



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 10:17 AM GMT

PDB ID : 1E9Y  
Title : CRYSTAL STRUCTURE OF HELICOBACTER PYLORI UREASE IN  
COMPLEX WITH ACETOHYDROXAMIC ACID  
Authors : Ha, N.-C.; Oh, S.-T.; Oh, B.-H.  
Deposited on : 2000-11-01  
Resolution : 3.00 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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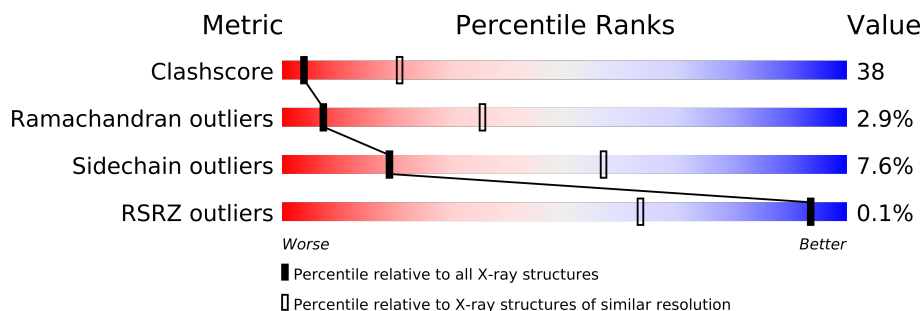
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	238	
2	B	569	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6272 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called UREASE SUBUNIT ALPHA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	238	Total	C	N	O	S	0	0	0
			1864	1175	333	348	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	170	ALA	SER	CONFLICT	UNP P14916

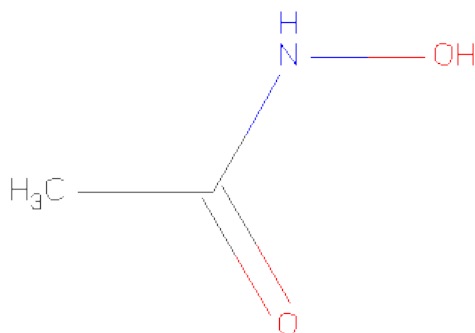
- Molecule 2 is a protein called UREASE SUBUNIT BETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	569	Total	C	N	O	S	0	0	0
			4335	2716	748	850	21			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	219	KCX	LYS	MODIFIED RESIDUE	UNP P69996
B	324	LYS	LEU	CONFLICT	UNP P69996
B	355	ALA	ILE	CONFLICT	UNP P69996
B	522	VAL	ILE	CONFLICT	UNP P69996
B	531	ASN	ASP	CONFLICT	UNP P69996

- Molecule 3 is ACETOHYDROXAMIC ACID (three-letter code: HAE) (formula: C<sub>2</sub>H<sub>5</sub>NO<sub>2</sub>).



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

- Molecule 4 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Ni	0	0
			2	2		

- Molecule 5 is water.

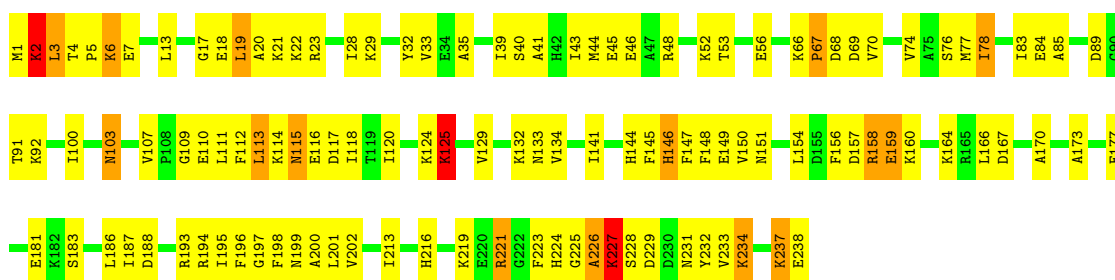
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	9	Total	O	0	0
			9	9		
5	B	57	Total	O	0	0
			57	57		

### 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.

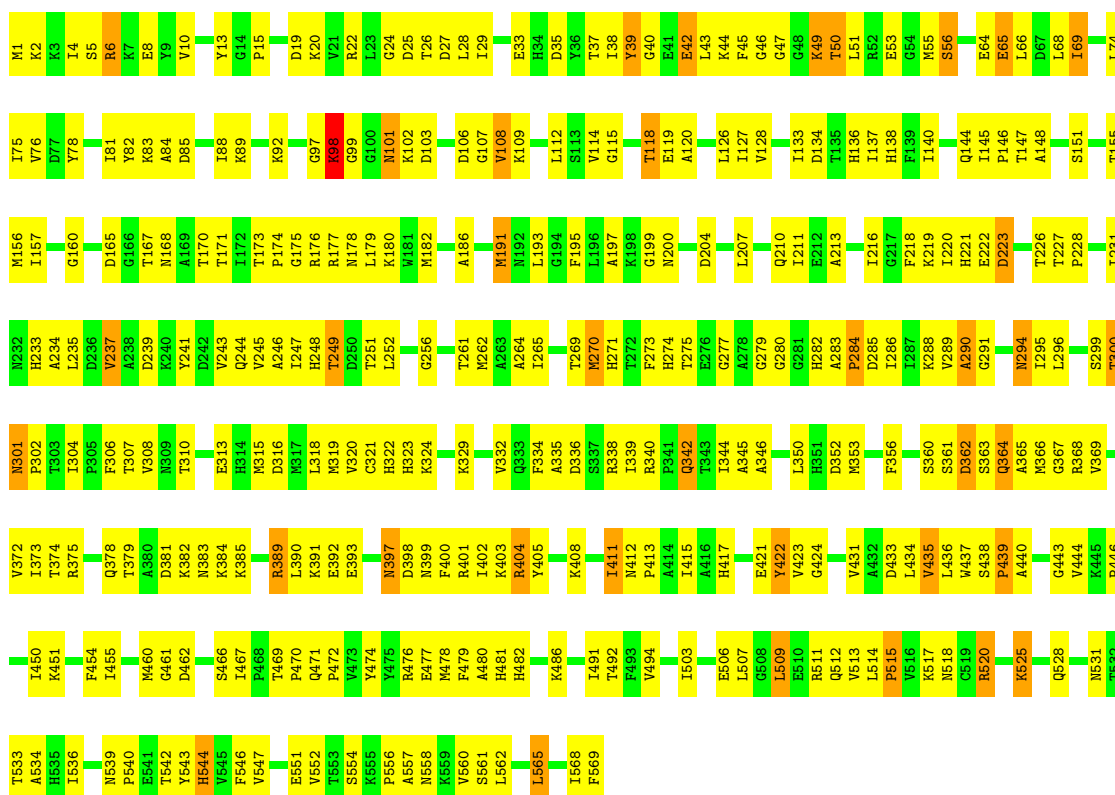
#### • Molecule 1: UREASE SUBUNIT ALPHA

Chain A:



