



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:09 PM GMT

PDB ID : 1E9Z
Title : CRYSTAL STRUCTURE OF HELICOBACTER PYLORI UREASE
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Deposited on : 2000-11-01
Resolution : 3.00 Å(reported)

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

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
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) : trunk26865

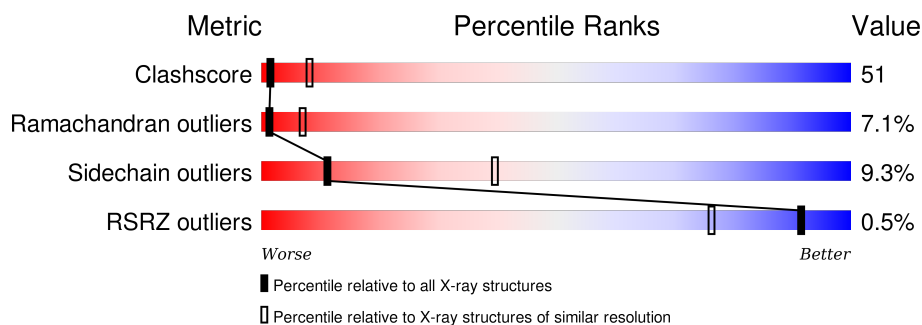
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (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 ≥ 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	238	<div> <div>32%</div> <div>59%</div> <div>8%</div> <div>.</div> </div>
2	B	569	<div> <div>%</div> <div>32%</div> <div>57%</div> <div>10%</div> <div>.</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6278 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 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
			4334	2716	747	850	21			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	219	KCX	LYS	MODIFIED RESIDUE	UNP P14917
B	355	ALA	ILE	CONFLICT	UNP P69996
B	522	VAL	ILE	CONFLICT	UNP P69996
B	531	ASN	ASP	CONFLICT	UNP P69996

- Molecule 3 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

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

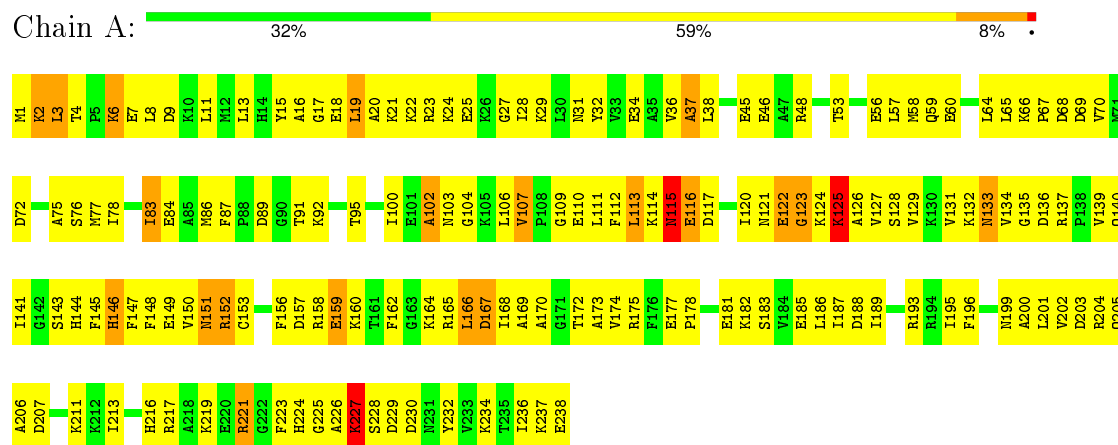
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	8	Total 8	O 8	0	0
4	B	70	Total 70	O 70	0	0

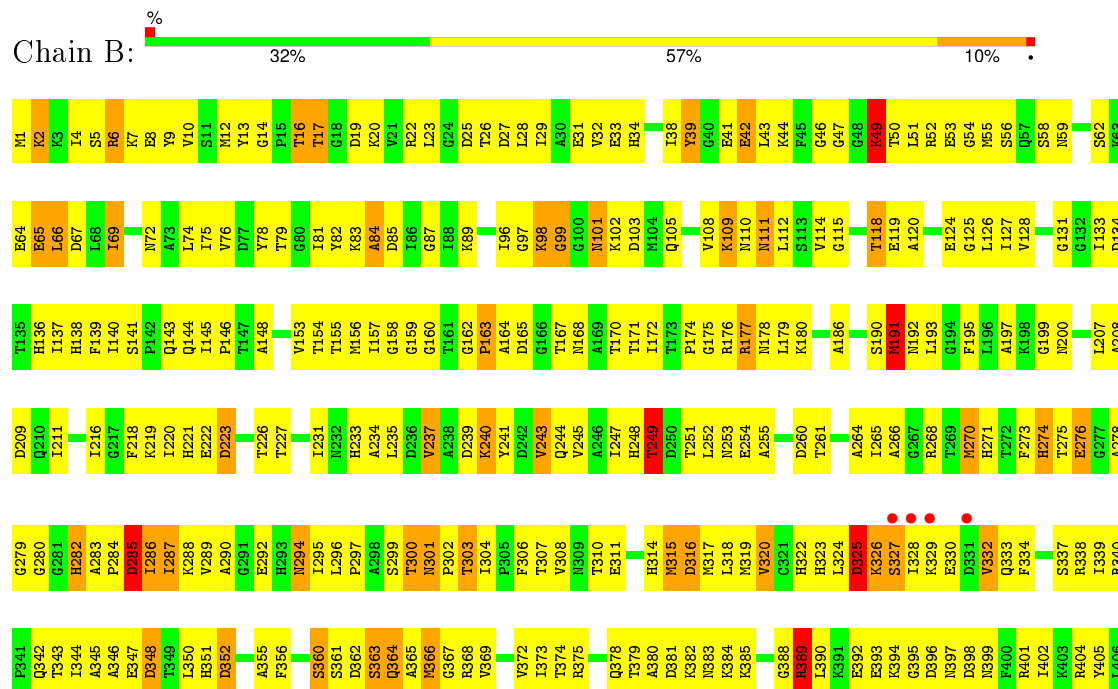
3 Residue-property plots

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: UREASE SUBUNIT ALPHA



• Molecule 2: UREASE SUBUNIT BETA





4 Data and refinement statistics

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α , β , γ	177.91Å 177.91Å 177.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 19.41 – 2.80	Depositor EDS
% Data completeness (in resolution range)	95.3 (20.00-3.00) 93.2 (19.41-2.80)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 2.79Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.212 , 0.284 0.216 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	24.1	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 18.6	EDS
Estimated twinning fraction	0.062 for -l,-k,-h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 21623 reflections	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	6278	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.88% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NI, 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	0.44	0/1892	0.63	0/2532
2	B	0.47	0/4405	0.67	0/5958
All	All	0.47	0/6297	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 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	1864	0	1909	165	0
2	B	4334	0	4261	486	0
3	B	2	0	0	0	0
4	A	8	0	0	2	0
4	B	70	0	0	14	0
All	All	6278	0	6170	634	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 51.

