	0.41
1:A:431:LEU:HD23	1:A:431:LEU:HA	1.89	0.41
1:A:164:LEU:HB2	1:A:175:LYS:HB2	2.03	0.41
1:A:728:VAL:O	1:B:750:HIS:HE1	2.04	0.41
1:A:562:ASN:O	1:A:565:THR:CB	2.67	0.41
1:A:134:ILE:HD11	1:A:164:LEU:CD1	2.50	0.41
1:B:159:PRO:HD3	1:B:216:TRP:CB	2.51	0.41
1:A:199:THR:OG1	1:A:204:GLU:HB2	2.21	0.41
1:A:384:ILE:HG23	1:A:407:ILE:HD11	2.03	0.41
1:B:621:ASN:ND2	1:B:621:ASN:N	2.69	0.41
1:A:615:LYS:O	1:A:616:MET:C	2.59	0.41
1:B:742:ILE:O	1:B:742:ILE:CG2	2.67	0.41
1:A:305:TRP:CE3	1:A:311:ILE:HG12	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:TRP:CG	1:A:462:SER:HA	2.56	0.41
1:B:103:ASN:O	1:B:104:ASP:HB2	2.21	0.40
1:A:177:GLU:HA	1:A:178:PRO:HD3	1.89	0.40
1:B:621:ASN:N	1:B:621:ASN:HD22	2.19	0.40
1:A:640:LEU:HA	1:A:640:LEU:HD23	1.82	0.40
1:A:420:ASN:H	1:A:420:ASN:ND2	2.20	0.40
1:A:385:CYS:HB3	1:A:387:PHE:CE1	2.56	0.40
1:B:64:SER:OG	1:B:65:ASP:N	2.54	0.40
1:A:554:LYS:HB3	1:A:577:SER:HB3	2.02	0.40
1:B:272:ASN:C	1:B:272:ASN:OD1	2.60	0.40
1:A:50:LYS:HD3	1:A:50:LYS:HA	1.94	0.40
1:A:530:LEU:HA	1:A:531:PRO:HD3	1.80	0.40
1:B:465:ALA:O	1:B:485:SER:OG	2.25	0.40
1:A:61:ARG:HB3	4:A:934:HOH:O	2.21	0.40
1:B:470:LEU:HD12	1:B:483:HIS:CE1	2.56	0.40
1:B:535:ASP:C	1:B:535:ASP:OD1	2.60	0.40
1:A:90:LEU:HD23	1:A:91:GLU:N	2.35	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%)	665 (92%)	54 (7%)	7 (1%)	19	16
1	B	726/728 (100%)	665 (92%)	58 (8%)	3 (0%)	39	42
All	All	1452/1456 (100%)	1330 (92%)	112 (8%)	10 (1%)	26	25

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	ARG

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Mol	Chain	Res	Type
1	A	488	ASP
1	B	111	GLY
1	B	242	SER
1	A	615	LYS
1	A	423	LYS
1	A	614	SER
1	B	108	SER
1	A	714	GLN
1	A	742	ILE

### 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	653/653 (100%)	596 (91%)	57 (9%)	13	12
1	B	653/653 (100%)	595 (91%)	58 (9%)	12	11
All	All	1306/1306 (100%)	1191 (91%)	115 (9%)	12	12

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	A	42	THR
1	A	49	LEU
1	A	60	LEU
1	A	87	SER
1	A	88	VAL
1	A	120	TYR
1	A	144	THR
1	A	156	THR
1	A	158	SER
1	A	169	ASN
1	A	180	LEU
1	A	195	TYR
1	A	202	VAL

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Mol	Chain	Res	Type
1	A	223	LEU
1	A	246	LEU
1	A	273	THR
1	A	278	SER
1	A	294	LEU
1	A	300	LEU
1	A	301	CYS
1	A	312	SER
1	A	316	LEU
1	A	326	ASP
1	A	334	SER
1	A	343	ARG
1	A	350	THR
1	A	377	ASN
1	A	378	GLU
1	A	385	CYS
1	A	389	ILE
1	A	392	LYS
1	A	399	LYS
1	A	410	LEU
1	A	420	ASN
1	A	431	LEU
1	A	435	GLN
1	A	448	GLU
1	A	452	GLU
1	A	471	ARG
1	A	472	CYS
1	A	479	LEU
1	A	482	LEU
1	A	502	LYS
1	A	514	LEU
1	A	517	ILE
1	A	540	TYR
1	A	543	LEU
1	A	544	LEU
1	A	566	TYR
1	A	594	ILE
1	A	621	ASN
1	A	677	GLU
1	A	684	ARG
1	A	704	HIS
1	A	715	GLN