#### • Molecule 2: UREASE SUBUNIT BETA

Chain B:



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	178.16Å 178.16Å 178.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 39.84 – 2.80	Depositor EDS
% Data completeness (in resolution range)	92.5 (20.00-3.00) 95.0 (39.84-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.07 (at 2.81Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.213 , 0.282 0.223 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	43.1	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 12.3	EDS
Estimated twinning fraction	0.027 for -l,-k,-h	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 22157 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	6272	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.78% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NI, HAE, KCX

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.42	0/1892	0.62	0/2532
2	B	0.45	0/4406	0.67	0/5958
All	All	0.44	0/6298	0.66	0/8490

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1864	0	1909	122	0
2	B	4335	0	4263	365	0
3	B	5	0	5	0	0
4	B	2	0	0	0	0
5	A	9	0	0	0	0
5	B	57	0	0	7	0
All	All	6272	0	6177	468	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 38.

All (468) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:274:HIS:HB3	2:B:300:THR:HB	1.41	1.02
2:B:140:ILE:HD12	2:B:364:GLN:HB3	1.43	0.98
2:B:6:ARG:HH11	2:B:6:ARG:HG2	1.25	0.97
2:B:284:PRO:HB2	2:B:340:ARG:HD3	1.43	0.96
2:B:244:GLN:NE2	2:B:245:VAL:H	1.67	0.92
2:B:363:SER:HB3	2:B:369:VAL:HB	1.51	0.91
2:B:200:ASN:HD21	2:B:221:HIS:H	1.15	0.91
2:B:44:LYS:H	2:B:50:THR:HG22	1.36	0.89
2:B:434:LEU:HD12	2:B:450:ILE:HD11	1.54	0.88
1:A:219:LYS:HE3	1:A:229:ASP:N	1.89	0.88
2:B:101:ASN:ND2	2:B:103:ASP:H	1.73	0.86
2:B:244:GLN:HE21	2:B:245:VAL:N	1.74	0.85
2:B:244:GLN:HE21	2:B:245:VAL:H	0.89	0.85
2:B:44:LYS:H	2:B:50:THR:CG2	1.91	0.84
2:B:136:HIS:HB3	2:B:360:SER:HB3	1.61	0.83
2:B:390:LEU:HB2	2:B:393:GLU:HG2	1.59	0.83
2:B:301:ASN:HB2	2:B:361:SER:HA	1.61	0.82
1:A:1:MET:HG3	1:A:3:LEU:HD13	1.62	0.82
1:A:125:LYS:N	1:A:125:LYS:HD3	1.97	0.79
2:B:275:THR:HG21	2:B:290:ALA:HB2	1.64	0.78
1:A:23:ARG:O	1:A:28:ILE:HG22	1.84	0.78
2:B:249:THR:HG21	2:B:286:ILE:HD13	1.65	0.78
2:B:466:SER:O	2:B:467:ILE:HG23	1.82	0.77
1:A:149:GLU:HG2	1:A:201:LEU:HD12	1.64	0.77
1:A:219:LYS:HE3	1:A:229:ASP:H	1.48	0.76
2:B:397:ASN:HD22	2:B:399:ASN:H	1.32	0.75
2:B:346:ALA:O	2:B:350:LEU:HG	1.87	0.75
2:B:301:ASN:HD22	2:B:368:ARG:H	1.34	0.74
1:A:109:GLY:HA2	2:B:22:ARG:O	1.87	0.74
2:B:492:THR:CG2	2:B:511:ARG:HD2	2.17	0.74
2:B:101:ASN:HD21	2:B:103:ASP:HB2	1.53	0.74
1:A:159:GLU:HG3	1:A:160:LYS:HD2	1.69	0.74
2:B:128:VAL:HG22	2:B:436:LEU:HD22	1.69	0.72
2:B:171:THR:OG1	2:B:219:KCX:HD3	1.89	0.72
1:A:2:LYS:HD3	1:A:2:LYS:H	1.54	0.72
2:B:46:GLY:HA3	2:B:49:LYS:HD3	1.71	0.72
2:B:211:ILE:HD13	2:B:243:VAL:HG21	1.71	0.72
2:B:284:PRO:CB	2:B:340:ARG:HD3	2.20	0.71
2:B:405:TYR:HA	2:B:408:LYS:HD2	1.71	0.71
2:B:423:VAL:HG22	2:B:424:GLY:H	1.53	0.71
1:A:118:ILE:HD11	2:B:6:ARG:NE	2.05	0.71
1:A:156:PHE:CE1	1:A:158:ARG:HD3	2.26	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:66:LEU:HD21	2:B:112:LEU:HA	1.74	0.70
2:B:329:LYS:HA	2:B:332:VAL:HG22	1.74	0.70
2:B:204:ASP:OD1	2:B:233:HIS:HD2	1.75	0.69
2:B:50:THR:O	2:B:56:SER:HB2	1.91	0.69
1:A:147:PHE:CE1	1:A:166:LEU:HD21	2.28	0.69
2:B:315:MET:O	2:B:319:MET:HG2	1.93	0.69
2:B:37:THR:HG22	5:B:2004:HOH:O	1.91	0.69
2:B:390:LEU:HD12	2:B:401:ARG:HB2	1.75	0.69
2:B:156:MET:N	2:B:191:MET:HE1	2.08	0.69
2:B:24:GLY:HA2	2:B:440:ALA:O	1.93	0.69
2:B:101:ASN:ND2	2:B:103:ASP:HB2	2.08	0.68
2:B:35:ASP:OD2	2:B:37:THR:HG23	1.93	0.68
2:B:423:VAL:HG22	5:B:2013:HOH:O	1.92	0.68
1:A:4:THR:HG1	1:A:7:GLU:HG3	1.59	0.68
2:B:25:ASP:OD1	2:B:561:SER:HB2	1.93	0.68
2:B:444:VAL:CG2	2:B:562:LEU:HD22	2.24	0.68
1:A:13:LEU:HB2	2:B:472:PRO:HG3	1.76	0.68
1:A:6:LYS:HB3	1:A:6:LYS:NZ	2.09	0.68
2:B:520:ARG:HH11	2:B:520:ARG:HA	1.58	0.67
2:B:492:THR:HG23	2:B:511:ARG:HD2	1.75	0.67
2:B:220:ILE:HB	2:B:247:ILE:HG13	1.75	0.67
2:B:398:ASP:O	2:B:402:ILE:HG12	1.95	0.67
2:B:365:ALA:O	2:B:366:MET:HB2	1.95	0.67
2:B:525:LYS:HE2	2:B:525:LYS:O	1.95	0.67
1:A:221:ARG:CG	1:A:221:ARG:HH11	2.08	0.67
1:A:219:LYS:HG2	1:A:229:ASP:OD2	1.95	0.67
2:B:470:PRO:HB2	5:B:2046:HOH:O	1.93	0.67
2:B:307:THR:OG1	2:B:310:THR:HG23	1.95	0.67
2:B:435:VAL:HG11	5:B:2018:HOH:O	1.94	0.67
