



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 15, 2016 – 11:23 AM EST

PDB ID : 1EAK  
Title : Catalytic domain of proMMP-2 E404Q mutant  
Authors : Bergmann, U.; Tuuttila, A.; Tryggvason, K.; Morgunova, E.  
Deposited on : 2001-07-12  
Resolution : 2.66 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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20028442  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20028442

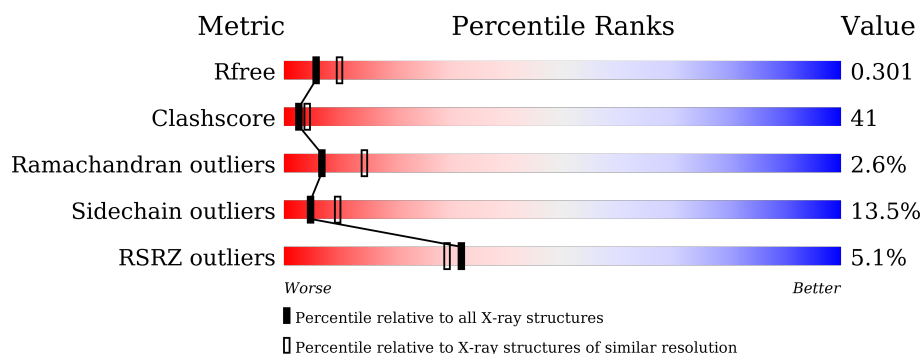
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.66 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3152 (2.70-2.62)
Clashscore	102246	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)
RSRZ outliers	91569	3161 (2.70-2.62)

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.

Mol	Chain	Length	Quality of chain
1	A	421	<div> <div>5%</div> <div> <div>46%</div> <div>43%</div> <div>10%</div> </div> </div>
1	B	421	<div> <div>3%</div> <div> <div>48%</div> <div>43%</div> <div>7%</div> </div> </div>
1	C	421	<div> <div>4%</div> <div> <div>50%</div> <div>41%</div> <div>8%</div> </div> </div>
1	D	421	<div> <div>5%</div> <div> <div>43%</div> <div>43%</div> <div>12%</div> </div> </div>
2	P	8	<div> <div>100%</div> <div> <div>25%</div> <div>25%</div> <div>50%</div> </div> </div>
2	R	8	<div> <div>100%</div> <div> <div>13%</div> <div>50%</div> <div>38%</div> </div> </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
3	SO4	B	853	-	-	-	X
3	SO4	C	850	-	-	X	-
3	SO4	D	857	-	-	X	-
5	CA	A	999	-	-	-	X
5	CA	B	999	-	-	-	X
5	CA	D	999	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13504 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 72 KDA TYPE IV COLLAGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	421	Total	C	N	O	S	0	0	0
			3330	2110	553	644	23			
1	B	419	Total	C	N	O	S	0	0	0
			3313	2100	551	639	23			
1	C	418	Total	C	N	O	S	0	0	0
			3305	2096	550	636	23			
1	D	419	Total	C	N	O	S	0	0	0
			3313	2100	551	639	23			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	404	GLN	GLU	ENGINEERED MUTATION	UNP P08253
B	404	GLN	GLU	ENGINEERED MUTATION	UNP P08253
C	404	GLN	GLU	ENGINEERED MUTATION	UNP P08253
D	404	GLN	GLU	ENGINEERED MUTATION	UNP P08253

- Molecule 2 is a protein called INHIBITOR PEPTIDE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	P	8	Total	C	N	O	0	0	0
			44	27	8	9			
2	R	8	Total	C	N	O	0	0	0
			44	27	8	9			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Zn	0	0
			2	2		
4	A	2	Total	Zn	0	0
			2	2		
4	D	2	Total	Zn	0	0
			2	2		
4	C	2	Total	Zn	0	0
			2	2		

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	2	Total Ca 2 2	0	0
5	A	2	Total Ca 2 2	0	0
5	D	2	Total Ca 2 2	0	0
5	C	2	Total Ca 2 2	0	0

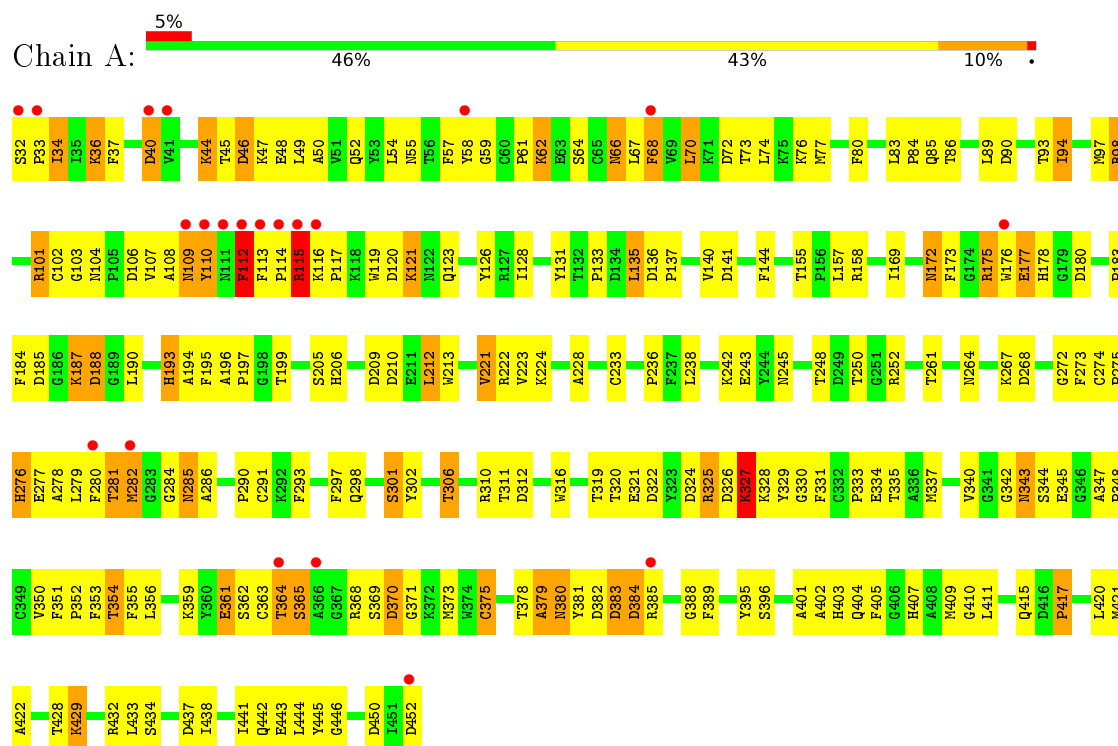
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	34	Total O 34 34	0	0
6	B	36	Total O 36 36	0	0
6	C	27	Total O 27 27	0	0
6	D	12	Total O 12 12	0	0

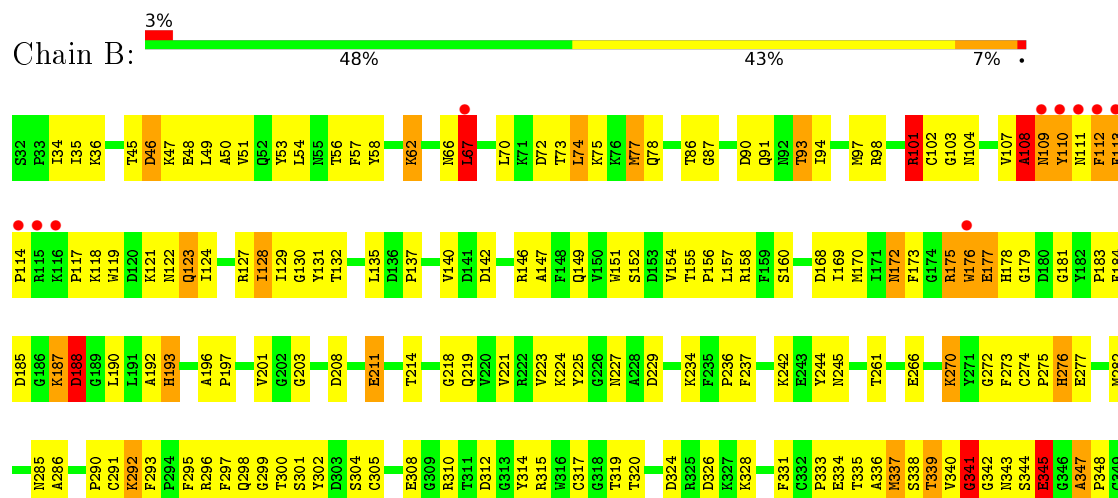
### 3 Residue-property plots

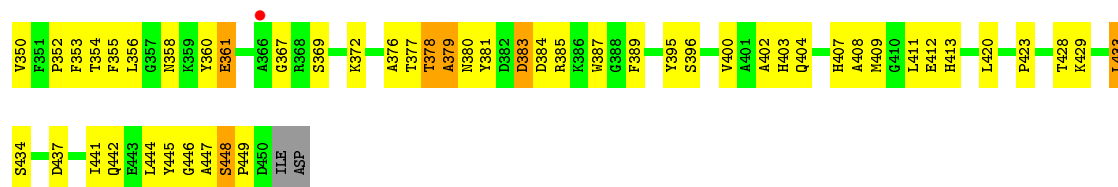
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

#### • Molecule 1: 72 KDA TYPE IV COLLAGENASE

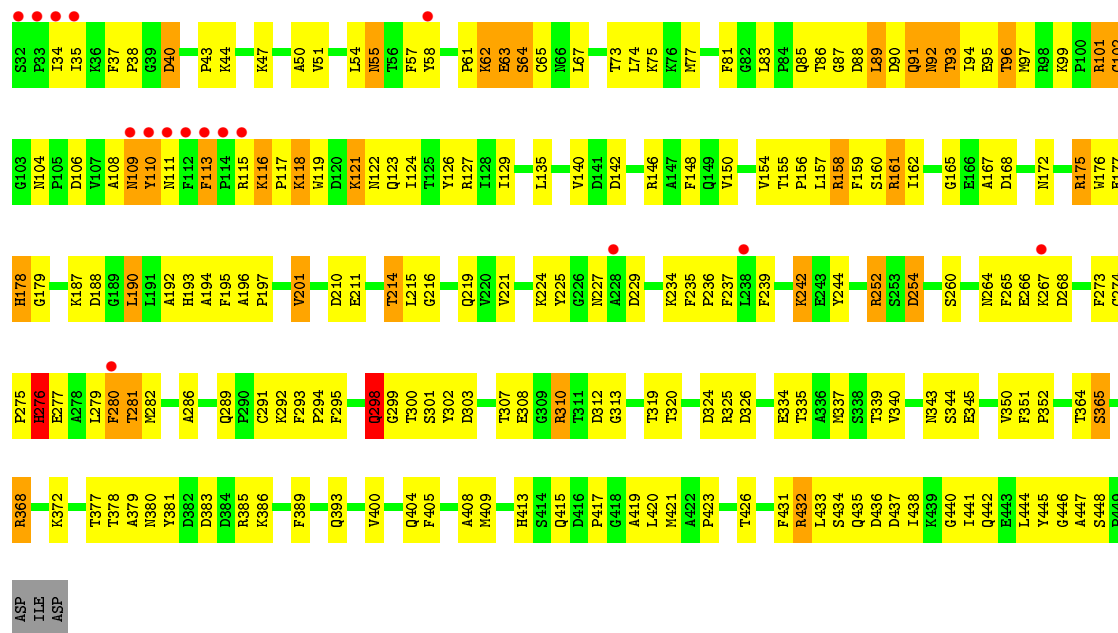


#### • Molecule 1: 72 KDA TYPE IV COLLAGENASE

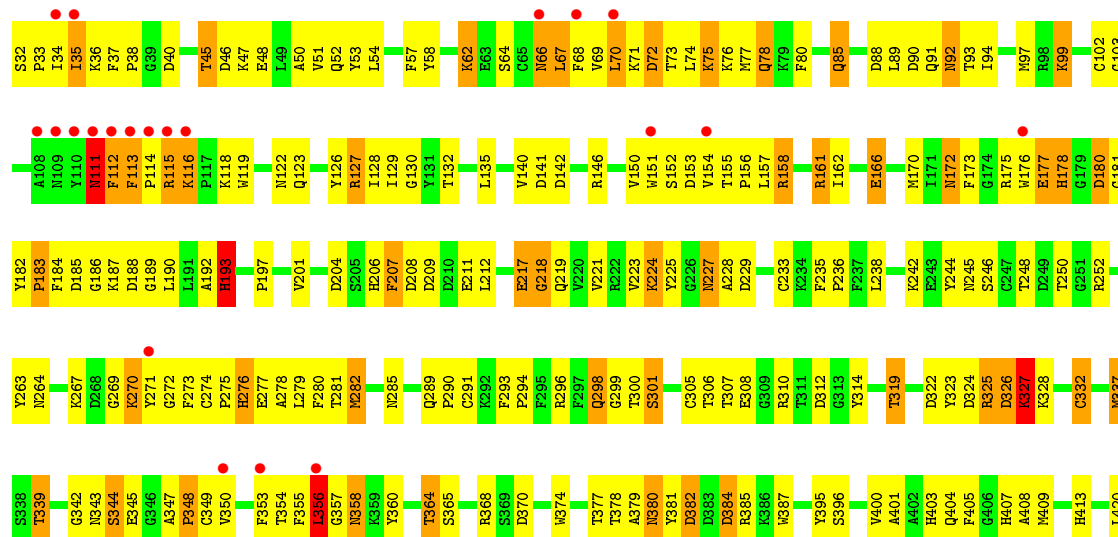
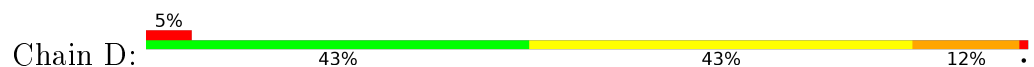




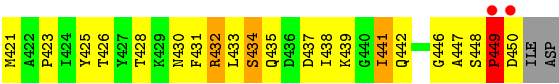
● Molecule 1: 72 KDA TYPE IV COLLAGENASE



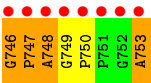
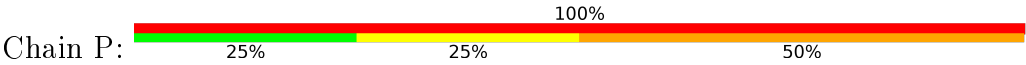
● Molecule 1: 72 KDA TYPE IV COLLAGENASE



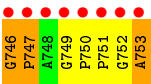
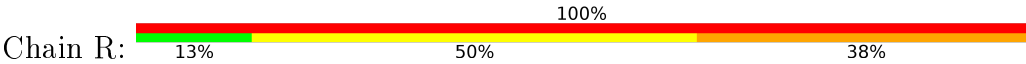




