Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 12:19 PM BST

PDB ID	:	1KBP
Title	:	KIDNEY BEAN PURPLE ACID PHOSPHATASE
Authors	:	Klabunde, T.; Strater, N.; Krebs, B.
Deposited on	:	1995-02-20
Resolution	:	2.65 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

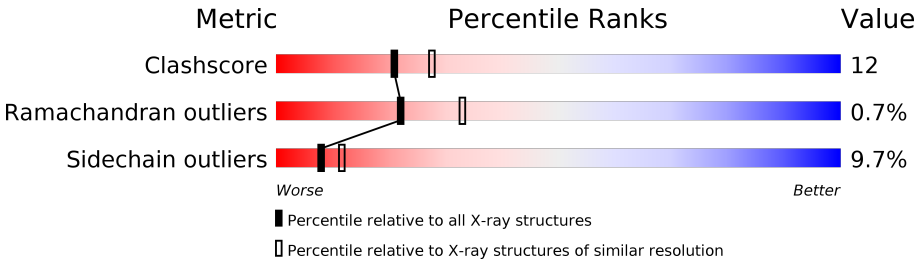
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	432	68% 25%
1	B	432	66% 27%
1	C	432	69% 23% 5%
1	D	432	67% 26% 5%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14334 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.

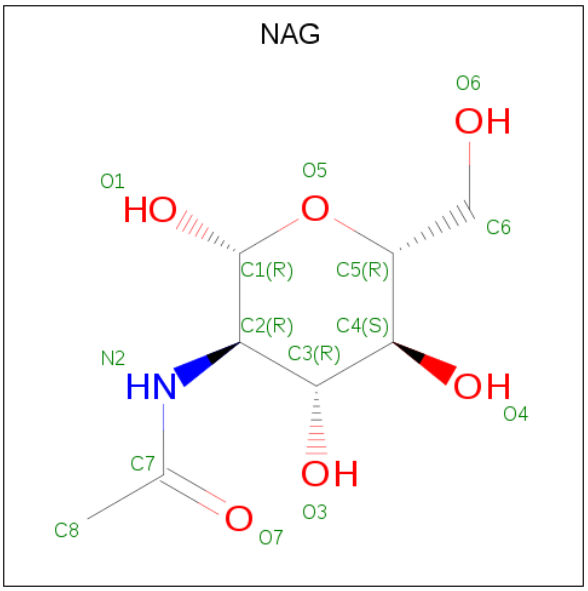
- Molecule 1 is a protein called PURPLE ACID PHOSPHATASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	424	Total	C	N	O	S	0	0	0
			3494	2243	605	636	10			
1	B	424	Total	C	N	O	S	0	0	0
			3494	2243	605	636	10			
1	C	424	Total	C	N	O	S	0	0	0
			3494	2243	605	636	10			
1	D	424	Total	C	N	O	S	0	0	0
			3494	2243	605	636	10			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	253	TYR	HIS	conflict	UNP P80366
A	254	SER	ILE	conflict	UNP P80366
B	253	TYR	HIS	conflict	UNP P80366
B	254	SER	ILE	conflict	UNP P80366
C	253	TYR	HIS	conflict	UNP P80366
C	254	SER	ILE	conflict	UNP P80366
D	253	TYR	HIS	conflict	UNP P80366
D	254	SER	ILE	conflict	UNP P80366

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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

- Molecule 3 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Fe 1 1	0	0
3	A	1	Total Fe 1 1	0	0
3	D	1	Total Fe 1 1	0	0
3	C	1	Total Fe 1 1	0	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Zn 1 1	0	0
4	A	1	Total Zn 1 1	0	0
4	D	1	Total Zn 1 1	0	0
4	C	1	Total Zn 1 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	18	Total O 18 18	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	17	Total O 17 17	0	0
5	C	17	Total O 17 17	0	0
5	D	18	Total O 18 18	0	0

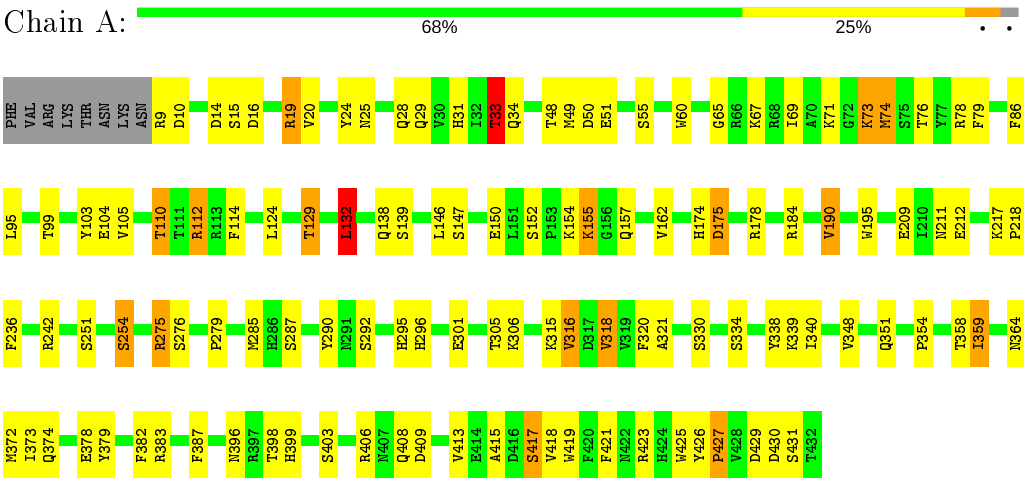
3 Residue-property plots (i)

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

Note EDS was not executed.

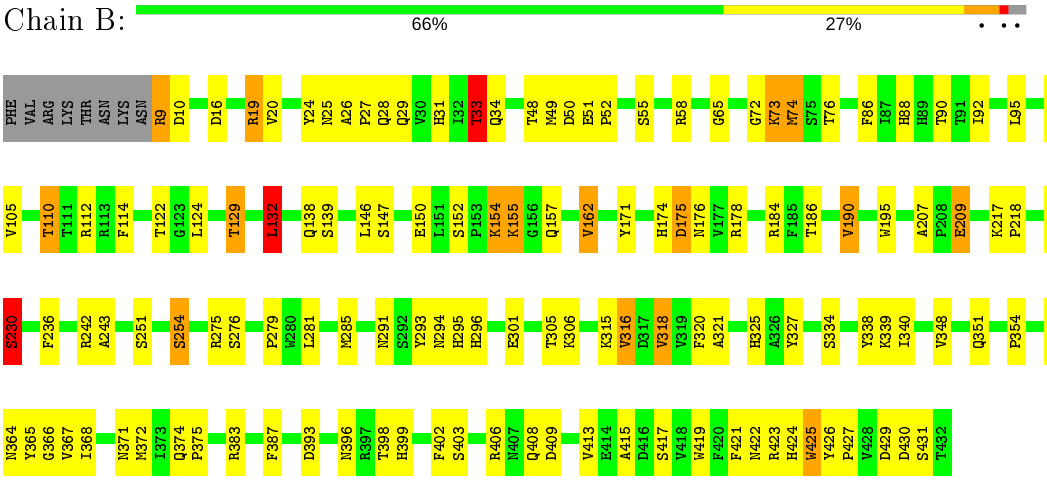
- Molecule 1: PURPLE ACID PHOSPHATASE

Chain A:



