Full wwPDB X-ray Structure Validation Report

Jan 31, 2016 – 09:04 PM GMT

PDB ID	:	1NEL
Title	:	FLUORIDE INHIBITION OF YEAST ENOLASE: CRYSTAL STRUCTURE OF THE ENOLASE-MG2+-F–PI COMPLEX AT 2.6-ANGSTROMS RESOLUTION
Authors	:	Lebioda, L.; Zhang, E.; Lewinski, K.; Brewer, M.J.
Deposited on	:	1993-08-20
Resolution	:	2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

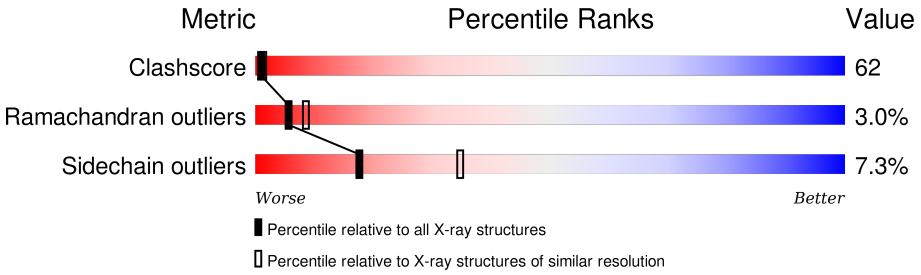
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.60 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	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	436	33% 49% 16%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3570 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 ENOLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	436	3289	2076	569	638	6	0	0	0

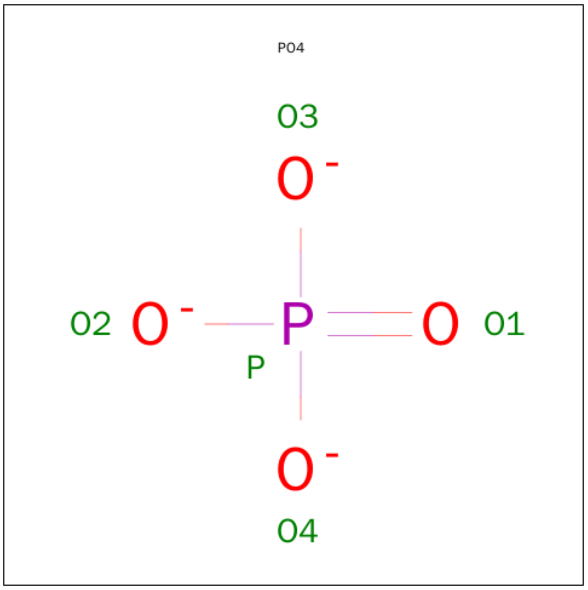
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	84	SER	LYS	CONFLICT	UNP P00924

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
2	A	1	1	1	0	0

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 5 4 1	0	0

- Molecule 4 is FLUORIDE ION (three-letter code: F) (formula: F).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total F 1 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	274	Total O 274 274	0	0

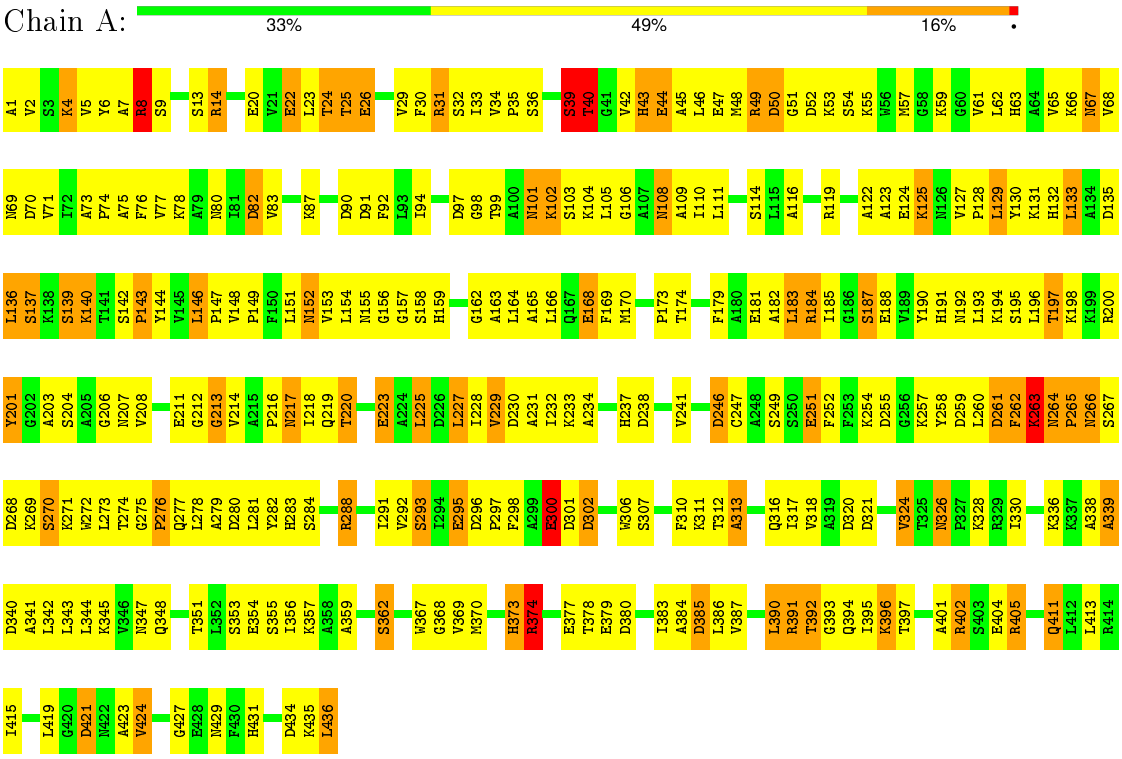
3 Residue-property plots (i)

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 was not executed.