● Molecule 2: INHIBITOR PEPTIDE



● Molecule 2: INHIBITOR PEPTIDE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	117.67Å 166.15Å 170.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.58 – 2.66 35.58 – 2.66	Depositor EDS
% Data completeness (in resolution range)	80.2 (35.58-2.66) 80.3 (35.58-2.66)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.00 (at 2.65Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.271 , 0.303 0.270 , 0.301	Depositor DCC
$R_{free}$ test set	3899 reflections (5.03%)	DCC
Wilson B-factor (Å <sup>2</sup> )	47.2	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 38.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	13504	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CA, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.49	1/3431 (0.0%)	0.94	9/4646 (0.2%)
1	B	0.51	0/3414	1.01	8/4624 (0.2%)
1	C	0.50	1/3406 (0.0%)	0.96	6/4613 (0.1%)
1	D	0.49	3/3414 (0.1%)	1.00	8/4624 (0.2%)
2	P	27.12	1/46 (2.2%)	1.58	2/62 (3.2%)
2	R	40.00	2/46 (4.3%)	1.10	0/62
All	All	2.84	8/13757 (0.1%)	0.98	33/18631 (0.2%)

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
1	B	0	1
1	D	0	3
All	All	0	5

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	R	753	ALA	C-OXT	271.21	6.38	1.23
2	P	753	ALA	C-OXT	183.83	4.72	1.23
1	C	435	GLN	CB-CG	-8.74	1.28	1.52
1	D	449	PRO	C-N	7.53	1.51	1.34
1	A	417	PRO	N-CD	7.47	1.58	1.47
1	D	348	PRO	N-CD	6.03	1.56	1.47
2	R	746	GLY	N-CA	5.37	1.54	1.46
1	D	449	PRO	N-CD	5.32	1.55	1.47

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	449	PRO	O-C-N	-21.55	88.23	122.70
1	D	193	HIS	CA-CB-CG	14.00	137.40	113.60
1	D	449	PRO	CA-C-N	13.63	147.19	117.20
1	C	435	GLN	CB-CG-CD	11.45	141.37	111.60
1	B	175	ARG	NE-CZ-NH1	-11.45	114.58	120.30
1	C	435	GLN	CA-CB-CG	8.79	132.75	113.40
1	B	175	ARG	NE-CZ-NH2	8.59	124.59	120.30
2	P	746	GLY	N-CA-C	-8.30	92.35	113.10
1	D	225	TYR	CB-CG-CD1	7.92	125.75	121.00
1	A	112	PHE	CA-C-O	-7.28	104.81	120.10
1	C	448	SER	N-CA-CB	6.62	120.42	110.50
1	B	146	ARG	NE-CZ-NH1	-6.50	117.05	120.30
1	D	161	ARG	NE-CZ-NH2	6.39	123.49	120.30
1	C	158	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	A	222	ARG	NE-CZ-NH2	6.12	123.36	120.30
1	D	225	TYR	CB-CG-CD2	-6.07	117.36	121.00
2	P	746	GLY	O-C-N	-5.97	109.77	121.10
1	D	382	ASP	CB-CG-OD1	-5.93	112.96	118.30
1	A	188	ASP	CB-CA-C	5.86	122.11	110.40
1	B	345	GLU	C-N-CA	5.83	134.55	122.30
1	A	115	ARG	O-C-N	5.64	131.72	122.70
1	D	225	TYR	CA-CB-CG	5.64	124.11	113.40
1	B	101	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	A	375	CYS	CA-CB-SG	-5.56	103.99	114.00
1	A	112	PHE	CA-CB-CG	5.43	126.93	113.90
1	B	108	ALA	O-C-N	5.22	131.05	122.70
1	B	336	ALA	CB-CA-C	-5.16	102.36	110.10
1	A	417	PRO	N-CA-CB	5.15	109.48	103.30
1	C	175	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	B	67	LEU	O-C-N	-5.05	114.61	122.70
1	A	222	ARG	NE-CZ-NH1	-5.05	117.77	120.30
1	C	298	GLN	CB-CA-C	5.05	120.50	110.40
1	A	59	GLY	N-CA-C	5.02	125.64	113.10

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	112	PHE	Mainchain
1	B	341	GLY	Mainchain
1	D	183	PRO	Mainchain

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Mol	Chain	Res	Type	Group
1	D	357	GLY	Mainchain
1	D	449	PRO	Mainchain

## 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	3330	0	3066	303	0
1	B	3313	0	3048	216	2
1	C	3305	0	3045	263	0
1	D	3313	0	3049	293	1
2	P	44	0	39	32	0
2	R	44	0	39	21	0
3	A	5	0	0	0	0
3	B	10	0	0	2	0
3	C	10	0	0	3	0
3	D	5	0	0	2	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	C	2	0	0	0	0
5	D	2	0	0	0	0
6	A	34	0	0	4	0
6	B	36	0	0	5	0
6	C	27	0	0	7	1
6	D	12	0	0	2	1
All	All	13504	0	12286	1047	3

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 41.