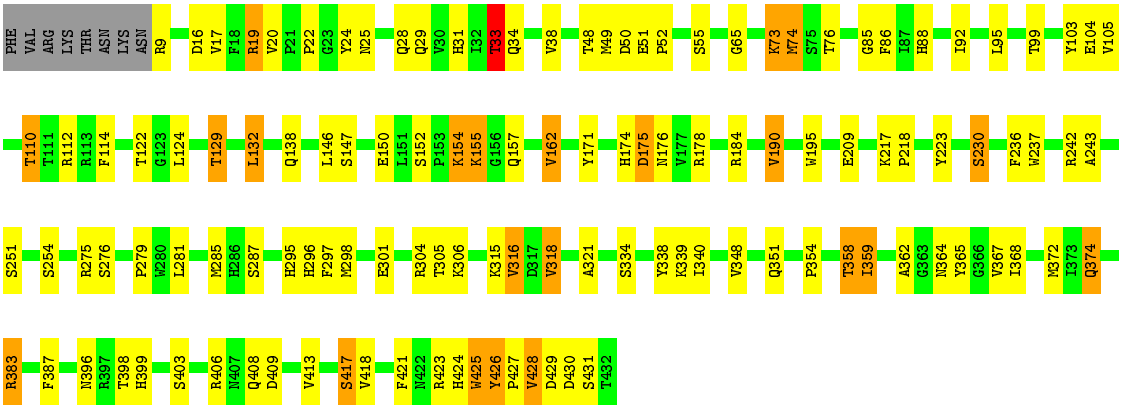
- Molecule 1: PURPLE ACID PHOSPHATASE

Chain B:



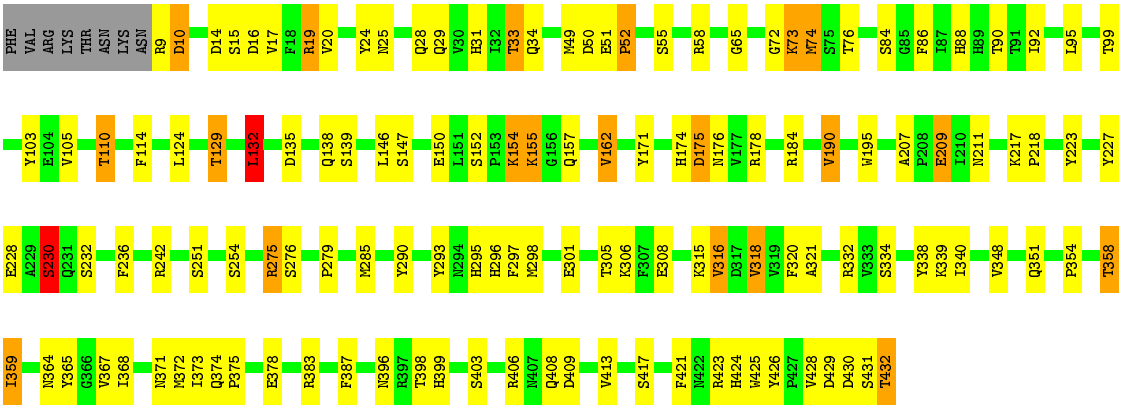
- Molecule 1: PURPLE ACID PHOSPHATASE

Chain C:



- Molecule 1: PURPLE ACID PHOSPHATASE

Chain D:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	132.70Å 347.30Å 128.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.65	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.65)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.195 , 0.233	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14334	wwPDB-VP
Average B, all atoms (Å^2)	39.0	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: ZN, NAG, FE

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	0.98	2/3613 (0.1%)	1.00	7/4912 (0.1%)
1	B	0.89	1/3613 (0.0%)	0.96	7/4912 (0.1%)
1	C	0.96	1/3613 (0.0%)	0.98	7/4912 (0.1%)
1	D	0.96	2/3613 (0.1%)	1.00	8/4912 (0.2%)
All	All	0.95	6/14452 (0.0%)	0.98	29/19648 (0.1%)

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	A	0	2
1	B	0	1
1	C	0	1
1	D	0	2
All	All	0	6

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	425	TRP	CB-CG	-5.76	1.39	1.50
1	A	372	MET	CG-SD	-5.57	1.66	1.81
1	B	425	TRP	CB-CG	-5.39	1.40	1.50
1	D	378	GLU	CG-CD	5.08	1.59	1.51
1	D	308	GLU	CD-OE2	5.04	1.31	1.25
1	A	378	GLU	CG-CD	5.01	1.59	1.51

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	132	LEU	CA-CB-CG	-8.03	96.83	115.30
1	C	132	LEU	CA-CB-CG	-7.59	97.84	115.30
1	C	230	SER	N-CA-C	-6.98	92.14	111.00
1	A	230	SER	N-CA-C	-6.96	92.21	111.00
1	D	230	SER	N-CA-C	-6.88	92.42	111.00
1	D	132	LEU	CA-CB-CG	-6.82	99.62	115.30
1	A	154	LYS	N-CA-C	-6.80	92.64	111.00
1	A	132	LEU	CA-CB-CG	-6.70	99.90	115.30
1	B	230	SER	N-CA-C	-6.65	93.04	111.00
1	C	154	LYS	N-CA-C	-6.31	93.97	111.00
1	A	318	VAL	CB-CA-C	-6.20	99.62	111.40
1	B	318	VAL	CB-CA-C	-6.16	99.69	111.40
1	D	154	LYS	N-CA-C	-6.15	94.40	111.00
1	D	318	VAL	CB-CA-C	-6.06	99.89	111.40
1	B	154	LYS	N-CA-C	-6.00	94.79	111.00
1	C	318	VAL	CB-CA-C	-5.71	100.56	111.40
1	C	33	THR	CB-CA-C	-5.70	96.21	111.60
1	A	275	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	D	135	ASP	CB-CG-OD1	5.54	123.29	118.30
1	D	10	ASP	CB-CG-OD1	5.32	123.09	118.30
1	C	33	THR	N-CA-CB	5.27	120.31	110.30
1	A	33	THR	CB-CA-C	-5.23	97.47	111.60
1	A	112	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	D	275	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	B	393	ASP	CB-CG-OD2	-5.12	113.69	118.30
1	C	38	VAL	N-CA-C	5.08	124.73	111.00
1	B	33	THR	CB-CA-C	-5.03	98.02	111.60
1	B	430	ASP	CB-CA-C	-5.02	100.36	110.40
1	D	332	ARG	NE-CZ-NH1	-5.00	117.80	120.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	223	TYR	Sidechain
1	A	290	TYR	Sidechain
1	B	223	TYR	Sidechain
1	C	223	TYR	Sidechain
1	D	223	TYR	Sidechain
1	D	290	TYR	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3494	0	3307	81	0
1	B	3494	0	3306	93	0
1	C	3494	0	3306	83	0
1	D	3494	0	3307	83	0
2	A	70	0	65	2	0
2	B	70	0	65	0	0
2	C	70	0	65	0	0
2	D	70	0	65	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	18	0	0	1	0
5	B	17	0	0	1	0
5	C	17	0	0	3	0
5	D	18	0	0	2	0
All	All	14334	0	13486	339	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 12.