- Molecule 1: ENOLASE

Chain A:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α, β, γ	122.50Å 122.50Å 67.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.169 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3570	wwPDB-VP
Average B, all atoms (Å^2)	20.0	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: PO4, MG, F

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	0.86	1/3349 (0.0%)	1.98	98/4531 (2.2%)

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	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	251	GLU	CD-OE2	-5.13	1.20	1.25

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	14	ARG	NE-CZ-NH2	-12.45	114.07	120.30
1	A	142	SER	N-CA-CB	-10.99	94.01	110.50
1	A	300	GLU	CA-CB-CG	10.77	137.09	113.40
1	A	184	ARG	NE-CZ-NH1	-10.74	114.93	120.30
1	A	405	ARG	NE-CZ-NH1	10.61	125.61	120.30
1	A	50	ASP	CB-CG-OD2	10.21	127.48	118.30
1	A	435	LYS	CB-CA-C	9.10	128.60	110.40
1	A	405	ARG	CD-NE-CZ	9.01	136.21	123.60
1	A	223	GLU	CA-CB-CG	8.89	132.96	113.40
1	A	402	ARG	NE-CZ-NH2	8.39	124.50	120.30
1	A	251	GLU	OE1-CD-OE2	8.34	133.31	123.30
1	A	396	LYS	CA-CB-CG	8.22	131.48	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	50	ASP	CB-CG-OD1	-8.21	110.91	118.30
1	A	301	ASP	CB-CG-OD2	8.16	125.64	118.30
1	A	340	ASP	CB-CG-OD2	-7.94	111.16	118.30
1	A	238	ASP	CB-CG-OD2	-7.86	111.23	118.30
1	A	255	ASP	CB-CG-OD1	-7.84	111.24	118.30
1	A	282	TYR	CB-CG-CD1	7.76	125.66	121.00
1	A	82	ASP	CB-CG-OD2	-7.72	111.35	118.30
1	A	435	LYS	CA-C-O	7.62	136.11	120.10
1	A	183	LEU	CB-CA-C	7.58	124.60	110.20
1	A	201	TYR	CB-CG-CD2	7.47	125.48	121.00
1	A	146	LEU	CB-CA-C	7.45	124.35	110.20
1	A	20	GLU	CG-CD-OE1	-7.42	103.47	118.30
1	A	8	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	A	405	ARG	NE-CZ-NH2	-7.06	116.77	120.30
1	A	288	ARG	CA-CB-CG	7.03	128.86	113.40
1	A	143	PRO	N-CA-C	7.01	130.33	112.10
1	A	201	TYR	CB-CG-CD1	-6.96	116.83	121.00
1	A	385	ASP	CB-CG-OD2	-6.92	112.07	118.30
1	A	49	ARG	NE-CZ-NH2	-6.92	116.84	120.30
1	A	4	LYS	N-CA-CB	-6.87	98.23	110.60
1	A	70	ASP	CB-CG-OD1	-6.82	112.17	118.30
1	A	282	TYR	CB-CG-CD2	-6.72	116.97	121.00
1	A	49	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	A	225	LEU	CB-CA-C	6.64	122.82	110.20
1	A	402	ARG	CG-CD-NE	6.57	125.59	111.80
1	A	184	ARG	NE-CZ-NH2	6.54	123.57	120.30
1	A	168	GLU	CG-CD-OE1	-6.52	105.26	118.30
1	A	340	ASP	CB-CG-OD1	6.51	124.16	118.30
1	A	47	GLU	N-CA-CB	6.46	122.22	110.60
1	A	184	ARG	CD-NE-CZ	-6.42	114.61	123.60
1	A	133	LEU	CB-CA-C	6.20	121.99	110.20
1	A	108	ASN	N-CA-CB	6.17	121.71	110.60
1	A	246	ASP	CB-CG-OD2	6.16	123.84	118.30
1	A	385	ASP	CB-CG-OD1	6.14	123.83	118.30
1	A	255	ASP	CB-CG-OD2	6.12	123.81	118.30
1	A	278	LEU	CB-CA-C	6.04	121.67	110.20
1	A	25	THR	N-CA-CB	5.91	121.53	110.30
1	A	183	LEU	CB-CG-CD2	-5.90	100.97	111.00
1	A	266	ASN	CB-CA-C	5.86	122.11	110.40
1	A	91	ASP	CB-CG-OD1	5.82	123.54	118.30
1	A	31	ARG	NE-CZ-NH1	-5.78	117.41	120.30
1	A	302	ASP	CB-CG-OD1	-5.73	113.14	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	261	ASP	CB-CG-OD2	5.72	123.45	118.30
1	A	142	SER	N-CA-C	5.71	126.41	111.00
1	A	146	LEU	N-CA-C	-5.62	95.83	111.00
1	A	14	ARG	NH1-CZ-NH2	5.62	125.58	119.40
1	A	374	ARG	NE-CZ-NH1	-5.58	117.51	120.30
1	A	397	THR	CA-CB-CG2	5.58	120.22	112.40
1	A	36	SER	N-CA-CB	5.58	118.86	110.50
1	A	168	GLU	CG-CD-OE2	5.56	129.41	118.30
1	A	229	VAL	CB-CA-C	5.55	121.95	111.40
1	A	435	LYS	CA-C-N	-5.54	105.01	117.20
1	A	47	GLU	CA-CB-CG	5.54	125.59	113.40
1	A	220	THR	N-CA-CB	-5.54	99.78	110.30
1	A	129	LEU	CB-CA-C	5.51	120.68	110.20
1	A	8	ARG	CA-CB-CG	5.50	125.50	113.40
1	A	223	GLU	CG-CD-OE2	-5.50	107.31	118.30
1	A	213	GLY	O-C-N	5.46	131.43	122.70
1	A	295	GLU	OE1-CD-OE2	5.45	129.84	123.30
1	A	137	SER	O-C-N	5.44	131.41	122.70
1	A	22	GLU	CB-CG-CD	5.43	128.86	114.20
1	A	391	ARG	N-CA-CB	-5.43	100.83	110.60
1	A	152	ASN	CA-C-O	-5.39	108.77	120.10
1	A	67	ASN	CB-CG-OD1	-5.35	110.91	121.60
1	A	435	LYS	C-N-CA	5.34	135.05	121.70
1	A	276	PRO	N-CD-CG	-5.33	95.21	103.20
1	A	192	ASN	CA-CB-CG	-5.31	101.73	113.40
1	A	261	ASP	O-C-N	5.30	131.18	122.70
1	A	246	ASP	N-CA-CB	5.29	120.12	110.60
1	A	82	ASP	CA-CB-CG	-5.26	101.83	113.40
1	A	311	LYS	CA-CB-CG	5.25	124.95	113.40
1	A	125	LYS	CA-CB-CG	5.25	124.95	113.40
1	A	25	THR	CA-CB-OG1	-5.20	98.07	109.00
1	A	251	GLU	CG-CD-OE1	-5.16	107.99	118.30
1	A	404	GLU	CG-CD-OE1	5.16	128.61	118.30
1	A	421	ASP	CB-CG-OD1	5.14	122.93	118.30
1	A	20	GLU	OE1-CD-OE2	5.14	129.47	123.30
1	A	47	GLU	CG-CD-OE2	5.13	128.57	118.30
1	A	339	ALA	CA-C-N	-5.12	105.93	117.20
1	A	142	SER	CA-C-N	5.11	131.41	117.10
1	A	424	VAL	CA-CB-CG1	5.11	118.56	110.90
1	A	411	GLN	N-CA-CB	5.11	119.79	110.60
1	A	251	GLU	CB-CA-C	-5.09	100.22	110.40
1	A	278	LEU	N-CA-C	-5.08	97.30	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	139	SER	N-CA-CB	-5.07	102.89	110.50
1	A	44	GLU	CG-CD-OE1	-5.07	108.17	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	374	ARG	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	3289	0	3293	410	11
2	A	1	0	0	0	0
3	A	5	0	0	0	0
4	A	1	0	0	0	0
5	A	274	0	0	109	10
All	All	3570	0	3293	410	11