2:B:350:LEU:HD23	2:B:353:MET:CE	2.25	0.66
2:B:422:TYR:O	2:B:431:VAL:HG22	1.96	0.66
2:B:6:ARG:NH1	2:B:6:ARG:HG2	2.03	0.66
2:B:342:GLN:NE2	2:B:342:GLN:H	1.93	0.66
1:A:40:SER:O	1:A:44:MET:HG3	1.96	0.65
2:B:412:ASN:HD21	2:B:528:GLN:N	1.95	0.65
1:A:164:LYS:HD3	1:A:186:LEU:CD1	2.27	0.65
2:B:200:ASN:HD21	2:B:221:HIS:N	1.93	0.65
2:B:467:ILE:HG13	2:B:470:PRO:HD3	1.79	0.65
2:B:391:LYS:HE2	2:B:392:GLU:OE2	1.96	0.65
2:B:444:VAL:HG22	2:B:562:LEU:HB3	1.77	0.64
2:B:339:ILE:HG22	2:B:339:ILE:O	1.96	0.64
2:B:156:MET:HG3	2:B:191:MET:HE1	1.79	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:525:LYS:HE3	2:B:531:ASN:HB2	1.77	0.64
1:A:164:LYS:HD3	1:A:186:LEU:HD12	1.79	0.64
2:B:151:SER:O	2:B:373:ILE:HD12	1.98	0.63
1:A:197:GLY:HA3	2:B:53:GLU:OE2	1.96	0.63
2:B:294:ASN:HD22	2:B:294:ASN:N	1.95	0.63
2:B:248:HIS:CE1	2:B:280:GLY:HA3	2.34	0.63
1:A:124:LYS:O	1:A:187:ILE:HG22	1.97	0.63
2:B:227:THR:O	2:B:231:ILE:HG13	1.99	0.63
2:B:382:LYS:HE3	2:B:560:VAL:HA	1.79	0.63
2:B:423:VAL:HG22	2:B:424:GLY:N	2.14	0.62
1:A:219:LYS:CE	1:A:228:SER:HA	2.29	0.62
1:A:4:THR:OG1	1:A:7:GLU:HG3	1.99	0.61
2:B:412:ASN:HD21	2:B:528:GLN:H	1.47	0.61
1:A:112:PHE:HB2	2:B:20:LYS:HB2	1.83	0.61
2:B:269:THR:HB	2:B:520:ARG:HH12	1.66	0.61
1:A:124:LYS:C	1:A:125:LYS:HD3	2.20	0.61
2:B:175:GLY:O	2:B:179:LEU:HG	2.00	0.61
2:B:397:ASN:ND2	2:B:399:ASN:H	1.99	0.61
2:B:434:LEU:HB2	2:B:450:ILE:HD11	1.83	0.60
2:B:318:LEU:HD22	2:B:339:ILE:HG13	1.83	0.60
1:A:237:LYS:O	1:A:237:LYS:HG3	2.00	0.60
2:B:568:ILE:HG23	2:B:569:PHE:HD1	1.67	0.60
2:B:133:ILE:HG12	2:B:155:THR:HB	1.83	0.60
1:A:221:ARG:HB3	1:A:221:ARG:HH11	1.65	0.60
1:A:129:VAL:O	1:A:183:SER:HA	2.02	0.60
1:A:6:LYS:HZ3	1:A:6:LYS:HB3	1.65	0.60
1:A:111:LEU:N	1:A:111:LEU:HD12	2.16	0.60
2:B:308:VAL:HG23	2:B:557:ALA:O	2.02	0.60
2:B:269:THR:HB	2:B:520:ARG:NH1	2.17	0.59
2:B:26:THR:HB	2:B:381:ASP:OD1	2.02	0.59
2:B:277:GLY:HA3	2:B:340:ARG:NH2	2.18	0.59
2:B:170:THR:HG22	2:B:221:HIS:CG	2.37	0.59
2:B:45:PHE:HB2	2:B:51:LEU:HD12	1.84	0.59
2:B:494:VAL:O	2:B:515:PRO:HA	2.02	0.59
1:A:70:VAL:HG21	1:A:100:ILE:HD12	1.84	0.59
2:B:6:ARG:CG	2:B:6:ARG:HH11	2.05	0.59
2:B:364:GLN:HE21	2:B:364:GLN:N	2.01	0.59
2:B:199:GLY:HA3	2:B:220:ILE:HD13	1.85	0.59
2:B:207:LEU:HD23	2:B:237:VAL:HG11	1.84	0.59
1:A:158:ARG:HG2	1:A:158:ARG:HH11	1.68	0.59
2:B:525:LYS:NZ	2:B:531:ASN:HD22	2.01	0.59
1:A:221:ARG:HH11	1:A:221:ARG:HG2	1.68	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:239:ASP:HA	2:B:520:ARG:HG2	1.85	0.58
2:B:294:ASN:HD22	2:B:294:ASN:H	1.49	0.58
2:B:274:HIS:HB3	2:B:300:THR:CB	2.27	0.58
2:B:148:ALA:HB2	2:B:369:VAL:HG22	1.86	0.58
2:B:434:LEU:O	2:B:450:ILE:HG12	2.03	0.58
2:B:318:LEU:HB2	2:B:339:ILE:HD11	1.86	0.58
2:B:361:SER:O	2:B:362:ASP:HB3	2.04	0.58
2:B:239:ASP:OD1	2:B:520:ARG:HG3	2.03	0.58
2:B:284:PRO:HG3	2:B:543:TYR:CE1	2.39	0.57
2:B:389:ARG:HG2	2:B:393:GLU:HG3	1.85	0.57
1:A:19:LEU:HD13	2:B:568:ILE:HD11	1.86	0.57
2:B:469:THR:N	2:B:470:PRO:HD2	2.19	0.57
2:B:115:GLY:H	2:B:118:THR:HG22	1.68	0.57
2:B:324:LYS:HE3	2:B:334:PHE:CD2	2.40	0.57
2:B:56:SER:O	2:B:101:ASN:HB2	2.05	0.57
2:B:114:VAL:HG13	2:B:118:THR:HG21	1.86	0.56
2:B:304:ILE:HG23	2:B:379:THR:OG1	2.04	0.56
1:A:83:ILE:HD12	1:A:84:GLU:H	1.70	0.56
2:B:66:LEU:O	2:B:118:THR:HB	2.04	0.56
2:B:249:THR:HB	2:B:282:HIS:H	1.70	0.56
2:B:301:ASN:HD21	2:B:368:ARG:HB2	1.71	0.56
1:A:221:ARG:CB	1:A:221:ARG:HH11	2.19	0.56
2:B:391:LYS:HG2	2:B:392:GLU:OE1	2.06	0.56
1:A:157:ASP:OD2	1:A:160:LYS:HD3	2.05	0.56
2:B:389:ARG:HH11	2:B:389:ARG:HG3	1.71	0.55
2:B:329:LYS:O	2:B:332:VAL:HG22	2.06	0.55
2:B:301:ASN:ND2	2:B:368:ARG:H	2.03	0.55
1:A:39:ILE:O	1:A:43:ILE:HG12	2.06	0.55
2:B:44:LYS:O	2:B:50:THR:HG22	2.07	0.55
2:B:340:ARG:O	2:B:344:ILE:HG13	2.07	0.55
1:A:158:ARG:NH1	1:A:224:HIS:O	2.39	0.55
2:B:109:LYS:HE3	2:B:109:LYS:HA	1.89	0.55
1:A:225:GLY:O	1:A:227:LYS:N	2.39	0.55
2:B:92:LYS:NZ	2:B:431:VAL:HG12	2.21	0.55
2:B:115:GLY:O	2:B:118:THR:HG22	2.06	0.55
2:B:467:ILE:HG13	2:B:470:PRO:CD	2.37	0.55
2:B:37:THR:O	2:B:38:ILE:HD13	2.07	0.55
1:A:33:VAL:HG11	2:B:568:ILE:HB	1.88	0.55
2:B:397:ASN:HD22	2:B:399:ASN:N	2.03	0.55
2:B:422:TYR:OH	2:B:515:PRO:O	2.20	0.54
2:B:542:THR:HG23	2:B:544:HIS:HB2	1.89	0.54
2:B:507:LEU:HB2	2:B:509:LEU:HD13	1.89	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:433:ASP:OD1	2:B:451:LYS:HD2	2.08	0.54
1:A:132:LYS:HB2	1:A:181:GLU:HG3	1.90	0.54