All (1047) 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:112:PHE:CE1	1:A:115:ARG:NH1	1.81	1.48
1:C:58:TYR:OH	1:C:77:MET:CG	1.72	1.36
1:A:176:TRP:CZ2	1:C:325:ARG:HA	1.61	1.32
1:A:176:TRP:CH2	1:C:325:ARG:HG3	1.64	1.31
1:A:176:TRP:CZ2	1:C:325:ARG:CB	2.16	1.28
1:B:107:VAL:O	1:B:109:ASN:N	1.71	1.23
1:D:184:PHE:HB3	1:D:208:ASP:OD2	1.36	1.22
1:A:176:TRP:CZ2	1:C:325:ARG:CA	2.22	1.22
1:A:112:PHE:CZ	1:A:115:ARG:NH1	1.99	1.20
1:A:175:ARG:HG2	1:C:298:GLN:OE1	1.36	1.20
1:D:176:TRP:CZ3	1:D:185:ASP:HA	1.56	1.18
1:D:426:THR:HA	6:D:2012:HOH:O	1.43	1.17
1:D:152:SER:HA	1:D:155:THR:OG1	1.39	1.17
1:C:58:TYR:CZ	1:C:77:MET:HB2	1.78	1.17
1:C:275:PRO:HA	1:C:280:PHE:CZ	1.80	1.15
1:B:187:LYS:O	1:B:188:ASP:OD1	1.64	1.15
1:A:276:HIS:NE2	2:P:747:PRO:O	1.78	1.15
1:A:112:PHE:HE1	1:A:115:ARG:CZ	1.36	1.14
1:C:58:TYR:CZ	1:C:77:MET:CB	2.31	1.13
1:A:58:TYR:CZ	1:A:77:MET:HA	1.83	1.13
1:C:276:HIS:CD2	1:C:335:THR:HG23	1.82	1.13
1:D:176:TRP:CZ3	1:D:185:ASP:CA	2.29	1.13
1:C:299:GLY:HA3	2:P:753:ALA:O	1.46	1.12
1:B:296:ARG:NH2	2:R:753:ALA:HB2	1.63	1.12
1:C:58:TYR:OH	1:C:77:MET:HG2	0.96	1.12
1:A:276:HIS:HE2	2:P:748:ALA:C	1.54	1.10
1:D:209:ASP:OD2	2:R:753:ALA:HB1	1.50	1.10
1:A:176:TRP:CH2	1:C:325:ARG:HA	1.85	1.10
1:B:286:ALA:HA	6:B:2022:HOH:O	1.53	1.09
1:A:176:TRP:HZ2	1:C:325:ARG:HB2	1.13	1.08
1:A:278:ALA:HB1	2:P:746:GLY:N	1.67	1.08
1:A:112:PHE:HE1	1:A:115:ARG:NH1	1.32	1.07
1:A:276:HIS:CE1	2:P:747:PRO:O	2.08	1.07
1:A:114:PRO:HB2	1:A:115:ARG:HE	1.20	1.06
1:C:58:TYR:CZ	1:C:77:MET:CG	2.39	1.06
1:B:299:GLY:HA2	2:R:753:ALA:HB3	1.09	1.06
1:A:176:TRP:CZ2	1:C:325:ARG:HB2	1.84	1.04
1:D:327:LYS:H	1:D:327:LYS:HE3	1.15	1.03
1:D:223:VAL:HG11	1:D:272:GLY:HA3	1.39	1.03
1:C:123:GLN:HG3	1:C:158:ARG:HH12	1.21	1.02
1:A:293:PHE:CE2	2:P:750:PRO:CG	2.42	1.02
1:A:117:PRO:CB	1:A:197:PRO:HD2	1.89	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:67:LEU:O	1:D:68:PHE:CD2	2.13	1.02
1:A:322:ASP:HB3	1:A:325:ARG:HH21	1.25	1.01
1:A:176:TRP:CH2	1:C:325:ARG:CG	2.44	1.00
1:D:112:PHE:O	1:D:113:PHE:O	1.79	0.99
1:B:320:THR:HG21	1:B:326:ASP:HB2	1.45	0.99
1:A:176:TRP:CE2	1:C:325:ARG:HA	1.98	0.99
1:B:187:LYS:C	1:B:188:ASP:OD1	2.01	0.99
1:D:276:HIS:HE1	2:R:749:GLY:HA2	1.27	0.98
1:A:113:PHE:HB2	1:A:114:PRO:HD3	1.45	0.98
1:A:293:PHE:CE2	2:P:750:PRO:HG2	1.99	0.98
1:C:58:TYR:CE1	1:C:77:MET:HB2	1.98	0.97
1:C:438:ILE:O	1:C:442:GLN:HG2	1.64	0.96
1:D:32:SER:N	1:D:33:PRO:HD3	1.79	0.96
1:A:58:TYR:CE1	1:A:77:MET:HA	2.01	0.95
1:B:299:GLY:CA	2:R:753:ALA:HB3	1.96	0.95
1:A:177:GLU:HA	1:A:177:GLU:OE1	1.65	0.95
1:C:109:ASN:ND2	1:C:113:PHE:CE2	2.35	0.94
1:B:54:LEU:HD11	1:B:74:LEU:HD13	1.49	0.93
1:C:299:GLY:CA	2:P:753:ALA:O	2.15	0.93
1:D:54:LEU:HD12	1:D:70:LEU:HD12	1.51	0.93
1:C:54:LEU:HA	1:C:58:TYR:HD2	1.32	0.92
1:D:111:ASN:H	1:D:111:ASN:HD22	1.15	0.92
1:A:176:TRP:CD1	1:C:324:ASP:HB3	2.05	0.92
1:C:214:THR:HG22	1:C:216:GLY:H	1.34	0.91
1:A:175:ARG:CG	1:C:298:GLN:OE1	2.17	0.91
1:D:176:TRP:CE3	1:D:185:ASP:HA	2.04	0.91
1:A:176:TRP:CZ2	1:C:325:ARG:CG	2.53	0.91
1:A:68:PHE:O	1:A:68:PHE:HD1	1.54	0.91
1:B:296:ARG:HH21	2:R:753:ALA:HB2	1.30	0.91
1:A:378:THR:HG21	1:A:384:ASP:HB2	1.52	0.90
1:D:112:PHE:CD2	1:D:113:PHE:HD1	1.90	0.90
1:A:293:PHE:CE2	2:P:750:PRO:HG3	2.02	0.90
1:C:119:TRP:HD1	1:C:409:MET:HE3	1.36	0.90
1:D:111:ASN:N	1:D:111:ASN:HD22	1.70	0.90
1:A:112:PHE:HZ	1:A:115:ARG:NH1	1.70	0.89
1:B:245:ASN:N	3:B:853:SO4:O4	2.05	0.89
1:C:264:ASN:HB3	1:C:267:LYS:HG2	1.55	0.89
1:C:58:TYR:OH	1:C:77:MET:CB	2.20	0.89
1:D:276:HIS:CE1	2:R:749:GLY:HA2	2.07	0.89
1:A:188:ASP:OD1	1:A:395:TYR:OH	1.91	0.88
1:A:175:ARG:HG2	1:C:298:GLN:CD	1.93	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:TRP:CZ2	1:C:325:ARG:HG3	2.09	0.88
1:A:157:LEU:HD13	1:A:409:MET:HE2	1.55	0.87
1:C:62:LYS:HD2	1:C:62:LYS:H	1.38	0.87
1:D:177:GLU:OE1	1:D:177:GLU:HA	1.70	0.87
1:A:176:TRP:HH2	1:C:325:ARG:HG3	1.01	0.87
1:D:62:LYS:HD3	1:D:62:LYS:H	1.40	0.87
1:D:221:VAL:HB	1:D:233:CYS:SG	2.15	0.86
1:D:112:PHE:O	1:D:113:PHE:C	2.10	0.85
1:A:117:PRO:HB3	1:A:197:PRO:HD2	1.58	0.85
1:D:152:SER:HA	1:D:155:THR:HG1	1.38	0.85
1:D:113:PHE:HD2	1:D:115:ARG:HG3	1.43	0.84
1:A:112:PHE:HZ	1:A:115:ARG:HH11	1.21	0.84
1:C:50:ALA:CB	1:C:89:LEU:HD11	2.08	0.84
1:D:355:PHE:HB3	1:D:360:TYR:CE2	2.11	0.84
1:C:432:ARG:HH11	1:C:432:ARG:HB3	1.41	0.83
1:D:327:LYS:N	1:D:327:LYS:HE3	1.93	0.83
1:A:57:PHE:HZ	1:A:190:LEU:HD22	1.43	0.83
1:D:355:PHE:HB3	1:D:360:TYR:HE2	1.43	0.83
1:B:341:GLY:CA	1:B:345:GLU:OE2	2.27	0.83
1:C:57:PHE:HZ	1:C:190:LEU:HD22	1.43	0.83
1:A:176:TRP:HZ2	1:C:325:ARG:CB	1.70	0.83
1:D:223:VAL:CG1	1:D:272:GLY:HA3	2.08	0.82
1:D:112:PHE:HD2	1:D:113:PHE:CD1	1.97	0.82
1:D:276:HIS:NE2	2:R:747:PRO:O	2.12	0.82
1:A:112:PHE:CE1	1:A:115:ARG:CZ	2.26	0.82
1:A:70:LEU:HD11	1:A:74:LEU:HD22	1.61	0.82
1:C:279:LEU:HB2	1:C:280:PHE:HD1	1.45	0.82
1:A:117:PRO:HB2	1:A:197:PRO:HD2	1.60	0.82
1:A:322:ASP:CB	1:A:325:ARG:HH21	1.92	0.81
1:A:276:HIS:CE1	2:P:749:GLY:HA2	2.15	0.81
1:B:62:LYS:HE3	1:B:62:LYS:H	1.45	0.81
1:C:123:GLN:HG3	1:C:158:ARG:NH1	1.94	0.81
1:A:285:ASN:HD21	1:A:329:TYR:H	1.26	0.81
1:D:71:LYS:O	1:D:75:LYS:HG2	1.81	0.81
1:D:184:PHE:CB	1:D:208:ASP:OD2	2.26	0.81
1:A:57:PHE:HZ	1:A:190:LEU:CD2	1.94	0.81
1:C:54:LEU:HA	1:C:58:TYR:CD2	2.15	0.81
1:A:223:VAL:CG1	1:A:272:GLY:HA3	2.10	0.80
1:A:223:VAL:HG11	1:A:272:GLY:HA3	1.62	0.80
1:A:327:LYS:H	1:A:327:LYS:HD2	1.45	0.80
1:A:280:PHE:HD1	1:A:281:THR:O	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:116:LYS:HD2	1:C:117:PRO:HD2	1.63	0.80
1:C:88:ASP:OD1	6:C:2004:HOH:O	1.99	0.80
1:D:242:LYS:HD3	1:D:244:TYR:CZ	2.16	0.80
1:A:175:ARG:N	1:C:298:GLN:OE1	2.14	0.80
1:A:58:TYR:CZ	1:A:77:MET:CA	2.65	0.80
1:A:176:TRP:CH2	1:C:325:ARG:CA	2.56	0.80
1:A:114:PRO:HB2	1:A:115:ARG:NE	1.96	0.80
1:B:297:PHE:HB3	1:B:302:TYR:HE2	1.46	0.79
1:A:325:ARG:O	1:A:327:LYS:HE3	1.83	0.79
1:A:278:ALA:CB	2:P:746:GLY:N	2.46	0.79
1:C:154:VAL:HG23	1:C:155:THR:HG23	1.64	0.79
1:D:112:PHE:CD2	1:D:113:PHE:CD1	2.70	0.79
1:C:277:GLU:HB2	1:C:291:CYS:SG	2.22	0.79
1:B:341:GLY:C	1:B:345:GLU:OE2	2.21	0.78
1:C:109:ASN:O	1:C:111:ASN:N	2.16	0.78
1:B:128:ILE:HD12	1:B:130:GLY:H	1.48	0.78
1:B:341:GLY:O	1:B:345:GLU:OE2	2.01	0.78
1:D:277:GLU:HG2	1:D:305:CYS:SG	2.24	0.78
1:C:58:TYR:HH	1:C:77:MET:HG2	0.95	0.77
1:C:58:TYR:CZ	1:C:77:MET:HG2	2.08	0.77
1:A:193:HIS:CD2	1:A:206:HIS:HB2	2.19	0.77
1:B:172:ASN:ND2	1:B:173:PHE:H	1.81	0.77
1:B:178:HIS:HB3	1:D:298:GLN:OE1	1.84	0.77
1:D:32:SER:N	1:D:33:PRO:CD	2.48	0.77
1:C:432:ARG:HB3	1:C:432:ARG:NH1	2.00	0.77
1:D:176:TRP:CZ2	1:D:186:GLY:HA3	2.20	0.76
1:D:356:LEU:HB2	1:D:382:ASP:OD1	1.86	0.76
1:C:58:TYR:HH	1:C:77:MET:CG	1.78	0.76
1:D:209:ASP:OD2	2:R:753:ALA:CB	2.30	0.75
1:C:276:HIS:HD2	1:C:335:THR:HG23	1.49	0.75
1:D:356:LEU:HD13	1:D:382:ASP:CG	2.08	0.74
1:A:353:PHE:HA	1:A:379:ALA:O	1.86	0.74
1:C:444:LEU:HB3	1:C:445:TYR:CD1	2.22	0.74
1:C:40:ASP:OD2	1:C:368:ARG:NH2	2.21	0.74
1:B:119:TRP:HD1	1:B:409:MET:HE3	1.53	0.74
1:D:449:PRO:O	1:D:450:ASP:OD1	2.04	0.74
1:C:58:TYR:CE1	1:C:77:MET:CB	2.66	0.74
1:A:117:PRO:HG2	1:A:196:ALA:HB1	1.70	0.73
1:A:432:ARG:NH1	1:A:433:LEU:O	2.22	0.73
1:A:58:TYR:OH	1:A:77:MET:HA	1.87	0.73
1:C:313:GLY:HA2	6:C:2021:HOH:O	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:252:ARG:HG3	1:C:252:ARG:HH11	1.54	0.73
1:A:344:SER:HB3	1:A:347:ALA:HB3	1.71	0.73
1:C:441:ILE:O	1:C:444:LEU:HB2	1.89	0.73
1:B:118:LYS:HE2	1:B:444:LEU:O	1.89	0.73
1:C:119:TRP:CD1	1:C:409:MET:HE3	2.23	0.73
1:C:320:THR:HG21	1:C:326:ASP:HB2	1.70	0.73
1:B:35:ILE:HD11	1:B:356:LEU:HD21	1.70	0.72
1:D:57:PHE:HZ	1:D:190:LEU:HD21	1.52	0.72
1:B:90:ASP:CG	6:B:2006:HOH:O	2.27	0.72
1:C:275:PRO:CA	1:C:280:PHE:CZ	2.68	0.72
1:B:181:GLY:O	1:B:183:PRO:HD3	1.89	0.72
1:B:121:LYS:NZ	1:B:168:ASP:OD1	2.21	0.72
1:C:57:PHE:CZ	1:C:101:ARG:HD2	2.24	0.72
1:B:299:GLY:HA2	2:R:752:GLY:O	1.88	0.72
1:A:236:PRO:HB3	1:A:245:ASN:OD1	1.89	0.72
1:D:111:ASN:H	1:D:111:ASN:ND2	1.88	0.72
1:A:115:ARG:HD2	1:A:115:ARG:N	2.04	0.72
1:A:187:LYS:HZ1	1:A:212:LEU:H	1.35	0.72
1:A:293:PHE:CZ	2:P:750:PRO:HG2	2.25	0.71
1:B:277:GLU:HB2	1:B:291:CYS:SG	2.30	0.71
1:B:157:LEU:HD21	1:B:445:TYR:CD1	2.25	0.71
1:A:285:ASN:ND2	1:A:329:TYR:H	1.89	0.71
1:A:209:ASP:OD2	2:P:753:ALA:HB3	1.91	0.71
1:A:177:GLU:OE1	1:A:177:GLU:CA	2.38	0.71
1:C:252:ARG:HH21	1:C:273:PHE:HZ	1.36	0.71
1:B:224:LYS:O	1:B:273:PHE:HB2	1.91	0.71
1:B:297:PHE:HB3	1:B:302:TYR:CE2	2.24	0.71
1:C:116:LYS:HD2	1:C:117:PRO:CD	2.21	0.71
1:D:58:TYR:OH	1:D:77:MET:HG2	1.90	0.71
1:A:322:ASP:HB3	1:A:325:ARG:NH2	2.03	0.71
1:C:122:ASN:ND2	1:C:156:PRO:HB2	2.06	0.71
1:A:112:PHE:CG	1:A:115:ARG:HB2	2.25	0.70
1:B:130:GLY:HA3	1:B:172:ASN:ND2	2.06	0.70
1:C:113:PHE:N	1:C:113:PHE:HD1	1.88	0.70
1:B:380:ASN:HB3	1:B:383:ASP:OD1	1.89	0.70
1:C:340:VAL:O	1:C:389:PHE:HB2	1.91	0.70
1:D:37:PHE:HE2	1:D:368:ARG:HG2	1.57	0.70
1:D:113:PHE:CD2	1:D:115:ARG:HG3	2.26	0.70
1:B:57:PHE:HZ	1:B:190:LEU:HD21	1.56	0.70
1:A:276:HIS:NE2	2:P:748:ALA:O	2.25	0.70
1:C:188:ASP:N	1:C:211:GLU:OE2	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:PHE:N	1:B:112:PHE:HD1	1.90	0.69
1:D:299:GLY:HA3	3:D:857:SO4:O2	1.91	0.69
1:C:298:GLN:NE2	1:C:324:ASP:CG	2.45	0.69
1:A:70:LEU:HD12	1:A:74:LEU:HB2	1.75	0.69
1:C:440:GLY:O	1:C:444:LEU:HD23	1.92	0.69
1:A:337:MET:CE	1:A:340:VAL:HG22	2.23	0.69
1:A:429:LYS:HB2	1:A:429:LYS:NZ	2.08	0.68
1:A:68:PHE:C	1:A:68:PHE:CD1	2.65	0.68
1:A:47:LYS:NZ	6:A:2001:HOH:O	2.26	0.68
1:C:156:PRO:HD3	1:C:446:GLY:O	1.93	0.68
1:C:58:TYR:CE1	1:C:77:MET:HA	2.29	0.68
1:D:227:ASN:HB3	1:D:270:LYS:HA	1.75	0.68
1:D:66:ASN:CG	1:D:67:LEU:H	1.97	0.68
1:C:58:TYR:CE1	1:C:77:MET:CA	2.77	0.68
1:B:35:ILE:CD1	1:B:356:LEU:HD21	2.24	0.68
1:B:62:LYS:CE	1:B:62:LYS:H	2.07	0.68
1:C:62:LYS:N	1:C:62:LYS:HD2	2.07	0.68
1:A:306:THR:HG23	1:C:300:THR:HG21	1.75	0.68
1:B:227:ASN:HD21	1:B:270:LYS:HA	1.58	0.68
1:B:119:TRP:CD1	1:B:409:MET:HE3	2.29	0.67
1:A:157:LEU:CD1	1:A:409:MET:HE2	2.24	0.67
1:D:154:VAL:HG23	1:D:155:THR:HG23	1.75	0.67
1:D:152:SER:CA	1:D:155:THR:OG1	2.30	0.67
1:D:156:PRO:HD3	1:D:446:GLY:O	1.95	0.67
1:A:131:TYR:O	2:P:753:ALA:OXT	2.11	0.67
1:B:122:ASN:ND2	1:B:156:PRO:HB2	2.10	0.67
1:C:62:LYS:CD	1:C:62:LYS:H	2.00	0.67
1:D:327:LYS:HD3	6:D:2009:HOH:O	1.93	0.67
1:A:172:ASN:ND2	1:A:173:PHE:H	1.91	0.67
1:A:361:GLU:H	1:A:361:GLU:CD	1.97	0.67
1:A:114:PRO:CB	1:A:115:ARG:HE	2.04	0.67
1:A:285:ASN:HD22	1:A:286:ALA:N	1.93	0.67
1:C:178:HIS:H	1:C:178:HIS:HD1	1.41	0.67
1:C:54:LEU:O	1:C:58:TYR:HB2	1.94	0.67
2:R:752:GLY:O	2:R:753:ALA:CB	2.42	0.67
1:C:299:GLY:CA	3:C:850:SO4:O1	2.42	0.67
1:D:35:ILE:HG13	1:D:36:LYS:H	1.58	0.67
1:A:68:PHE:C	1:A:68:PHE:HD1	1.98	0.67
1:A:184:PHE:O	6:A:2009:HOH:O	2.11	0.67
1:A:187:LYS:HG2	1:A:210:ASP:O	1.95	0.67
1:B:176:TRP:CZ3	1:B:185:ASP:HA	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:HIS:NE2	1:A:206:HIS:HB2	2.10	0.66
1:B:117:PRO:HB2	1:B:196:ALA:HB1	1.77	0.66
1:D:279:LEU:O	1:D:290:PRO:HG3	1.95	0.66
1:D:342:GLY:HA2	1:D:387:TRP:CH2	2.30	0.66
1:B:112:PHE:HD1	1:B:112:PHE:H	1.44	0.66
1:C:127:ARG:NH1	1:C:165:GLY:H	1.93	0.66
1:D:54:LEU:CD1	1:D:70:LEU:HD12	2.24	0.66
1:C:101:ARG:HD3	1:C:102:CYS:O	1.96	0.66
1:C:298:GLN:NE2	1:C:324:ASP:OD1	2.28	0.66
1:D:50:ALA:HB2	1:D:89:LEU:HD11	1.78	0.66
1:A:278:ALA:HB3	2:P:746:GLY:O	1.96	0.66
1:A:280:PHE:CD1	1:A:281:THR:O	2.47	0.66
1:C:276:HIS:NE2	1:C:335:THR:HG23	2.10	0.66