All (339) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:LYS:HA	1:A:73:LYS:HE2	1.50	0.93
1:B:129:THR:HG21	1:B:155:LYS:HE3	1.53	0.91
1:D:73:LYS:HE2	1:D:73:LYS:HA	1.52	0.91
1:C:73:LYS:HE2	1:C:73:LYS:HA	1.53	0.89
1:A:359:ILE:H	1:A:359:ILE:HD13	1.35	0.89
1:A:129:THR:HG21	1:A:155:LYS:HE3	1.53	0.88
1:B:73:LYS:HA	1:B:73:LYS:HE2	1.55	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:ILE:N	1:A:359:ILE:HD13	1.90	0.86
1:D:129:THR:HG21	1:D:155:LYS:HE3	1.61	0.82
1:B:359:ILE:H	1:B:359:ILE:HD13	1.44	0.82
1:C:359:ILE:N	1:C:359:ILE:HD13	1.95	0.82
1:C:129:THR:HG21	1:C:155:LYS:HE3	1.60	0.81
1:C:359:ILE:H	1:C:359:ILE:HD13	1.45	0.79
1:D:359:ILE:H	1:D:359:ILE:HD13	1.47	0.78
1:B:359:ILE:HD13	1:B:359:ILE:N	1.97	0.77
1:A:426:TYR:N	1:A:427:PRO:HD3	1.99	0.76
1:A:33:THR:HG23	1:A:195:TRP:O	1.87	0.74
1:B:426:TYR:N	1:B:427:PRO:HD3	2.03	0.74
1:B:74:MET:HE3	1:B:86:PHE:HD1	1.54	0.73
1:D:359:ILE:HD13	1:D:359:ILE:N	2.03	0.73
1:D:275:ARG:NH2	1:D:315:LYS:O	2.23	0.71
1:C:74:MET:HE3	1:C:86:PHE:HD1	1.56	0.70
1:C:358:THR:HG21	5:C:452:HOH:O	1.91	0.70
1:D:421:PHE:CD2	1:D:430:ASP:HB3	2.27	0.70
1:C:33:THR:HG21	5:C:450:HOH:O	1.90	0.70
1:C:217:LYS:HB3	1:C:218:PRO:HD3	1.74	0.69
1:B:24:TYR:O	1:B:110:THR:HG23	1.93	0.69
1:B:275:ARG:NH2	1:B:315:LYS:O	2.26	0.68
1:C:138:GLN:NE2	1:C:178:ARG:HH11	1.92	0.68
1:B:33:THR:HG23	1:B:195:TRP:O	1.93	0.68
1:A:24:TYR:O	1:A:110:THR:HG23	1.94	0.68
1:C:275:ARG:NH2	1:C:315:LYS:O	2.27	0.67
1:D:190:VAL:HG13	1:D:195:TRP:CD1	2.29	0.67
1:B:9:ARG:HG2	1:B:366:GLY:HA3	1.74	0.67
1:C:33:THR:HG23	1:C:195:TRP:O	1.93	0.67
1:A:138:GLN:NE2	1:A:178:ARG:HH11	1.93	0.67
1:C:301:GLU:O	1:C:305:THR:HG23	1.96	0.66
1:A:368:ILE:HG12	1:A:387:PHE:CZ	2.32	0.65
1:C:338:TYR:CZ	1:C:340:ILE:HA	2.31	0.65
1:A:275:ARG:NH2	1:A:315:LYS:O	2.29	0.64
1:B:29:GLN:O	1:B:31:HIS:HD2	1.80	0.64
1:B:338:TYR:CZ	1:B:340:ILE:HA	2.33	0.64
1:D:24:TYR:O	1:D:110:THR:HG23	1.98	0.63
1:D:217:LYS:HB3	1:D:218:PRO:HD3	1.80	0.63
1:B:217:LYS:HB3	1:B:218:PRO:HD3	1.81	0.63
1:C:374:GLN:HE22	1:C:383:ARG:HH12	1.44	0.62
1:D:74:MET:HE3	1:D:86:PHE:HD1	1.63	0.62
1:B:28:GLN:HG3	1:B:29:GLN:HG3	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:GLN:NE2	1:B:178:ARG:HH11	1.98	0.62
1:D:33:THR:HG23	1:D:195:TRP:O	1.99	0.62
1:B:301:GLU:O	1:B:305:THR:HG23	1.99	0.62
1:D:368:ILE:HG12	1:D:387:PHE:CZ	2.35	0.62
1:A:217:LYS:HB3	1:A:218:PRO:HD3	1.81	0.61
1:B:10:ASP:HA	1:B:139:SER:HA	1.81	0.61
1:A:338:TYR:CZ	1:A:340:ILE:HA	2.36	0.60
1:D:16:ASP:HA	1:D:19:ARG:HD3	1.83	0.60
1:D:55:SER:OG	1:D:88:HIS:HD2	1.83	0.60
1:C:421:PHE:CD2	1:C:430:ASP:HB3	2.37	0.60
1:A:55:SER:OG	1:A:88:HIS:HD2	1.85	0.60
1:B:316:VAL:HG22	1:B:354:PRO:HB3	1.84	0.60
1:D:129:THR:H	1:D:157:GLN:HE21	1.49	0.60
1:A:409:ASP:HB3	1:A:413:VAL:HB	1.83	0.59
1:D:409:ASP:HB3	1:D:413:VAL:HB	1.83	0.59
1:A:74:MET:HE3	1:A:86:PHE:HD1	1.67	0.59
1:D:138:GLN:NE2	1:D:178:ARG:HH11	1.99	0.59
1:B:33:THR:HG21	5:B:449:HOH:O	2.02	0.59
1:C:368:ILE:HG12	1:C:387:PHE:CZ	2.36	0.59
1:A:25:ASN:ND2	1:A:51:GLU:H	2.00	0.59
1:A:129:THR:H	1:A:157:GLN:HE21	1.50	0.59
1:B:368:ILE:HG12	1:B:387:PHE:CZ	2.38	0.58
1:A:421:PHE:CD2	1:A:430:ASP:HB3	2.38	0.58
1:C:129:THR:H	1:C:157:GLN:HE21	1.52	0.57
1:A:74:MET:CE	1:A:76:THR:HG23	2.33	0.57
1:A:28:GLN:HG3	1:A:29:GLN:HG3	1.86	0.57
1:D:146:LEU:O	1:D:150:GLU:HG3	2.03	0.57
1:A:301:GLU:O	1:A:305:THR:HG23	2.05	0.57
1:A:10:ASP:HA	1:A:139:SER:HA	1.87	0.57
1:B:399:HIS:CE1	1:B:421:PHE:HE1	2.23	0.56
1:C:28:GLN:NE2	1:C:184:ARG:HE	2.03	0.56
1:A:316:VAL:HG22	1:A:354:PRO:HB3	1.87	0.56
1:A:406:ARG:HB3	1:A:408:GLN:OE1	2.05	0.56
1:C:316:VAL:HG22	1:C:354:PRO:HB3	1.87	0.56
1:B:129:THR:H	1:B:157:GLN:HE21	1.52	0.56
1:C:74:MET:CE	1:C:76:THR:HG23	2.36	0.56
1:C:24:TYR:O	1:C:110:THR:HG23	2.05	0.56