2:B:437:TRP:CZ3	2:B:446:PRO:HB3	2.43	0.54
2:B:43:LEU:HA	2:B:50:THR:HG21	1.90	0.54
2:B:249:THR:HG21	2:B:286:ILE:CD1	2.37	0.54
1:A:134:VAL:HG12	1:A:134:VAL:O	2.06	0.54
2:B:300:THR:HG23	2:B:302:PRO:CG	2.38	0.54
2:B:389:ARG:HG3	2:B:389:ARG:NH1	2.23	0.54
2:B:186:ALA:HB1	2:B:193:LEU:HD12	1.89	0.54
2:B:461:GLY:HA2	2:B:472:PRO:O	2.08	0.54
2:B:539:ASN:CG	2:B:542:THR:HG22	2.28	0.54
2:B:197:ALA:HB1	2:B:210:GLN:OE1	2.08	0.54
2:B:492:THR:HG22	2:B:511:ARG:HH11	1.72	0.54
1:A:177:GLU:HA	1:A:177:GLU:OE1	2.07	0.54
2:B:222:GLU:HB2	2:B:248:HIS:HD2	1.73	0.53
2:B:302:PRO:HG3	2:B:366:MET:O	2.08	0.53
2:B:450:ILE:O	2:B:450:ILE:HG13	2.07	0.53
2:B:76:VAL:HG23	2:B:127:ILE:HG23	1.90	0.53
2:B:74:LEU:HD12	2:B:82:TYR:O	2.07	0.53
2:B:492:THR:HG22	2:B:511:ARG:NH1	2.23	0.53
1:A:144:HIS:C	2:B:55:MET:HE3	2.28	0.53
2:B:361:SER:O	2:B:362:ASP:CB	2.57	0.53
2:B:284:PRO:HB2	2:B:340:ARG:CD	2.29	0.53
2:B:207:LEU:HD21	2:B:234:ALA:HA	1.90	0.53
2:B:411:ILE:O	2:B:415:ILE:HG13	2.09	0.53
2:B:114:VAL:HG13	2:B:118:THR:CG2	2.39	0.52
2:B:75:ILE:HD12	2:B:82:TYR:CE1	2.44	0.52
2:B:200:ASN:ND2	2:B:221:HIS:H	1.95	0.52
2:B:69:ILE:HD13	2:B:114:VAL:CG2	2.39	0.52
1:A:114:LYS:O	1:A:115:ASN:C	2.48	0.52
2:B:126:LEU:N	2:B:126:LEU:HD12	2.25	0.52
2:B:101:ASN:HD22	2:B:102:LYS:N	2.08	0.52
2:B:492:THR:HG21	5:B:2024:HOH:O	2.09	0.51
1:A:150:VAL:HG21	1:A:154:LEU:HD12	1.93	0.51
2:B:136:HIS:CB	2:B:360:SER:HB3	2.36	0.51
1:A:107:VAL:HG23	1:A:110:GLU:HB3	1.93	0.51
2:B:301:ASN:ND2	2:B:368:ARG:HB2	2.26	0.51
1:A:221:ARG:NH1	1:A:221:ARG:HG2	2.24	0.51
2:B:285:ASP:O	2:B:288:LYS:HG2	2.11	0.51
2:B:390:LEU:H	2:B:393:GLU:HG3	1.74	0.51
2:B:156:MET:N	2:B:191:MET:CE	2.73	0.51
1:A:117:ASP:OD1	2:B:5:SER:HA	2.11	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:17:GLY:HA3	1:A:41:ALA:HB2	1.93	0.51
2:B:234:ALA:O	2:B:237:VAL:HG13	2.10	0.51
2:B:156:MET:CG	2:B:191:MET:HE1	2.40	0.51
1:A:4:THR:HB	1:A:5:PRO:HD2	1.91	0.51
2:B:221:HIS:CE1	2:B:223:ASP:H	2.27	0.51
1:A:125:LYS:N	1:A:125:LYS:CD	2.73	0.51
2:B:241:TYR:O	2:B:243:VAL:HG13	2.10	0.51
2:B:102:LYS:HA	2:B:108:VAL:HG11	1.93	0.51
1:A:199:ASN:O	1:A:200:ALA:HB3	2.11	0.51
2:B:115:GLY:H	2:B:118:THR:CG2	2.23	0.51
1:A:21:LYS:HG3	1:A:22:LYS:N	2.26	0.51
2:B:165:ASP:HA	2:B:168:ASN:HD22	1.75	0.51
2:B:6:ARG:CG	2:B:6:ARG:NH1	2.68	0.51
2:B:319:MET:HE1	2:B:335:ALA:HB2	1.92	0.50
1:A:6:LYS:HD2	1:A:6:LYS:C	2.31	0.50
1:A:186:LEU:O	1:A:186:LEU:HD12	2.11	0.50
1:A:74:VAL:HG12	1:A:100:ILE:HD11	1.92	0.50
2:B:533:THR:O	2:B:534:ALA:HB2	2.11	0.50
2:B:511:ARG:O	2:B:513:VAL:HG23	2.11	0.50
2:B:98:LYS:HE3	2:B:99:GLY:O	2.11	0.50
1:A:53:THR:HG23	1:A:56:GLU:OE1	2.11	0.50
2:B:222:GLU:OE1	2:B:251:THR:HB	2.11	0.50
2:B:476:ARG:O	2:B:478:MET:HE2	2.11	0.50
2:B:78:TYR:HA	2:B:403:LYS:HG2	1.93	0.50
2:B:364:GLN:HE21	2:B:364:GLN:CA	2.23	0.50
2:B:299:SER:HB2	2:B:356:PHE:CD2	2.47	0.50
2:B:51:LEU:HD23	2:B:56:SER:HB3	1.94	0.50
1:A:158:ARG:CG	1:A:158:ARG:HH11	2.25	0.50
1:A:21:LYS:HG3	1:A:22:LYS:H	1.77	0.50
1:A:78:ILE:O	1:A:78:ILE:HG22	2.10	0.50
1:A:120:ILE:HG23	2:B:40:GLY:HA2	1.94	0.50
2:B:302:PRO:HD3	2:B:367:GLY:HA2	1.94	0.50
1:A:213:ILE:HG12	1:A:232:TYR:OH	2.11	0.49
2:B:108:VAL:HG22	2:B:108:VAL:O	2.11	0.49
2:B:26:THR:HG22	2:B:561:SER:OG	2.11	0.49
1:A:156:PHE:CZ	1:A:158:ARG:HD3	2.48	0.49
2:B:114:VAL:HA	2:B:118:THR:HG21	1.94	0.49
2:B:220:ILE:CG2	2:B:226:THR:HG23	2.43	0.49
1:A:17:GLY:HA3	1:A:41:ALA:CB	2.42	0.49
2:B:315:MET:HA	2:B:339:ILE:HD12	1.95	0.49
2:B:539:ASN:OD1	2:B:542:THR:HG22	2.12	0.49
2:B:119:GLU:HG3	2:B:120:ALA:N	2.26	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:374:THR:HA	2:B:443:GLY:O	2.13	0.49
2:B:352:ASP:OD2	2:B:383:ASN:HB3	2.12	0.49
2:B:316:ASP:O	2:B:320:VAL:HG23	2.12	0.49
2:B:384:LYS:HA	2:B:401:ARG:HH12	1.77	0.49
1:A:2:LYS:CD	1:A:2:LYS:H	2.23	0.49
2:B:145:ILE:HB	2:B:146:PRO:CD	2.42	0.49
2:B:33:GLU:OE1	2:B:81:ILE:N	2.32	0.49
2:B:44:LYS:N	2:B:50:THR:HG22	2.16	0.49
1:A:45:GLU:O	1:A:48:ARG:HB3	2.13	0.49
1:A:219:LYS:HE3	1:A:228:SER:HA	1.95	0.49
2:B:324:LYS:HE3	2:B:334:PHE:HD2	1.76	0.49
2:B:273:PHE:O	2:B:274:HIS:C	2.51	0.48
2:B:466:SER:O	2:B:467:ILE:CG2	2.57	0.48
2:B:404:ARG:HH11	2:B:404:ARG:CG	2.26	0.48
2:B:78:TYR:CE2	2:B:411:ILE:HG13	2.47	0.48
2:B:301:ASN:N	2:B:302:PRO:HD2	2.28	0.48
2:B:19:ASP:N	2:B:19:ASP:OD2	2.46	0.48
2:B:109:LYS:HD2	2:B:109:LYS:N	2.28	0.48
1:A:156:PHE:O	1:A:225:GLY:HA3	2.12	0.48
2:B:520:ARG:N	2:B:520:ARG:HD2	2.28	0.48