All (634) 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)
2:B:301:ASN:ND2	2:B:368:ARG:H	1.55	1.02
2:B:109:LYS:H	2:B:109:LYS:HE3	1.23	1.02
2:B:200:ASN:HD21	2:B:221:HIS:H	1.01	1.00
2:B:140:ILE:HD12	2:B:364:GLN:HB3	1.42	0.99
2:B:244:GLN:HE21	2:B:245:VAL:H	1.07	0.96
2:B:211:ILE:HD13	2:B:243:VAL:HG21	1.47	0.95
2:B:244:GLN:NE2	2:B:245:VAL:H	1.65	0.94
2:B:405:TYR:HA	2:B:408:LYS:HD2	1.48	0.94
2:B:286:ILE:HG23	2:B:287:ILE:H	1.32	0.94
2:B:115:GLY:H	2:B:118:THR:CG2	1.79	0.93
2:B:300:THR:HG23	2:B:301:ASN:H	1.30	0.93
2:B:165:ASP:HA	2:B:168:ASN:HD22	1.33	0.91
2:B:44:LYS:H	2:B:50:THR:CG2	1.84	0.89
1:A:67:PRO:HB2	1:A:103:ASN:HB2	1.53	0.89
2:B:20:LYS:HG2	2:B:31:GLU:HG3	1.52	0.89
2:B:156:MET:N	2:B:191:MET:HE1	1.88	0.89
2:B:109:LYS:CE	2:B:109:LYS:H	1.86	0.87
2:B:249:THR:HG21	2:B:286:ILE:HD13	1.57	0.87
2:B:318:LEU:HD21	2:B:339:ILE:HD11	1.57	0.85
2:B:299:SER:HB2	2:B:351:HIS:HE1	1.37	0.85
2:B:44:LYS:O	2:B:50:THR:HG22	1.79	0.82
2:B:301:ASN:HD22	2:B:368:ARG:H	1.26	0.82
2:B:361:SER:O	2:B:367:GLY:HA3	1.81	0.81
1:A:46:GLU:HG2	1:A:57:LEU:HD21	1.62	0.81
2:B:411:ILE:HG21	2:B:528:GLN:HG3	1.63	0.81
2:B:44:LYS:H	2:B:50:THR:HG22	1.45	0.79
1:A:121:ASN:HD21	1:A:165:ARG:HH22	1.30	0.79
2:B:347:GLU:HA	2:B:350:LEU:HD12	1.63	0.79
1:A:129:VAL:O	1:A:183:SER:HA	1.83	0.79
2:B:507:LEU:HB2	2:B:509:LEU:CD2	2.12	0.79
1:A:141:ILE:O	1:A:173:ALA:HB1	1.84	0.78
2:B:287:ILE:HD11	2:B:350:LEU:HD11	1.66	0.78
2:B:286:ILE:HG23	2:B:287:ILE:N	1.99	0.77
2:B:101:ASN:ND2	2:B:103:ASP:H	1.83	0.77
2:B:422:TYR:O	2:B:431:VAL:HG22	1.85	0.77
1:A:125:LYS:N	1:A:125:LYS:HD3	1.99	0.77
2:B:148:ALA:HB2	2:B:369:VAL:HG22	1.65	0.77
2:B:235:LEU:CD1	2:B:265:ILE:HA	2.15	0.76
2:B:507:LEU:HB2	2:B:509:LEU:HD21	1.67	0.76
2:B:381:ASP:HB3	2:B:382:LYS:HZ3	1.51	0.75
1:A:149:GLU:HG2	1:A:201:LEU:HD12	1.67	0.75
1:A:159:GLU:HG3	1:A:160:LYS:HD2	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:390:LEU:H	2:B:393:GLU:HG3	1.50	0.75
1:A:21:LYS:HG3	1:A:22:LYS:N	2.01	0.75
2:B:76:VAL:HG22	2:B:81:ILE:HG23	1.66	0.75
2:B:398:ASP:O	2:B:402:ILE:HG12	1.87	0.74
2:B:136:HIS:HB3	2:B:360:SER:HB3	1.69	0.74
2:B:274:HIS:CB	2:B:279:GLY:HA3	2.18	0.74
2:B:200:ASN:HD21	2:B:221:HIS:N	1.80	0.74
2:B:294:ASN:HD22	2:B:294:ASN:H	1.35	0.74
2:B:186:ALA:HB1	2:B:193:LEU:HD12	1.69	0.73
2:B:294:ASN:HD22	2:B:294:ASN:N	1.84	0.73
2:B:144:GLN:HE22	2:B:364:GLN:HB2	1.52	0.73
2:B:153:VAL:HG21	4:B:2014:HOH:O	1.89	0.73
2:B:433:ASP:OD1	2:B:451:LYS:HD2	1.89	0.72
1:A:45:GLU:HG3	4:A:2003:HOH:O	1.88	0.72
2:B:390:LEU:HD21	2:B:401:ARG:NH2	2.04	0.72
2:B:72:ASN:HB2	2:B:124:GLU:HB3	1.69	0.72
1:A:124:LYS:C	1:A:125:LYS:HD3	2.09	0.72
1:A:4:THR:OG1	1:A:7:GLU:HG3	1.89	0.72
2:B:27:ASP:N	2:B:381:ASP:OD1	2.23	0.71
2:B:448:MET:HB3	2:B:458:SER:HB2	1.71	0.71
2:B:389:ARG:HH11	2:B:389:ARG:HG3	1.56	0.71
2:B:467:ILE:HG13	2:B:470:PRO:HD3	1.72	0.71
2:B:378:GLN:O	2:B:382:LYS:HG2	1.91	0.71
2:B:390:LEU:HG	4:B:2039:HOH:O	1.91	0.71
2:B:119:GLU:HG3	2:B:120:ALA:N	2.06	0.70
2:B:66:LEU:HD21	2:B:87:GLY:HA3	1.72	0.70
2:B:278:ALA:O	2:B:366:MET:HE1	1.92	0.70
1:A:109:GLY:HA2	2:B:22:ARG:O	1.92	0.70
2:B:365:ALA:O	2:B:366:MET:HB2	1.92	0.69
2:B:115:GLY:H	2:B:118:THR:HG23	1.56	0.69
1:A:72:ASP:OD1	1:A:106:LEU:HB3	1.92	0.69
2:B:444:VAL:HG11	2:B:562:LEU:HB3	1.74	0.69
1:A:67:PRO:HB2	1:A:103:ASN:CB	2.22	0.69
2:B:322:HIS:HB2	2:B:324:LEU:HG	1.73	0.69
2:B:454:PHE:HD1	2:B:480:ALA:HB2	1.58	0.69
2:B:318:LEU:H	2:B:318:LEU:HD22	1.58	0.68
2:B:176:ARG:HD2	2:B:209:ASP:OD1	1.93	0.68
1:A:46:GLU:HB3	1:A:57:LEU:HD11	1.75	0.68
1:A:132:LYS:HG3	1:A:181:GLU:HB2	1.76	0.67
1:A:87:PHE:CE2	1:A:92:LYS:HB2	2.29	0.67
1:A:66:LYS:HG2	1:A:69:ASP:CG	2.15	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:397:ASN:HD22	2:B:399:ASN:H	1.42	0.67
2:B:423:VAL:HG22	4:B:2012:HOH:O	1.93	0.67
1:A:157:ASP:CG	1:A:160:LYS:HD3	2.15	0.67
2:B:467:ILE:HD12	2:B:469:THR:CG2	2.26	0.66
2:B:275:THR:HG21	2:B:290:ALA:HB2	1.75	0.66
2:B:23:LEU:HD13	2:B:442:PHE:CE2	2.30	0.66
2:B:467:ILE:HD12	2:B:469:THR:HG23	1.76	0.66
2:B:304:ILE:O	2:B:375:ARG:HD3	1.96	0.66
2:B:144:GLN:NE2	2:B:364:GLN:HB2	2.10	0.66
2:B:235:LEU:HD11	2:B:265:ILE:HA	1.78	0.66
1:A:217:ARG:O	1:A:221:ARG:HD3	1.96	0.66
2:B:299:SER:HB2	2:B:351:HIS:CE1	2.25	0.66
2:B:239:ASP:OD1	2:B:520:ARG:HG3	1.96	0.66
2:B:520:ARG:N	2:B:520:ARG:HD2	2.09	0.66
2:B:276:GLU:CD	2:B:278:ALA:H	2.00	0.65
2:B:78:TYR:CE2	2:B:411:ILE:HG13	2.32	0.65
2:B:274:HIS:HB3	2:B:300:THR:HB	1.77	0.65
2:B:534:ALA:O	2:B:536:ILE:HG22	1.96	0.65
2:B:504:LYS:HA	2:B:509:LEU:HD23	1.79	0.65
1:A:75:ALA:HA	1:A:100:ILE:HG13	1.78	0.65
2:B:176:ARG:NH1	2:B:209:ASP:OD2	2.30	0.65
2:B:374:THR:OG1	2:B:444:VAL:HG12	1.97	0.64
2:B:520:ARG:HH11	2:B:520:ARG:HA	1.62	0.64
2:B:546:PHE:CE2	2:B:551:GLU:HB2	2.33	0.64
2:B:285:ASP:HB3	2:B:288:LYS:HE3	1.79	0.64
2:B:27:ASP:HB2	2:B:385:LYS:NZ	2.12	0.64
2:B:381:ASP:HB3	2:B:382:LYS:NZ	2.12	0.64
2:B:157:ILE:HG23	2:B:216:ILE:HD11	1.78	0.64
2:B:9:TYR:CZ	2:B:13:TYR:HD2	2.15	0.64
2:B:361:SER:O	2:B:362:ASP:HB2	1.97	0.64
2:B:99:GLY:HA2	2:B:108:VAL:HG23	1.79	0.64
2:B:145:ILE:HB	2:B:146:PRO:CD	2.26	0.64
2:B:412:ASN:HD21	2:B:528:GLN:H	1.44	0.64
1:A:83:ILE:HD12	1:A:84:GLU:N	2.12	0.64
2:B:319:MET:HG3	2:B:326:LYS:CE	2.28	0.64
2:B:444:VAL:CG1	2:B:562:LEU:HB3	2.27	0.64
1:A:75:ALA:HA	1:A:100:ILE:CD1	2.28	0.64
2:B:98:LYS:H	2:B:109:LYS:NZ	1.95	0.64
2:B:25:ASP:OD1	2:B:561:SER:HB2	1.97	0.64
1:A:23:ARG:O	1:A:28:ILE:HG22	1.97	0.64
2:B:390:LEU:HB2	2:B:393:GLU:HG2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:287:ILE:HD11	2:B:350:LEU:CD1	2.28	0.63
2:B:550:LYS:HG2	2:B:551:GLU:N	2.12	0.63
1:A:131:VAL:N	1:A:182:LYS:O	2.32	0.63
2:B:301:ASN:ND2	2:B:368:ARG:N	2.38	0.63
2:B:469:THR:N	2:B:470:PRO:HD2	2.12	0.63
2:B:115:GLY:H	2:B:118:THR:HG21	1.62	0.63
2:B:66:LEU:O	2:B:118:THR:HB	1.98	0.63
2:B:101:ASN:C	2:B:101:ASN:HD22	2.02	0.63
2:B:27:ASP:HB2	2:B:385:LYS:HZ3	1.63	0.62
2:B:422:TYR:O	2:B:430:LYS:HB3	2.00	0.62
2:B:467:ILE:HG13	2:B:470:PRO:CD	2.28	0.62
1:A:158:ARG:HD3	1:A:224:HIS:O	1.99	0.62
2:B:98:LYS:HE3	2:B:99:GLY:O	1.99	0.62
2:B:304:ILE:HG23	2:B:379:THR:OG1	2.00	0.62
2:B:44:LYS:H	2:B:50:THR:HG21	1.61	0.62
2:B:128:VAL:HG22	2:B:436:LEU:HD22	1.82	0.62
1:A:134:VAL:HG12	1:A:134:VAL:O	1.99	0.61
2:B:318:LEU:HB3	2:B:324:LEU:HD12	1.81	0.61
2:B:381:ASP:O	2:B:385:LYS:HG2	2.00	0.61
1:A:167:ASP:HB2	1:A:187:ILE:HG23	1.83	0.61
2:B:115:GLY:O	2:B:118:THR:HG23	2.01	0.60
2:B:4:ILE:HD11	2:B:8:GLU:CB	2.31	0.60
1:A:115:ASN:O	1:A:116:GLU:HB2	2.00	0.60
2:B:6:ARG:HG2	2:B:6:ARG:HH11	1.64	0.60
2:B:52:ARG:HH21	2:B:55:MET:HE1	1.64	0.60
2:B:423:VAL:HG22	2:B:424:GLY:H	1.66	0.60
2:B:308:VAL:HG23	2:B:557:ALA:O	2.00	0.60
2:B:300:THR:HG23	2:B:301:ASN:N	2.10	0.60
2:B:404:ARG:CZ	4:B:2042:HOH:O	2.48	0.60
2:B:352:ASP:OD1	2:B:383:ASN:HB3	2.01	0.60
2:B:218:PHE:HB2	2:B:245:VAL:HG13	1.84	0.60
2:B:411:ILE:HG21	2:B:528:GLN:CG	2.30	0.60
2:B:171:THR:OG1	2:B:219:KCX:HE2	2.02	0.60