1:C:396:ASN:HB2	1:C:398:THR:H	1.70	0.56
1:D:28:GLN:HG3	1:D:29:GLN:HG3	1.87	0.55
1:A:146:LEU:O	1:A:150:GLU:HG3	2.06	0.55
1:D:25:ASN:HD22	1:D:50:ASP:H	1.54	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:VAL:HG13	1:A:195:TRP:CD1	2.42	0.54
1:B:409:ASP:HB3	1:B:413:VAL:HB	1.90	0.54
1:A:28:GLN:NE2	1:A:184:ARG:HE	2.06	0.54
1:C:174:HIS:O	1:C:175:ASP:C	2.46	0.54
1:A:285:MET:O	1:A:321:ALA:HA	2.08	0.53
1:D:396:ASN:HB2	1:D:398:THR:H	1.73	0.53
1:B:174:HIS:O	1:B:175:ASP:C	2.47	0.53
1:A:174:HIS:O	1:A:175:ASP:C	2.46	0.53
1:B:146:LEU:O	1:B:150:GLU:HG3	2.09	0.53
1:B:171:TYR:CE1	1:B:178:ARG:HG3	2.43	0.53
1:C:34:GLN:NE2	1:C:242:ARG:HE	2.06	0.53
1:C:74:MET:HE1	1:C:76:THR:HG23	1.90	0.53
1:C:421:PHE:CD2	1:C:428:VAL:HG22	2.44	0.53
1:D:29:GLN:O	1:D:31:HIS:HD2	1.92	0.53
1:C:33:THR:CG2	1:C:195:TRP:O	2.57	0.52
1:D:34:GLN:NE2	1:D:242:ARG:HE	2.07	0.52
1:A:33:THR:CG2	1:A:195:TRP:O	2.57	0.52
1:B:129:THR:HG23	1:B:157:GLN:HE21	1.72	0.52
1:B:190:VAL:HG13	1:B:195:TRP:CD1	2.44	0.52
1:B:25:ASN:ND2	1:B:51:GLU:H	2.08	0.52
1:D:301:GLU:O	1:D:305:THR:HG23	2.09	0.52
1:D:364:ASN:ND2	1:D:367:VAL:H	2.08	0.52
1:A:25:ASN:HD21	1:A:51:GLU:H	1.58	0.52
1:D:171:TYR:CE1	1:D:178:ARG:HG3	2.45	0.52
1:B:421:PHE:HB3	1:B:426:TYR:HD2	1.73	0.52
1:B:406:ARG:HB3	1:B:408:GLN:OE1	2.10	0.52
1:C:359:ILE:N	1:C:359:ILE:CD1	2.71	0.52
1:B:421:PHE:HB3	1:B:426:TYR:O	2.09	0.52
1:C:28:GLN:HG3	1:C:29:GLN:HG3	1.92	0.52
1:B:28:GLN:NE2	1:B:184:ARG:HE	2.07	0.51
1:D:398:THR:HG22	1:D:426:TYR:HB2	1.91	0.51
1:B:73:LYS:HA	1:B:73:LYS:CE	2.34	0.51
1:D:431:SER:O	1:D:432:THR:HG23	2.10	0.51
1:A:417:SER:C	1:A:418:VAL:HG23	2.31	0.51
1:B:55:SER:OG	1:B:88:HIS:HD2	1.92	0.51
1:C:29:GLN:O	1:C:31:HIS:HD2	1.93	0.51
1:C:364:ASN:HD21	1:C:367:VAL:H	1.56	0.51
1:B:365:TYR:CD1	1:B:365:TYR:N	2.78	0.51
1:C:364:ASN:ND2	1:C:367:VAL:H	2.08	0.51
1:D:129:THR:HG23	1:D:157:GLN:HE21	1.76	0.51
1:D:399:HIS:CE1	1:D:421:PHE:HE1	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:316:VAL:HG22	1:D:354:PRO:HB3	1.91	0.51
1:A:351:GLN:OE1	1:A:429:ASP:HA	2.10	0.51
1:B:34:GLN:NE2	1:B:242:ARG:HE	2.09	0.51
1:C:424:HIS:HD2	1:C:425:TRP:CD1	2.28	0.51
1:A:29:GLN:O	1:A:31:HIS:HD2	1.92	0.50
1:B:295:HIS:O	1:B:296:HIS:HB2	2.10	0.50
1:C:406:ARG:HB3	1:C:408:GLN:OE1	2.11	0.50
1:B:281:LEU:HD23	1:B:316:VAL:HA	1.93	0.50
1:B:327:TYR:OH	1:B:402:PHE:HE2	1.94	0.50
1:C:409:ASP:HB3	1:C:413:VAL:HB	1.93	0.50
1:D:338:TYR:CZ	1:D:340:ILE:HA	2.46	0.50
1:C:362:ALA:HB2	5:C:444:HOH:O	2.11	0.50
1:B:359:ILE:CD1	1:B:359:ILE:N	2.72	0.50
1:B:423:ARG:HA	1:B:423:ARG:NE	2.27	0.50
1:D:338:TYR:O	1:D:339:LYS:HG2	2.11	0.50
1:D:297:PHE:CE2	1:D:298:MET:HG3	2.47	0.50
1:C:351:GLN:OE1	1:C:429:ASP:HA	2.12	0.49
1:C:73:LYS:HA	1:C:73:LYS:CE	2.32	0.49
1:B:16:ASP:HA	1:B:19:ARG:HD3	1.95	0.49
1:B:207:ALA:HA	1:B:209:GLU:OE2	2.13	0.49
1:C:155:LYS:HE2	1:C:155:LYS:N	2.27	0.49
1:C:297:PHE:CE2	1:C:298:MET:HG3	2.47	0.49
1:D:174:HIS:O	1:D:175:ASP:C	2.50	0.49
1:D:406:ARG:HB3	1:D:408:GLN:OE1	2.12	0.49
1:D:351:GLN:OE1	1:D:429:ASP:HA	2.12	0.49
1:D:74:MET:CE	1:D:76:THR:HG23	2.43	0.49
1:A:16:ASP:HA	1:A:19:ARG:HD3	1.94	0.49
1:A:33:THR:HG21	5:A:449:HOH:O	2.13	0.49
1:A:359:ILE:CD1	1:A:359:ILE:N	2.67	0.49
1:C:374:GLN:NE2	1:C:383:ARG:HH12	2.09	0.49
1:D:190:VAL:HG13	1:D:195:TRP:CG	2.47	0.49
1:D:72:GLY:HA3	1:D:90:THR:OG1	2.13	0.49
1:B:422:ASN:OD1	1:B:425:TRP:N	2.43	0.49
1:C:426:TYR:O	1:C:426:TYR:CG	2.64	0.49
1:A:129:THR:HG23	1:A:157:GLN:HE21	1.78	0.49
1:A:396:ASN:HB2	1:A:398:THR:H	1.78	0.48
1:B:155:LYS:N	1:B:155:LYS:HE2	2.28	0.48
1:D:364:ASN:HD21	1:D:367:VAL:H	1.59	0.48
1:D:25:ASN:ND2	1:D:50:ASP:H	2.11	0.48
1:D:155:LYS:HE2	1:D:155:LYS:N	2.28	0.48
1:D:14:ASP:O	1:D:15:SER:C	2.50	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:25:ASN:ND2	1:D:51:GLU:H	2.10	0.48