1:D:152:SER:HB3	1:D:157:LEU:HD12	1.77	0.66
1:C:109:ASN:ND2	1:C:113:PHE:CZ	2.64	0.66
1:C:279:LEU:HB2	1:C:280:PHE:CD1	2.30	0.66
2:R:752:GLY:O	2:R:753:ALA:HB3	1.96	0.66
1:A:334:GLU:HG3	1:A:335:THR:N	2.11	0.66
1:B:413:HIS:CG	1:B:423:PRO:HG3	2.31	0.66
1:A:80:PHE:HA	1:A:415:GLN:HE21	1.61	0.65
1:B:310:ARG:HH21	1:B:312:ASP:CG	1.99	0.65
1:C:113:PHE:CD1	1:C:113:PHE:N	2.60	0.65
1:D:119:TRP:CD2	1:D:197:PRO:HB3	2.31	0.65
1:D:327:LYS:CE	1:D:327:LYS:H	2.01	0.65
1:A:62:LYS:HD2	1:A:62:LYS:H	1.60	0.65
1:C:302:TYR:OH	1:C:308:GLU:HG2	1.96	0.65
1:D:123:GLN:HB3	1:D:158:ARG:HH11	1.61	0.65
1:A:403:HIS:ND1	1:A:420:LEU:O	2.30	0.65
1:D:264:ASN:HB3	1:D:267:LYS:HB2	1.78	0.65
1:B:112:PHE:N	1:B:112:PHE:CD1	2.61	0.65
1:D:37:PHE:CE2	1:D:368:ARG:HG2	2.32	0.65
1:D:127:ARG:HG2	1:D:162:ILE:O	1.96	0.65
1:C:225:TYR:N	1:C:229:ASP:HB2	2.13	0.64
1:D:57:PHE:HZ	1:D:190:LEU:CD2	2.11	0.64
1:A:114:PRO:C	1:A:115:ARG:HD2	2.18	0.64
1:C:242:LYS:HE2	1:C:244:TYR:CE1	2.32	0.64
1:D:188:ASP:OD1	1:D:395:TYR:OH	2.07	0.64
1:C:275:PRO:HA	1:C:280:PHE:HZ	1.56	0.64
1:A:176:TRP:CE2	1:C:325:ARG:CA	2.70	0.64
1:A:172:ASN:HD22	1:A:173:PHE:H	1.44	0.64
1:A:368:ARG:NH2	1:A:389:PHE:HZ	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:ASN:OD1	1:A:383:ASP:HB2	1.98	0.64
1:D:176:TRP:CE3	1:D:184:PHE:O	2.51	0.64
1:A:54:LEU:HD12	1:A:70:LEU:HD13	1.80	0.63
1:B:121:LYS:NZ	1:B:168:ASP:CG	2.50	0.63
1:A:301:SER:OG	1:C:303:ASP:HB3	1.99	0.63
1:D:176:TRP:HZ3	1:D:185:ASP:HA	1.51	0.63
1:A:276:HIS:HE2	2:P:749:GLY:N	1.96	0.63
1:A:58:TYR:CE1	1:A:77:MET:CA	2.81	0.63
1:C:277:GLU:OE1	1:C:277:GLU:N	2.31	0.63
1:D:201:VAL:HA	1:D:204:ASP:OD2	1.98	0.63
1:D:276:HIS:HB3	1:D:279:LEU:HD12	1.81	0.63
1:D:281:THR:HG22	1:D:289:GLN:O	1.99	0.63
1:D:75:LYS:HA	1:D:78:GLN:CG	2.29	0.63
1:A:84:PRO:O	1:A:86:THR:HG23	1.99	0.63
1:B:344:SER:CB	1:B:377:THR:HG21	2.29	0.63
1:B:434:SER:HB3	1:B:437:ASP:OD2	1.97	0.63
1:D:57:PHE:CZ	1:D:190:LEU:HD21	2.33	0.63
1:D:122:ASN:O	1:D:157:LEU:HA	1.99	0.62
1:D:344:SER:HB3	1:D:347:ALA:HB3	1.80	0.62
1:D:75:LYS:HA	1:D:78:GLN:HG2	1.81	0.62
1:D:53:TYR:CE2	1:D:97:MET:HA	2.34	0.62
1:B:101:ARG:HD3	1:B:102:CYS:O	1.99	0.62
1:C:313:GLY:CA	6:C:2021:HOH:O	2.46	0.62
1:D:355:PHE:O	1:D:356:LEU:C	2.37	0.62
1:D:344:SER:CB	1:D:377:THR:HG21	2.29	0.62
1:B:109:ASN:OD1	1:B:110:TYR:N	2.32	0.62
1:D:356:LEU:CB	1:D:382:ASP:OD1	2.47	0.62
1:C:118:LYS:HD2	1:C:444:LEU:O	1.99	0.62
1:C:405:PHE:O	1:C:409:MET:HG2	2.00	0.62
1:D:277:GLU:HB3	1:D:291:CYS:SG	2.39	0.62
1:D:45:THR:HG22	1:D:48:GLU:HB2	1.82	0.62
1:A:355:PHE:CD1	1:A:356:LEU:HD13	2.35	0.62
1:B:178:HIS:CB	1:D:298:GLN:OE1	2.46	0.62
1:D:285:ASN:OD1	1:D:328:LYS:HD2	2.00	0.62
1:A:276:HIS:CE1	2:P:749:GLY:CA	2.83	0.61
1:B:129:ILE:HD13	1:B:170:MET:HE3	1.81	0.61
1:A:334:GLU:CG	1:A:335:THR:N	2.63	0.61
1:B:117:PRO:HB2	1:B:197:PRO:HD2	1.81	0.61
1:C:242:LYS:HE2	1:C:244:TYR:CZ	2.35	0.61
1:A:34:ILE:HD11	1:A:369:SER:HB2	1.82	0.61
1:C:101:ARG:NH2	1:C:106:ASP:OD2	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:320:THR:OG1	1:C:326:ASP:OD2	2.18	0.61
1:C:188:ASP:OD2	1:C:372:LYS:HE2	2.00	0.61
1:A:176:TRP:HH2	1:C:325:ARG:CG	1.93	0.61
1:A:37:PHE:CE2	1:A:368:ARG:HD3	2.36	0.61
1:B:172:ASN:HD22	1:B:173:PHE:H	1.47	0.61
1:D:354:THR:HB	1:D:380:ASN:ND2	2.15	0.61
2:P:746:GLY:O	2:P:747:PRO:O	2.19	0.61
1:B:62:LYS:HE3	1:B:62:LYS:N	2.16	0.60
1:D:238:LEU:HB2	1:D:263:TYR:CE1	2.36	0.60
1:A:285:ASN:HD21	1:A:329:TYR:N	1.99	0.60
1:B:107:VAL:O	1:B:108:ALA:C	2.34	0.60
1:A:276:HIS:NE2	2:P:748:ALA:C	2.39	0.60
1:C:178:HIS:HD1	1:C:178:HIS:N	2.00	0.60
1:D:177:GLU:OE1	1:D:177:GLU:CA	2.46	0.60
1:D:356:LEU:HD13	1:D:382:ASP:OD2	2.01	0.60
1:B:34:ILE:HD12	1:B:369:SER:HB3	1.83	0.60
1:A:40:ASP:OD2	1:A:368:ARG:NH2	2.34	0.60
1:B:128:ILE:HD11	1:B:131:TYR:CE1	2.36	0.60
1:B:187:LYS:HZ1	1:B:340:VAL:HG11	1.66	0.60
1:D:219:GLN:HE22	1:D:337:MET:H	1.49	0.60
1:B:275:PRO:HG2	1:B:334:GLU:OE1	2.01	0.60
1:D:38:PRO:HD2	1:D:381:TYR:OH	2.01	0.60
1:D:356:LEU:HA	1:D:382:ASP:OD2	2.00	0.60
1:A:40:ASP:OD2	1:A:368:ARG:CZ	2.50	0.60
1:B:129:ILE:HG21	1:B:170:MET:HE3	1.82	0.60
1:A:276:HIS:HE1	2:P:749:GLY:HA2	1.61	0.60
1:A:221:VAL:HG13	1:A:233:CYS:HB2	1.83	0.60
1:A:284:GLY:N	6:A:2021:HOH:O	2.31	0.60
1:A:324:ASP:O	1:A:327:LYS:HE2	2.01	0.60
1:B:355:PHE:HB3	1:B:360:TYR:CE1	2.37	0.60
1:A:310:ARG:HD2	1:A:316:TRP:CD1	2.36	0.59
1:B:340:VAL:O	1:B:389:PHE:HB2	2.02	0.59
1:D:154:VAL:O	1:D:448:SER:N	2.34	0.59
1:D:72:ASP:O	1:D:76:LYS:HG3	2.02	0.59
1:B:299:GLY:C	2:R:753:ALA:OXT	2.36	0.59
1:B:305:CYS:SG	1:B:317:CYS:HB3	2.41	0.59
1:C:124:ILE:O	1:C:159:PHE:HA	2.02	0.59
1:C:142:ASP:OD2	1:C:146:ARG:HD3	2.03	0.59
1:D:342:GLY:HA2	1:D:387:TRP:CZ2	2.37	0.59
1:B:236:PRO:HB3	1:B:245:ASN:OD1	2.02	0.59
1:C:122:ASN:HA	1:C:157:LEU:HD23	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:VAL:HG11	1:A:379:ALA:HA	1.83	0.59
1:A:45:THR:OG1	1:A:48:GLU:HG2	2.03	0.59
1:A:57:PHE:CZ	1:A:101:ARG:HD2	2.37	0.59
1:D:343:ASN:O	1:D:345:GLU:N	2.35	0.59
1:B:54:LEU:HD22	1:B:73:THR:HG22	1.85	0.59
1:A:306:THR:HG23	1:C:300:THR:CG2	2.33	0.59
1:D:227:ASN:HB2	1:D:271:TYR:CD1	2.37	0.59
1:D:326:ASP:O	1:D:328:LYS:N	2.33	0.59
1:D:58:TYR:CZ	1:D:77:MET:CB	2.86	0.59
1:D:219:GLN:NE2	1:D:337:MET:H	2.01	0.58
1:A:119:TRP:C	1:A:121:LYS:H	2.05	0.58
1:D:187:LYS:NZ	1:D:211:GLU:OE1	2.35	0.58
1:C:409:MET:O	1:C:445:TYR:OH	2.17	0.58
1:A:108:ALA:O	1:A:110:TYR:N	2.34	0.58
1:A:381:TYR:CD1	1:A:385:ARG:HA	2.38	0.58
1:A:405:PHE:O	1:A:409:MET:HG2	2.03	0.58
1:C:419:ALA:HA	1:C:434:SER:HB3	1.86	0.58
1:A:223:VAL:HG13	1:A:272:GLY:HA3	1.86	0.58
1:A:50:ALA:HB2	1:A:97:MET:HE1	1.84	0.58
1:B:172:ASN:ND2	1:B:173:PHE:N	2.51	0.58
1:C:413:HIS:CE1	1:C:423:PRO:HB3	2.38	0.58
1:B:176:TRP:O	1:B:177:GLU:C	2.41	0.58
1:B:50:ALA:HB2	1:B:97:MET:HE1	1.85	0.58
1:C:177:GLU:OE2	1:C:179:GLY:N	2.35	0.58
1:D:235:PHE:CE1	1:D:246:SER:HA	2.38	0.58
1:B:103:GLY:HA2	1:B:190:LEU:HD22	1.83	0.58
1:D:176:TRP:CZ2	1:D:186:GLY:CA	2.86	0.58
1:B:310:ARG:NH2	1:B:312:ASP:OD2	2.37	0.58
1:B:47:LYS:O	1:B:51:VAL:HG23	2.03	0.58
1:A:293:PHE:CD2	2:P:750:PRO:HG3	2.39	0.57
1:D:152:SER:O	1:D:155:THR:N	2.38	0.57
1:D:435:GLN:O	1:D:439:LYS:HG3	2.04	0.57
1:D:69:VAL:HG12	1:D:69:VAL:O	2.02	0.57
1:C:57:PHE:CZ	1:C:190:LEU:HD22	2.32	0.57
1:A:58:TYR:CE2	1:A:77:MET:CG	2.87	0.57
1:B:214:THR:O	1:B:396:SER:HA	2.04	0.57
1:D:40:ASP:HB3	1:D:387:TRP:HH2	1.69	0.57
1:D:396:SER:O	1:D:400:VAL:HG23	2.03	0.57
1:A:68:PHE:O	1:A:68:PHE:CD1	2.44	0.57
1:B:324:ASP:HB2	1:D:175:ARG:NH1	2.19	0.57
1:C:178:HIS:ND1	1:C:178:HIS:N	2.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:70:LEU:O	1:D:74:LEU:HB2	2.04	0.57
1:A:364:THR:OG1	1:A:365:SER:N	2.38	0.57
1:C:444:LEU:CB	1:C:445:TYR:CD1	2.87	0.57
1:D:277:GLU:OE1	2:R:750:PRO:HD2	2.04	0.57
1:A:119:TRP:HD1	1:A:409:MET:HE3	1.69	0.57
1:D:150:VAL:O	1:D:150:VAL:HG12	2.04	0.57
1:A:331:PHE:O	1:A:333:PRO:HD3	2.05	0.57
1:A:403:HIS:HE1	1:A:422:ALA:O	1.87	0.57
1:B:224:LYS:HE3	1:B:282:MET:SD	2.45	0.57
1:C:58:TYR:HE1	1:C:77:MET:HA	1.68	0.57
1:D:155:THR:HG21	1:D:441:ILE:HG12	1.86	0.57
1:C:83:LEU:CD1	1:C:93:THR:HA	2.35	0.57
1:D:172:ASN:ND2	1:D:173:PHE:H	2.03	0.57
1:D:180:ASP:OD1	1:D:181:GLY:N	2.38	0.57
1:D:322:ASP:CG	1:D:325:ARG:HB2	2.25	0.57
1:D:54:LEU:HD12	1:D:70:LEU:CD1	2.31	0.56
1:A:58:TYR:CE2	1:A:77:MET:HG2	2.40	0.56
1:B:157:LEU:HD21	1:B:445:TYR:CE1	2.39	0.56
2:P:747:PRO:O	2:P:748:ALA:C	2.43	0.56
1:B:301:SER:HB2	2:R:751:PRO:HB2	1.85	0.56
1:C:117:PRO:HG2	1:C:196:ALA:HB1	1.87	0.56
1:D:67:LEU:O	1:D:68:PHE:CG	2.57	0.56
1:A:334:GLU:HG3	1:A:335:THR:H	1.69	0.56
1:C:101:ARG:HH22	1:C:106:ASP:CG	2.08	0.56
1:A:176:TRP:C	1:A:184:PHE:H	2.09	0.56
1:D:420:LEU:HB2	1:D:431:PHE:HZ	1.70	0.56
1:C:299:GLY:HA2	2:P:753:ALA:H	1.71	0.56
1:A:57:PHE:CZ	1:A:190:LEU:HD22	2.33	0.56
1:A:32:SER:N	1:A:33:PRO:CD	2.67	0.56
1:D:58:TYR:CZ	1:D:77:MET:HB2	2.40	0.56
1:A:188:ASP:OD1	1:A:395:TYR:CE2	2.59	0.56
1:B:312:ASP:OD2	1:B:314:TYR:HD2	1.88	0.56
1:C:54:LEU:HD23	1:C:58:TYR:CD2	2.41	0.56
2:P:747:PRO:O	2:P:749:GLY:N	2.39	0.56
1:B:442:GLN:O	1:B:446:GLY:N	2.36	0.56
1:C:298:GLN:HE22	1:C:324:ASP:CG	2.08	0.56
1:C:157:LEU:HD11	1:C:445:TYR:CD2	2.40	0.56
1:C:50:ALA:HB2	1:C:89:LEU:HD21	1.88	0.56
1:D:238:LEU:HG	1:D:242:LYS:O	2.06	0.56
1:B:121:LYS:HZ2	1:B:168:ASP:CG	2.08	0.56
1:B:187:LYS:NZ	1:B:340:VAL:HG11	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:119:TRP:CE2	1:D:197:PRO:HB3	2.41	0.56
1:B:57:PHE:CZ	1:B:190:LEU:HD21	2.38	0.56
1:D:45:THR:CG2	1:D:48:GLU:H	2.18	0.56
1:A:102:CYS:SG	1:A:103:GLY:N	2.79	0.55
1:A:337:MET:HE3	1:A:340:VAL:HG22	1.88	0.55
1:B:214:THR:HG22	1:B:219:GLN:HA	1.88	0.55
1:C:89:LEU:HD21	1:C:97:MET:CE	2.37	0.55
1:D:38:PRO:HG3	1:D:385:ARG:HB3	1.88	0.55
1:B:350:VAL:HG22	1:B:376:ALA:O	2.06	0.55
1:D:193:HIS:C	1:D:404:GLN:OE1	2.44	0.55
1:A:285:ASN:HD21	1:A:328:LYS:HA	1.71	0.55
1:A:342:GLY:HA3	1:A:388:GLY:HA2	1.87	0.55
1:B:221:VAL:HA	1:B:334:GLU:OE2	2.07	0.55
1:D:66:ASN:CG	1:D:67:LEU:N	2.58	0.55
1:A:194:ALA:HB2	1:A:205:SER:HA	1.86	0.55
1:A:117:PRO:CG	1:A:196:ALA:HB1	2.35	0.55
1:B:127:ARG:HG2	1:B:129:ILE:HG23	1.89	0.55
1:A:175:ARG:CG	1:C:298:GLN:CD	2.71	0.55
1:A:380:ASN:HD21	1:A:382:ASP:HB2	1.72	0.55
1:B:286:ALA:C	6:B:2022:HOH:O	2.43	0.55
1:C:123:GLN:HG2	1:C:158:ARG:HH22	1.72	0.55
1:B:225:TYR:H	1:B:229:ASP:HB2	1.71	0.55
1:D:45:THR:HG22	1:D:48:GLU:H	1.71	0.55
1:B:442:GLN:HG2	1:B:447:ALA:HA	1.88	0.55
1:D:45:THR:HG22	1:D:48:GLU:CB	2.36	0.55
1:D:58:TYR:CE1	1:D:77:MET:HA	2.42	0.55
1:A:310:ARG:NH1	1:A:312:ASP:OD2	2.40	0.55
1:A:188:ASP:OD1	1:A:395:TYR:CZ	2.58	0.55
1:A:58:TYR:O	1:A:107:VAL:HG21	2.07	0.55
1:C:313:GLY:N	6:C:2021:HOH:O	2.38	0.55
1:D:166:GLU:HG2	1:D:170:MET:HE2	1.89	0.55
1:A:187:LYS:NZ	1:A:212:LEU:H	2.02	0.55
1:A:83:LEU:CD1	1:A:93:THR:HA	2.37	0.55
1:C:344:SER:CB	1:C:377:THR:HG21	2.36	0.55
1:A:74:LEU:HD21	1:A:89:LEU:HD12	1.89	0.55
1:C:310:ARG:NH1	1:C:312:ASP:OD2	2.40	0.55
1:A:176:TRP:CZ3	1:C:325:ARG:HA	2.39	0.55
1:C:415:GLN:O	1:C:417:PRO:HD3	2.07	0.55
1:C:61:PRO:O	1:C:65:CYS:HB2	2.07	0.55
1:A:343:ASN:C	1:A:343:ASN:OD1	2.45	0.54
1:C:89:LEU:CD2	1:C:94:ILE:HG12	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:TYR:O	1:C:161:ARG:HA	2.06	0.54
1:D:227:ASN:HB2	1:D:271:TYR:H	1.71	0.54
1:D:70:LEU:O	1:D:74:LEU:CB	2.55	0.54
1:A:104:ASN:OD1	1:A:193:HIS:HB2	2.07	0.54
1:A:128:ILE:HD12	1:A:144:PHE:HD2	1.73	0.54
1:C:54:LEU:HD23	1:C:58:TYR:CE2	2.41	0.54
1:C:299:GLY:C	3:C:850:SO4:O1	2.46	0.54
1:A:34:ILE:CD1	1:A:369:SER:HB2	2.38	0.54
1:C:91:GLN:HE21	1:C:95:GLU:HG3	1.71	0.54
1:A:57:PHE:CZ	1:A:190:LEU:CD2	2.84	0.54
1:D:312:ASP:CG	1:D:314:TYR:HD1	2.11	0.54
1:D:192:ALA:HB3	1:D:404:GLN:NE2	2.23	0.54
1:B:299:GLY:O	2:R:753:ALA:OXT	2.25	0.54
1:B:350:VAL:HG23	1:B:350:VAL:O	2.07	0.54
1:C:378:THR:HG23	1:C:380:ASN:O	2.07	0.54
1:D:276:HIS:NE2	2:R:747:PRO:C	2.61	0.54
1:D:40:ASP:HB3	1:D:387:TRP:CH2	2.42	0.54
1:D:433:LEU:HD11	1:D:437:ASP:CB	2.37	0.54
1:A:276:HIS:O	1:A:279:LEU:HB2	2.08	0.54
1:B:381:TYR:O	1:B:385:ARG:N	2.40	0.54
1:C:219:GLN:NE2	1:C:337:MET:H	2.05	0.54
1:D:252:ARG:NH1	1:D:273:PHE:HZ	2.06	0.54
1:A:285:ASN:C	1:A:285:ASN:HD22	2.10	0.54
1:A:52:GLN:HA	1:A:52:GLN:HE21	1.72	0.54
1:A:155:THR:OG1	1:A:157:LEU:HB2	2.08	0.54
1:B:237:PHE:CE2	1:B:244:TYR:HB2	2.42	0.54
1:C:176:TRP:O	1:C:178:HIS:ND1	2.40	0.53
1:D:197:PRO:HG3	1:D:408:ALA:O	2.08	0.53
1:D:404:GLN:O	1:D:407:HIS:HB2	2.09	0.53