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 62.

All (410) 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:345:LYS:HD3	1:A:374:ARG:NH1	1.19	1.47
1:A:101:ASN:ND2	1:A:103:SER:HB3	1.52	1.24
1:A:257:LYS:NZ	1:A:269:LYS:HE2	1.54	1.22
1:A:345:LYS:CD	1:A:374:ARG:NH1	2.03	1.21
1:A:262:PHE:O	1:A:263:LYS:HG3	1.40	1.17
1:A:99:THR:HG21	1:A:104:LYS:HB2	1.23	1.15
1:A:97:ASP:O	1:A:99:THR:HG23	1.48	1.10
1:A:383:ILE:HG23	5:A:495:HOH:O	1.55	1.07
1:A:101:ASN:HD21	1:A:103:SER:HB3	0.94	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:LYS:CD	1:A:374:ARG:HH12	1.62	1.03
1:A:125:LYS:HE3	1:A:132:HIS:CE1	1.94	1.02
1:A:379:GLU:HG3	5:A:504:HOH:O	1.57	1.01
1:A:413:LEU:HD22	5:A:490:HOH:O	1.58	1.01
1:A:254:LYS:HA	5:A:622:HOH:O	1.62	1.00
1:A:257:LYS:HZ1	1:A:269:LYS:HE2	1.17	0.99
1:A:391:ARG:NH1	1:A:434:ASP:O	1.96	0.98
1:A:385:ASP:OD1	5:A:633:HOH:O	1.82	0.98
1:A:227:LEU:HD13	5:A:749:HOH:O	1.64	0.96
1:A:252:PHE:HB3	1:A:262:PHE:CD1	2.01	0.96
1:A:200:ARG:HD2	5:A:749:HOH:O	1.63	0.96
1:A:300:GLU:HG3	5:A:619:HOH:O	1.65	0.96
1:A:261:ASP:OD2	1:A:264:ASN:CA	2.14	0.94
1:A:345:LYS:CE	1:A:374:ARG:HH12	1.80	0.94
1:A:143:PRO:HB2	1:A:424:VAL:HG22	1.50	0.93
1:A:46:LEU:HD22	1:A:103:SER:HA	1.49	0.93
1:A:261:ASP:OD2	1:A:264:ASN:HA	1.69	0.92
1:A:345:LYS:HD3	1:A:374:ARG:HH12	1.11	0.91
1:A:324:VAL:HG13	1:A:348:GLN:HG2	1.51	0.91
1:A:257:LYS:CE	1:A:269:LYS:HE2	2.00	0.91
1:A:391:ARG:O	1:A:434:ASP:HA	1.71	0.91
1:A:267:SER:HA	5:A:581:HOH:O	1.69	0.91
1:A:257:LYS:HZ2	1:A:269:LYS:HG2	1.36	0.90
1:A:51:GLY:N	5:A:689:HOH:O	2.04	0.89
1:A:99:THR:CG2	1:A:104:LYS:HB2	2.02	0.89
1:A:345:LYS:HD3	1:A:374:ARG:HH11	1.37	0.88
1:A:313:ALA:HB3	5:A:482:HOH:O	1.72	0.87
1:A:125:LYS:HE3	1:A:132:HIS:HE1	1.40	0.87
1:A:268:ASP:OD2	1:A:270:SER:HB2	1.76	0.86
1:A:326:ASN:ND2	1:A:328:LYS:HB3	1.92	0.85
1:A:257:LYS:HZ2	1:A:269:LYS:CG	1.89	0.85
1:A:261:ASP:HB3	1:A:264:ASN:HD22	1.42	0.85
1:A:193:LEU:O	1:A:197:THR:HG23	1.76	0.84
1:A:78:LYS:HD2	5:A:679:HOH:O	1.78	0.83
1:A:187:SER:HB2	5:A:549:HOH:O	1.77	0.83
1:A:25:THR:HG21	5:A:721:HOH:O	1.78	0.83
1:A:101:ASN:HD21	1:A:103:SER:CB	1.88	0.82
1:A:200:ARG:NH1	5:A:602:HOH:O	2.13	0.82
1:A:173:PRO:HG2	1:A:182:ALA:HB1	1.61	0.82
1:A:401:ALA:O	1:A:402:ARG:HB2	1.79	0.79
1:A:166:LEU:HD22	1:A:247:CYS:HA	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:ASP:CG	1:A:270:SER:HB2	2.04	0.78
1:A:261:ASP:O	1:A:263:LYS:N	2.16	0.78
1:A:262:PHE:O	1:A:263:LYS:CG	2.27	0.78
1:A:379:GLU:OE2	5:A:508:HOH:O	2.02	0.78
1:A:211:GLU:OE2	5:A:529:HOH:O	2.02	0.77
1:A:326:ASN:HD22	1:A:328:LYS:H	1.28	0.77
1:A:97:ASP:OD1	1:A:105:LEU:N	2.16	0.77
1:A:257:LYS:NZ	1:A:269:LYS:CE	2.42	0.77
1:A:33:ILE:HG22	1:A:378:THR:HG21	1.67	0.77
1:A:320:ASP:HA	5:A:650:HOH:O	1.83	0.76
1:A:391:ARG:HD2	5:A:486:HOH:O	1.86	0.76
1:A:73:ALA:HB1	5:A:625:HOH:O	1.85	0.76
1:A:163:ALA:H	1:A:217:ASN:ND2	1.82	0.76
1:A:50:ASP:OD2	1:A:62:LEU:HB2	1.86	0.75
1:A:320:ASP:OD1	5:A:650:HOH:O	2.04	0.75
1:A:344:LEU:O	1:A:344:LEU:HD23	1.87	0.75
1:A:195:SER:HA	5:A:675:HOH:O	1.87	0.74
1:A:48:MET:CE	5:A:572:HOH:O	2.34	0.74
1:A:144:TYR:HD2	1:A:419:LEU:HD13	1.52	0.74
1:A:139:SER:HA	5:A:485:HOH:O	1.87	0.74
1:A:131:LYS:HG2	5:A:724:HOH:O	1.88	0.73
1:A:59:LYS:HE3	5:A:559:HOH:O	1.89	0.73
1:A:4:LYS:O	1:A:4:LYS:HG2	1.87	0.73
1:A:257:LYS:NZ	1:A:269:LYS:HG2	2.03	0.73
1:A:143:PRO:HG3	1:A:424:VAL:CG1	2.20	0.72
1:A:42:VAL:HG23	1:A:43:HIS:N	2.04	0.71
1:A:344:LEU:HD23	1:A:344:LEU:C	2.09	0.71
1:A:293:SER:CB	5:A:446:HOH:O	2.31	0.71
1:A:50:ASP:OD2	1:A:62:LEU:N	2.23	0.71