1:A:364:ASN:ND2	1:A:367:VAL:H	2.11	0.48
1:C:25:ASN:ND2	1:C:51:GLU:H	2.12	0.48
1:B:122:THR:HG23	1:B:243:ALA:O	2.14	0.48
1:C:16:ASP:HA	1:C:19:ARG:HD3	1.96	0.48
1:B:25:ASN:HD22	1:B:50:ASP:H	1.60	0.47
1:C:301:GLU:OE1	1:C:304:ARG:NH1	2.47	0.47
1:B:396:ASN:HB2	1:B:398:THR:H	1.79	0.47
1:D:171:TYR:CD1	1:D:178:ARG:HG3	2.48	0.47
1:A:74:MET:HE3	1:A:76:THR:HG23	1.97	0.47
1:B:124:LEU:O	1:B:279:PRO:HG3	2.15	0.47
1:B:24:TYR:N	1:B:110:THR:HG21	2.30	0.47
1:B:285:MET:O	1:B:321:ALA:HA	2.15	0.47
1:C:104:GLU:HA	1:C:112:ARG:O	2.15	0.47
1:A:92:ILE:CG2	1:A:95:LEU:HD21	2.45	0.47
1:B:162:VAL:HG11	1:B:321:ALA:C	2.35	0.47
1:C:423:ARG:NE	1:C:423:ARG:HA	2.30	0.47
1:C:103:TYR:CE1	1:C:114:PHE:HB2	2.50	0.47
1:A:190:VAL:HG13	1:A:195:TRP:CG	2.50	0.47
1:B:104:GLU:HA	1:B:112:ARG:O	2.15	0.47
1:B:316:VAL:O	1:B:354:PRO:HB3	2.16	0.46
1:D:10:ASP:HA	1:D:139:SER:HA	1.96	0.46
1:D:92:ILE:CG2	1:D:95:LEU:HD21	2.45	0.46
1:B:399:HIS:HB3	1:B:419:TRP:CZ3	2.50	0.46
1:C:146:LEU:O	1:C:150:GLU:HG3	2.15	0.46
1:C:9:ARG:HG2	1:C:9:ARG:HH11	1.79	0.46
1:A:364:ASN:HD21	1:A:367:VAL:H	1.63	0.46
1:A:103:TYR:CE1	1:A:114:PHE:HB2	2.51	0.46
1:B:291:ASN:ND2	1:B:293:TYR:H	2.13	0.46
1:C:398:THR:OG1	1:C:399:HIS:HD2	1.99	0.46
1:A:398:THR:OG1	1:A:399:HIS:HD2	1.99	0.46
1:B:351:GLN:OE1	1:B:429:ASP:HA	2.15	0.46
1:C:295:HIS:O	1:C:296:HIS:HB2	2.16	0.46
1:D:132:LEU:HD22	1:D:320:PHE:CD1	2.50	0.46
1:D:162:VAL:HG11	1:D:321:ALA:C	2.36	0.46
1:A:48:THR:OG1	1:A:88:HIS:HE1	1.99	0.46
1:D:423:ARG:NE	1:D:423:ARG:HA	2.30	0.46
1:B:399:HIS:CE1	1:B:421:PHE:CE1	3.04	0.46
1:C:138:GLN:HE21	1:C:178:ARG:HH11	1.59	0.46
1:D:103:TYR:CE2	1:D:114:PHE:HB2	2.51	0.46
1:A:155:LYS:N	1:A:155:LYS:HE2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:ASN:HD22	1:A:50:ASP:H	1.64	0.46
1:B:364:ASN:ND2	1:B:367:VAL:H	2.14	0.46
1:A:34:GLN:HE22	1:A:242:ARG:HE	1.64	0.45
1:A:421:PHE:HB3	1:A:426:TYR:O	2.16	0.45
1:B:422:ASN:OD1	1:B:424:HIS:HB3	2.16	0.45
1:B:294:ASN:ND2	1:B:372:MET:O	2.49	0.45
1:C:285:MET:O	1:C:321:ALA:HA	2.15	0.45
1:C:281:LEU:HD23	1:C:316:VAL:HA	1.98	0.45
1:C:374:GLN:NE2	1:C:374:GLN:HA	2.31	0.45
1:D:34:GLN:HE22	1:D:242:ARG:HE	1.64	0.45
1:D:295:HIS:O	1:D:296:HIS:HB2	2.17	0.45
1:A:399:HIS:CE1	1:A:421:PHE:HE1	2.35	0.45
1:A:34:GLN:NE2	1:A:242:ARG:HE	2.15	0.45
1:A:251:SER:HB3	1:A:254:SER:HB2	1.97	0.45
1:B:33:THR:CG2	1:B:195:TRP:O	2.62	0.45
1:A:295:HIS:O	1:A:296:HIS:HB2	2.17	0.45
1:A:429:ASP:OD1	1:A:431:SER:HB2	2.17	0.45
1:B:171:TYR:CD1	1:B:178:ARG:HG3	2.52	0.45
1:D:236:PHE:O	1:D:251:SER:HB2	2.17	0.45
1:A:73:LYS:CE	1:A:73:LYS:HA	2.30	0.44
1:B:103:TYR:CZ	1:B:114:PHE:HB2	2.52	0.44
1:B:364:ASN:HD21	1:B:367:VAL:H	1.64	0.44
1:D:33:THR:HG21	5:D:450:HOH:O	2.17	0.44
1:D:92:ILE:HG22	1:D:95:LEU:HD21	1.98	0.44
1:C:48:THR:OG1	1:C:88:HIS:HE1	1.99	0.44
1:D:421:PHE:CD2	1:D:428:VAL:CG2	3.00	0.44
1:A:132:LEU:HD22	1:A:320:PHE:CD1	2.52	0.44
1:B:425:TRP:O	1:B:426:TYR:HB2	2.15	0.44
1:B:228:GLU:C	1:B:230:SER:O	2.56	0.44
1:B:316:VAL:CG2	1:B:354:PRO:HB3	2.46	0.44
1:B:368:ILE:HG12	1:B:387:PHE:CE1	2.52	0.44
1:D:28:GLN:HE21	1:D:29:GLN:HE21	1.65	0.44
1:C:25:ASN:ND2	1:C:50:ASP:HB2	2.33	0.44
1:D:124:LEU:O	1:D:279:PRO:HG3	2.17	0.44
1:D:74:MET:HE1	1:D:76:THR:HG23	1.99	0.44
1:D:103:TYR:CZ	1:D:114:PHE:HB2	2.53	0.44
1:D:424:HIS:HD2	1:D:425:TRP:CD1	2.35	0.44
1:A:60:TRP:HB3	1:A:67:LYS:HA	2.00	0.44
1:B:103:TYR:CE2	1:B:114:PHE:HB2	2.52	0.44
1:D:162:VAL:CG1	1:D:162:VAL:O	2.66	0.44
1:D:207:ALA:HA	1:D:209:GLU:OE2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:228:GLU:C	1:D:230:SER:O	2.56	0.44
1:D:368:ILE:HG12	1:D:387:PHE:CE1	2.52	0.44
1:A:338:TYR:O	1:A:339:LYS:HG2	2.18	0.43
1:B:190:VAL:HG13	1:B:195:TRP:CG	2.53	0.43
1:B:398:THR:OG1	1:B:399:HIS:HD2	2.01	0.43
1:D:33:THR:CG2	1:D:195:TRP:O	2.65	0.43