2:B:520:ARG:HH11	2:B:520:ARG:CG	2.14	0.60
2:B:271:HIS:HA	2:B:296:LEU:HB2	1.82	0.60
1:A:170:ALA:HB3	2:B:42:GLU:HG2	1.83	0.60
2:B:412:ASN:HD21	2:B:528:GLN:N	2.00	0.60
1:A:213:ILE:HD13	1:A:238:GLU:HB3	1.83	0.60
1:A:227:LYS:HE2	1:A:227:LYS:HA	1.84	0.60
2:B:58:SER:HB2	2:B:101:ASN:ND2	2.17	0.60
2:B:159:GLY:H	2:B:171:THR:HB	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:286:ILE:CG2	2:B:287:ILE:H	2.11	0.59
2:B:141:SER:O	2:B:144:GLN:HG3	2.01	0.59
2:B:46:GLY:HA3	2:B:49:LYS:HD3	1.84	0.59
2:B:43:LEU:HD22	2:B:56:SER:OG	2.02	0.59
2:B:394:LYS:HD2	2:B:395:GLY:N	2.17	0.59
2:B:52:ARG:HH21	2:B:55:MET:CE	2.14	0.59
2:B:220:ILE:HB	2:B:247:ILE:HG13	1.84	0.59
2:B:490:ASN:C	2:B:491:ILE:HD12	2.22	0.59
2:B:261:THR:O	2:B:265:ILE:HG13	2.02	0.59
1:A:121:ASN:ND2	1:A:165:ARG:HH22	1.97	0.59
1:A:145:PHE:HB2	2:B:55:MET:HE3	1.84	0.59
2:B:423:VAL:HG22	2:B:424:GLY:N	2.18	0.59
2:B:520:ARG:NH1	2:B:520:ARG:HA	2.18	0.59
2:B:74:LEU:HD23	2:B:127:ILE:HG12	1.85	0.59
2:B:319:MET:HG3	2:B:326:LYS:NZ	2.18	0.58
2:B:492:THR:HG23	2:B:513:VAL:HG22	1.85	0.58
2:B:288:LYS:HA	2:B:536:ILE:HG12	1.85	0.58
1:A:76:SER:CB	1:A:107:VAL:HG12	2.34	0.58
2:B:346:ALA:HB1	2:B:552:VAL:HG23	1.85	0.58
1:A:143:SER:O	1:A:165:ARG:HB2	2.02	0.58
2:B:297:PRO:HG3	2:B:524:LYS:HE3	1.85	0.58
2:B:38:ILE:O	2:B:38:ILE:HG22	2.04	0.58
2:B:539:ASN:O	2:B:543:TYR:HA	2.04	0.58
1:A:144:HIS:O	2:B:55:MET:HG2	2.04	0.58
2:B:180:LYS:HG3	2:B:507:LEU:HD22	1.85	0.58
1:A:221:ARG:HD2	1:A:221:ARG:N	2.19	0.58
2:B:83:LYS:O	2:B:84:ALA:HB2	2.04	0.58
2:B:144:GLN:OE1	2:B:363:SER:HB2	2.04	0.58
2:B:200:ASN:ND2	2:B:221:HIS:H	1.86	0.58
1:A:107:VAL:HG23	1:A:110:GLU:CD	2.24	0.58
2:B:75:ILE:HD12	2:B:82:TYR:CE1	2.39	0.58
2:B:539:ASN:CG	2:B:542:THR:HG22	2.24	0.58
2:B:334:PHE:HA	2:B:337:SER:OG	2.04	0.58
2:B:136:HIS:CB	2:B:360:SER:HB3	2.33	0.58
2:B:176:ARG:HA	2:B:179:LEU:HD12	1.85	0.58
2:B:285:ASP:O	2:B:287:ILE:HG22	2.03	0.58
2:B:240:LYS:HD2	2:B:240:LYS:H	1.69	0.57
2:B:316:ASP:O	2:B:319:MET:HG2	2.04	0.57
2:B:26:THR:HB	2:B:381:ASP:CG	2.24	0.57
2:B:319:MET:HG3	2:B:326:LYS:HE3	1.85	0.57
1:A:193:ARG:HB2	1:A:205:GLN:HE22	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:6:ARG:NH1	2:B:19:ASP:OD2	2.37	0.57
2:B:507:LEU:HB2	2:B:509:LEU:HD22	1.85	0.57
2:B:380:ALA:HB2	2:B:405:TYR:CD2	2.40	0.57
2:B:397:ASN:ND2	4:B:2040:HOH:O	2.36	0.57
1:A:18:GLU:O	1:A:22:LYS:HG3	2.03	0.57
2:B:32:VAL:HG22	2:B:74:LEU:HD13	1.87	0.57
2:B:207:LEU:HD21	2:B:234:ALA:HA	1.87	0.57
2:B:288:LYS:HA	2:B:536:ILE:CD1	2.35	0.57
2:B:547:VAL:C	2:B:549:GLY:H	2.08	0.57
1:A:164:LYS:HG2	1:A:188:ASP:HA	1.87	0.57
2:B:75:ILE:O	2:B:81:ILE:HA	2.05	0.57
2:B:145:ILE:HB	2:B:146:PRO:HD3	1.87	0.56
2:B:220:ILE:CG2	2:B:226:THR:HG23	2.35	0.56
2:B:542:THR:O	2:B:543:TYR:HB2	2.05	0.56
2:B:274:HIS:HB2	2:B:279:GLY:HA3	1.86	0.56
2:B:211:ILE:CD1	2:B:243:VAL:HG21	2.28	0.56
2:B:26:THR:HG22	2:B:561:SER:OG	2.05	0.56
2:B:542:THR:OG1	2:B:544:HIS:ND1	2.39	0.56
1:A:8:LEU:HD22	1:A:8:LEU:H	1.70	0.56
2:B:158:GLY:O	2:B:195:PHE:HA	2.06	0.56
2:B:109:LYS:N	2:B:109:LYS:HE3	2.08	0.56
2:B:66:LEU:HD23	2:B:69:ILE:HG23	1.88	0.56
2:B:539:ASN:OD1	2:B:541:GLU:HB2	2.06	0.56
2:B:530:ASN:HD22	2:B:530:ASN:H	1.53	0.56
2:B:285:ASP:O	2:B:287:ILE:N	2.39	0.55
2:B:133:ILE:HG12	2:B:155:THR:HB	1.86	0.55
1:A:32:TYR:O	1:A:36:VAL:HG23	2.05	0.55
2:B:520:ARG:HG3	2:B:520:ARG:NH1	2.21	0.55
2:B:4:ILE:HG12	2:B:5:SER:N	2.22	0.55
2:B:479:PHE:C	2:B:481:HIS:H	2.10	0.55
1:A:31:ASN:OD1	1:A:34:GLU:HG3	2.07	0.55
2:B:286:ILE:O	2:B:288:LYS:N	2.39	0.55
1:A:46:GLU:CG	1:A:57:LEU:HD21	2.35	0.55
1:A:3:LEU:HD23	1:A:8:LEU:HD11	1.88	0.55
1:A:13:LEU:HB2	2:B:472:PRO:HG3	1.88	0.55
2:B:316:ASP:O	2:B:318:LEU:N	2.40	0.55
1:A:76:SER:HB3	1:A:107:VAL:HG12	1.87	0.55
1:A:45:GLU:O	1:A:48:ARG:HB3	2.06	0.55
2:B:329:LYS:HB3	4:B:2031:HOH:O	2.06	0.55
2:B:16:THR:OG1	2:B:17:THR:N	2.40	0.55
2:B:394:LYS:HD2	2:B:395:GLY:H	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4:ILE:HD11	2:B:8:GLU:HB2	1.89	0.55
2:B:101:ASN:C	2:B:101:ASN:ND2	2.58	0.55
2:B:46:GLY:CA	2:B:49:LYS:HD3	2.37	0.55
2:B:249:THR:HB	2:B:282:HIS:H	1.71	0.54
2:B:454:PHE:CD1	2:B:480:ALA:HB2	2.40	0.54
2:B:542:THR:HG23	2:B:544:HIS:H	1.72	0.54
2:B:51:LEU:HA	2:B:56:SER:HB3	1.90	0.54
1:A:196:PHE:HA	1:A:203:ASP:HA	1.90	0.54
1:A:78:ILE:HD12	1:A:78:ILE:N	2.23	0.54
2:B:6:ARG:O	2:B:7:LYS:C	2.46	0.54
1:A:186:LEU:O	1:A:186:LEU:HD12	2.08	0.54
2:B:346:ALA:O	2:B:350:LEU:HG	2.07	0.54
1:A:204:ARG:NH2	1:A:238:GLU:HA	2.22	0.54
2:B:328:ILE:O	2:B:332:VAL:HG22	2.08	0.54
2:B:278:ALA:HB3	2:B:303:THR:HG21	1.90	0.53
2:B:411:ILE:O	2:B:415:ILE:HG13	2.08	0.53
2:B:384:LYS:O	2:B:388:GLY:N	2.36	0.53
2:B:134:ASP:HB2	4:B:2014:HOH:O	2.08	0.53
2:B:220:ILE:HG21	2:B:226:THR:HG23	1.89	0.53
2:B:162:GLY:O	2:B:164:ALA:N	2.37	0.53
2:B:407:SER:HA	2:B:410:THR:OG1	2.08	0.53
1:A:115:ASN:O	1:A:116:GLU:CB	2.56	0.53
2:B:62:SER:C	2:B:64:GLU:H	2.11	0.53
2:B:306:PHE:HB3	4:B:2029:HOH:O	2.09	0.53
2:B:279:GLY:HA2	2:B:366:MET:HE2	1.90	0.53
2:B:191:MET:O	2:B:193:LEU:HG	2.08	0.53
2:B:568:ILE:HG12	2:B:568:ILE:O	2.08	0.53
2:B:471:GLN:HA	2:B:473:VAL:HG23	1.90	0.53
2:B:525:LYS:HG2	4:B:2062:HOH:O	2.07	0.53
2:B:72:ASN:O	2:B:124:GLU:HA	2.09	0.53
1:A:78:ILE:O	1:A:78:ILE:HG22	2.09	0.53
1:A:140:GLN:HE21	1:A:175:ARG:NH1	2.06	0.53
1:A:66:LYS:HG2	1:A:69:ASP:OD1	2.09	0.53
1:A:156:PHE:O	1:A:225:GLY:HA3	2.09	0.53
2:B:467:ILE:CD1	2:B:469:THR:HG23	2.39	0.53
2:B:345:ALA:CB	2:B:553:THR:HG23	2.39	0.53
2:B:126:LEU:CD1	2:B:126:LEU:N	2.72	0.53
2:B:136:HIS:CE1	2:B:362:ASP:OD1	2.62	0.52
2:B:339:ILE:HG22	2:B:339:ILE:O	2.09	0.52
2:B:294:ASN:ND2	2:B:294:ASN:N	2.57	0.52
2:B:320:VAL:HG12	2:B:320:VAL:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:247:ILE:HB	2:B:270:MET:SD	2.50	0.52
1:A:127:VAL:HG22	1:A:186:LEU:O	2.09	0.52
2:B:32:VAL:HG22	2:B:74:LEU:CD1	2.38	0.52
1:A:19:LEU:HD13	2:B:568:ILE:HD11	1.92	0.52
2:B:482:HIS:O	2:B:485:ALA:HB3	2.08	0.52
1:A:110:GLU:HG2	2:B:22:ARG:HD2	1.91	0.52
2:B:491:ILE:N	2:B:491:ILE:HD12	2.24	0.52
1:A:195:ILE:HD13	1:A:195:ILE:N	2.25	0.52
2:B:301:ASN:HD22	2:B:368:ARG:N	2.02	0.52
2:B:26:THR:HB	2:B:381:ASP:OD1	2.10	0.52
2:B:233:HIS:O	2:B:237:VAL:HG12	2.10	0.52
2:B:44:LYS:N	2:B:50:THR:HG22	2.21	0.51
1:A:122:GLU:O	1:A:123:GLY:C	2.48	0.51
1:A:24:LYS:O	1:A:27:GLY:N	2.39	0.51
2:B:111:ASN:C	2:B:111:ASN:ND2	2.63	0.51
2:B:12:MET:HG2	2:B:13:TYR:CE1	2.45	0.51
2:B:251:THR:O	2:B:253:ASN:N	2.44	0.51
2:B:447:ASN:O	2:B:459:GLN:HG2	2.09	0.51
2:B:46:GLY:C	2:B:49:LYS:HD3	2.31	0.51
1:A:185:GLU:HG3	2:B:2:LYS:CE	2.41	0.51
1:A:120:ILE:HD13	1:A:169:ALA:HA	1.92	0.51
1:A:147:PHE:O	1:A:150:VAL:HG22	2.11	0.51
2:B:474:TYR:OH	2:B:476:ARG:NH1	2.43	0.51
2:B:85:ASP:OD2	2:B:98:LYS:O	2.29	0.50
2:B:302:PRO:C	2:B:304:ILE:H	2.14	0.50
1:A:19:LEU:CD1	2:B:568:ILE:HD11	2.42	0.50
1:A:177:GLU:O	1:A:178:PRO:C	2.50	0.50
2:B:434:LEU:HD12	2:B:450:ILE:HD11	1.93	0.50
2:B:111:ASN:HD22	2:B:111:ASN:C	2.11	0.50