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Mol	Chain	Res	Type
1	A	736	THR
1	B	41	LYS
1	B	42	THR
1	B	49	LEU
1	B	60	LEU
1	B	63	ILE
1	B	71	LYS
1	B	86	SER
1	B	87	SER
1	B	90	LEU
1	B	91	GLU
1	B	93	SER
1	B	143	ILE
1	B	180	LEU
1	B	202	VAL
1	B	214	LEU
1	B	223	LEU
1	B	236	ILE
1	B	242	SER
1	B	246	LEU
1	B	273	THR
1	B	279	VAL
1	B	295	ILE
1	B	300	LEU
1	B	311	ILE
1	B	314	GLN
1	B	332	GLU
1	B	375	ILE
1	B	377	ASN
1	B	390	ASP
1	B	392	LYS
1	B	397	ILE
1	B	405	ILE
1	B	420	ASN
1	B	435	GLN
1	B	452	GLU
1	B	471	ARG
1	B	472	CYS
1	B	479	LEU
1	B	480	TYR
1	B	500	LEU
1	B	514	LEU

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Mol	Chain	Res	Type
1	B	517	ILE
1	B	543	LEU
1	B	546	VAL
1	B	562	ASN
1	B	566	TYR
1	B	594	ILE
1	B	600	THR
1	B	620	ASP
1	B	621	ASN
1	B	627	TRP
1	B	677	GLU
1	B	680	LEU
1	B	684	ARG
1	B	715	GLN
1	B	726	VAL
1	B	731	GLN
1	B	759	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	GLN
1	A	263	ASN
1	A	298	HIS
1	A	363	HIS
1	A	377	ASN
1	A	420	ASN
1	A	483	HIS
1	A	508	GLN
1	A	533	HIS
1	A	586	GLN
1	A	592	HIS
1	A	621	ASN
1	A	679	ASN
1	A	715	GLN
1	A	748	HIS
1	A	750	HIS
1	B	66	HIS
1	B	126	HIS
1	B	150	ASN
1	B	263	ASN
1	B	286	GLN

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Mol	Chain	Res	Type
1	B	298	HIS
1	B	363	HIS
1	B	377	ASN
1	B	383	HIS
1	B	420	ASN
1	B	430	ASN
1	B	435	GLN
1	B	450	ASN
1	B	483	HIS
1	B	562	ASN
1	B	621	ASN
1	B	679	ASN
1	B	715	GLN
1	B	750	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

10 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	793	1	14,14,15	0.69	1 (7%)	15,19,21	2.56	6 (40%)
2	NAG	A	794	1	14,14,15	0.97	1 (7%)	15,19,21	2.03	5 (33%)
2	NAG	A	795	1	14,14,15	0.70	0	15,19,21	2.31	3 (20%)
2	NAG	A	796	1	14,14,15	0.72	0	15,19,21	1.99	4 (26%)
3	5AP	A	900	-	28,29,29	2.06	5 (17%)	34,41,41	2.40	11 (32%)
3	5AP	B	1900	-	28,29,29	1.54	5 (17%)	34,41,41	2.34	12 (35%)
2	NAG	B	793	1	14,14,15	0.66	1 (7%)	15,19,21	1.17	1 (6%)
2	NAG	B	794	1	14,14,15	0.69	0	15,19,21	1.44	2 (13%)
2	NAG	B	796	1	14,14,15	0.87	1 (7%)	15,19,21	1.58	4 (26%)
2	NAG	B	797	1	14,14,15	0.60	0	15,19,21	1.78	3 (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	NAG	A	793	1	-	0/6/23/26	0/1/1/1
2	NAG	A	794	1	-	0/6/23/26	0/1/1/1
2	NAG	A	795	1	-	0/6/23/26	0/1/1/1
2	NAG	A	796	1	-	0/6/23/26	0/1/1/1
3	5AP	A	900	-	-	0/12/14/14	0/3/3/3
3	5AP	B	1900	-	-	0/12/14/14	0/3/3/3
2	NAG	B	793	1	-	0/6/23/26	0/1/1/1
2	NAG	B	794	1	-	0/6/23/26	0/1/1/1
2	NAG	B	796	1	-	0/6/23/26	0/1/1/1
2	NAG	B	797	1	1/1/5/7	0/6/23/26	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	900	5AP	C11-C10	-7.97	1.41	1.49
3	B	1900	5AP	C10-N9	-3.78	1.28	1.34
3	B	1900	5AP	C12-C11	-2.80	1.35	1.39
3	B	1900	5AP	C8-C3	-2.45	1.35	1.39
3	A	900	5AP	C11-C17	-2.38	1.35	1.40
3	A	900	5AP	C16-C17	-2.30	1.34	1.38
3	B	1900	5AP	C22-N1	-2.17	1.31	1.35
2	A	794	NAG	O5-C1	-2.05	1.40	1.43
3	A	900	5AP	C12-C11	-2.03	1.36	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	793	NAG	O5-C1	-2.03	1.40	1.43
2	B	793	NAG	O5-C1	-2.00	1.40	1.43
2	B	796	NAG	C1-C2	2.27	1.55	1.52
3	B	1900	5AP	C10-C19	3.97	1.46	1.40
3	A	900	5AP	C10-C19	4.72	1.47	1.40