1:A:436:LEU:O	1:A:436:LEU:HG	1.90	0.71
1:A:1:ALA:N	5:A:463:HOH:O	2.19	0.71
1:A:345:LYS:NZ	1:A:374:ARG:HH12	1.88	0.71
1:A:30:PHE:CE2	1:A:123:ALA:HB2	2.26	0.71
1:A:48:MET:HE3	5:A:572:HOH:O	1.89	0.70
1:A:30:PHE:HE2	1:A:123:ALA:HB2	1.56	0.70
1:A:268:ASP:O	1:A:271:LYS:HB2	1.92	0.70
1:A:49:ARG:O	5:A:689:HOH:O	2.09	0.70
1:A:228:ILE:O	1:A:232:ILE:HG13	1.90	0.70
1:A:111:LEU:HB2	5:A:761:HOH:O	1.90	0.69
1:A:9:SER:HB3	5:A:695:HOH:O	1.90	0.69
1:A:104:LYS:HG2	5:A:683:HOH:O	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:ASP:CB	1:A:264:ASN:HD22	2.05	0.68
1:A:362:SER:O	1:A:367:TRP:HB2	1.93	0.68
1:A:295:GLU:OE1	1:A:396:LYS:NZ	2.25	0.68
1:A:194:LYS:HG2	1:A:198:LYS:HE2	1.76	0.68
1:A:227:LEU:CD1	5:A:749:HOH:O	2.32	0.68
1:A:261:ASP:C	1:A:263:LYS:H	1.96	0.68
1:A:208:VAL:HB	1:A:213:GLY:O	1.94	0.68
1:A:300:GLU:HB2	1:A:321:ASP:O	1.93	0.68
1:A:148:VAL:HG11	1:A:174:THR:HG22	1.74	0.68
1:A:196:LEU:HD12	1:A:231:ALA:HB2	1.74	0.67
1:A:143:PRO:HG3	1:A:424:VAL:HG13	1.74	0.67
1:A:390:LEU:O	1:A:391:ARG:HB3	1.93	0.67
1:A:57:MET:HE2	5:A:552:HOH:O	1.94	0.67
1:A:326:ASN:O	1:A:330:ILE:HG13	1.94	0.67
1:A:61:VAL:HA	5:A:573:HOH:O	1.94	0.66
1:A:9:SER:C	5:A:535:HOH:O	2.34	0.66
1:A:155:ASN:OD1	5:A:795:HOH:O	2.13	0.66
1:A:140:LYS:O	5:A:486:HOH:O	2.13	0.66
1:A:63:HIS:O	1:A:66:LYS:N	2.29	0.66
1:A:330:ILE:CD1	1:A:342:LEU:HD22	2.26	0.65
1:A:312:THR:HG21	5:A:629:HOH:O	1.94	0.65
1:A:181:GLU:OE1	5:A:790:HOH:O	2.12	0.65
1:A:373:HIS:CD2	1:A:373:HIS:H	2.14	0.65
1:A:262:PHE:HE2	5:A:525:HOH:O	1.79	0.65
1:A:97:ASP:OD2	1:A:99:THR:OG1	2.07	0.64
1:A:288:ARG:HD2	5:A:638:HOH:O	1.97	0.64
1:A:49:ARG:NH2	5:A:591:HOH:O	2.30	0.64
1:A:257:LYS:HE3	1:A:269:LYS:HE2	1.76	0.64
1:A:317:ILE:HG22	1:A:339:ALA:CB	2.26	0.64
1:A:218:ILE:HG23	1:A:223:GLU:HG2	1.80	0.64
1:A:22:GLU:OE2	1:A:31:ARG:NH2	2.31	0.64
1:A:324:VAL:HG12	1:A:324:VAL:O	1.99	0.63
1:A:44:GLU:HA	1:A:324:VAL:HG11	1.80	0.63
1:A:144:TYR:CD2	1:A:419:LEU:HD13	2.33	0.63
1:A:261:ASP:OD2	1:A:264:ASN:CB	2.45	0.63
1:A:131:LYS:HD3	1:A:131:LYS:O	1.99	0.63
1:A:82:ASP:OD1	1:A:82:ASP:C	2.35	0.63
1:A:49:ARG:CZ	5:A:591:HOH:O	2.46	0.62
1:A:14:ARG:NH1	5:A:553:HOH:O	2.32	0.62
1:A:306:TRP:HE3	1:A:338:ALA:O	1.82	0.62
1:A:163:ALA:H	1:A:217:ASN:HD22	1.45	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:LYS:CE	1:A:374:ARG:NH1	2.52	0.62
1:A:42:VAL:CG2	1:A:43:HIS:N	2.62	0.62
1:A:326:ASN:ND2	1:A:328:LYS:H	1.97	0.62
1:A:156:GLY:O	1:A:164:LEU:O	2.17	0.62
1:A:34:VAL:HG13	1:A:35:PRO:HD2	1.82	0.62
1:A:80:ASN:ND2	1:A:80:ASN:O	2.33	0.62
1:A:14:ARG:CZ	5:A:553:HOH:O	2.47	0.62
1:A:316:GLN:OE1	1:A:431:HIS:ND1	2.32	0.62
1:A:330:ILE:HD13	1:A:342:LEU:HD22	1.82	0.61
1:A:384:ALA:O	1:A:387:VAL:HG12	1.99	0.61
1:A:326:ASN:HD22	1:A:328:LYS:N	1.99	0.61
1:A:166:LEU:CD2	1:A:247:CYS:HA	2.29	0.61
1:A:274:THR:OG1	1:A:276:PRO:HD2	2.01	0.61
1:A:262:PHE:C	1:A:263:LYS:HG3	2.19	0.60
1:A:25:THR:OG1	1:A:26:GLU:N	2.29	0.60
1:A:103:SER:CB	5:A:734:HOH:O	2.49	0.60
1:A:257:LYS:HZ1	1:A:269:LYS:CE	2.04	0.60
1:A:143:PRO:CB	1:A:424:VAL:HG22	2.26	0.60
1:A:218:ILE:HG23	1:A:223:GLU:CG	2.32	0.60
1:A:268:ASP:OD1	1:A:270:SER:HB2	2.01	0.60
1:A:30:PHE:CE2	1:A:123:ALA:CB	2.84	0.60
1:A:34:VAL:HG12	1:A:35:PRO:O	2.01	0.60
1:A:44:GLU:HA	1:A:324:VAL:CG1	2.32	0.60
1:A:144:TYR:CD2	1:A:419:LEU:CD1	2.84	0.60
1:A:252:PHE:HB2	1:A:259:ASP:O	2.02	0.59
1:A:317:ILE:HG22	1:A:339:ALA:HB2	1.83	0.59
1:A:343:LEU:HD23	1:A:345:LYS:HE3	1.83	0.59
1:A:44:GLU:OE1	5:A:470:HOH:O	2.15	0.59
1:A:269:LYS:C	1:A:271:LYS:N	2.52	0.59