1:A:32:TYR:CD1	1:A:77:MET:HE2	2.48	0.48
1:A:120:ILE:HG23	2:B:40:GLY:CA	2.43	0.48
2:B:6:ARG:HH12	2:B:19:ASP:CG	2.17	0.48
2:B:69:ILE:HD13	2:B:114:VAL:HG21	1.95	0.48
2:B:381:ASP:O	2:B:385:LYS:HG3	2.13	0.48
2:B:306:PHE:CE2	2:B:345:ALA:HB2	2.49	0.48
2:B:83:LYS:O	2:B:84:ALA:HB2	2.13	0.48
2:B:102:LYS:HG2	2:B:102:LYS:O	2.13	0.48
2:B:450:ILE:HG22	2:B:455:ILE:HG12	1.94	0.48
2:B:66:LEU:HD12	2:B:88:ILE:N	2.28	0.48
2:B:300:THR:C	2:B:302:PRO:HD2	2.34	0.48
2:B:361:SER:O	2:B:367:GLY:HA3	2.14	0.48
2:B:517:LYS:O	2:B:518:ASN:HB2	2.14	0.47
2:B:101:ASN:C	2:B:101:ASN:HD22	2.16	0.47
2:B:233:HIS:O	2:B:237:VAL:HG12	2.14	0.47
1:A:233:VAL:HG12	1:A:233:VAL:O	2.14	0.47
2:B:218:PHE:HE1	2:B:237:VAL:HG13	1.78	0.47
1:A:141:ILE:O	1:A:173:ALA:HB1	2.14	0.47
1:A:118:ILE:HD11	2:B:6:ARG:HE	1.78	0.47
1:A:1:MET:HG3	1:A:1:MET:O	2.15	0.47
1:A:35:ALA:HB3	1:A:78:ILE:HD11	1.96	0.47
2:B:492:THR:HG23	2:B:511:ARG:CD	2.42	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:85:ALA:O	1:A:91:THR:HA	2.14	0.47
1:A:118:ILE:CD1	2:B:6:ARG:HE	2.28	0.47
2:B:321:CYS:O	2:B:322:HIS:HB2	2.13	0.47
1:A:145:PHE:HB2	2:B:55:MET:HE1	1.97	0.47
2:B:313:GLU:O	2:B:316:ASP:HB3	2.15	0.47
2:B:64:GLU:O	2:B:89:LYS:HD2	2.14	0.47
2:B:182:MET:HB3	2:B:195:PHE:CE2	2.48	0.47
2:B:275:THR:HB	2:B:356:PHE:CZ	2.49	0.47
2:B:227:THR:HB	2:B:228:PRO:HD2	1.96	0.47
2:B:252:LEU:N	2:B:252:LEU:HD12	2.30	0.47
2:B:101:ASN:C	2:B:101:ASN:ND2	2.68	0.47
2:B:393:GLU:OE1	2:B:398:ASP:HA	2.15	0.47
2:B:226:THR:HG22	2:B:231:ILE:HD11	1.97	0.47
2:B:252:LEU:H	2:B:252:LEU:HD12	1.80	0.46
2:B:544:HIS:HB3	2:B:546:PHE:HE1	1.80	0.46
2:B:207:LEU:HD23	2:B:237:VAL:CG1	2.45	0.46
2:B:404:ARG:O	2:B:408:LYS:HG3	2.16	0.46
2:B:525:LYS:HE2	2:B:525:LYS:CA	2.46	0.46
2:B:27:ASP:O	2:B:29:ILE:HD13	2.16	0.46
2:B:138:HIS:HB3	2:B:140:ILE:HG13	1.96	0.46
2:B:235:LEU:CD1	2:B:265:ILE:HA	2.46	0.46
1:A:150:VAL:O	1:A:151:ASN:C	2.53	0.46
2:B:300:THR:HG23	2:B:302:PRO:HG2	1.98	0.46
1:A:226:ALA:O	1:A:227:LYS:C	2.54	0.46
2:B:145:ILE:HB	2:B:146:PRO:HD3	1.97	0.45
2:B:352:ASP:HB2	2:B:383:ASN:OD1	2.16	0.45
2:B:300:THR:HG23	2:B:302:PRO:HD2	1.96	0.45
2:B:444:VAL:HG22	2:B:562:LEU:HD22	1.96	0.45
2:B:211:ILE:HD11	2:B:218:PHE:CZ	2.52	0.45
2:B:568:ILE:HG12	2:B:568:ILE:O	2.16	0.45
2:B:174:PRO:O	2:B:178:ASN:HB2	2.16	0.45
1:A:76:SER:HB3	1:A:107:VAL:HG12	1.99	0.45
2:B:207:LEU:CD2	2:B:234:ALA:HA	2.47	0.45
1:A:53:THR:OG1	1:A:56:GLU:HG3	2.15	0.45
1:A:115:ASN:O	1:A:116:GLU:HG3	2.17	0.45
2:B:289:VAL:HG12	2:B:295:ILE:HG13	1.97	0.45
2:B:503:ILE:HA	2:B:506:GLU:HB2	1.99	0.45
2:B:115:GLY:O	2:B:118:THR:CG2	2.64	0.45
2:B:365:ALA:HB2	5:B:2021:HOH:O	2.16	0.45
2:B:434:LEU:HB2	2:B:450:ILE:CD1	2.47	0.45
1:A:113:LEU:HG	2:B:10:VAL:HG21	1.98	0.44
2:B:6:ARG:O	2:B:10:VAL:HG23	2.17	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:342:GLN:HE21	2:B:342:GLN:H	1.62	0.44
2:B:271:HIS:ND1	2:B:417:HIS:HE1	2.15	0.44
1:A:118:ILE:CD1	2:B:6:ARG:NE	2.78	0.44
2:B:221:HIS:ND1	2:B:222:GLU:N	2.65	0.44
2:B:455:ILE:HG22	2:B:478:MET:HG3	1.99	0.44
2:B:270:MET:O	2:B:296:LEU:HB2	2.17	0.44
2:B:491:ILE:HG21	2:B:514:LEU:HD23	1.98	0.44
2:B:244:GLN:HG3	2:B:245:VAL:N	2.33	0.44
1:A:17:GLY:O	1:A:20:ALA:HB3	2.18	0.44
1:A:66:LYS:HG2	1:A:69:ASP:OD1	2.18	0.44
1:A:227:LYS:HA	1:A:227:LYS:CE	2.48	0.44
2:B:92:LYS:HZ2	2:B:431:VAL:HG12	1.81	0.44
2:B:160:GLY:HA3	2:B:167:THR:HG23	1.99	0.44
2:B:15:PRO:O	2:B:83:LYS:HD3	2.18	0.44
2:B:10:VAL:HG12	2:B:10:VAL:O	2.17	0.44
1:A:67:PRO:HB2	1:A:103:ASN:CB	2.47	0.44
2:B:421:GLU:O	2:B:421:GLU:HG2	2.16	0.44
2:B:140:ILE:HD11	2:B:168:ASN:HA	2.00	0.44
2:B:221:HIS:HE1	2:B:223:ASP:OD1	2.01	0.43
2:B:405:TYR:O	2:B:408:LYS:HB2	2.18	0.43
2:B:134:ASP:OD1	2:B:137:ILE:HD11	2.17	0.43
2:B:412:ASN:N	2:B:413:PRO:HD2	2.32	0.43
1:A:33:VAL:CG1	2:B:568:ILE:HB	2.48	0.43
2:B:382:LYS:HE2	2:B:560:VAL:HG12	2.00	0.43
2:B:222:GLU:HB2	2:B:248:HIS:CD2	2.52	0.43
2:B:389:ARG:HH11	2:B:389:ARG:CG	2.32	0.43
2:B:176:ARG:HA	2:B:179:LEU:HD12	2.00	0.43
1:A:91:THR:O	1:A:92:LYS:HD3	2.19	0.43
2:B:248:HIS:HE1	2:B:279:GLY:O	2.01	0.43
2:B:438:SER:HA	2:B:439:PRO:HD2	1.70	0.43
2:B:338:ARG:HA	2:B:340:ARG:HH12	1.83	0.43
2:B:28:LEU:C	2:B:29:ILE:HD12	2.39	0.43
2:B:289:VAL:C	2:B:291:GLY:H	2.22	0.43
2:B:39:TYR:HA	2:B:42:GLU:OE2	2.18	0.43
2:B:369:VAL:O	2:B:369:VAL:HG22	2.19	0.43
2:B:397:ASN:ND2	2:B:399:ASN:HB2	2.34	0.43
2:B:306:PHE:HE2	2:B:556:PRO:HD3	1.83	0.43