2:B:408:LYS:HE2	2:B:530:ASN:OD1	2.11	0.50
2:B:69:ILE:HD13	2:B:114:VAL:CG2	2.40	0.50
1:A:75:ALA:HA	1:A:100:ILE:CG1	2.39	0.50
1:A:110:GLU:OE1	1:A:112:PHE:HE2	1.95	0.50
1:A:32:TYR:CD1	1:A:77:MET:HE2	2.47	0.50
2:B:404:ARG:O	2:B:408:LYS:HG3	2.12	0.50
2:B:52:ARG:NH1	4:B:2003:HOH:O	2.44	0.50
1:A:189:ILE:O	1:A:193:ARG:HG2	2.12	0.49
2:B:186:ALA:CB	2:B:193:LEU:HD12	2.40	0.49
1:A:87:PHE:CD2	1:A:92:LYS:HB2	2.47	0.49
2:B:244:GLN:HE21	2:B:245:VAL:N	1.92	0.49
1:A:147:PHE:O	1:A:150:VAL:HG13	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:450:ILE:HG13	2:B:450:ILE:O	2.10	0.49
2:B:226:THR:HG22	2:B:231:ILE:HD11	1.93	0.49
1:A:70:VAL:HG21	1:A:100:ILE:HD12	1.94	0.49
2:B:392:GLU:H	2:B:392:GLU:CD	2.16	0.49
1:A:124:LYS:O	1:A:125:LYS:C	2.51	0.49
1:A:116:GLU:O	2:B:6:ARG:HD2	2.12	0.49
2:B:208:ALA:HB1	2:B:241:TYR:OH	2.12	0.49
2:B:138:HIS:HA	2:B:171:THR:HG22	1.95	0.49
1:A:2:LYS:HD3	1:A:2:LYS:H	1.78	0.49
2:B:520:ARG:CA	2:B:520:ARG:HH11	2.23	0.49
2:B:240:LYS:HD2	2:B:240:LYS:N	2.27	0.49
1:A:128:SER:HB3	1:A:183:SER:OG	2.13	0.49
2:B:520:ARG:HH11	2:B:520:ARG:HG3	1.77	0.49
1:A:1:MET:HE2	1:A:3:LEU:HD22	1.93	0.49
2:B:101:ASN:HD22	2:B:102:LYS:N	2.11	0.49
1:A:144:HIS:NE2	2:B:41:GLU:OE1	2.41	0.49
2:B:340:ARG:HE	2:B:343:THR:HG21	1.77	0.49
2:B:494:VAL:O	2:B:515:PRO:HA	2.13	0.49
2:B:234:ALA:O	2:B:237:VAL:HG13	2.13	0.49
2:B:417:HIS:O	2:B:419:ILE:HG23	2.13	0.49
2:B:172:ILE:HG12	2:B:219:KCX:HB2	1.95	0.48
2:B:227:THR:O	2:B:231:ILE:HG13	2.13	0.48
1:A:144:HIS:HA	1:A:165:ARG:HD2	1.93	0.48
2:B:448:MET:CB	2:B:458:SER:HB2	2.40	0.48
2:B:136:HIS:HB2	2:B:360:SER:OG	2.14	0.48
1:A:86:MET:HA	1:A:91:THR:HA	1.95	0.48
2:B:220:ILE:HG22	2:B:226:THR:OG1	2.13	0.48
1:A:202:VAL:O	1:A:204:ARG:HG3	2.14	0.48
2:B:520:ARG:HH11	2:B:520:ARG:CB	2.26	0.48
1:A:232:TYR:CE1	1:A:234:LYS:HA	2.49	0.48
2:B:286:ILE:CG2	2:B:287:ILE:N	2.70	0.48
1:A:232:TYR:HE1	1:A:234:LYS:HA	1.78	0.48
1:A:38:LEU:CD2	1:A:65:LEU:HD21	2.43	0.48
2:B:565:LEU:CD2	2:B:565:LEU:O	2.62	0.48
1:A:17:GLY:O	1:A:20:ALA:HB3	2.13	0.48
1:A:8:LEU:HD22	1:A:8:LEU:N	2.28	0.48
2:B:389:ARG:HG3	2:B:389:ARG:NH1	2.26	0.48
2:B:156:MET:HG3	2:B:191:MET:CE	2.44	0.48
2:B:528:GLN:O	2:B:529:PHE:HB2	2.14	0.48
2:B:268:ARG:HG2	4:B:2026:HOH:O	2.14	0.48
2:B:301:ASN:HB3	2:B:302:PRO:CD	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:LYS:O	1:A:237:LYS:HG3	2.13	0.48
2:B:85:ASP:HB2	2:B:97:GLY:O	2.14	0.47
1:A:29:LYS:HA	1:A:69:ASP:O	2.13	0.47
2:B:126:LEU:N	2:B:126:LEU:HD12	2.28	0.47
2:B:467:ILE:O	2:B:470:PRO:HD2	2.15	0.47
1:A:1:MET:CE	1:A:3:LEU:HD22	2.43	0.47
1:A:53:THR:OG1	1:A:56:GLU:HG3	2.13	0.47
2:B:98:LYS:N	2:B:109:LYS:NZ	2.60	0.47
2:B:160:GLY:HA3	2:B:167:THR:HG23	1.95	0.47
2:B:345:ALA:HB1	2:B:553:THR:HG23	1.97	0.47
2:B:109:LYS:C	2:B:111:ASN:N	2.68	0.47
2:B:547:VAL:O	2:B:549:GLY:N	2.48	0.47
1:A:117:ASP:OD1	2:B:5:SER:HA	2.14	0.47
1:A:216:HIS:O	1:A:219:LYS:HB3	2.14	0.47
1:A:133:ASN:ND2	1:A:135:GLY:H	2.13	0.47
2:B:274:HIS:HB3	2:B:279:GLY:HA3	1.95	0.47
2:B:338:ARG:HA	2:B:340:ARG:NH1	2.29	0.47
2:B:530:ASN:H	2:B:530:ASN:ND2	2.12	0.47
2:B:138:HIS:O	2:B:140:ILE:N	2.44	0.47
2:B:46:GLY:N	2:B:49:LYS:HB2	2.30	0.47
2:B:319:MET:HA	2:B:324:LEU:HB2	1.96	0.47
2:B:299:SER:CB	2:B:351:HIS:HE1	2.20	0.47
2:B:562:LEU:HA	2:B:566:PHE:CE1	2.50	0.47
1:A:25:GLU:C	1:A:27:GLY:H	2.18	0.47
2:B:29:ILE:HD12	2:B:29:ILE:N	2.29	0.47
2:B:244:GLN:HG2	2:B:416:ALA:O	2.15	0.47
2:B:239:ASP:HA	2:B:520:ARG:HG2	1.96	0.47
1:A:32:TYR:HB2	1:A:77:MET:HE1	1.97	0.47
2:B:62:SER:HB3	2:B:110:ASN:ND2	2.30	0.47
2:B:140:ILE:O	2:B:163:PRO:HD3	2.15	0.47
2:B:172:ILE:CG1	2:B:219:KCX:HB2	2.45	0.47
2:B:324:LEU:O	2:B:325:ASP:C	2.53	0.47
2:B:455:ILE:HG22	2:B:478:MET:CB	2.45	0.47
1:A:114:LYS:O	2:B:6:ARG:HD3	2.15	0.47
2:B:374:THR:HA	2:B:443:GLY:O	2.15	0.47
2:B:114:VAL:HA	2:B:118:THR:HG21	1.97	0.46
2:B:53:GLU:HG2	2:B:59:ASN:HD21	1.80	0.46
2:B:176:ARG:HH11	2:B:209:ASP:CG	2.17	0.46
2:B:297:PRO:HB2	2:B:356:PHE:HD1	1.79	0.46
2:B:460:MET:HB3	2:B:476:ARG:HB2	1.96	0.46
2:B:311:GLU:N	4:B:2030:HOH:O	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:285:ASP:HB3	2:B:288:LYS:CE	2.45	0.46
2:B:23:LEU:HB3	2:B:442:PHE:CD2	2.50	0.46
1:A:217:ARG:O	1:A:221:ARG:CD	2.62	0.46
2:B:286:ILE:O	2:B:287:ILE:C	2.54	0.46
2:B:165:ASP:CA	2:B:168:ASN:HD22	2.15	0.46
2:B:384:LYS:HA	2:B:401:ARG:NH1	2.30	0.46
1:A:13:LEU:O	1:A:16:ALA:HB3	2.16	0.46
1:A:148:PHE:C	1:A:148:PHE:CD1	2.89	0.46
2:B:96:ILE:HG13	2:B:428:VAL:HG23	1.96	0.46
2:B:98:LYS:CB	2:B:109:LYS:HZ3	2.28	0.46
2:B:109:LYS:C	2:B:111:ASN:H	2.18	0.46
2:B:275:THR:HB	2:B:356:PHE:CE1	2.50	0.46
2:B:164:ALA:O	2:B:168:ASN:ND2	2.49	0.46
1:A:2:LYS:CD	1:A:2:LYS:H	2.27	0.46
2:B:461:GLY:O	2:B:462:ASP:C	2.54	0.46
2:B:144:GLN:O	2:B:145:ILE:C	2.53	0.46
2:B:145:ILE:H	2:B:145:ILE:HG12	1.60	0.46
2:B:20:LYS:HE2	2:B:396:ASP:O	2.15	0.46
2:B:314:HIS:O	2:B:315:MET:C	2.53	0.46
2:B:457:LEU:HA	2:B:478:MET:HG2	1.97	0.46
2:B:9:TYR:CE2	2:B:13:TYR:HD2	2.33	0.46
2:B:4:ILE:CG1	2:B:5:SER:N	2.78	0.46
2:B:539:ASN:HB3	2:B:542:THR:HG23	1.98	0.46
2:B:33:GLU:O	2:B:34:HIS:CD2	2.68	0.46
2:B:530:ASN:ND2	2:B:530:ASN:N	2.63	0.46
2:B:288:LYS:HA	2:B:536:ILE:CG1	2.46	0.46
2:B:222:GLU:OE1	2:B:251:THR:HB	2.16	0.46
2:B:264:ALA:C	2:B:266:ALA:N	2.69	0.46
2:B:111:ASN:O	2:B:111:ASN:ND2	2.46	0.46
2:B:285:ASP:N	2:B:285:ASP:OD1	2.49	0.46
2:B:197:ALA:HB3	2:B:218:PHE:HD2	1.80	0.46
1:A:66:LYS:HE2	1:A:69:ASP:OD2	2.16	0.46
2:B:137:ILE:HG13	2:B:156:MET:HE2	1.97	0.46
1:A:141:ILE:HD13	1:A:141:ILE:N	2.31	0.46
1:A:125:LYS:O	1:A:125:LYS:HG2	2.16	0.46
2:B:486:LYS:HG3	2:B:487:TYR:N	2.31	0.46
2:B:164:ALA:C	2:B:168:ASN:ND2	2.70	0.45
2:B:43:LEU:HA	2:B:50:THR:HG21	1.98	0.45
2:B:350:LEU:HB3	2:B:355:ALA:HB3	1.99	0.45
2:B:479:PHE:HB2	4:B:2048:HOH:O	2.16	0.45
2:B:302:PRO:HD3	2:B:367:GLY:HA2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:467:ILE:HD12	2:B:469:THR:HG21	1.98	0.45
1:A:185:GLU:HG3	2:B:2:LYS:HE2	1.98	0.45
1:A:64:LEU:O	1:A:65:LEU:HD23	2.15	0.45
2:B:283:ALA:HA	2:B:284:PRO:HA	1.75	0.45
2:B:138:HIS:CD2	2:B:171:THR:CG2	3.00	0.45
2:B:314:HIS:CB	2:B:339:ILE:HD13	2.46	0.45
2:B:177:ARG:NH1	2:B:180:LYS:HD3	2.30	0.45
1:A:139:VAL:HG12	1:A:141:ILE:HD11	1.98	0.45
1:A:58:MET:HG3	1:A:95:THR:O	2.16	0.45
2:B:148:ALA:HB2	2:B:369:VAL:CG2	2.41	0.45
2:B:363:SER:CB	2:B:369:VAL:HB	2.46	0.45
2:B:137:ILE:HG21	2:B:156:MET:HE2	1.98	0.45
1:A:102:ALA:C	1:A:104:GLY:H	2.19	0.45
2:B:294:ASN:ND2	2:B:294:ASN:H	2.08	0.45
1:A:156:PHE:CE1	1:A:158:ARG:HA	2.51	0.45
2:B:28:LEU:C	2:B:29:ILE:HD12	2.37	0.45
2:B:136:HIS:HB2	2:B:273:PHE:CE1	2.51	0.45
2:B:340:ARG:O	2:B:344:ILE:HG13	2.17	0.45
2:B:299:SER:CB	2:B:351:HIS:CE1	2.98	0.45
2:B:4:ILE:HD11	2:B:8:GLU:HB3	1.96	0.45
1:A:111:LEU:CD2	2:B:10:VAL:HG11	2.47	0.45
2:B:10:VAL:O	2:B:14:GLY:N	2.48	0.45
2:B:405:TYR:HA	2:B:408:LYS:CD	2.34	0.45
2:B:407:SER:O	2:B:412:ASN:HB2	2.17	0.45
2:B:172:ILE:O	2:B:174:PRO:HD3	2.17	0.45
1:A:107:VAL:HG23	1:A:110:GLU:OE2	2.17	0.45