1:A:251:SER:CB	1:A:254:SER:HB2	2.48	0.43
1:B:236:PHE:O	1:B:251:SER:HB2	2.17	0.43
1:B:424:HIS:HD2	1:B:425:TRP:NE1	2.17	0.43
1:B:58:ARG:O	1:B:103:TYR:HA	2.19	0.43
1:B:325:HIS:HA	1:B:360:GLY:O	2.19	0.43
1:C:122:THR:HG23	1:C:243:ALA:O	2.18	0.43
1:C:34:GLN:HE22	1:C:242:ARG:HE	1.65	0.43
1:C:368:ILE:HG12	1:C:387:PHE:CE1	2.54	0.43
1:D:316:VAL:CG2	1:D:354:PRO:HB3	2.47	0.43
1:C:237:TRP:O	1:C:237:TRP:CD1	2.71	0.43
1:A:78:ARG:NH2	1:D:84:SER:O	2.52	0.43
1:B:374:GLN:HA	1:B:375:PRO:HA	1.69	0.43
1:D:162:VAL:HG13	1:D:162:VAL:O	2.18	0.43
1:A:365:TYR:N	1:A:365:TYR:CD1	2.86	0.43
1:A:292:SER:O	1:A:373:ILE:HB	2.19	0.43
1:C:426:TYR:N	1:C:427:PRO:CD	2.81	0.43
1:D:28:GLN:NE2	1:D:184:ARG:HE	2.17	0.43
1:D:365:TYR:CD1	1:D:365:TYR:N	2.86	0.43
1:B:124:LEU:HD12	1:B:279:PRO:HD3	2.00	0.43
1:A:79:PHE:O	1:A:212:GLU:OE2	2.36	0.42
1:B:251:SER:HB3	1:B:254:SER:HB2	2.00	0.42
1:D:358:THR:HG21	5:D:453:HOH:O	2.18	0.42
1:A:24:TYR:N	1:A:110:THR:HG21	2.33	0.42
1:A:330:SER:HB2	1:A:379:TYR:O	2.18	0.42
1:B:74:MET:CE	1:B:76:THR:HG23	2.48	0.42
1:B:92:ILE:HG22	1:B:95:LEU:HD21	1.99	0.42
1:C:92:ILE:CG2	1:C:95:LEU:HD21	2.49	0.42
1:B:426:TYR:N	1:B:427:PRO:CD	2.76	0.42
1:C:171:TYR:CE1	1:C:178:ARG:HG3	2.55	0.42
1:B:92:ILE:CG2	1:B:95:LEU:HD21	2.49	0.42
1:D:25:ASN:ND2	1:D:50:ASP:HB2	2.35	0.42
1:A:124:LEU:HD12	1:A:279:PRO:HD3	2.02	0.42
1:B:132:LEU:HD22	1:B:320:PHE:CD1	2.54	0.42
1:C:92:ILE:HG22	1:C:95:LEU:HD21	2.02	0.42
1:A:104:GLU:HA	1:A:112:ARG:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:TRP:C	1:A:427:PRO:HD3	2.39	0.41
1:A:55:SER:HB2	1:A:71:LYS:HZ3	1.84	0.41
1:D:297:PHE:CD1	1:D:373:ILE:HD11	2.55	0.41
1:C:155:LYS:HG3	1:C:155:LYS:H	1.58	0.41
1:C:34:GLN:HE21	1:C:242:ARG:HH21	1.68	0.41
1:D:285:MET:O	1:D:321:ALA:HA	2.20	0.41
1:A:211:ASN:OD1	2:A:436(A):NAG:N2	2.54	0.41
1:A:423:ARG:NE	1:A:423:ARG:HA	2.34	0.41
1:B:72:GLY:HA3	1:B:90:THR:OG1	2.20	0.41
1:C:399:HIS:CE1	1:C:421:PHE:HE1	2.38	0.41
1:C:55:SER:OG	1:C:88:HIS:HD2	2.03	0.41
1:A:399:HIS:HB3	1:A:419:TRP:CZ3	2.56	0.41
1:D:293:TYR:HA	1:D:372:MET:HA	2.02	0.41
1:A:211:ASN:OD1	2:A:436(A):NAG:C2	2.68	0.41
1:A:251:SER:OG	1:A:254:SER:HB2	2.20	0.41
1:C:124:LEU:O	1:C:279:PRO:HG3	2.20	0.41
1:A:406:ARG:HG3	1:A:415:ALA:CB	2.51	0.41
1:C:236:PHE:O	1:C:251:SER:HB2	2.19	0.41
1:C:338:TYR:O	1:C:339:LYS:HG2	2.20	0.41
1:C:25:ASN:HD22	1:C:50:ASP:H	1.67	0.41
1:D:51:GLU:HB2	1:D:52:PRO:HD2	2.01	0.41
1:D:374:GLN:HA	1:D:375:PRO:HA	1.79	0.41
1:C:171:TYR:CD1	1:C:178:ARG:HG3	2.55	0.41
1:C:365:TYR:N	1:C:365:TYR:CD1	2.87	0.41
1:A:14:ASP:O	1:A:15:SER:C	2.59	0.41
1:A:236:PHE:O	1:A:251:SER:HB2	2.21	0.41
1:A:382:PHE:CD1	1:A:382:PHE:C	2.93	0.41
1:C:374:GLN:HE21	1:C:374:GLN:HA	1.86	0.41
1:B:26:ALA:HA	1:B:27:PRO:HD3	1.90	0.40
1:B:338:TYR:O	1:B:339:LYS:HG2	2.21	0.40
1:C:162:VAL:O	1:C:162:VAL:HG13	2.21	0.40
1:C:428:VAL:HG23	1:C:429:ASP:N	2.34	0.40
1:D:58:ARG:O	1:D:103:TYR:HA	2.21	0.40
1:C:190:VAL:HG13	1:C:195:TRP:CD1	2.56	0.40
1:B:129:THR:H	1:B:157:GLN:NE2	2.17	0.40
1:B:178:ARG:HD3	1:B:178:ARG:HA	2.00	0.40
1:C:316:VAL:CG2	1:C:354:PRO:HB3	2.51	0.40
1:C:417:SER:C	1:C:418:VAL:HG23	2.41	0.40
1:B:186:THR:O	1:B:190:VAL:HG23	2.22	0.40
1:B:406:ARG:HG3	1:B:415:ALA:CB	2.52	0.40
1:B:48:THR:OG1	1:B:88:HIS:HE1	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:227:TYR:O	1:D:232:SER:HB3	2.21	0.40
1:A:368:ILE:HG12	1:A:387:PHE:CE1	2.56	0.40
1:C:76:THR:HG22	1:C:85:GLY:O	2.22	0.40
1:D:211:ASN:OD1	2:D:436(A):NAG:C2	2.69	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	422/432 (98%)	387 (92%)	32 (8%)	3 (1%)	22	33
1	B	422/432 (98%)	380 (90%)	39 (9%)	3 (1%)	22	33
1	C	422/432 (98%)	386 (92%)	32 (8%)	4 (1%)	17	26
1	D	422/432 (98%)	388 (92%)	32 (8%)	2 (0%)	29	43
All	All	1688/1728 (98%)	1541 (91%)	135 (8%)	12 (1%)	22	33