1:A:195:ILE:HG23	1:A:198:PHE:HE1	1.84	0.43
2:B:361:SER:HB3	2:B:372:VAL:CG2	2.48	0.42
2:B:405:TYR:HA	2:B:408:LYS:CD	2.43	0.42
2:B:437:TRP:CE3	2:B:446:PRO:HB3	2.54	0.42
1:A:232:TYR:CE1	1:A:234:LYS:HA	2.54	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:481:HIS:HB3	2:B:482:HIS:ND1	2.34	0.42
2:B:539:ASN:HA	2:B:540:PRO:HD3	1.87	0.42
2:B:546:PHE:HA	2:B:551:GLU:HA	2.00	0.42
2:B:4:ILE:HD11	2:B:8:GLU:HB3	2.01	0.42
2:B:261:THR:O	2:B:264:ALA:HB3	2.18	0.42
2:B:434:LEU:CD1	2:B:450:ILE:HD11	2.35	0.42
1:A:110:GLU:HG2	2:B:22:ARG:HD2	2.01	0.42
1:A:195:ILE:HG23	1:A:198:PHE:CE1	2.54	0.42
1:A:1:MET:O	1:A:2:LYS:C	2.58	0.42
1:A:2:LYS:N	1:A:2:LYS:HD3	2.27	0.42
2:B:299:SER:HB2	2:B:356:PHE:HD2	1.84	0.42
2:B:13:TYR:CE1	2:B:42:GLU:HG3	2.54	0.42
1:A:229:ASP:C	1:A:231:ASN:H	2.23	0.42
1:A:149:GLU:HB3	1:A:199:ASN:HB2	2.01	0.42
2:B:173:THR:CG2	2:B:179:LEU:HD23	2.50	0.42
1:A:83:ILE:HD12	1:A:84:GLU:N	2.33	0.42
1:A:232:TYR:HE1	1:A:238:GLU:OE1	2.03	0.42
1:A:167:ASP:HB2	1:A:187:ILE:HG23	2.01	0.42
2:B:369:VAL:HG12	5:B:2032:HOH:O	2.19	0.42
1:A:66:LYS:HB2	1:A:67:PRO:HD2	2.02	0.42
1:A:28:ILE:HG23	1:A:28:ILE:O	2.18	0.42
2:B:353:MET:HE1	2:B:552:VAL:HG11	2.02	0.42
2:B:68:LEU:HD12	2:B:88:ILE:HD12	2.02	0.42
2:B:544:HIS:HB3	2:B:546:PHE:CE1	2.55	0.42
2:B:491:ILE:HA	2:B:512:GLN:O	2.20	0.42
1:A:89:ASP:N	1:A:89:ASP:OD2	2.53	0.42
2:B:277:GLY:HA3	2:B:340:ARG:HH21	1.85	0.41
1:A:158:ARG:NH2	1:A:223:PHE:HD2	2.16	0.41
2:B:165:ASP:HA	2:B:168:ASN:ND2	2.33	0.41
2:B:375:ARG:HA	2:B:378:GLN:OE1	2.20	0.41
2:B:128:VAL:HG22	2:B:436:LEU:CD2	2.44	0.41
2:B:191:MET:O	2:B:193:LEU:HG	2.20	0.41
2:B:378:GLN:O	2:B:382:LYS:HG2	2.21	0.41
2:B:176:ARG:HB2	2:B:213:ALA:CB	2.50	0.41
1:A:194:ARG:HB3	1:A:196:PHE:HE1	1.85	0.41
2:B:283:ALA:HA	2:B:284:PRO:HA	1.79	0.41
2:B:144:GLN:O	2:B:147:THR:HB	2.19	0.41
2:B:460:MET:HB3	2:B:476:ARG:HB2	2.02	0.41
2:B:547:VAL:CG1	2:B:552:VAL:HG13	2.50	0.41
2:B:115:GLY:N	2:B:118:THR:CG2	2.83	0.41
1:A:145:PHE:O	1:A:147:PHE:N	2.53	0.41
2:B:145:ILE:HG23	2:B:191:MET:HG3	2.02	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:85:ASP:HB2	2:B:97:GLY:O	2.21	0.41
2:B:134:ASP:OD1	2:B:361:SER:HB3	2.19	0.41
1:A:124:LYS:O	1:A:125:LYS:C	2.58	0.41
2:B:319:MET:CE	2:B:335:ALA:HB2	2.50	0.41
2:B:525:LYS:HE3	2:B:531:ASN:CB	2.47	0.41
1:A:29:LYS:HG2	1:A:29:LYS:H	1.68	0.41
2:B:144:GLN:OE1	2:B:363:SER:HB2	2.21	0.41
2:B:101:ASN:ND2	2:B:103:ASP:N	2.56	0.41
2:B:477:GLU:HB3	2:B:482:HIS:HE1	1.86	0.41
2:B:382:LYS:CE	2:B:560:VAL:HA	2.49	0.41
1:A:29:LYS:HA	1:A:69:ASP:O	2.20	0.41
1:A:216:HIS:O	1:A:219:LYS:HB3	2.21	0.41
2:B:404:ARG:CG	2:B:404:ARG:NH1	2.83	0.41
1:A:227:LYS:NZ	1:A:227:LYS:HA	2.35	0.41
2:B:304:ILE:HA	2:B:304:ILE:HD13	1.93	0.41
2:B:246:ALA:HB1	2:B:273:PHE:CE2	2.56	0.41
2:B:25:ASP:OD2	2:B:565:LEU:HD12	2.21	0.41
2:B:471:GLN:HA	2:B:472:PRO:C	2.41	0.41
2:B:412:ASN:ND2	2:B:528:GLN:H	2.17	0.41
2:B:322:HIS:O	2:B:323:HIS:HB2	2.21	0.41
1:A:170:ALA:HB3	2:B:42:GLU:HG2	2.03	0.41
2:B:479:PHE:C	2:B:481:HIS:H	2.23	0.41
2:B:454:PHE:HB3	2:B:480:ALA:HB2	2.03	0.41
1:A:188:ASP:HB3	1:A:193:ARG:HH12	1.86	0.41
1:A:148:PHE:O	1:A:148:PHE:CD1	2.74	0.41
2:B:256:GLY:O	2:B:282:HIS:HE1	2.04	0.40
2:B:157:ILE:HD13	2:B:216:ILE:CD1	2.50	0.40
2:B:520:ARG:HG3	2:B:520:ARG:NH1	2.37	0.40
2:B:411:ILE:HG21	2:B:528:GLN:HG3	2.03	0.40
2:B:294:ASN:ND2	2:B:294:ASN:N	2.66	0.40
2:B:173:THR:HG22	2:B:179:LEU:HD23	2.03	0.40
2:B:451:LYS:HA	2:B:451:LYS:HD2	1.91	0.40
2:B:345:ALA:HB1	2:B:554:SER:O	2.20	0.40
2:B:4:ILE:HD11	2:B:8:GLU:CB	2.52	0.40
2:B:400:PHE:CD1	2:B:400:PHE:C	2.95	0.40
1:A:18:GLU:HA	1:A:21:LYS:HG2	2.02	0.40
2:B:134:ASP:CG	2:B:137:ILE:HD11	2.41	0.40
2:B:136:HIS:HD2	2:B:171:THR:HG21	1.87	0.40
2:B:220:ILE:HG22	2:B:226:THR:HG23	2.02	0.40
2:B:308:VAL:HG21	2:B:558:ASN:OD1	2.22	0.40
2:B:539:ASN:HB3	2:B:542:THR:HG23	2.04	0.40
2:B:64:GLU:O	2:B:65:GLU:C	2.60	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:262:MET:HE1	2:B:289:VAL:HG22	2.04	0.40
2:B:477:GLU:CB	2:B:482:HIS:HE1	2.34	0.40
1:A:146:HIS:CE1	1:A:202:VAL:HG21	2.57	0.40
2:B:474:TYR:HE1	2:B:476:ARG:HD3	1.87	0.40
1:A:158:ARG:CG	1:A:158:ARG:NH1	2.85	0.40
2:B:177:ARG:O	2:B:180:LYS:HB3	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	236/238 (99%)	190 (80%)	37 (16%)	9 (4%)	5	27
2	B	566/569 (100%)	483 (85%)	69 (12%)	14 (2%)	9	40
All	All	802/807 (99%)	673 (84%)	106 (13%)	23 (3%)	7	35