1:C:252:ARG:HG3	1:C:252:ARG:NH1	2.22	0.53
1:D:343:ASN:OD1	1:D:344:SER:N	2.41	0.53
1:D:339:THR:HB	1:D:347:ALA:O	2.08	0.53
1:A:119:TRP:O	1:A:121:LYS:N	2.42	0.53
1:A:157:LEU:O	1:A:158:ARG:NH1	2.41	0.53
1:D:285:ASN:OD1	1:D:328:LYS:HA	2.07	0.53
1:A:177:GLU:OE1	1:A:178:HIS:N	2.39	0.53
1:A:176:TRP:O	1:A:184:PHE:N	2.42	0.53
1:A:415:GLN:O	1:A:417:PRO:HD3	2.09	0.53
1:B:286:ALA:CA	6:B:2022:HOH:O	2.31	0.53
1:B:147:ALA:HB1	1:B:402:ALA:HA	1.89	0.53
1:C:214:THR:HG21	1:C:393:GLN:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:433:LEU:HD22	1:C:437:ASP:CB	2.39	0.53
1:A:73:THR:O	1:A:76:LYS:N	2.40	0.53
1:B:49:LEU:HD21	1:B:98:ARG:HG2	1.89	0.53
1:C:146:ARG:O	1:C:150:VAL:HG23	2.09	0.53
1:A:275:PRO:HA	1:A:280:PHE:CE2	2.44	0.53
1:B:292:LYS:O	1:B:295:PHE:HB3	2.09	0.53
1:B:45:THR:OG1	1:B:48:GLU:HG3	2.09	0.53
1:B:75:LYS:HG2	1:B:87:GLY:HA2	1.91	0.53
1:C:58:TYR:CE2	1:C:77:MET:HG3	2.44	0.53
1:A:101:ARG:NH2	1:A:106:ASP:OD2	2.41	0.53
1:B:154:VAL:HG23	1:B:155:THR:HG23	1.91	0.53
1:D:157:LEU:HD12	1:D:157:LEU:O	2.09	0.53
1:D:278:ALA:HB1	2:R:746:GLY:O	2.09	0.53
1:A:297:PHE:HB3	1:A:302:TYR:CE1	2.44	0.53
1:A:34:ILE:HG13	1:A:368:ARG:O	2.08	0.53
1:D:356:LEU:HD22	1:D:382:ASP:OD1	2.09	0.53
1:A:128:ILE:HD12	1:A:144:PHE:CD2	2.43	0.53
1:A:58:TYR:CZ	1:A:77:MET:CB	2.92	0.53
1:B:175:ARG:HD3	1:D:298:GLN:HA	1.91	0.53
1:B:341:GLY:HA2	1:B:345:GLU:OE2	2.07	0.52
1:D:180:ASP:CG	1:D:182:TYR:H	2.12	0.52
1:B:75:LYS:HA	1:B:78:GLN:OE1	2.09	0.52
1:C:58:TYR:CE2	1:C:77:MET:CG	2.91	0.52
1:D:150:VAL:HG11	1:D:431:PHE:HE2	1.74	0.52
1:D:129:ILE:HD12	1:D:170:MET:HB3	1.92	0.52
1:A:40:ASP:OD2	1:A:368:ARG:NH1	2.43	0.52
1:B:223:VAL:HG21	1:B:272:GLY:HA3	1.90	0.52
1:C:89:LEU:HD21	1:C:97:MET:HE1	1.90	0.52
1:A:113:PHE:CB	1:A:114:PRO:HD3	2.25	0.52
1:A:310:ARG:HD2	1:A:316:TRP:HD1	1.74	0.52
1:C:292:LYS:HB3	1:C:320:THR:O	2.09	0.52
1:C:38:PRO:HG3	1:C:385:ARG:NH2	2.24	0.52
1:C:47:LYS:O	1:C:51:VAL:HG23	2.09	0.52
1:D:322:ASP:OD2	1:D:325:ARG:HB2	2.09	0.52
1:D:420:LEU:HB2	1:D:431:PHE:CZ	2.44	0.52
1:B:344:SER:HB3	1:B:377:THR:HG21	1.89	0.52
1:B:344:SER:O	1:B:345:GLU:C	2.48	0.52
1:B:378:THR:O	1:B:380:ASN:N	2.43	0.52
1:D:35:ILE:HG13	1:D:36:LYS:N	2.24	0.52
1:A:45:THR:HG23	1:A:48:GLU:OE2	2.09	0.52
1:B:107:VAL:O	1:B:109:ASN:CA	2.56	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:PRO:HD3	1:B:333:PRO:O	2.09	0.52
1:D:187:LYS:HZ3	1:D:212:LEU:H	1.57	0.52
1:A:278:ALA:CB	2:P:746:GLY:O	2.58	0.52
1:C:441:ILE:O	1:C:445:TYR:HD1	1.93	0.52
1:D:296:ARG:HG2	1:D:296:ARG:HH11	1.75	0.52
1:A:58:TYR:CZ	1:A:77:MET:HG2	2.46	0.51
1:D:152:SER:C	1:D:154:VAL:N	2.63	0.51
1:D:207:PHE:CD1	1:D:207:PHE:N	2.78	0.51
1:D:276:HIS:CE1	2:R:749:GLY:CA	2.88	0.51
1:D:306:THR:HG23	1:D:308:GLU:H	1.73	0.51
1:D:58:TYR:CZ	1:D:77:MET:CG	2.93	0.51
1:A:293:PHE:HE2	2:P:750:PRO:CG	2.14	0.51
1:A:113:PHE:HB2	1:A:114:PRO:CD	2.31	0.51
1:A:310:ARG:HH21	1:A:331:PHE:HZ	1.58	0.51
1:C:50:ALA:HA	1:C:97:MET:SD	2.51	0.51
1:D:324:ASP:O	1:D:327:LYS:HE2	2.10	0.51
1:D:142:ASP:O	1:D:146:ARG:HG3	2.11	0.51
1:A:62:LYS:CD	1:A:62:LYS:H	2.21	0.51
1:C:175:ARG:HB2	1:C:210:ASP:OD2	2.10	0.51
1:C:219:GLN:HE22	1:C:337:MET:H	1.58	0.51
1:A:172:ASN:ND2	1:A:173:PHE:N	2.59	0.51
1:C:61:PRO:HB2	1:C:64:SER:HB3	1.92	0.51
1:D:47:LYS:O	1:D:51:VAL:HG23	2.11	0.51
1:A:101:ARG:HH22	1:A:106:ASP:CG	2.14	0.51
1:C:110:TYR:HA	1:C:113:PHE:HB2	1.93	0.51
1:D:448:SER:OG	1:D:450:ASP:OD2	2.26	0.51
1:A:381:TYR:CE1	1:A:385:ARG:HA	2.45	0.51
1:D:310:ARG:NH2	1:D:312:ASP:OD2	2.36	0.51
1:C:162:ILE:HD11	1:C:167:ALA:HB2	1.93	0.51
1:D:115:ARG:O	1:D:116:LYS:HG3	2.11	0.51
1:A:176:TRP:O	1:A:183:PRO:HA	2.11	0.50
1:A:337:MET:HE2	1:A:340:VAL:HG22	1.92	0.50
1:B:169:ILE:HG23	1:B:203:GLY:O	2.11	0.50
1:B:192:ALA:O	1:B:193:HIS:HB3	2.11	0.50
1:C:109:ASN:C	1:C:111:ASN:N	2.64	0.50
1:C:37:PHE:HD1	1:C:381:TYR:HH	1.60	0.50
1:D:122:ASN:O	1:D:157:LEU:CA	2.59	0.50
1:D:289:GLN:HB2	1:D:319:THR:HG21	1.94	0.50
1:A:228:ALA:CB	1:A:261:THR:HG21	2.42	0.50
1:C:378:THR:O	1:C:379:ALA:C	2.47	0.50
1:D:122:ASN:O	1:D:157:LEU:CB	2.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:185:ASP:OD2	1:D:189:GLY:HA3	2.10	0.50
1:B:117:PRO:CB	1:B:196:ALA:HB1	2.41	0.50
1:C:224:LYS:HE3	1:C:282:MET:CE	2.41	0.50
1:D:152:SER:C	1:D:155:THR:H	2.13	0.50
1:D:432:ARG:NH1	1:D:434:SER:HA	2.27	0.50
1:C:298:GLN:NE2	1:C:324:ASP:OD2	2.44	0.50
1:C:58:TYR:CZ	1:C:77:MET:CA	2.93	0.50
1:C:81:PHE:HZ	1:C:101:ARG:HH21	1.59	0.50
1:D:112:PHE:CG	1:D:113:PHE:N	2.79	0.50
1:B:350:VAL:HG21	1:B:378:THR:C	2.32	0.50
1:C:292:LYS:O	1:C:295:PHE:HB3	2.11	0.50
1:D:378:THR:HG21	1:D:384:ASP:HB2	1.93	0.50
1:A:112:PHE:CZ	1:A:115:ARG:HG2	2.44	0.50
1:A:429:LYS:HB2	1:A:429:LYS:HZ2	1.76	0.50
1:B:434:SER:O	1:B:437:ASP:N	2.44	0.50
1:B:57:PHE:HZ	1:B:190:LEU:CD2	2.24	0.50
1:C:118:LYS:O	1:C:119:TRP:C	2.48	0.50
1:C:433:LEU:HD22	1:C:437:ASP:HB3	1.93	0.50
1:D:275:PRO:HA	1:D:280:PHE:CZ	2.46	0.50
1:B:227:ASN:O	1:B:270:LYS:HE2	2.11	0.50
1:B:286:ALA:CB	1:B:319:THR:HG21	2.41	0.50
1:C:444:LEU:HB3	1:C:445:TYR:CE1	2.46	0.50
1:D:296:ARG:HG2	1:D:296:ARG:NH1	2.27	0.50
1:A:275:PRO:O	1:A:276:HIS:HB2	2.12	0.49
1:A:340:VAL:O	1:A:389:PHE:HB2	2.11	0.49
1:C:43:PRO:O	1:C:44:LYS:HE2	2.11	0.49
1:C:157:LEU:HD11	1:C:445:TYR:CE2	2.47	0.49
1:C:197:PRO:HG3	1:C:408:ALA:O	2.12	0.49
1:D:193:HIS:CD2	1:D:206:HIS:HB2	2.47	0.49
1:D:353:PHE:HE1	1:D:355:PHE:HB2	1.77	0.49
1:D:438:ILE:O	1:D:442:GLN:HG3	2.12	0.49
1:B:211:GLU:HG3	1:B:395:TYR:CE1	2.48	0.49
1:B:296:ARG:HH21	2:R:753:ALA:CB	2.13	0.49
1:C:350:VAL:HG11	1:C:379:ALA:N	2.27	0.49
1:C:135:LEU:HB2	1:C:140:VAL:HG23	1.94	0.49
1:C:237:PHE:CE1	1:C:244:TYR:HB2	2.48	0.49
1:A:62:LYS:HD2	1:A:62:LYS:N	2.26	0.49
1:B:341:GLY:N	1:B:345:GLU:OE2	2.44	0.49
1:C:58:TYR:OH	1:C:77:MET:CA	2.59	0.49
1:B:298:GLN:N	1:B:324:ASP:OD2	2.33	0.49
1:C:155:THR:HB	1:C:156:PRO:HD2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:282:MET:O	1:B:331:PHE:HB2	2.13	0.49
1:C:148:PHE:HB3	1:C:159:PHE:CD2	2.47	0.49
1:A:364:THR:O	1:A:373:MET:HA	2.12	0.49
1:C:50:ALA:HB3	1:C:89:LEU:HD11	1.91	0.49
1:D:111:ASN:N	1:D:111:ASN:ND2	2.44	0.49
1:A:281:THR:HG21	1:A:330:GLY:HA3	1.94	0.49
1:B:350:VAL:HG21	1:B:379:ALA:N	2.28	0.49
1:A:243:GLU:OE1	1:D:91:GLN:HG2	2.13	0.49
1:A:121:LYS:HD3	1:A:123:GLN:O	2.13	0.49
1:B:77:MET:CE	1:B:93:THR:HB	2.42	0.49
1:C:34:ILE:HG23	1:C:368:ARG:HA	1.95	0.49
1:D:350:VAL:HG11	1:D:379:ALA:HA	1.94	0.49
1:D:54:LEU:HD22	1:D:73:THR:HG22	1.94	0.49
1:A:442:GLN:O	1:A:446:GLY:N	2.40	0.48
1:A:444:LEU:HD23	1:A:445:TYR:CE2	2.48	0.48
1:B:184:PHE:CD2	1:B:208:ASP:HA	2.47	0.48
1:C:123:GLN:CG	1:C:158:ARG:HH22	2.25	0.48
1:A:117:PRO:HB3	1:A:197:PRO:CD	2.37	0.48
1:C:129:ILE:HD11	1:C:172:ASN:HB2	1.95	0.48
1:A:46:ASP:OD1	1:A:94:ILE:HD13	2.12	0.48
1:B:188:ASP:OD2	1:B:372:LYS:NZ	2.43	0.48
1:B:197:PRO:HG3	1:B:408:ALA:O	2.13	0.48
1:D:89:LEU:HD13	1:D:94:ILE:HD11	1.95	0.48
1:A:381:TYR:O	1:A:385:ARG:N	2.42	0.48
1:B:121:LYS:HE3	1:B:124:ILE:HD13	1.95	0.48
1:C:299:GLY:N	3:C:850:SO4:O1	2.46	0.48
1:D:102:CYS:SG	1:D:103:GLY:N	2.86	0.48
1:B:107:VAL:C	1:B:109:ASN:N	2.57	0.48
1:C:117:PRO:HB2	1:C:197:PRO:HD2	1.95	0.48
1:C:420:LEU:HD13	1:C:431:PHE:CZ	2.48	0.48
1:D:300:THR:HG22	1:D:301:SER:N	2.28	0.48
1:D:368:ARG:NH1	1:D:368:ARG:HB3	2.29	0.48
1:A:302:TYR:CD1	1:A:302:TYR:N	2.81	0.48
1:A:354:THR:OG1	1:A:380:ASN:HB2	2.14	0.48
1:B:188:ASP:OD2	1:B:372:LYS:CE	2.61	0.48
1:C:86:THR:HG22	1:C:88:ASP:H	1.79	0.48
1:C:96:THR:HA	1:C:99:LYS:HG3	1.94	0.48
1:D:327:LYS:CE	1:D:327:LYS:N	2.69	0.48
1:A:185:ASP:OD1	1:A:185:ASP:N	2.46	0.48
1:C:90:ASP:OD2	1:C:92:ASN:HB2	2.12	0.48
1:D:37:PHE:O	1:D:40:ASP:OD1	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:78:GLN:HG3	1:D:85:GLN:HA	1.96	0.48
1:A:44:LYS:HB2	1:A:48:GLU:HG3	1.96	0.48
1:B:185:ASP:OD2	1:B:190:LEU:HG	2.13	0.48
1:C:308:GLU:HG2	6:C:2020:HOH:O	2.14	0.48
1:D:152:SER:O	1:D:154:VAL:N	2.47	0.48
2:P:746:GLY:O	2:P:747:PRO:C	2.52	0.48
1:A:37:PHE:CD2	1:A:368:ARG:HD3	2.49	0.48
1:B:175:ARG:C	1:B:176:TRP:O	2.51	0.48
1:B:66:ASN:O	1:B:67:LEU:C	2.53	0.48
1:C:155:THR:HB	1:C:156:PRO:CD	2.43	0.48
1:B:127:ARG:HG2	1:B:129:ILE:CG2	2.43	0.47
1:B:339:THR:HB	1:B:347:ALA:O	2.14	0.47
1:B:90:ASP:O	1:B:93:THR:N	2.47	0.47
1:C:381:TYR:O	1:C:385:ARG:N	2.38	0.47
1:A:140:VAL:O	1:A:141:ASP:C	2.52	0.47
1:A:285:ASN:ND2	1:A:285:ASN:C	2.67	0.47
1:A:36:LYS:O	1:A:36:LYS:HG2	2.14	0.47
1:B:227:ASN:ND2	1:B:270:LYS:HA	2.28	0.47
1:B:35:ILE:CG2	1:B:36:LYS:N	2.76	0.47
1:D:151:TRP:CE3	1:D:441:ILE:HD13	2.50	0.47
1:B:57:PHE:CZ	1:B:101:ARG:HD2	2.49	0.47
1:C:55:ASN:OD1	1:C:62:LYS:HG3	2.14	0.47
1:D:127:ARG:HD2	1:D:129:ILE:HG13	1.96	0.47
1:B:175:ARG:O	1:B:176:TRP:O	2.32	0.47
1:B:225:TYR:OH	1:B:282:MET:CE	2.63	0.47
1:C:275:PRO:CA	1:C:280:PHE:HZ	2.22	0.47
1:C:83:LEU:HD13	1:C:93:THR:HA	1.97	0.47
1:C:77:MET:CE	1:C:97:MET:HG3	2.45	0.47
1:D:368:ARG:NH1	1:D:370:ASP:OD1	2.47	0.47
1:A:355:PHE:CE1	1:A:356:LEU:HD13	2.49	0.47
1:A:55:ASN:HD21	1:A:62:LYS:HG3	1.80	0.47
1:B:132:THR:O	1:B:132:THR:HG23	2.15	0.47
1:B:403:HIS:ND1	1:B:420:LEU:O	2.45	0.47
1:C:104:ASN:HD21	1:C:194:ALA:H	1.62	0.47
1:C:279:LEU:CB	1:C:280:PHE:HD1	2.22	0.47
1:D:223:VAL:CG1	1:D:224:LYS:N	2.78	0.47
1:D:74:LEU:HD11	1:D:93:THR:HG21	1.96	0.47
1:A:375:CYS:SG	1:A:375:CYS:O	2.68	0.47
1:D:211:GLU:HA	1:D:211:GLU:OE1	2.14	0.47
1:D:92:ASN:HA	1:D:92:ASN:HD22	1.54	0.47
1:B:285:ASN:OD1	1:B:285:ASN:C	2.53	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:ARG:O	1:B:176:TRP:C	2.50	0.47
1:C:109:ASN:C	1:C:111:ASN:H	2.18	0.47
1:D:58:TYR:CE2	1:D:77:MET:HG3	2.50	0.47
1:D:217:GLU:O	1:D:218:GLY:O	2.33	0.47
1:D:57:PHE:CZ	1:D:190:LEU:CD2	2.94	0.47
1:A:407:HIS:O	1:A:410:GLY:N	2.41	0.46
1:C:214:THR:CG2	1:C:216:GLY:H	2.19	0.46
1:D:123:GLN:HB3	1:D:158:ARG:HD3	1.97	0.46
1:D:337:MET:CE	1:D:337:MET:HA	2.44	0.46
1:B:312:ASP:CG	1:B:314:TYR:HD2	2.19	0.46
1:B:343:ASN:OD1	1:B:387:TRP:N	2.49	0.46
1:C:89:LEU:HD23	1:C:94:ILE:HG12	1.96	0.46
1:A:52:GLN:HA	1:A:52:GLN:NE2	2.29	0.46
1:B:275:PRO:O	1:B:276:HIS:HB2	2.15	0.46
1:C:117:PRO:O	1:C:118:LYS:HB2	2.15	0.46
1:C:252:ARG:NH2	1:C:273:PHE:CZ	2.79	0.46
1:D:58:TYR:CE2	1:D:77:MET:HB2	2.50	0.46
1:B:74:LEU:O	1:B:78:GLN:HG3	2.16	0.46
1:C:281:THR:OG1	1:C:289:GLN:O	2.22	0.46
1:D:152:SER:CB	1:D:157:LEU:O	2.63	0.46
1:D:235:PHE:CZ	1:D:246:SER:HA	2.51	0.46
1:D:312:ASP:OD1	1:D:314:TYR:HD1	1.98	0.46
1:D:403:HIS:CE1	1:D:421:MET:HA	2.50	0.46
1:C:116:LYS:HA	1:C:117:PRO:HD3	1.76	0.46
1:C:299:GLY:HA2	2:P:753:ALA:O	2.08	0.46
1:A:316:TRP:HA	1:A:331:PHE:HA	1.98	0.46
1:C:221:VAL:HA	1:C:334:GLU:OE2	2.16	0.46
1:D:123:GLN:CB	1:D:158:ARG:HH11	2.27	0.46
1:D:193:HIS:HD2	1:D:206:HIS:HB2	1.79	0.46
1:A:428:THR:O	1:A:429:LYS:C	2.53	0.46
1:B:102:CYS:SG	1:B:104:ASN:HB2	2.56	0.46
1:B:344:SER:HB3	1:B:347:ALA:HB3	1.98	0.46
1:B:54:LEU:HD11	1:B:74:LEU:CD1	2.35	0.46
1:C:109:ASN:HB2	1:C:113:PHE:CG	2.50	0.46
1:B:184:PHE:CE2	1:B:208:ASP:HA	2.50	0.46
1:C:35:ILE:HD11	1:C:37:PHE:CE1	2.51	0.46
1:D:368:ARG:HD2	1:D:374:TRP:CD1	2.50	0.46
1:D:407:HIS:HE2	1:D:413:HIS:CD2	2.34	0.46
1:A:117:PRO:HG2	1:A:196:ALA:CB	2.43	0.46
1:A:382:ASP:HA	1:A:385:ARG:HE	1.81	0.46
1:A:90:ASP:O	1:A:93:THR:HB	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:MET:HG3	1:B:78:GLN:N	2.31	0.46
1:C:121:LYS:NZ	1:C:168:ASP:OD1	2.47	0.46
1:C:122:ASN:HB3	1:C:156:PRO:O	2.16	0.46
1:D:152:SER:CA	1:D:155:THR:HG1	2.21	0.46
1:D:180:ASP:OD1	1:D:182:TYR:N	2.41	0.46