2:B:393:GLU:OE1	2:B:398:ASP:HA	2.17	0.45
1:A:150:VAL:O	1:A:151:ASN:C	2.55	0.45
2:B:143:GLN:O	2:B:146:PRO:HG2	2.17	0.44
2:B:286:ILE:C	2:B:288:LYS:N	2.69	0.44
1:A:6:LYS:O	1:A:9:ASP:HB2	2.17	0.44
2:B:289:VAL:HG12	2:B:295:ILE:HG21	1.98	0.44
1:A:162:PHE:CE1	1:A:211:LYS:HA	2.52	0.44
2:B:361:SER:HB3	2:B:372:VAL:CG2	2.46	0.44
2:B:9:TYR:CZ	2:B:13:TYR:CD2	3.02	0.44
1:A:219:LYS:HG2	1:A:229:ASP:OD2	2.17	0.44
2:B:318:LEU:HB2	2:B:319:MET:CE	2.47	0.44
1:A:87:PHE:HB2	1:A:89:ASP:OD2	2.17	0.44
2:B:411:ILE:CG2	2:B:528:GLN:CG	2.96	0.44
2:B:422:TYR:OH	2:B:515:PRO:O	2.29	0.44
2:B:490:ASN:O	2:B:512:GLN:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:LEU:HD23	1:A:8:LEU:CD1	2.47	0.44
2:B:226:THR:O	2:B:226:THR:HG22	2.17	0.44
2:B:69:ILE:HD13	2:B:114:VAL:HG21	1.99	0.44
1:A:111:LEU:HD21	2:B:10:VAL:HG11	1.99	0.44
1:A:152:ARG:HB2	1:A:223:PHE:HA	1.99	0.44
2:B:325:ASP:OD1	2:B:327:SER:HB3	2.17	0.44
2:B:382:LYS:HE3	2:B:560:VAL:HA	1.99	0.44
2:B:550:LYS:CG	2:B:551:GLU:N	2.81	0.44
2:B:332:VAL:O	2:B:333:GLN:HG3	2.18	0.44
1:A:60:GLU:O	1:A:60:GLU:HG2	2.17	0.44
2:B:197:ALA:HB3	2:B:218:PHE:CD2	2.53	0.44
2:B:207:LEU:HD23	2:B:237:VAL:HG11	1.99	0.44
2:B:547:VAL:HG12	2:B:552:VAL:HG13	2.00	0.44
2:B:420:SER:O	2:B:430:LYS:HE2	2.18	0.44
1:A:147:PHE:CE1	1:A:166:LEU:HD21	2.53	0.44
2:B:318:LEU:CD2	2:B:339:ILE:HD11	2.38	0.44
2:B:6:ARG:HG2	2:B:6:ARG:NH1	2.32	0.44
1:A:140:GLN:HE21	1:A:175:ARG:HH11	1.64	0.44
2:B:67:ASP:OD2	2:B:89:LYS:HA	2.18	0.44
2:B:155:THR:C	2:B:191:MET:HE1	2.38	0.43
2:B:136:HIS:O	2:B:362:ASP:HA	2.17	0.43
2:B:156:MET:HG3	2:B:191:MET:HE1	2.00	0.43
2:B:279:GLY:HA2	2:B:366:MET:CE	2.48	0.43
2:B:156:MET:H	2:B:191:MET:HE1	1.73	0.43
2:B:412:ASN:N	2:B:413:PRO:HD2	2.33	0.43
2:B:519:CYS:C	2:B:520:ARG:HD2	2.38	0.43
1:A:166:LEU:HD13	1:A:174:VAL:CG2	2.47	0.43
2:B:308:VAL:HG21	2:B:558:ASN:OD1	2.18	0.43
2:B:307:THR:H	2:B:310:THR:HG23	1.84	0.43
2:B:363:SER:HB3	2:B:369:VAL:HB	2.00	0.43
2:B:133:ILE:HG23	2:B:155:THR:HB	2.01	0.43
2:B:64:GLU:O	2:B:65:GLU:C	2.56	0.43
2:B:438:SER:HA	2:B:439:PRO:HD2	1.78	0.43
2:B:275:THR:HB	2:B:356:PHE:HE1	1.83	0.43
1:A:150:VAL:O	1:A:158:ARG:NH2	2.49	0.43
1:A:8:LEU:H	1:A:8:LEU:CD2	2.30	0.43
2:B:144:GLN:OE1	2:B:363:SER:CB	2.67	0.43
2:B:352:ASP:OD1	2:B:401:ARG:NH2	2.50	0.43
1:A:37:ALA:O	1:A:38:LEU:C	2.56	0.43
2:B:467:ILE:CG1	2:B:469:THR:HG23	2.49	0.43
2:B:455:ILE:O	2:B:480:ALA:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:ALA:O	1:A:227:LYS:C	2.57	0.43
1:A:72:ASP:O	1:A:106:LEU:HD23	2.18	0.43
2:B:49:LYS:HB3	2:B:50:THR:H	1.61	0.43
2:B:53:GLU:C	2:B:55:MET:H	2.22	0.43
2:B:125:GLY:C	2:B:126:LEU:HD12	2.39	0.43
2:B:565:LEU:O	2:B:565:LEU:HD22	2.17	0.43
2:B:254:GLU:HG3	2:B:255:ALA:N	2.34	0.43
1:A:152:ARG:HA	1:A:223:PHE:CD2	2.54	0.43
2:B:248:HIS:CG	2:B:274:HIS:CE1	3.07	0.42
2:B:300:THR:O	2:B:301:ASN:HB2	2.18	0.42
2:B:115:GLY:N	2:B:118:THR:HG23	2.27	0.42
2:B:78:TYR:CE2	2:B:79:THR:HG23	2.53	0.42
1:A:1:MET:O	1:A:2:LYS:C	2.58	0.42
2:B:547:VAL:C	2:B:549:GLY:N	2.72	0.42
2:B:318:LEU:HB2	2:B:319:MET:HE1	2.01	0.42
1:A:151:ASN:C	1:A:153:CYS:H	2.22	0.42
1:A:202:VAL:HG12	1:A:204:ARG:H	1.84	0.42
1:A:2:LYS:N	1:A:2:LYS:HD3	2.33	0.42
1:A:38:LEU:HD23	1:A:65:LEU:HD21	2.02	0.42
2:B:174:PRO:O	2:B:178:ASN:ND2	2.41	0.42
2:B:369:VAL:O	2:B:369:VAL:HG22	2.18	0.42
2:B:191:MET:O	2:B:192:ASN:C	2.57	0.42
1:A:219:LYS:HD3	1:A:228:SER:HA	2.01	0.42
2:B:523:THR:O	2:B:526:ASP:HB2	2.18	0.42
2:B:280:GLY:HA2	2:B:338:ARG:CZ	2.50	0.42
1:A:146:HIS:HE1	1:A:202:VAL:HG21	1.85	0.42
2:B:219:KCX:OQ2	2:B:221:HIS:HD2	2.03	0.42
2:B:245:VAL:HG12	2:B:270:MET:HE1	2.02	0.42
1:A:199:ASN:O	1:A:200:ALA:HB3	2.20	0.42
2:B:301:ASN:HD22	2:B:367:GLY:HA2	1.84	0.42
2:B:192:ASN:ND2	2:B:451:LYS:HE2	2.34	0.42
2:B:527:MET:O	2:B:531:ASN:HB3	2.20	0.42
1:A:126:ALA:O	1:A:127:VAL:HG13	2.20	0.42
1:A:136:ASP:OD1	1:A:137:ARG:NE	2.53	0.42
2:B:138:HIS:CD2	2:B:171:THR:HG23	2.55	0.42
2:B:297:PRO:CG	2:B:524:LYS:HE3	2.50	0.42
2:B:248:HIS:NE2	2:B:280:GLY:HA3	2.35	0.42
2:B:49:LYS:HD2	2:B:49:LYS:N	2.35	0.42
1:A:112:PHE:HB2	2:B:20:LYS:HB2	2.01	0.41
2:B:314:HIS:O	2:B:316:ASP:N	2.53	0.41
2:B:407:SER:HA	2:B:410:THR:HG1	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:THR:O	1:A:7:GLU:N	2.53	0.41
1:A:114:LYS:O	1:A:114:LYS:HG3	2.20	0.41
2:B:332:VAL:O	2:B:332:VAL:HG23	2.20	0.41
1:A:106:LEU:HD12	1:A:107:VAL:H	1.84	0.41
2:B:348:ASP:OD1	2:B:348:ASP:N	2.48	0.41
2:B:360:SER:HB3	2:B:361:SER:H	1.68	0.41
2:B:134:ASP:OD1	2:B:361:SER:HB3	2.19	0.41
2:B:568:ILE:HG23	2:B:569:PHE:HD1	1.85	0.41
2:B:273:PHE:O	2:B:274:HIS:ND1	2.53	0.41
2:B:69:ILE:HD13	2:B:114:VAL:HG22	2.01	0.41
2:B:389:ARG:HH21	2:B:396:ASP:C	2.22	0.41
2:B:389:ARG:HH21	2:B:397:ASN:N	2.18	0.41
2:B:99:GLY:HA3	2:B:112:LEU:HB3	2.02	0.41
2:B:318:LEU:H	2:B:318:LEU:CD2	2.30	0.41
1:A:227:LYS:HG3	1:A:228:SER:H	1.86	0.41
1:A:166:LEU:HD13	1:A:174:VAL:HG23	2.01	0.41
2:B:251:THR:C	2:B:253:ASN:N	2.73	0.41
2:B:102:LYS:HA	2:B:108:VAL:CG1	2.51	0.41
2:B:99:GLY:N	2:B:109:LYS:HZ1	2.19	0.41
1:A:139:VAL:HG12	1:A:141:ILE:CD1	2.51	0.41
1:A:166:LEU:O	1:A:168:ILE:HG12	2.21	0.41
1:A:236:ILE:O	1:A:236:ILE:HG12	2.21	0.41
2:B:301:ASN:HD21	2:B:368:ARG:H	1.54	0.41
1:A:125:LYS:N	1:A:125:LYS:CD	2.79	0.41
2:B:471:GLN:HA	2:B:472:PRO:C	2.41	0.41
1:A:11:LEU:O	1:A:15:TYR:HD2	2.03	0.41
2:B:136:HIS:CE1	2:B:273:PHE:CG	3.09	0.41
2:B:412:ASN:ND2	2:B:528:GLN:H	2.16	0.41
1:A:122:GLU:HG3	1:A:123:GLY:N	2.36	0.41
2:B:175:GLY:O	2:B:179:LEU:HG	2.21	0.41
1:A:91:THR:HG23	4:A:2005:HOH:O	2.20	0.41
2:B:199:GLY:HA3	2:B:220:ILE:HD13	2.03	0.41
1:A:66:LYS:HB2	1:A:67:PRO:HD2	2.03	0.41
2:B:373:ILE:HB	4:B:2036:HOH:O	2.21	0.41
2:B:131:GLY:HA3	2:B:154:THR:HG23	2.03	0.41
2:B:220:ILE:HG22	2:B:226:THR:HG23	2.03	0.40
2:B:533:THR:O	2:B:534:ALA:HB2	2.20	0.40
1:A:46:GLU:HB3	1:A:57:LEU:CD1	2.47	0.40
2:B:469:THR:N	2:B:470:PRO:CD	2.81	0.40
2:B:445:LYS:HA	2:B:446:PRO:HD2	1.92	0.40
2:B:109:LYS:O	2:B:111:ASN:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:221:HIS:CE1	2:B:223:ASP:OD1	2.75	0.40
1:A:122:GLU:O	1:A:124:LYS:HG2	2.21	0.40
2:B:466:SER:O	2:B:467:ILE:HG23	2.21	0.40
2:B:99:GLY:H	2:B:109:LYS:HZ1	1.70	0.40
2:B:25:ASP:OD1	2:B:25:ASP:C	2.60	0.40
2:B:124:GLU:HG2	2:B:124:GLU:O	2.22	0.40
1:A:23:ARG:C	1:A:28:ILE:HG22	2.42	0.40
2:B:511:ARG:O	2:B:513:VAL:HG23	2.21	0.40
2:B:251:THR:C	2:B:253:ASN:H	2.23	0.40
2:B:441:PHE:CD1	2:B:441:PHE:N	2.89	0.40
2:B:191:MET:HE3	2:B:191:MET:C	2.41	0.40
2:B:38:ILE:O	2:B:39:TYR:C	2.60	0.40
2:B:110:ASN:HA	2:B:110:ASN:HD22	1.69	0.40
2:B:525:LYS:HD3	2:B:531:ASN:HD22	1.86	0.40
2:B:26:THR:HG22	2:B:561:SER:CB	2.52	0.40
1:A:21:LYS:HG3	1:A:22:LYS:H	1.84	0.40
1:A:1:MET:O	1:A:3:LEU:N	2.54	0.40
1:A:113:LEU:HD12	1:A:113:LEU:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	236/238 (99%)	183 (78%)	37 (16%)	16 (7%)	1	7
2	B	566/569 (100%)	428 (76%)	97 (17%)	41 (7%)	1	7
All	All	802/807 (99%)	611 (76%)	134 (17%)	57 (7%)	1	7