1:A:159:HIS:CD2	1:A:159:HIS:N	2.70	0.59
1:A:129:LEU:O	1:A:132:HIS:N	2.35	0.59
1:A:265:PRO:HD2	1:A:266:ASN:H	1.66	0.59
1:A:261:ASP:OD2	1:A:264:ASN:N	2.35	0.58
1:A:103:SER:HB3	5:A:734:HOH:O	2.04	0.58
1:A:265:PRO:C	1:A:267:SER:H	2.07	0.58
1:A:33:ILE:CG2	1:A:378:THR:HG21	2.32	0.57
1:A:71:VAL:O	1:A:74:PRO:HG2	2.04	0.57
1:A:144:TYR:HD2	1:A:419:LEU:CD1	2.18	0.57
1:A:387:VAL:HG21	1:A:395:ILE:HB	1.86	0.57
1:A:111:LEU:CB	5:A:761:HOH:O	2.51	0.57
1:A:68:VAL:O	1:A:73:ALA:HB2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:ASP:C	1:A:52:ASP:OD1	2.42	0.57
1:A:269:LYS:C	1:A:271:LYS:H	2.07	0.57
1:A:265:PRO:CD	1:A:266:ASN:N	2.68	0.57
1:A:201:TYR:HD1	5:A:593:HOH:O	1.87	0.57
1:A:194:LYS:CG	1:A:198:LYS:HE2	2.35	0.57
1:A:373:HIS:H	1:A:373:HIS:HD2	1.53	0.57
1:A:101:ASN:C	1:A:101:ASN:HD22	2.08	0.57
1:A:383:ILE:HG13	1:A:395:ILE:HD11	1.86	0.57
1:A:173:PRO:CG	1:A:182:ALA:HB1	2.34	0.56
1:A:249:SER:OG	1:A:298:PHE:C	2.43	0.56
1:A:251:GLU:HA	5:A:791:HOH:O	2.06	0.56
1:A:324:VAL:CG1	1:A:324:VAL:O	2.53	0.56
1:A:101:ASN:ND2	1:A:103:SER:CB	2.47	0.56
1:A:343:LEU:CD2	1:A:345:LYS:HE3	2.35	0.56
1:A:252:PHE:HD2	1:A:262:PHE:CE1	2.23	0.56
1:A:369:VAL:O	1:A:392:THR:HB	2.06	0.56
1:A:201:TYR:CA	5:A:593:HOH:O	2.54	0.56
1:A:4:LYS:HE2	5:A:605:HOH:O	2.06	0.56
1:A:4:LYS:O	1:A:4:LYS:CG	2.51	0.56
1:A:140:LYS:HB2	1:A:391:ARG:NE	2.20	0.56
1:A:43:HIS:HD2	5:A:733:HOH:O	1.88	0.55
1:A:50:ASP:HB2	5:A:574:HOH:O	2.06	0.55
1:A:194:LYS:O	1:A:198:LYS:HE3	2.06	0.55
1:A:42:VAL:CG2	1:A:43:HIS:H	2.19	0.55
1:A:271:LYS:O	1:A:272:TRP:C	2.45	0.55
1:A:320:ASP:CA	5:A:650:HOH:O	2.50	0.55
1:A:280:ASP:HB2	5:A:637:HOH:O	2.06	0.55
1:A:261:ASP:C	1:A:263:LYS:N	2.55	0.55
1:A:373:HIS:ND1	1:A:405:ARG:NH1	2.54	0.55
1:A:101:ASN:HD22	1:A:103:SER:H	1.55	0.55
1:A:257:LYS:CE	1:A:269:LYS:CE	2.81	0.55
1:A:390:LEU:O	1:A:391:ARG:CB	2.55	0.55
1:A:67:ASN:O	1:A:71:VAL:HB	2.06	0.55
1:A:185:ILE:HG12	1:A:237:HIS:CE1	2.42	0.55
1:A:225:LEU:HD11	1:A:291:ILE:HD11	1.89	0.55
1:A:32:SER:OG	1:A:116:ALA:HB2	2.07	0.55
1:A:49:ARG:C	5:A:689:HOH:O	2.44	0.54
1:A:190:TYR:O	1:A:193:LEU:HB3	2.07	0.54
1:A:229:VAL:O	1:A:232:ILE:N	2.40	0.54
1:A:281:LEU:O	1:A:281:LEU:HD12	2.07	0.54
1:A:262:PHE:C	1:A:263:LYS:HE3	2.28	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:ALA:N	1:A:26:GLU:OE2	2.36	0.54
1:A:312:THR:CG2	5:A:629:HOH:O	2.54	0.54
1:A:163:ALA:N	1:A:217:ASN:ND2	2.55	0.54
1:A:94:ILE:HG23	5:A:690:HOH:O	2.08	0.54
1:A:216:PRO:HG2	1:A:218:ILE:HG13	1.89	0.54
1:A:273:LEU:HA	1:A:277:GLN:OE1	2.08	0.54
1:A:201:TYR:HE2	1:A:227:LEU:CD2	2.21	0.54
1:A:153:VAL:HB	1:A:193:LEU:HD23	1.88	0.54
1:A:219:GLN:N	1:A:223:GLU:OE1	2.37	0.54
1:A:201:TYR:HA	5:A:593:HOH:O	2.08	0.53
1:A:2:VAL:HG22	1:A:23:LEU:HD21	1.90	0.53
1:A:111:LEU:O	1:A:114:SER:HB3	2.08	0.53
1:A:48:MET:HE2	5:A:572:HOH:O	2.01	0.53
1:A:69:ASN:HB2	5:A:681:HOH:O	2.09	0.53
1:A:110:ILE:O	1:A:111:LEU:C	2.47	0.53
1:A:146:LEU:HD21	1:A:415:ILE:HG22	1.91	0.53
1:A:265:PRO:CD	1:A:266:ASN:H	2.21	0.52
1:A:211:GLU:CD	1:A:373:HIS:HE1	2.12	0.52
1:A:261:ASP:CB	1:A:264:ASN:ND2	2.72	0.52
1:A:104:LYS:CG	5:A:683:HOH:O	2.53	0.52
1:A:200:ARG:NH1	5:A:642:HOH:O	2.43	0.52
1:A:166:LEU:HD22	1:A:247:CYS:SG	2.50	0.52
1:A:246:ASP:HA	1:A:295:GLU:HB3	1.91	0.52
1:A:252:PHE:O	1:A:258:TYR:HA	2.09	0.52
1:A:32:SER:HA	1:A:380:ASP:OD2	2.09	0.52
1:A:43:HIS:C	1:A:324:VAL:HG11	2.30	0.52
1:A:268:ASP:OD2	1:A:270:SER:CB	2.55	0.52
1:A:257:LYS:HE3	1:A:269:LYS:CE	2.38	0.52
1:A:102:LYS:NZ	1:A:354:GLU:OE2	2.42	0.52
1:A:87:LYS:NZ	5:A:739:HOH:O	2.35	0.52