1:A:243:GLU:CD	1:D:91:GLN:HG2	2.36	0.45
1:A:277:GLU:HB2	1:A:291:CYS:SG	2.56	0.45
1:A:286:ALA:HB2	1:A:319:THR:OG1	2.16	0.45
1:A:361:GLU:CD	1:A:361:GLU:N	2.65	0.45
1:B:135:LEU:HB2	1:B:140:VAL:CG2	2.46	0.45
1:B:352:PRO:HB3	1:B:361:GLU:OE2	2.16	0.45
1:C:400:VAL:O	1:C:404:GLN:HG2	2.15	0.45
1:D:152:SER:HB3	1:D:157:LEU:O	2.16	0.45
1:D:350:VAL:O	1:D:353:PHE:HB3	2.16	0.45
1:A:248:THR:CG2	1:A:250:THR:HG22	2.46	0.45
1:A:356:LEU:HD12	1:A:382:ASP:OD1	2.16	0.45
1:A:433:LEU:HD22	1:A:437:ASP:CB	2.46	0.45
1:A:80:PHE:HA	1:A:415:GLN:NE2	2.28	0.45
1:D:154:VAL:HB	1:D:442:GLN:NE2	2.31	0.45
1:B:177:GLU:OE2	1:B:179:GLY:N	2.46	0.45
1:B:234:LYS:O	1:B:237:PHE:HB3	2.16	0.45
1:B:400:VAL:O	1:B:404:GLN:HG2	2.16	0.45
1:C:413:HIS:HA	1:C:421:MET:O	2.16	0.45
1:A:176:TRP:CD1	1:C:324:ASP:CB	2.90	0.45
1:C:447:ALA:HB1	6:C:2027:HOH:O	2.16	0.45
1:D:176:TRP:HA	1:D:184:PHE:O	2.17	0.45
1:A:113:PHE:N	1:A:114:PRO:CD	2.80	0.45
1:A:74:LEU:HD21	1:A:89:LEU:CD1	2.47	0.45
1:D:242:LYS:HD3	1:D:244:TYR:CE2	2.51	0.45
1:D:299:GLY:HA3	3:D:857:SO4:S	2.57	0.45
1:D:62:LYS:H	1:D:62:LYS:CD	2.13	0.45
1:D:78:GLN:NE2	1:D:93:THR:OG1	2.50	0.45
1:B:214:THR:CG2	1:B:219:GLN:HA	2.45	0.45
1:B:46:ASP:OD2	1:B:94:ILE:HG21	2.17	0.45
1:B:53:TYR:CD1	1:B:57:PHE:HD2	2.34	0.45
1:D:224:LYS:HA	1:D:229:ASP:OD1	2.17	0.45
1:D:154:VAL:O	1:D:447:ALA:HA	2.17	0.45
1:A:438:ILE:O	1:A:442:GLN:HG3	2.17	0.45
1:A:84:PRO:O	1:A:86:THR:N	2.49	0.45
1:B:121:LYS:NZ	1:B:168:ASP:OD2	2.46	0.45
1:B:433:LEU:HA	1:B:433:LEU:HD23	1.78	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:ASP:OD1	1:B:93:THR:CG2	2.64	0.45
1:C:192:ALA:O	1:C:193:HIS:HB3	2.17	0.45
1:C:57:PHE:HZ	1:C:190:LEU:CD2	2.22	0.45
1:D:364:THR:OG1	1:D:365:SER:N	2.49	0.45
1:D:442:GLN:HA	1:D:446:GLY:H	1.82	0.45
1:A:172:ASN:HD22	1:A:173:PHE:N	2.14	0.45
1:B:348:PRO:O	1:B:377:THR:HG22	2.17	0.45
1:D:176:TRP:O	1:D:183:PRO:HA	2.17	0.45
1:D:176:TRP:CZ2	1:D:186:GLY:N	2.82	0.45
1:D:178:HIS:N	1:D:178:HIS:ND1	2.65	0.45
1:D:228:ALA:HB2	1:D:270:LYS:HB3	1.99	0.45
1:A:279:LEU:C	1:A:290:PRO:HB3	2.37	0.44
1:A:347:ALA:HA	1:A:348:PRO:HD3	1.80	0.44
1:A:351:PHE:HA	1:A:352:PRO:HA	1.80	0.44
1:A:324:ASP:HB2	1:C:175:ARG:NH1	2.31	0.44
1:C:63:GLU:H	1:C:63:GLU:CD	2.18	0.44
1:D:128:ILE:HD13	1:D:141:ASP:OD1	2.17	0.44
1:D:217:GLU:HG2	1:D:217:GLU:H	1.55	0.44
1:D:368:ARG:HH12	1:D:370:ASP:CG	2.20	0.44
1:A:58:TYR:OH	1:A:77:MET:HG2	2.16	0.44
1:B:315:ARG:HH11	1:B:315:ARG:HG3	1.81	0.44
1:B:34:ILE:HA	1:B:367:GLY:O	2.17	0.44
1:D:112:PHE:CE2	1:D:113:PHE:HD1	2.33	0.44
1:A:119:TRP:HD1	1:A:409:MET:CE	2.30	0.44
1:B:130:GLY:HA3	1:B:172:ASN:HD22	1.81	0.44
1:C:252:ARG:NH1	1:C:254:ASP:OD1	2.50	0.44
1:C:154:VAL:O	1:C:447:ALA:HA	2.17	0.44
1:D:135:LEU:HB2	1:D:140:VAL:HG22	1.99	0.44
1:D:53:TYR:CD2	1:D:97:MET:HG2	2.52	0.44
1:A:126:TYR:HA	1:A:169:ILE:O	2.18	0.44
1:A:368:ARG:NH2	1:A:389:PHE:CZ	2.81	0.44
1:D:353:PHE:CD1	1:D:353:PHE:C	2.91	0.44
1:D:358:ASN:ND2	1:D:358:ASN:N	2.63	0.44
1:D:74:LEU:O	1:D:78:GLN:HG2	2.17	0.44
1:A:362:SER:OG	1:A:363:CYS:N	2.51	0.44
1:B:274:CYS:HA	1:B:275:PRO:HD3	1.83	0.44
1:C:124:ILE:HB	1:C:159:PHE:CD1	2.53	0.44
1:D:401:ALA:HB1	1:D:405:PHE:CE2	2.53	0.44
1:A:113:PHE:CB	1:A:114:PRO:CD	2.94	0.44
1:C:211:GLU:OE1	1:C:211:GLU:HA	2.18	0.44
1:D:395:TYR:CD1	1:D:395:TYR:N	2.85	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:ILE:HG21	1:A:131:TYR:CE1	2.52	0.44
1:C:260:SER:HG	1:C:265:PHE:HD1	1.61	0.44
1:C:54:LEU:CD2	1:C:58:TYR:CD2	3.00	0.44
1:D:154:VAL:HB	1:D:442:GLN:HE21	1.82	0.44
1:A:196:ALA:HB1	1:A:197:PRO:HD2	1.98	0.44
1:A:55:ASN:ND2	1:A:62:LYS:HG3	2.33	0.44
1:B:128:ILE:HD11	1:B:131:TYR:CD1	2.51	0.44
1:B:184:PHE:HB3	1:B:208:ASP:OD2	2.18	0.44
1:B:302:TYR:OH	1:B:308:GLU:HG2	2.18	0.44
1:C:109:ASN:HB2	1:C:113:PHE:CD1	2.53	0.44
1:D:152:SER:O	1:D:153:ASP:C	2.54	0.44
1:D:271:TYR:CD2	1:D:272:GLY:N	2.85	0.44
1:D:54:LEU:HA	1:D:58:TYR:HD2	1.83	0.44
1:B:187:LYS:HA	1:B:211:GLU:OE1	2.18	0.44
1:B:380:ASN:CB	1:B:383:ASP:OD1	2.63	0.44
1:C:225:TYR:CA	1:C:229:ASP:HB2	2.48	0.44
1:D:413:HIS:HD1	1:D:423:PRO:HG3	1.83	0.44
1:A:411:LEU:HB2	1:A:421:MET:HE1	2.00	0.43
1:B:188:ASP:OD2	1:B:372:LYS:HE2	2.17	0.43
1:B:342:GLY:O	1:B:345:GLU:HG2	2.18	0.43
1:B:86:THR:HG21	6:B:2006:HOH:O	2.17	0.43
1:B:90:ASP:O	1:B:91:GLN:C	2.56	0.43
1:A:37:PHE:HE2	1:A:368:ARG:HD3	1.78	0.43
1:B:175:ARG:HD2	1:B:175:ARG:HH11	1.49	0.43
1:B:353:PHE:CG	1:B:376:ALA:HB3	2.54	0.43
1:B:404:GLN:O	1:B:407:HIS:HB2	2.18	0.43
1:C:104:ASN:ND2	1:C:193:HIS:HB2	2.33	0.43
1:D:343:ASN:ND2	1:D:385:ARG:O	2.51	0.43
1:D:433:LEU:HD11	1:D:437:ASP:HB2	2.00	0.43
1:D:89:LEU:HB3	1:D:94:ILE:HD11	1.99	0.43
1:A:133:PRO:HG2	2:P:753:ALA:HA	2.01	0.43
1:A:327:LYS:H	1:A:327:LYS:CD	2.24	0.43
1:C:239:PHE:CD1	1:C:265:PHE:HD2	2.36	0.43
1:C:420:LEU:HD13	1:C:431:PHE:CE1	2.53	0.43
1:D:282:MET:HA	1:D:282:MET:CE	2.48	0.43
1:B:109:ASN:ND2	1:B:110:TYR:CE1	2.86	0.43
1:B:285:ASN:OD1	1:B:328:LYS:HA	2.18	0.43
1:A:136:ASP:O	1:A:140:VAL:HG23	2.18	0.43
1:A:248:THR:HG23	1:A:250:THR:HG22	2.00	0.43
1:A:119:TRP:CD1	1:A:409:MET:HE3	2.52	0.43
1:A:411:LEU:HD11	1:A:441:ILE:HB	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:381:TYR:C	1:C:381:TYR:CD1	2.92	0.43
1:D:248:THR:OG1	1:D:250:THR:HG22	2.18	0.43
1:A:119:TRP:CD1	1:A:409:MET:CE	3.02	0.43
1:A:194:ALA:CB	1:A:205:SER:HA	2.48	0.43
1:B:123:GLN:NE2	1:B:158:ARG:HD3	2.33	0.43
1:B:193:HIS:C	1:B:193:HIS:CD2	2.90	0.43
1:B:58:TYR:CE1	1:B:77:MET:HB2	2.54	0.43
1:D:130:GLY:HA3	1:D:172:ASN:ND2	2.34	0.43
1:A:140:VAL:HG12	1:A:144:PHE:CE2	2.54	0.43
1:B:300:THR:OG1	3:B:852:SO4:O1	2.35	0.43
1:D:344:SER:HB3	1:D:377:THR:HG21	2.01	0.43
1:B:261:THR:O	1:B:261:THR:HG22	2.18	0.43
1:A:276:HIS:NE2	2:P:749:GLY:CA	2.82	0.43
1:C:239:PHE:HD1	1:C:265:PHE:HD2	1.67	0.43
1:A:378:THR:HG21	1:A:384:ASP:CB	2.37	0.43
1:B:113:PHE:CZ	1:B:114:PRO:CG	2.91	0.43
1:B:298:GLN:NE2	1:B:324:ASP:OD1	2.47	0.43
1:A:176:TRP:CD2	1:C:325:ARG:HA	2.50	0.43
1:A:57:PHE:CZ	1:A:190:LEU:HD21	2.54	0.42
1:C:276:HIS:CD2	1:C:335:THR:CG2	2.76	0.42
1:C:364:THR:OG1	1:C:365:SER:N	2.52	0.42
1:D:176:TRP:HE3	1:D:184:PHE:O	2.01	0.42
1:D:58:TYR:CZ	1:D:77:MET:HA	2.54	0.42
1:A:175:ARG:O	1:A:176:TRP:C	2.57	0.42
1:B:293:PHE:CE1	1:B:304:SER:HA	2.54	0.42
1:C:434:SER:OG	1:C:436:ASP:HB3	2.19	0.42
1:D:129:ILE:HD11	1:D:170:MET:CE	2.49	0.42
1:C:109:ASN:CG	1:C:113:PHE:CZ	2.92	0.42
1:C:275:PRO:O	1:C:276:HIS:HB2	2.19	0.42
1:D:54:LEU:O	1:D:58:TYR:HB2	2.19	0.42
1:D:99:LYS:HE3	1:D:99:LYS:HA	2.01	0.42
1:A:135:LEU:HD13	1:A:213:TRP:O	2.19	0.42
1:A:238:LEU:HD12	1:A:242:LYS:O	2.20	0.42
1:A:354:THR:H	1:A:380:ASN:HA	1.83	0.42
1:B:448:SER:HA	1:B:449:PRO:HD3	1.79	0.42
1:C:126:TYR:CZ	1:C:161:ARG:HB2	2.54	0.42
1:D:40:ASP:OD1	1:D:40:ASP:N	2.53	0.42
1:A:119:TRP:C	1:A:121:LYS:N	2.73	0.42
1:B:135:LEU:HB2	1:B:140:VAL:HG23	2.01	0.42
1:B:70:LEU:O	1:B:74:LEU:HD22	2.19	0.42
1:C:227:ASN:C	6:C:2012:HOH:O	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:437:ASP:O	1:C:441:ILE:HG22	2.19	0.42
1:D:293:PHE:HA	1:D:294:PRO:HA	1.83	0.42
1:D:155:THR:HA	1:D:446:GLY:O	2.20	0.42
1:B:151:TRP:CZ3	1:B:441:ILE:HB	2.55	0.42
1:A:355:PHE:O	1:A:356:LEU:HB2	2.19	0.42
1:B:196:ALA:HB1	1:B:197:PRO:HD2	2.01	0.42
1:B:223:VAL:CG2	1:B:272:GLY:HA3	2.49	0.42
1:C:351:PHE:HA	1:C:352:PRO:HA	1.75	0.42
1:C:75:LYS:HG3	1:C:87:GLY:HA2	2.00	0.42
1:D:350:VAL:HG11	1:D:379:ALA:CA	2.49	0.42
1:D:58:TYR:OH	1:D:77:MET:CG	2.61	0.42
1:D:58:TYR:CE2	1:D:77:MET:CG	3.03	0.42
1:A:429:LYS:HB2	1:A:429:LYS:HZ3	1.80	0.42
1:B:193:HIS:O	1:B:193:HIS:HD2	2.01	0.42
1:C:150:VAL:HG12	1:C:150:VAL:O	2.20	0.42
1:C:343:ASN:OD1	1:C:386:LYS:HA	2.20	0.42
1:C:50:ALA:HB1	1:C:89:LEU:HD11	1.96	0.42
1:D:72:ASP:O	1:D:75:LYS:HG3	2.20	0.42
1:A:321:GLU:HG2	6:A:2027:HOH:O	2.19	0.42
1:B:149:GLN:HA	1:B:152:SER:OG	2.19	0.42
1:D:151:TRP:HA	1:D:151:TRP:CE3	2.55	0.42
1:D:350:VAL:CG1	1:D:379:ALA:HA	2.49	0.42
1:D:53:TYR:CG	1:D:97:MET:HG2	2.55	0.42
1:D:80:PHE:C	1:D:80:PHE:CD1	2.93	0.42
1:A:58:TYR:CE2	1:A:77:MET:CB	3.02	0.42
1:B:292:LYS:HA	1:B:292:LYS:HD3	1.79	0.42
1:B:335:THR:HG22	1:B:337:MET:HE3	2.01	0.42
1:C:108:ALA:HB1	1:C:110:TYR:HD1	1.85	0.42
1:C:195:PHE:CD2	1:C:201:VAL:HG13	2.55	0.42
1:C:343:ASN:OD1	1:C:386:LYS:HD2	2.20	0.42
1:C:81:PHE:HE1	1:C:423:PRO:HG2	1.84	0.42
1:A:101:ARG:HD3	1:A:102:CYS:O	2.20	0.41
1:A:224:LYS:O	1:A:273:PHE:HB2	2.20	0.41
1:C:188:ASP:OD2	1:C:372:LYS:CE	2.67	0.41
1:C:286:ALA:CB	1:C:319:THR:HG21	2.50	0.41
1:D:432:ARG:HD3	1:D:432:ARG:O	2.20	0.41
1:B:344:SER:CB	1:B:377:THR:HG1	2.26	0.41
1:D:235:PHE:CE1	1:D:246:SER:CA	3.03	0.41
1:A:196:ALA:HB1	1:A:197:PRO:CD	2.49	0.41
1:B:285:ASN:OD1	1:B:328:LYS:HD2	2.20	0.41
1:B:342:GLY:HA2	1:B:387:TRP:CZ2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:ALA:O	1:C:109:ASN:OD1	2.38	0.41
1:D:89:LEU:HD13	1:D:94:ILE:CD1	2.51	0.41
1:B:35:ILE:HG22	1:B:36:LYS:N	2.36	0.41
1:B:353:PHE:HB2	1:B:376:ALA:HB3	2.02	0.41
1:C:274:CYS:O	1:C:280:PHE:CE1	2.74	0.41
1:D:274:CYS:HA	1:D:275:PRO:HD3	1.78	0.41
1:D:405:PHE:O	1:D:409:MET:HG2	2.21	0.41
1:B:378:THR:OG1	1:B:384:ASP:OD2	2.38	0.41
1:D:347:ALA:HA	1:D:348:PRO:HD3	1.85	0.41
1:A:176:TRP:CA	1:A:184:PHE:H	2.33	0.41
1:D:122:ASN:H	1:D:123:GLN:NE2	2.19	0.41
1:D:129:ILE:HD11	1:D:170:MET:HE1	2.01	0.41
1:D:178:HIS:CE1	1:D:182:TYR:O	2.73	0.41
1:D:72:ASP:N	1:D:72:ASP:OD1	2.43	0.41
1:B:151:TRP:CH2	1:B:411:LEU:CD1	3.03	0.41
1:B:49:LEU:CD2	1:B:98:ARG:HG2	2.51	0.41
1:D:227:ASN:OD1	1:D:269:GLY:O	2.39	0.41
1:D:435:GLN:HG3	1:D:439:LYS:HE3	2.03	0.41
1:A:187:LYS:HE3	1:A:212:LEU:HB2	2.03	0.41
1:B:58:TYR:CZ	1:B:77:MET:HB2	2.55	0.41
1:D:126:TYR:CZ	1:D:161:ARG:HB2	2.56	0.41
1:A:401:ALA:O	1:A:402:ALA:C	2.58	0.41
1:A:73:THR:HA	1:A:76:LYS:HG3	2.02	0.41
1:D:312:ASP:O	1:D:314:TYR:CD1	2.74	0.41
1:A:434:SER:HB3	1:A:437:ASP:OD2	2.21	0.41
1:B:110:TYR:HB2	1:B:111:ASN:H	1.26	0.41
1:C:148:PHE:C	1:C:150:VAL:H	2.24	0.41
1:A:193:HIS:CD2	1:A:193:HIS:C	2.94	0.41
1:A:274:CYS:HA	1:A:275:PRO:HD3	1.91	0.41
1:A:282:MET:HG2	1:A:333:PRO:HG2	2.02	0.41
1:A:298:GLN:NE2	1:A:324:ASP:OD1	2.53	0.41
1:B:123:GLN:OE1	1:B:158:ARG:NH1	2.54	0.41
1:B:75:LYS:HG2	1:B:87:GLY:CA	2.51	0.41
1:C:92:ASN:HD22	1:C:92:ASN:HA	1.62	0.41
1:D:277:GLU:HG3	1:D:332:CYS:HB3	2.03	0.41
1:D:307:THR:O	1:D:308:GLU:C	2.57	0.41
1:D:395:TYR:HD2	1:D:425:TYR:CD2	2.39	0.41
1:A:276:HIS:NE2	2:P:749:GLY:N	2.66	0.41
1:A:264:ASN:CG	1:A:267:LYS:HG3	2.41	0.40
1:A:49:LEU:HD21	1:A:98:ARG:HD2	2.03	0.40
1:D:312:ASP:CG	1:D:314:TYR:CD1	2.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:ASN:HD22	1:A:66:ASN:HA	1.65	0.40
1:A:70:LEU:CD1	1:A:74:LEU:HB2	2.48	0.40
1:C:275:PRO:HB2	1:C:334:GLU:O	2.21	0.40
1:C:293:PHE:HA	1:C:294:PRO:HA	1.63	0.40
1:C:92:ASN:O	1:C:96:THR:HG23	2.22	0.40
1:D:227:ASN:CB	1:D:270:LYS:HA	2.48	0.40
1:A:180:ASP:OD2	1:A:195:PHE:HZ	2.04	0.40
1:A:320:THR:OG1	1:A:321:GLU:N	2.54	0.40
1:A:193:HIS:CA	1:A:404:GLN:OE1	2.69	0.40
1:A:433:LEU:HD22	1:A:437:ASP:HB2	2.02	0.40
1:C:73:THR:O	1:C:74:LEU:C	2.58	0.40
1:D:236:PRO:HB3	1:D:245:ASN:OD1	2.22	0.40
2:R:749:GLY:HA2	2:R:750:PRO:HD3	1.94	0.40
1:C:124:ILE:HB	1:C:159:PHE:HD1	1.86	0.40
1:C:307:THR:O	1:C:308:GLU:C	2.60	0.40
1:D:323:TYR:O	1:D:327:LYS:HA	2.21	0.40
1:A:137:PRO:HD3	1:A:333:PRO:O	2.22	0.40
1:B:242:LYS:HD3	1:B:244:TYR:CZ	2.57	0.40
1:C:127:ARG:NH1	1:C:165:GLY:N	2.67	0.40
1:C:235:PHE:HA	1:C:236:PRO:HA	1.80	0.40
1:D:151:TRP:O	1:D:155:THR:HG23	2.21	0.40