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	125	LYS
1	A	227	LYS
1	A	226	ALA
1	A	234	LYS
2	B	65	GLU
2	B	107	GLY
2	B	290	ALA
2	B	439	PRO
1	A	146	HIS
2	B	49	LYS
1	A	115	ASN
2	B	98	LYS
2	B	191	MET

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Mol	Chain	Res	Type
2	B	362	ASP
1	A	67	PRO
1	A	78	ILE
2	B	2	LYS
2	B	39	TYR
2	B	47	GLY
2	B	462	ASP
2	B	301	ASN
2	B	515	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	197/197 (100%)	181 (92%)	16 (8%)	17	53
2	B	458/458 (100%)	424 (93%)	34 (7%)	20	58
All	All	655/655 (100%)	605 (92%)	50 (8%)	19	57

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	3	LEU
1	A	6	LYS
1	A	19	LEU
1	A	46	GLU
1	A	52	LYS
1	A	68	ASP
1	A	103	ASN
1	A	113	LEU
1	A	125	LYS
1	A	133	ASN
1	A	158	ARG
1	A	159	GLU
1	A	221	ARG
1	A	227	LYS
1	A	237	LYS

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Mol	Chain	Res	Type
2	B	1	MET
2	B	6	ARG
2	B	42	GLU
2	B	50	THR
2	B	56	SER
2	B	69	ILE
2	B	98	LYS
2	B	101	ASN
2	B	106	ASP
2	B	108	VAL
2	B	118	THR
2	B	223	ASP
2	B	237	VAL
2	B	249	THR
2	B	270	MET
2	B	284	PRO
2	B	294	ASN
2	B	300	THR
2	B	336	ASP
2	B	342	GLN
2	B	364	GLN
2	B	389	ARG
2	B	397	ASN
2	B	404	ARG
2	B	411	ILE
2	B	422	TYR
2	B	435	VAL
2	B	486	LYS
2	B	509	LEU
2	B	520	ARG
2	B	525	LYS
2	B	536	ILE
2	B	544	HIS
2	B	565	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	HIS
1	A	103	ASN
1	A	121	ASN
1	A	133	ASN