1:A:44:GLU:CA	1:A:324:VAL:HG11	2.39	0.52
1:A:386:LEU:HG	1:A:390:LEU:HD12	1.91	0.51
1:A:265:PRO:C	1:A:267:SER:N	2.64	0.51
1:A:411:GLN:NE2	5:A:487:HOH:O	2.42	0.51
1:A:55:LYS:HE3	5:A:697:HOH:O	2.10	0.51
1:A:73:ALA:HB3	1:A:74:PRO:CD	2.40	0.51
1:A:220:THR:HA	5:A:555:HOH:O	2.10	0.51
1:A:165:ALA:HB2	1:A:260:LEU:O	2.11	0.51
1:A:57:MET:CE	5:A:552:HOH:O	2.54	0.50
1:A:292:VAL:O	5:A:645:HOH:O	2.19	0.50
1:A:127:VAL:HG23	1:A:128:PRO:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:PHE:HB2	1:A:306:TRP:CD1	2.46	0.50
1:A:164:LEU:HD21	1:A:169:PHE:CE2	2.47	0.50
1:A:251:GLU:CA	5:A:791:HOH:O	2.59	0.50
1:A:165:ALA:N	5:A:773:HOH:O	2.41	0.50
1:A:83:VAL:HG22	5:A:722:HOH:O	2.12	0.50
1:A:343:LEU:HD11	1:A:396:LYS:HD2	1.94	0.50
1:A:200:ARG:NH2	1:A:230:ASP:OD2	2.39	0.50
1:A:76:PHE:O	1:A:77:VAL:C	2.50	0.50
1:A:257:LYS:HZ2	1:A:269:LYS:HE2	1.67	0.50
1:A:279:ALA:O	1:A:283:HIS:HD2	1.94	0.50
1:A:373:HIS:CD2	1:A:396:LYS:O	2.65	0.49
1:A:24:THR:HG23	1:A:29:VAL:HG22	1.94	0.49
1:A:268:ASP:O	1:A:271:LYS:N	2.37	0.49
1:A:281:LEU:O	1:A:284:SER:HB3	2.12	0.49
1:A:257:LYS:HB3	1:A:272:TRP:HB3	1.94	0.49
1:A:208:VAL:HG21	1:A:212:GLY:HA2	1.94	0.49
1:A:31:ARG:O	1:A:119:ARG:NH1	2.45	0.49
1:A:227:LEU:HD22	5:A:749:HOH:O	2.12	0.49
1:A:152:ASN:OD1	1:A:155:ASN:ND2	2.45	0.49
1:A:218:ILE:HG23	1:A:223:GLU:HB3	1.94	0.49
1:A:268:ASP:C	1:A:270:SER:N	2.65	0.49
1:A:4:LYS:CE	5:A:471:HOH:O	2.59	0.49
1:A:111:LEU:HD22	1:A:347:ASN:HA	1.95	0.49
1:A:429:ASN:HA	5:A:630:HOH:O	2.12	0.49
1:A:42:VAL:CG2	1:A:43:HIS:CE1	2.95	0.49
1:A:149:PRO:HG2	1:A:151:LEU:HD11	1.95	0.48
1:A:194:LYS:HE3	1:A:206:GLY:O	2.13	0.48
1:A:380:ASP:OD2	5:A:498:HOH:O	2.19	0.48
1:A:263:LYS:N	1:A:263:LYS:HE3	2.29	0.48
1:A:155:ASN:CG	5:A:795:HOH:O	2.51	0.48
1:A:201:TYR:CB	5:A:593:HOH:O	2.62	0.48
1:A:154:LEU:HD11	1:A:218:ILE:HD12	1.95	0.48
1:A:252:PHE:CD2	1:A:262:PHE:CE1	3.02	0.48
1:A:257:LYS:CB	1:A:272:TRP:HB3	2.43	0.48
1:A:52:ASP:CB	5:A:583:HOH:O	2.61	0.48
1:A:265:PRO:HD2	1:A:266:ASN:N	2.29	0.47
1:A:30:PHE:CZ	1:A:123:ALA:CB	2.97	0.47
1:A:251:GLU:CD	5:A:791:HOH:O	2.51	0.47
1:A:211:GLU:OE1	1:A:373:HIS:HE1	1.98	0.47
1:A:184:ARG:HD3	1:A:184:ARG:HH11	1.34	0.47
1:A:218:ILE:HG22	1:A:219:GLN:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:GLU:OE1	5:A:702:HOH:O	2.19	0.47
1:A:75:ALA:HB1	1:A:92:PHE:HZ	1.80	0.47
1:A:125:LYS:CE	1:A:132:HIS:CE1	2.84	0.47
1:A:300:GLU:HB3	1:A:321:ASP:HB3	1.96	0.47
1:A:73:ALA:HB3	1:A:74:PRO:HD2	1.96	0.47
1:A:351:THR:OG1	1:A:354:GLU:HG3	2.15	0.47
1:A:157:GLY:O	1:A:158:SER:C	2.53	0.47
1:A:139:SER:C	1:A:140:LYS:O	2.52	0.47
1:A:324:VAL:HG12	5:A:467:HOH:O	2.14	0.46
1:A:97:ASP:O	1:A:99:THR:CG2	2.41	0.46
1:A:14:ARG:HG2	5:A:595:HOH:O	2.14	0.46
1:A:106:GLY:O	1:A:109:ALA:HB3	2.15	0.46
1:A:208:VAL:CB	1:A:213:GLY:O	2.62	0.46
1:A:208:VAL:HA	1:A:213:GLY:O	2.14	0.46
1:A:368:GLY:CA	5:A:587:HOH:O	2.62	0.46
1:A:159:HIS:N	1:A:159:HIS:HD2	2.14	0.46
1:A:139:SER:O	1:A:140:LYS:O	2.34	0.46
1:A:280:ASP:OD2	5:A:753:HOH:O	2.21	0.46
1:A:211:GLU:CD	1:A:373:HIS:CE1	2.89	0.46
1:A:101:ASN:HD22	1:A:103:SER:N	2.14	0.46
1:A:157:GLY:C	1:A:159:HIS:N	2.68	0.46
1:A:154:LEU:HD11	1:A:218:ILE:CD1	2.46	0.46
1:A:143:PRO:HG3	1:A:424:VAL:HG11	1.95	0.46
1:A:65:VAL:HG12	5:A:681:HOH:O	2.15	0.45
1:A:30:PHE:N	1:A:30:PHE:CD1	2.84	0.45
1:A:216:PRO:HG2	1:A:218:ILE:CD1	2.46	0.45
1:A:90:ASP:OD2	1:A:353:SER:HB2	2.16	0.45
1:A:46:LEU:O	1:A:46:LEU:HD23	2.16	0.45
1:A:131:LYS:NZ	1:A:135:ASP:OD1	2.49	0.45
1:A:111:LEU:CD2	1:A:347:ASN:HA	2.46	0.45
1:A:170:MET:HE1	1:A:246:ASP:HB2	1.98	0.45