All (57) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	102	ALA
1	A	116	GLU
1	A	125	LYS
1	A	172	THR
1	A	227	LYS
2	B	49	LYS
2	B	249	THR
2	B	285	ASP
2	B	286	ILE
2	B	300	THR
2	B	301	ASN
2	B	317	MET
1	A	2	LYS
1	A	122	GLU
1	A	123	GLY
1	A	151	ASN
1	A	167	ASP
2	B	2	LYS
2	B	47	GLY
2	B	191	MET
2	B	282	HIS
2	B	327	SER
2	B	389	ARG
2	B	462	ASP
2	B	39	TYR
2	B	65	GLU
2	B	84	ALA
2	B	139	PHE
2	B	163	PRO
2	B	252	LEU
2	B	274	HIS
2	B	287	ILE
2	B	360	SER
2	B	363	SER
2	B	439	PRO
2	B	480	ALA
2	B	548	ASP
2	B	564	GLN
1	A	152	ARG
1	A	166	LEU
1	A	206	ALA
2	B	315	MET
2	B	326	LYS

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Mol	Chain	Res	Type
2	B	366	MET
1	A	37	ALA
1	A	146	HIS
2	B	17	THR
2	B	303	THR
2	B	316	ASP
2	B	332	VAL
1	A	115	ASN
2	B	54	GLY
2	B	99	GLY
2	B	320	VAL
2	B	325	ASP
2	B	444	VAL
2	B	426	VAL