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	793	NAG	C4-C3-C2	-5.68	102.40	111.23
2	A	796	NAG	C2-N2-C7	-5.30	116.23	123.04
2	A	795	NAG	C2-N2-C7	-4.98	116.64	123.04
2	A	795	NAG	C4-C3-C2	-4.86	103.67	111.23
3	A	900	5AP	C17-C16-C14	-4.80	113.36	118.69
2	B	797	NAG	C2-N2-C7	-4.39	117.40	123.04
3	A	900	5AP	C11-C17-CL2	-3.98	114.57	120.67
3	B	1900	5AP	C17-C16-C14	-3.65	114.63	118.69
2	B	794	NAG	C4-C3-C2	-3.49	105.81	111.23
2	B	797	NAG	C3-C4-C5	-3.30	104.44	110.20
2	A	796	NAG	C3-C4-C5	-3.29	104.46	110.20
3	B	1900	5AP	C19-C10-N9	-3.21	118.38	122.73
2	B	796	NAG	C3-C2-N2	-3.11	103.11	110.56
2	B	793	NAG	C4-C3-C2	-2.64	107.12	111.23
2	A	794	NAG	C4-C3-C2	-2.56	107.24	111.23
2	B	796	NAG	O7-C7-C8	-2.56	117.36	122.06
3	A	900	5AP	C13-C12-C11	-2.54	115.80	120.23
2	A	794	NAG	C3-C2-N2	-2.49	104.59	110.56
2	A	794	NAG	C6-C5-C4	-2.44	106.99	113.02
3	A	900	5AP	C10-C11-C17	-2.44	118.48	121.10
3	B	1900	5AP	C16-C17-CL2	-2.40	114.80	118.50
3	B	1900	5AP	C13-C12-C11	-2.36	116.12	120.23
2	A	796	NAG	C4-C3-C2	-2.36	107.56	111.23
2	A	793	NAG	C3-C4-C5	-2.33	106.13	110.20
3	B	1900	5AP	C12-C11-C10	-2.14	116.48	119.62
3	A	900	5AP	C29-O26-C7	-2.13	112.52	117.51
2	B	796	NAG	C6-C5-C4	-2.10	107.83	113.02
3	A	900	5AP	N1-C2-N9	-2.05	122.10	125.37
3	A	900	5AP	C4-C3-C2	2.20	123.11	120.17
2	A	794	NAG	O7-C7-N2	2.25	126.46	121.86
2	B	796	NAG	C8-C7-N2	2.40	120.70	116.11
2	B	797	NAG	O5-C5-C6	2.51	112.77	107.35
2	B	794	NAG	O5-C5-C6	2.57	112.91	107.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	793	NAG	O4-C4-C5	2.58	116.07	109.24
3	B	1900	5AP	N23-C22-N1	2.61	120.73	116.95
3	B	1900	5AP	C10-C11-C17	2.62	123.92	121.10
3	B	1900	5AP	C8-C3-C4	2.78	122.57	118.29
2	A	796	NAG	O4-C4-C5	2.83	116.74	109.24
2	A	793	NAG	C3-C2-N2	3.63	119.25	110.56
3	B	1900	5AP	C12-C13-C14	3.87	123.53	119.23
2	A	793	NAG	O3-C3-C2	4.03	117.10	109.11
2	A	793	NAG	C2-N2-C7	4.12	128.33	123.04
3	A	900	5AP	N23-C22-N1	4.33	123.22	116.95
3	B	1900	5AP	C16-C17-C11	4.33	124.92	121.76
3	B	1900	5AP	C11-C10-N9	4.42	118.98	114.63
2	A	794	NAG	C2-N2-C7	4.43	128.73	123.04
2	A	795	NAG	C1-O5-C5	4.81	118.35	112.25
3	A	900	5AP	C11-C10-N9	5.02	119.57	114.63
3	A	900	5AP	C10-N9-C2	5.08	120.40	117.05
3	A	900	5AP	C16-C17-C11	5.72	125.94	121.76
3	B	1900	5AP	C10-N9-C2	6.95	121.64	117.05

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	797	NAG	C1

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	793	NAG	1	0
2	A	795	NAG	1	0
3	A	900	5AP	5	0
2	B	793	NAG	5	0
2	B	794	NAG	1	0
2	B	797	NAG	2	0

## 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 was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.