1:A:46:LEU:HD13	5:A:736:HOH:O	2.17	0.45
1:A:5:VAL:HB	5:A:625:HOH:O	2.17	0.45
1:A:4:LYS:HD3	5:A:471:HOH:O	2.17	0.45
1:A:164:LEU:HD21	1:A:169:PHE:HE2	1.80	0.45
1:A:392:THR:OG1	1:A:393:GLY:N	2.50	0.45
1:A:266:ASN:HA	1:A:266:ASN:HD22	1.66	0.45
1:A:166:LEU:CD2	1:A:247:CYS:SG	3.05	0.45
1:A:201:TYR:HB3	5:A:593:HOH:O	2.17	0.44
1:A:162:GLY:HA2	1:A:217:ASN:ND2	2.33	0.44
1:A:168:GLU:OE1	1:A:170:MET:CE	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:LEU:HD23	1:A:386:LEU:HA	1.98	0.44
1:A:359:ALA:CB	1:A:390:LEU:CD2	2.95	0.44
1:A:127:VAL:HB	1:A:128:PRO:HD2	1.99	0.44
1:A:283:HIS:O	1:A:284:SER:C	2.56	0.44
1:A:318:VAL:HA	1:A:341:ALA:HB3	1.99	0.44
1:A:39:SER:O	1:A:40:THR:O	2.36	0.44
1:A:13:SER:N	1:A:377:GLU:O	2.40	0.44
1:A:6:TYR:HE1	1:A:8:ARG:HB3	1.81	0.44
1:A:391:ARG:CD	5:A:486:HOH:O	2.55	0.44
1:A:344:LEU:CD2	1:A:344:LEU:C	2.85	0.44
1:A:144:TYR:CD2	1:A:419:LEU:HD11	2.52	0.44
1:A:233:LYS:O	1:A:234:ALA:C	2.56	0.44
1:A:261:ASP:OD2	1:A:264:ASN:CG	2.57	0.43
1:A:310:PHE:CD1	1:A:310:PHE:C	2.92	0.43
1:A:370:MET:HA	1:A:394:GLN:O	2.18	0.43
1:A:140:LYS:N	5:A:485:HOH:O	2.24	0.43
1:A:69:ASN:O	1:A:73:ALA:HB3	2.18	0.43
1:A:6:TYR:CD1	1:A:7:ALA:N	2.86	0.43
1:A:43:HIS:CD2	5:A:733:HOH:O	2.69	0.43
1:A:42:VAL:HG23	1:A:43:HIS:CG	2.53	0.43
1:A:269:LYS:HD2	5:A:747:HOH:O	2.18	0.43
1:A:5:VAL:N	5:A:625:HOH:O	2.52	0.43
1:A:281:LEU:C	1:A:281:LEU:HD12	2.39	0.43
1:A:266:ASN:CG	5:A:793:HOH:O	2.57	0.43
1:A:330:ILE:HD11	1:A:342:LEU:HD22	1.97	0.43
1:A:247:CYS:HB2	1:A:296:ASP:O	2.19	0.43
1:A:275:GLY:N	1:A:276:PRO:CD	2.81	0.43
1:A:220:THR:HG23	5:A:707:HOH:O	2.17	0.43
1:A:129:LEU:O	1:A:130:TYR:C	2.57	0.42
1:A:179:PHE:HE1	1:A:183:LEU:CD2	2.32	0.42
1:A:46:LEU:CD1	5:A:736:HOH:O	2.66	0.42
1:A:369:VAL:O	1:A:392:THR:CB	2.66	0.42
1:A:184:ARG:NH1	5:A:541:HOH:O	2.52	0.42
1:A:9:SER:CB	5:A:535:HOH:O	2.67	0.42
1:A:139:SER:CA	5:A:485:HOH:O	2.59	0.42
1:A:174:THR:HB	1:A:427:GLY:O	2.20	0.42
1:A:136:LEU:N	1:A:136:LEU:HD23	2.34	0.42
1:A:275:GLY:N	1:A:276:PRO:HD3	2.35	0.42
1:A:232:ILE:HD13	1:A:241:VAL:HG12	2.02	0.42
1:A:345:LYS:HB2	1:A:348:GLN:HB2	2.01	0.42
1:A:166:LEU:HD22	1:A:247:CYS:CA	2.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:SER:OG	1:A:336:LYS:O	2.30	0.42
1:A:44:GLU:CD	1:A:348:GLN:HG3	2.40	0.42
1:A:262:PHE:C	1:A:263:LYS:CE	2.88	0.42
1:A:119:ARG:HA	1:A:129:LEU:HD13	2.00	0.42
1:A:153:VAL:O	1:A:214:VAL:HG22	2.19	0.42
1:A:279:ALA:O	1:A:283:HIS:CD2	2.73	0.42
1:A:357:LYS:CE	5:A:799:HOH:O	2.68	0.42
1:A:52:ASP:O	1:A:54:SER:N	2.53	0.41
1:A:326:ASN:ND2	1:A:328:LYS:CB	2.74	0.41
1:A:137:SER:HB3	1:A:356:ILE:HG23	2.01	0.41
1:A:201:TYR:HE2	1:A:227:LEU:HD22	1.83	0.41
1:A:168:GLU:OE2	1:A:396:LYS:CE	2.68	0.41
1:A:188:GLU:OE1	1:A:237:HIS:NE2	2.26	0.41
1:A:146:LEU:CD1	1:A:423:ALA:HB1	2.50	0.41
1:A:26:GLU:HG2	1:A:26:GLU:H	1.46	0.41
1:A:218:ILE:CG2	1:A:223:GLU:HB3	2.51	0.41
1:A:75:ALA:HB1	1:A:92:PHE:CZ	2.56	0.41
1:A:227:LEU:CD2	5:A:749:HOH:O	2.68	0.41
1:A:35:PRO:HG2	1:A:347:ASN:HB3	2.03	0.41
1:A:14:ARG:HD3	1:A:14:ARG:HH11	1.67	0.41
1:A:80:ASN:HA	5:A:561:HOH:O	2.21	0.41
1:A:424:VAL:O	1:A:424:VAL:HG23	2.21	0.41
1:A:436:LEU:O	1:A:436:LEU:CG	2.65	0.41
1:A:122:ALA:C	1:A:124:GLU:N	2.73	0.41
1:A:43:HIS:O	1:A:324:VAL:HG11	2.21	0.40
1:A:90:ASP:CG	1:A:351:THR:HB	2.41	0.40
1:A:98:GLY:C	1:A:99:THR:CG2	2.88	0.40
1:A:391:ARG:O	1:A:391:ARG:HG2	2.21	0.40
1:A:297:PRO:HD2	1:A:306:TRP:CH2	2.56	0.40
1:A:266:ASN:ND2	5:A:793:HOH:O	2.54	0.40
1:A:44:GLU:N	1:A:324:VAL:HG11	2.36	0.40
1:A:254:LYS:HD3	1:A:272:TRP:CH2	2.57	0.40