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%)	15	47
2	B	458/458 (100%)	413 (90%)	45 (10%)	10	36
All	All	655/655 (100%)	594 (91%)	61 (9%)	11	39

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	6	LYS
1	A	19	LEU
1	A	59	GLN
1	A	68	ASP
1	A	83	ILE
1	A	107	VAL
1	A	113	LEU
1	A	115	ASN

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Mol	Chain	Res	Type
1	A	125	LYS
1	A	133	ASN
1	A	159	GLU
1	A	207	ASP
1	A	221	ARG
1	A	227	LYS
1	A	230	ASP
2	B	1	MET
2	B	6	ARG
2	B	16	THR
2	B	42	GLU
2	B	49	LYS
2	B	66	LEU
2	B	69	ILE
2	B	98	LYS
2	B	101	ASN
2	B	105	GLN
2	B	109	LYS
2	B	111	ASN
2	B	118	THR
2	B	170	THR
2	B	177	ARG
2	B	190	SER
2	B	191	MET
2	B	223	ASP
2	B	237	VAL
2	B	240	LYS
2	B	243	VAL
2	B	249	THR
2	B	260	ASP
2	B	270	MET
2	B	276	GLU
2	B	285	ASP
2	B	292	GLU
2	B	294	ASN
2	B	323	HIS
2	B	325	ASP
2	B	330	GLU
2	B	342	GLN
2	B	348	ASP
2	B	352	ASP
2	B	364	GLN