All (3) 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)
6:C:2007:HOH:O	6:D:2007:HOH:O[4_555]	1.89	0.31
1:B:67:LEU:CD1	1:B:290:PRO:CG[4_465]	2.16	0.04
1:B:361:GLU:O	1:D:68:PHE:CE1[4_465]	2.19	0.01

## 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	419/421 (100%)	376 (90%)	33 (8%)	10 (2%)	7	16
1	B	417/421 (99%)	374 (90%)	31 (7%)	12 (3%)	6	12
1	C	416/421 (99%)	378 (91%)	31 (8%)	7 (2%)	11	25
1	D	417/421 (99%)	370 (89%)	35 (8%)	12 (3%)	6	12
2	P	6/8 (75%)	4 (67%)	0	2 (33%)	0	0
2	R	6/8 (75%)	1 (17%)	4 (67%)	1 (17%)	0	0
All	All	1681/1700 (99%)	1503 (89%)	134 (8%)	44 (3%)	7	14

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	67	LEU
1	A	120	ASP
1	B	67	LEU
1	B	108	ALA
1	B	379	ALA
1	C	110	TYR
1	D	66	ASN
1	D	111	ASN
1	D	113	PHE
1	D	218	GLY
1	D	344	SER
2	P	747	PRO
2	P	748	ALA
1	A	276	HIS
1	B	176	TRP
1	B	177	GLU
1	B	276	HIS
1	B	345	GLU
1	C	118	LYS
1	D	327	LYS
2	R	747	PRO
1	A	327	LYS
1	A	370	ASP
1	B	218	GLY
1	C	85	GLN
1	C	345	GLU
1	A	109	ASN
1	B	113	PHE
1	C	109	ASN
1	C	276	HIS