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Mol	Chain	Res	Type
1	A	140	GLN
1	A	192	ASN
2	B	101	ASN
2	B	110	ASN
2	B	136	HIS
2	B	200	ASN
2	B	233	HIS
2	B	244	GLN
2	B	294	ASN
2	B	301	ASN
2	B	322	HIS
2	B	342	GLN
2	B	351	HIS
2	B	364	GLN
2	B	383	ASN
2	B	397	ASN
2	B	412	ASN
2	B	417	HIS
2	B	471	GLN
2	B	490	ASN
2	B	496	GLN
2	B	531	ASN
2	B	564	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	KCX	B	219	2,4	11,11,12	5.43	3 (27%)	10,12,14	2.19	5 (50%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	KCX	B	219	2,4	-	0/8/10/12	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	219	KCX	O-C	17.58	1.23	1.11
2	B	219	KCX	CB-CA	-2.65	1.51	1.53
2	B	219	KCX	OQ1-CX	2.45	1.26	1.21

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	219	KCX	OQ2-CX-OQ1	-3.67	117.59	122.17
2	B	219	KCX	OQ2-CX-NZ	3.43	120.61	116.33
2	B	219	KCX	C-CA-N	-2.54	111.30	113.83
2	B	219	KCX	CB-CA-N	2.29	117.38	110.67
2	B	219	KCX	CG-CB-CA	-2.15	105.63	113.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	HAE	B	800	4	4,4,4	4.15	1 (25%)	4,4,4	1.67	1 (25%)

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	HAE	B	800	4	-	0/1/2/2	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	800	HAE	O-N	-8.08	1.25	1.39

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	800	HAE	C1-C2-N	2.60	117.45	114.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	238/238 (100%)	-0.40	0 100 100	21, 43, 60, 80	0
2	B	569/569 (100%)	-0.43	0 100 100	11, 31, 71, 110	0
All	All	807/807 (100%)	-0.42	0 93 100	11, 35, 65, 110	0

There are no RSRZ outliers to report.

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

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	KCX	B	219	12/13	0.22	1.52	29,34,50,53	0

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	HAE	B	800	5/5	0.21	0.75	60,60,61,61	0
4	NI	B	3001	1/1	0.12	-2.34	55,55,55,55	0
4	NI	B	3002	1/1	0.10	-3.41	42,42,42,42	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.