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	175	ASP
1	C	175	ASP
1	A	65	GLY
1	B	175	ASP
1	C	65	GLY
1	C	431	SER
1	D	65	GLY
1	D	175	ASP
1	B	431	SER
1	A	427	PRO
1	B	65	GLY

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Mol	Chain	Res	Type
1	C	426	TYR

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	373/381 (98%)	339 (91%)	34 (9%)	9 13
1	B	373/381 (98%)	338 (91%)	35 (9%)	8 13
1	C	373/381 (98%)	334 (90%)	39 (10%)	7 10
1	D	373/381 (98%)	336 (90%)	37 (10%)	8 11
All	All	1492/1524 (98%)	1347 (90%)	145 (10%)	8 11

All (145) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ARG
1	A	19	ARG
1	A	20	VAL
1	A	33	THR
1	A	49	MET
1	A	69	ILE
1	A	73	LYS
1	A	74	MET
1	A	99	THR
1	A	105	VAL
1	A	110	THR
1	A	129	THR
1	A	132	LEU
1	A	147	SER
1	A	152	SER
1	A	155	LYS
1	A	162	VAL
1	A	190	VAL
1	A	209	GLU
1	A	230	SER

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Mol	Chain	Res	Type
1	A	254	SER
1	A	276	SER
1	A	287	SER
1	A	306	LYS
1	A	316	VAL
1	A	318	VAL
1	A	334	SER
1	A	348	VAL
1	A	358	THR
1	A	359	ILE
1	A	374	GLN
1	A	383	ARG
1	A	403	SER
1	A	417	SER
1	B	9	ARG
1	B	19	ARG
1	B	20	VAL
1	B	33	THR
1	B	49	MET
1	B	52	PRO
1	B	73	LYS
1	B	74	MET
1	B	99	THR
1	B	105	VAL
1	B	110	THR
1	B	129	THR
1	B	132	LEU
1	B	147	SER
1	B	152	SER
1	B	154	LYS
1	B	155	LYS
1	B	162	VAL
1	B	176	ASN
1	B	190	VAL
1	B	209	GLU
1	B	230	SER
1	B	254	SER
1	B	276	SER
1	B	306	LYS
1	B	316	VAL
1	B	318	VAL
1	B	334	SER

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Mol	Chain	Res	Type
1	B	348	VAL
1	B	358	THR
1	B	359	ILE
1	B	371	ASN
1	B	383	ARG
1	B	403	SER
1	B	417	SER
1	C	17	VAL
1	C	19	ARG
1	C	20	VAL
1	C	22	PRO
1	C	33	THR
1	C	49	MET
1	C	52	PRO
1	C	73	LYS
1	C	74	MET
1	C	99	THR
1	C	105	VAL
1	C	110	THR
1	C	129	THR
1	C	132	LEU
1	C	147	SER
1	C	152	SER
1	C	154	LYS
1	C	155	LYS
1	C	162	VAL
1	C	176	ASN
1	C	190	VAL
1	C	209	GLU
1	C	230	SER
1	C	254	SER
1	C	276	SER
1	C	287	SER
1	C	306	LYS
1	C	316	VAL
1	C	318	VAL
1	C	334	SER
1	C	348	VAL
1	C	358	THR
1	C	359	ILE
1	C	372	MET
1	C	374	GLN

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Mol	Chain	Res	Type
1	C	383	ARG
1	C	403	SER
1	C	417	SER
1	C	428	VAL
1	D	9	ARG
1	D	17	VAL
1	D	19	ARG
1	D	20	VAL
1	D	33	THR
1	D	49	MET
1	D	52	PRO
1	D	73	LYS
1	D	74	MET
1	D	99	THR
1	D	105	VAL
1	D	110	THR
1	D	129	THR
1	D	132	LEU
1	D	147	SER
1	D	152	SER
1	D	154	LYS
1	D	155	LYS
1	D	162	VAL
1	D	176	ASN
1	D	190	VAL
1	D	209	GLU
1	D	230	SER
1	D	254	SER
1	D	276	SER
1	D	306	LYS
1	D	316	VAL
1	D	318	VAL
1	D	334	SER
1	D	348	VAL
1	D	358	THR
1	D	359	ILE
1	D	371	ASN
1	D	383	ARG
1	D	403	SER
1	D	417	SER
1	D	432	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	28	GLN
1	A	31	HIS
1	A	34	GLN
1	A	88	HIS
1	A	138	GLN
1	A	157	GLN
1	A	291	ASN
1	A	294	ASN
1	A	364	ASN
1	A	371	ASN
1	A	399	HIS
1	A	424	HIS
1	B	25	ASN
1	B	28	GLN
1	B	31	HIS
1	B	34	GLN
1	B	88	HIS
1	B	138	GLN
1	B	157	GLN
1	B	291	ASN
1	B	294	ASN
1	B	364	ASN
1	B	399	HIS
1	B	424	HIS
1	C	25	ASN
1	C	28	GLN
1	C	31	HIS
1	C	34	GLN
1	C	88	HIS
1	C	138	GLN
1	C	157	GLN
1	C	291	ASN
1	C	294	ASN
1	C	364	ASN
1	C	374	GLN
1	C	399	HIS
1	C	424	HIS
1	D	25	ASN
1	D	28	GLN
1	D	31	HIS
1	D	34	GLN

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Mol	Chain	Res	Type
1	D	88	HIS
1	D	138	GLN
1	D	157	GLN
1	D	224	HIS
1	D	291	ASN
1	D	294	ASN
1	D	364	ASN
1	D	399	HIS
1	D	424	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 28 ligands modelled in this entry, 8 are monoatomic - leaving 20 for Mogul analysis.

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	436(A)	1	14,14,15	1.30	2 (14%)	17,19,21	1.10	2 (11%)
2	NAG	D	434(A)	1	14,14,15	1.03	1 (7%)	17,19,21	1.77	4 (23%)
2	NAG	A	437(A)	1	14,14,15	1.29	2 (14%)	17,19,21	0.84	0
2	NAG	B	433(A)	1	14,14,15	0.86	0	17,19,21	1.46	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	C	437(A)	1	14,14,15	1.15	1 (7%)	17,19,21	0.74	0
2	NAG	D	433(A)	1	14,14,15	1.00	0	17,19,21	1.43	3 (17%)
2	NAG	A	433(A)	1	14,14,15	1.13	1 (7%)	17,19,21	1.52	3 (17%)
2	NAG	C	436(A)	1	14,14,15	1.32	2 (14%)	17,19,21	1.14	2 (11%)
2	NAG	C	433(A)	1	14,14,15	0.91	0	17,19,21	1.32	2 (11%)
2	NAG	D	437(A)	1	14,14,15	1.92	5 (35%)	17,19,21	1.12	3 (17%)
2	NAG	B	436(A)	1	14,14,15	1.35	2 (14%)	17,19,21	1.14	2 (11%)
2	NAG	C	434(A)	1	14,14,15	1.09	1 (7%)	17,19,21	1.77	3 (17%)
2	NAG	D	436(A)	1	14,14,15	1.20	1 (7%)	17,19,21	1.05	2 (11%)
2	NAG	B	437(A)	1	14,14,15	1.24	1 (7%)	17,19,21	0.78	0
2	NAG	C	435(A)	1	14,14,15	0.48	0	17,19,21	0.65	0
2	NAG	D	435(A)	1	14,14,15	0.68	0	17,19,21	0.92	0
2	NAG	A	435(A)	1	14,14,15	0.72	0	17,19,21	0.84	0
2	NAG	B	435(A)	1	14,14,15	0.69	0	17,19,21	0.55	0
2	NAG	A	434(A)	1	14,14,15	1.01	1 (7%)	17,19,21	1.71	3 (17%)
2	NAG	B	434(A)	1	14,14,15	0.93	1 (7%)	17,19,21	1.60	2 (11%)