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Mol	Chain	Res	Type
2	B	389	ARG
2	B	411	ILE
2	B	435	VAL
2	B	457	LEU
2	B	469	THR
2	B	492	THR
2	B	520	ARG
2	B	530	ASN
2	B	536	ILE
2	B	565	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	HIS
1	A	59	GLN
1	A	121	ASN
1	A	133	ASN
1	A	140	GLN
1	A	192	ASN
1	A	205	GLN
2	B	34	HIS
2	B	59	ASN
2	B	101	ASN
2	B	110	ASN
2	B	111	ASN
2	B	168	ASN
2	B	200	ASN
2	B	244	GLN
2	B	294	ASN
2	B	301	ASN
2	B	333	GLN
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

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Mol	Chain	Res	Type
2	B	512	GLN
2	B	518	ASN
2	B	564	GLN

5.3.3 RNA ⓘ

There are no RNA molecules 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	3,2	7,11,12	0.87	0	7,12,14	1.08	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
2	KCX	B	219	3,2	-	0/6/10/12	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	219	KCX	4	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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, 95th 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 ²)	Q<0.9
1	A	238/238 (100%)	-0.78	0 100 100	6, 26, 47, 79	0
2	B	568/569 (99%)	-0.82	4 (0%) 89 70	1, 13, 55, 100	0
All	All	806/807 (99%)	-0.81	4 (0%) 91 76	1, 17, 50, 100	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	331	ASP	3.3
2	B	327	SER	2.3
2	B	329	LYS	2.2
2	B	328	ILE	2.1

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, 95th 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 ²)	Q<0.9
2	KCX	B	219	12/13	0.92	0.17	-	18,24,39,41	0

6.3 Carbohydrates

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, 95th 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(\AA^2)	Q<0.9
3	NI	B	3001	1/1	0.98	0.09	-1.22	56,56,56,56	0
3	NI	B	3002	1/1	0.98	0.08	-2.09	74,74,74,74	0

6.5 Other polymers [i](#)

There are no such residues in this entry.