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Mol	Chain	Res	Type
1	D	112	PHE
1	D	356	LEU
1	A	85	GLN
1	A	379	ALA
1	B	188	ASP
1	C	91	GLN
1	D	85	GLN
1	D	180	ASP
1	B	347	ALA
1	A	61	PRO
1	B	341	GLY
1	A	371	GLY
1	D	114	PRO
1	D	449	PRO

### 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	351/351 (100%)	295 (84%)	56 (16%)	3	6
1	B	349/351 (99%)	312 (89%)	37 (11%)	8	17
1	C	348/351 (99%)	306 (88%)	42 (12%)	6	12
1	D	349/351 (99%)	294 (84%)	55 (16%)	3	6
2	P	3/3 (100%)	3 (100%)	0	100	100
2	R	3/3 (100%)	3 (100%)	0	100	100
All	All	1403/1410 (100%)	1213 (86%)	190 (14%)	5	9

All (190) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	ILE
1	A	36	LYS
1	A	40	ASP
1	A	44	LYS

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Mol	Chain	Res	Type
1	A	46	ASP
1	A	62	LYS
1	A	64	SER
1	A	66	ASN
1	A	68	PHE
1	A	70	LEU
1	A	72	ASP
1	A	94	ILE
1	A	98	ARG
1	A	101	ARG
1	A	109	ASN
1	A	110	TYR
1	A	112	PHE
1	A	115	ARG
1	A	116	LYS
1	A	121	LYS
1	A	135	LEU
1	A	172	ASN
1	A	175	ARG
1	A	177	GLU
1	A	187	LYS
1	A	193	HIS
1	A	199	THR
1	A	212	LEU
1	A	221	VAL
1	A	252	ARG
1	A	268	ASP
1	A	281	THR
1	A	282	MET
1	A	285	ASN
1	A	301	SER
1	A	306	THR
1	A	311	THR
1	A	325	ARG
1	A	326	ASP
1	A	327	LYS
1	A	343	ASN
1	A	345	GLU
1	A	354	THR
1	A	359	LYS
1	A	361	GLU
1	A	364	THR

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Mol	Chain	Res	Type
1	A	365	SER
1	A	370	ASP
1	A	380	ASN
1	A	383	ASP
1	A	384	ASP
1	A	396	SER
1	A	429	LYS
1	A	443	GLU
1	A	450	ASP
1	A	452	ASP
1	B	46	ASP
1	B	56	THR
1	B	62	LYS
1	B	72	ASP
1	B	74	LEU
1	B	77	MET
1	B	93	THR
1	B	101	ARG
1	B	109	ASN
1	B	110	TYR
1	B	112	PHE
1	B	123	GLN
1	B	128	ILE
1	B	142	ASP
1	B	160	SER
1	B	172	ASN
1	B	187	LYS
1	B	188	ASP
1	B	193	HIS
1	B	201	VAL
1	B	211	GLU
1	B	266	GLU
1	B	270	LYS
1	B	292	LYS
1	B	337	MET
1	B	338	SER
1	B	339	THR
1	B	354	THR
1	B	358	ASN
1	B	361	GLU
1	B	378	THR
1	B	383	ASP

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Mol	Chain	Res	Type
1	B	412	GLU
1	B	428	THR
1	B	429	LYS
1	B	433	LEU
1	B	448	SER
1	C	40	ASP
1	C	55	ASN
1	C	62	LYS
1	C	63	GLU
1	C	64	SER
1	C	67	LEU
1	C	89	LEU
1	C	92	ASN
1	C	93	THR
1	C	96	THR
1	C	101	ARG
1	C	102	CYS
1	C	113	PHE
1	C	115	ARG
1	C	116	LYS
1	C	121	LYS
1	C	160	SER
1	C	161	ARG
1	C	178	HIS
1	C	187	LYS
1	C	190	LEU
1	C	201	VAL
1	C	214	THR
1	C	215	LEU
1	C	234	LYS
1	C	242	LYS
1	C	252	ARG
1	C	254	ASP
1	C	266	GLU
1	C	268	ASP
1	C	276	HIS
1	C	280	PHE
1	C	281	THR
1	C	298	GLN
1	C	301	SER
1	C	310	ARG
1	C	339	THR

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Mol	Chain	Res	Type
1	C	365	SER
1	C	368	ARG
1	C	383	ASP
1	C	426	THR
1	C	432	ARG
1	D	34	ILE
1	D	35	ILE
1	D	45	THR
1	D	46	ASP
1	D	52	GLN
1	D	62	LYS
1	D	64	SER
1	D	67	LEU
1	D	70	LEU
1	D	72	ASP
1	D	75	LYS
1	D	78	GLN
1	D	88	ASP
1	D	90	ASP
1	D	92	ASN
1	D	99	LYS
1	D	111	ASN
1	D	115	ARG
1	D	116	LYS
1	D	118	LYS
1	D	127	ARG
1	D	132	THR
1	D	158	ARG
1	D	166	GLU
1	D	172	ASN
1	D	177	GLU
1	D	178	HIS
1	D	193	HIS
1	D	207	PHE
1	D	217	GLU
1	D	224	LYS
1	D	227	ASN
1	D	270	LYS
1	D	276	HIS
1	D	282	MET
1	D	298	GLN
1	D	301	SER

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Mol	Chain	Res	Type
1	D	319	THR
1	D	325	ARG
1	D	326	ASP
1	D	327	LYS
1	D	332	CYS
1	D	337	MET
1	D	339	THR
1	D	349	CYS
1	D	356	LEU
1	D	358	ASN
1	D	364	THR
1	D	380	ASN
1	D	384	ASP
1	D	428	THR
1	D	430	ASN
1	D	432	ARG
1	D	434	SER
1	D	441	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	GLN
1	A	55	ASN
1	A	66	ASN
1	A	172	ASN
1	A	285	ASN
1	A	415	GLN
1	B	172	ASN
1	B	407	HIS
1	B	415	GLN
1	C	91	GLN
1	C	92	ASN
1	C	104	ASN
1	C	219	GLN
1	C	240	ASN
1	C	276	HIS
1	C	403	HIS
1	C	407	HIS
1	C	430	ASN
1	D	85	GLN
1	D	92	ASN

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Mol	Chain	Res	Type
1	D	111	ASN
1	D	123	GLN
1	D	172	ASN
1	D	219	GLN
1	D	227	ASN
1	D	358	ASN
1	D	380	ASN
1	D	442	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 22 ligands modelled in this entry, 16 are monoatomic - leaving 6 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	SO4	A	851	-	4,4,4	0.82	0	6,6,6	0.15	0
3	SO4	B	852	-	4,4,4	0.88	0	6,6,6	0.44	0
3	SO4	B	853	-	4,4,4	1.50	0	6,6,6	0.22	0
3	SO4	C	850	-	4,4,4	1.00	0	6,6,6	0.60	0
3	SO4	C	856	-	4,4,4	1.08	0	6,6,6	0.36	0
3	SO4	D	857	-	4,4,4	1.56	1 (25%)	6,6,6	0.52	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	SO4	A	851	-	-	0/0/0/0	0/0/0/0
3	SO4	B	852	-	-	0/0/0/0	0/0/0/0
3	SO4	B	853	-	-	0/0/0/0	0/0/0/0
3	SO4	C	850	-	-	0/0/0/0	0/0/0/0
3	SO4	C	856	-	-	0/0/0/0	0/0/0/0
3	SO4	D	857	-	-	0/0/0/0	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	857	SO4	O3-S	2.23	1.55	1.47

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	852	SO4	1	0
3	B	853	SO4	1	0
3	C	850	SO4	3	0
3	D	857	SO4	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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	421/421 (100%)	0.24	21 (4%) 32 30	16, 34, 78, 100	0
1	B	419/421 (99%)	0.08	11 (2%) 59 58	15, 31, 60, 100	0
1	C	418/421 (99%)	0.20	16 (3%) 44 42	17, 37, 71, 100	0
1	D	419/421 (99%)	0.38	23 (5%) 29 26	21, 47, 83, 100	0
2	P	8/8 (100%)	7.49	8 (100%) 0 0	78, 81, 90, 95	0
2	R	8/8 (100%)	4.08	8 (100%) 0 0	71, 74, 78, 80	0
All	All	1693/1700 (99%)	0.28	87 (5%) 32 29	15, 38, 78, 100	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	P	746	GLY	14.3
1	C	115	ARG	11.7
1	D	113	PHE	9.8
1	C	112	PHE	9.4
1	D	114	PRO	9.3
1	B	109	ASN	9.0
2	P	753	ALA	8.9
2	P	750	PRO	8.7
1	A	114	PRO	8.6
1	B	110	TYR	8.5
1	C	114	PRO	8.3
1	B	114	PRO	8.2
1	B	112	PHE	8.1
1	A	110	TYR	8.1
1	A	111	ASN	7.8
1	B	113	PHE	7.7
2	R	750	PRO	7.7
1	A	113	PHE	7.5
1	D	112	PHE	7.2

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Mol	Chain	Res	Type	RSRZ
2	P	751	PRO	7.1
1	D	110	TYR	6.9
1	C	113	PHE	6.7
1	D	111	ASN	6.7
2	P	747	PRO	6.6
1	B	115	ARG	6.5
1	A	176	TRP	6.1
1	C	110	TYR	6.0
1	D	115	ARG	5.6
1	D	450	ASP	5.6
2	P	748	ALA	5.3
2	R	752	GLY	5.2
1	D	356	LEU	5.2
2	P	749	GLY	5.1
1	C	109	ASN	5.0
1	D	109	ASN	4.7
2	R	751	PRO	4.5
1	A	112	PHE	4.5
2	R	749	GLY	4.4
1	B	111	ASN	4.4
1	C	111	ASN	4.3
1	D	66	ASN	4.2
2	P	752	GLY	3.9
1	A	115	ARG	3.9
1	D	176	TRP	3.8
1	A	452	ASP	3.8
1	C	35	ILE	3.8
2	R	747	PRO	3.7
1	C	32	SER	3.6
1	D	35	ILE	3.6
1	C	58	TYR	3.5
1	C	33	PRO	3.5
1	D	353	PHE	3.2
1	A	32	SER	3.1
1	D	449	PRO	3.0
1	B	116	LYS	2.9
1	C	280	PHE	2.9
1	B	67	LEU	2.9
1	A	40	ASP	2.9
1	A	41	VAL	2.8
1	C	267	LYS	2.8
1	A	33	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	34	ILE	2.7
1	A	280	PHE	2.6
1	B	176	TRP	2.6
2	R	746	GLY	2.5
1	D	154	VAL	2.5
1	D	271	TYR	2.5
1	D	350	VAL	2.5
2	R	753	ALA	2.5
1	D	70	LEU	2.4
1	D	116	LYS	2.4
1	B	366	ALA	2.4
1	D	108	ALA	2.4
1	D	151	TRP	2.3
1	C	34	ILE	2.3
1	A	58	TYR	2.3
1	A	364	THR	2.3
1	D	68	PHE	2.2
1	C	228	ALA	2.2
1	A	385	ARG	2.1
1	A	68	PHE	2.1
2	R	748	ALA	2.1
1	A	282	MET	2.1
1	A	109	ASN	2.1
1	A	116	LYS	2.1
1	C	238	LEU	2.1
1	A	366	ALA	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	CA	B	999	1/1	0.21	0.32	5.77	100,100,100,100	0
5	CA	D	999	1/1	0.46	0.32	3.83	100,100,100,100	0
5	CA	A	999	1/1	0.75	0.24	2.58	76,76,76,76	0
3	SO4	B	853	5/5	0.89	0.22	2.03	72,72,74,75	0
3	SO4	C	856	5/5	0.77	0.24	1.78	75,77,77,79	0
3	SO4	B	852	5/5	0.93	0.24	0.81	64,65,66,67	0
3	SO4	A	851	5/5	0.97	0.20	0.63	40,41,44,45	0
3	SO4	D	857	5/5	0.96	0.19	0.19	46,47,48,49	0
5	CA	D	998	1/1	0.91	0.19	0.17	34,34,34,34	0
5	CA	C	999	1/1	0.86	0.13	-0.17	94,94,94,94	0
3	SO4	C	850	5/5	0.96	0.16	-0.57	41,41,43,44	0
4	ZN	D	997	1/1	0.98	0.15	-0.79	40,40,40,40	0
5	CA	A	998	1/1	0.94	0.14	-1.14	20,20,20,20	0
5	CA	C	998	1/1	0.96	0.16	-1.61	30,30,30,30	0
5	CA	B	998	1/1	0.87	0.15	-1.63	20,20,20,20	0
4	ZN	C	997	1/1	1.00	0.15	-2.18	26,26,26,26	0
4	ZN	B	997	1/1	0.98	0.14	-2.46	23,23,23,23	0
4	ZN	A	997	1/1	0.99	0.14	-2.90	20,20,20,20	0
4	ZN	C	996	1/1	0.98	0.12	-3.21	32,32,32,32	0
4	ZN	A	996	1/1	0.99	0.07	-3.66	26,26,26,26	0
4	ZN	D	996	1/1	0.99	0.10	-4.34	35,35,35,35	0
4	ZN	B	996	1/1	0.99	0.11	-4.41	24,24,24,24	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.