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	436(A)	1	-	2/6/23/26	0/1/1/1
2	NAG	D	434(A)	1	-	3/6/23/26	0/1/1/1
2	NAG	A	437(A)	1	-	2/6/23/26	0/1/1/1
2	NAG	B	433(A)	1	-	2/6/23/26	0/1/1/1
2	NAG	C	437(A)	1	-	2/6/23/26	0/1/1/1
2	NAG	D	433(A)	1	-	2/6/23/26	0/1/1/1
2	NAG	A	433(A)	1	-	2/6/23/26	0/1/1/1
2	NAG	C	436(A)	1	-	2/6/23/26	0/1/1/1
2	NAG	C	433(A)	1	-	2/6/23/26	0/1/1/1
2	NAG	D	437(A)	1	-	2/6/23/26	0/1/1/1
2	NAG	B	436(A)	1	-	2/6/23/26	0/1/1/1
2	NAG	C	434(A)	1	-	3/6/23/26	0/1/1/1
2	NAG	D	436(A)	1	-	2/6/23/26	0/1/1/1
2	NAG	B	437(A)	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	435(A)	1	-	2/6/23/26	0/1/1/1
2	NAG	D	435(A)	1	-	2/6/23/26	0/1/1/1
2	NAG	A	435(A)	1	-	2/6/23/26	0/1/1/1
2	NAG	B	435(A)	1	-	1/6/23/26	0/1/1/1
2	NAG	A	434(A)	1	-	3/6/23/26	0/1/1/1
2	NAG	B	434(A)	1	-	4/6/23/26	0/1/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	437(A)	NAG	C4-C3	4.02	1.62	1.52
2	B	436(A)	NAG	C1-C2	3.37	1.57	1.52
2	C	436(A)	NAG	C1-C2	3.26	1.57	1.52
2	A	436(A)	NAG	C1-C2	2.98	1.56	1.52
2	D	437(A)	NAG	C4-C5	2.96	1.59	1.53
2	B	437(A)	NAG	C4-C5	2.89	1.59	1.53
2	D	437(A)	NAG	C1-C2	2.80	1.56	1.52
2	D	436(A)	NAG	C1-C2	2.66	1.56	1.52
2	A	434(A)	NAG	C4-C5	2.60	1.58	1.53
2	D	437(A)	NAG	C3-C2	2.53	1.57	1.52
2	D	434(A)	NAG	C4-C5	2.50	1.58	1.53
2	B	434(A)	NAG	C4-C5	2.43	1.58	1.53
2	C	434(A)	NAG	C4-C5	2.38	1.58	1.53
2	A	433(A)	NAG	C1-C2	2.38	1.55	1.52
2	A	437(A)	NAG	C4-C3	2.37	1.58	1.52
2	C	437(A)	NAG	C4-C3	2.31	1.58	1.52
2	A	436(A)	NAG	O5-C5	2.16	1.47	1.43
2	D	437(A)	NAG	C8-C7	2.16	1.55	1.50
2	C	436(A)	NAG	O5-C5	2.07	1.47	1.43
2	A	437(A)	NAG	C4-C5	2.05	1.57	1.53
2	B	436(A)	NAG	O5-C5	2.02	1.47	1.43

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	434(A)	NAG	C4-C3-C2	-5.07	103.58	111.02
2	C	434(A)	NAG	C4-C3-C2	-4.94	103.77	111.02
2	D	434(A)	NAG	C4-C3-C2	-4.78	104.01	111.02
2	B	434(A)	NAG	C4-C3-C2	-4.63	104.24	111.02
2	B	433(A)	NAG	C4-C3-C2	-3.29	106.19	111.02
2	C	433(A)	NAG	C4-C3-C2	-3.24	106.27	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	433(A)	NAG	C4-C3-C2	-3.13	106.43	111.02
2	A	433(A)	NAG	C4-C3-C2	-3.11	106.46	111.02
2	D	434(A)	NAG	O5-C5-C6	-2.92	102.62	107.20
2	A	433(A)	NAG	C2-N2-C7	-2.81	118.90	122.90
2	A	436(A)	NAG	C4-C3-C2	-2.78	106.94	111.02
2	C	434(A)	NAG	O5-C1-C2	-2.77	106.91	111.29
2	C	436(A)	NAG	C4-C3-C2	-2.72	107.03	111.02
2	D	436(A)	NAG	C4-C3-C2	-2.67	107.11	111.02
2	D	433(A)	NAG	C2-N2-C7	-2.65	119.13	122.90
2	B	436(A)	NAG	C4-C3-C2	-2.61	107.19	111.02
2	A	433(A)	NAG	C1-O5-C5	2.57	115.67	112.19
2	B	434(A)	NAG	O5-C1-C2	-2.46	107.41	111.29
2	B	436(A)	NAG	C1-O5-C5	2.37	115.40	112.19
2	A	434(A)	NAG	O5-C5-C6	-2.31	103.58	107.20
2	D	434(A)	NAG	C1-O5-C5	2.31	115.32	112.19
2	D	437(A)	NAG	C4-C3-C2	-2.29	107.66	111.02
2	C	436(A)	NAG	C1-O5-C5	2.29	115.29	112.19
2	B	433(A)	NAG	C2-N2-C7	-2.29	119.65	122.90
2	A	434(A)	NAG	O5-C1-C2	-2.24	107.75	111.29
2	D	437(A)	NAG	O3-C3-C4	2.23	115.50	110.35
2	A	436(A)	NAG	C1-O5-C5	2.19	115.16	112.19
2	D	436(A)	NAG	C1-O5-C5	2.17	115.13	112.19
2	C	434(A)	NAG	O5-C5-C6	-2.16	103.82	107.20
2	B	433(A)	NAG	C1-O5-C5	2.15	115.11	112.19
2	C	433(A)	NAG	C2-N2-C7	-2.12	119.88	122.90
2	D	434(A)	NAG	O5-C1-C2	-2.03	108.08	111.29
2	D	437(A)	NAG	O4-C4-C3	2.03	115.04	110.35
2	B	433(A)	NAG	C3-C4-C5	-2.03	106.63	110.24
2	D	433(A)	NAG	C3-C4-C5	-2.01	106.65	110.24

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	434(A)	NAG	O5-C5-C6-O6
2	A	434(A)	NAG	O5-C5-C6-O6
2	C	434(A)	NAG	O5-C5-C6-O6
2	D	434(A)	NAG	O5-C5-C6-O6
2	D	433(A)	NAG	O5-C5-C6-O6
2	C	433(A)	NAG	O5-C5-C6-O6
2	A	433(A)	NAG	O5-C5-C6-O6
2	B	433(A)	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	A	437(A)	NAG	O5-C5-C6-O6
2	C	435(A)	NAG	O5-C5-C6-O6
2	C	437(A)	NAG	O5-C5-C6-O6
2	A	437(A)	NAG	C4-C5-C6-O6
2	D	433(A)	NAG	C4-C5-C6-O6
2	A	435(A)	NAG	O5-C5-C6-O6
2	C	437(A)	NAG	C4-C5-C6-O6
2	D	437(A)	NAG	C4-C5-C6-O6
2	C	433(A)	NAG	C4-C5-C6-O6
2	B	437(A)	NAG	C4-C5-C6-O6
2	D	435(A)	NAG	O5-C5-C6-O6
2	D	437(A)	NAG	O5-C5-C6-O6
2	B	437(A)	NAG	O5-C5-C6-O6
2	D	434(A)	NAG	C4-C5-C6-O6
2	C	434(A)	NAG	C4-C5-C6-O6
2	B	435(A)	NAG	O5-C5-C6-O6
2	B	433(A)	NAG	C4-C5-C6-O6
2	A	433(A)	NAG	C4-C5-C6-O6
2	B	434(A)	NAG	C4-C5-C6-O6
2	A	434(A)	NAG	C4-C5-C6-O6
2	C	436(A)	NAG	O5-C5-C6-O6
2	A	436(A)	NAG	O5-C5-C6-O6
2	B	436(A)	NAG	O5-C5-C6-O6
2	D	436(A)	NAG	O5-C5-C6-O6
2	C	435(A)	NAG	C4-C5-C6-O6
2	A	435(A)	NAG	C4-C5-C6-O6
2	B	436(A)	NAG	C3-C2-N2-C7
2	A	434(A)	NAG	C3-C2-N2-C7
2	C	434(A)	NAG	C3-C2-N2-C7
2	C	436(A)	NAG	C3-C2-N2-C7
2	D	436(A)	NAG	C3-C2-N2-C7
2	A	436(A)	NAG	C3-C2-N2-C7
2	D	434(A)	NAG	C3-C2-N2-C7
2	D	435(A)	NAG	C4-C5-C6-O6
2	B	434(A)	NAG	C3-C2-N2-C7
2	B	434(A)	NAG	C1-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	436(A)	NAG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	436(A)	NAG	1	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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.