All (11) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:GLY:C	5:A:754:HOH:O[3_644]	0.95	1.25
1:A:99:THR:N	5:A:754:HOH:O[3_644]	1.02	1.18
1:A:204:SER:N	5:A:449:HOH:O[8_666]	1.03	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:HIS:CD2	5:A:557:HOH:O[8_666]	1.62	0.58
1:A:207:ASN:ND2	5:A:763:HOH:O[8_666]	1.72	0.48
1:A:98:GLY:O	5:A:754:HOH:O[3_644]	1.86	0.34
1:A:98:GLY:CA	5:A:754:HOH:O[3_644]	1.92	0.28
1:A:203:ALA:C	5:A:449:HOH:O[8_666]	2.03	0.17
1:A:204:SER:CA	5:A:449:HOH:O[8_666]	2.09	0.11
1:A:302:ASP:OD2	1:A:421:ASP:OD2[4_564]	2.16	0.04
1:A:99:THR:CA	5:A:754:HOH:O[3_644]	2.17	0.03

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	434/436 (100%)	369 (85%)	52 (12%)	13 (3%)	5 8

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	THR
1	A	39	SER
1	A	43	HIS
1	A	140	LYS
1	A	263	LYS
1	A	300	GLU
1	A	45	ALA
1	A	262	PHE
1	A	53	LYS
1	A	136	LEU
1	A	313	ALA
1	A	102	LYS
1	A	324	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	344/344 (100%)	319 (93%)	25 (7%)	17 35

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ARG
1	A	24	THR
1	A	26	GLU
1	A	39	SER
1	A	40	THR
1	A	101	ASN
1	A	108	ASN
1	A	147	PRO
1	A	187	SER
1	A	197	THR
1	A	217	ASN
1	A	227	LEU
1	A	263	LYS
1	A	264	ASN
1	A	265	PRO
1	A	270	SER
1	A	293	SER
1	A	300	GLU
1	A	326	ASN
1	A	355	SER
1	A	362	SER
1	A	373	HIS
1	A	390	LEU
1	A	392	THR
1	A	436	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	HIS
1	A	101	ASN
1	A	207	ASN
1	A	217	ASN
1	A	264	ASN
1	A	266	ASN
1	A	283	HIS
1	A	326	ASN
1	A	411	GLN

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)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	$\#\|Z\| > 2$
3	PO4	A	444	-	4,4,4	0.84	0	6,6,6	0.28	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
3	PO4	A	444	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.