



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:40 AM UTC

PDB ID : 3V0B / pdb_00003v0b
Title : 3.9 angstrom crystal structure of BoNT/Ai in complex with NTNHA
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Deposited on : 2011-12-07
Resolution : 3.90 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

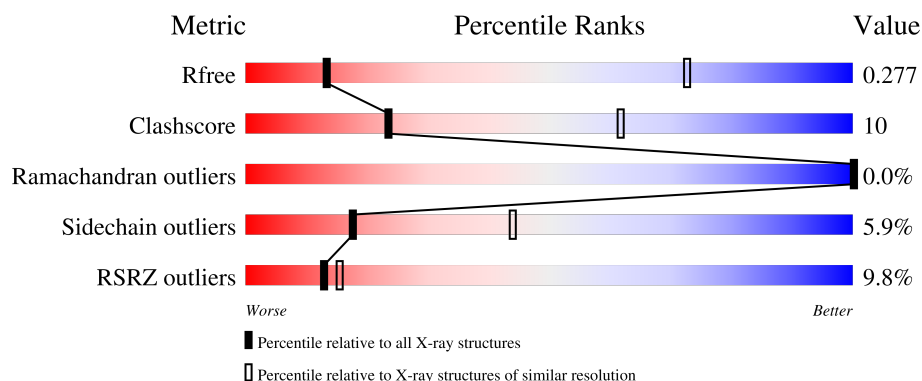
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.90 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}	180053	1270 (4.10-3.70)
Clashscore	190562	1034 (4.08-3.72)
Ramachandran outliers	187476	1251 (4.10-3.70)
Sidechain outliers	187428	1243 (4.10-3.70)
RSRZ outliers	180081	1269 (4.10-3.70)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	1296	8% 78% 20% ..
2	B	1196	12% 70% 22% ..

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 19830 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 BoNT/A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1280	Total	C	N	O	S	36	0	0
			10418	6681	1721	1983	33			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	224	GLN	GLU	engineered mutation	UNP Q7B8V4
A	363	ALA	ARG	engineered mutation	UNP Q7B8V4
A	366	PHE	TYR	engineered mutation	UNP Q7B8V4
A	1158	ALA	THR	conflict	UNP Q7B8V4

- Molecule 2 is a protein called NTN1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1150	Total	C	N	O	S	46	0	0
			9410	6022	1515	1841	32			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	expression tag	UNP Q45914
B	0	SER	-	expression tag	UNP Q45914
B	1194	PRO	-	expression tag	UNP Q45914

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

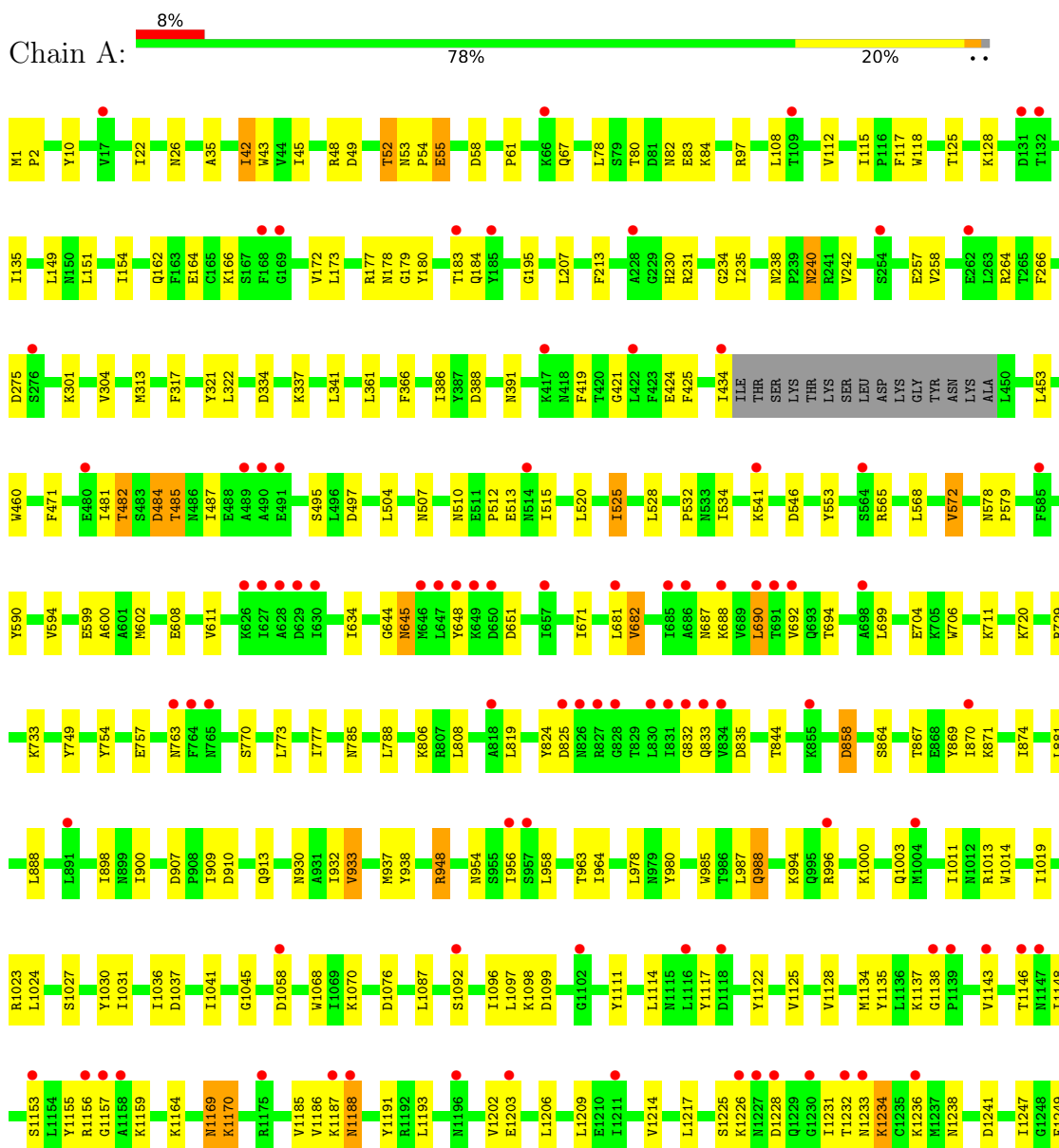
- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

3 Residue-property plots

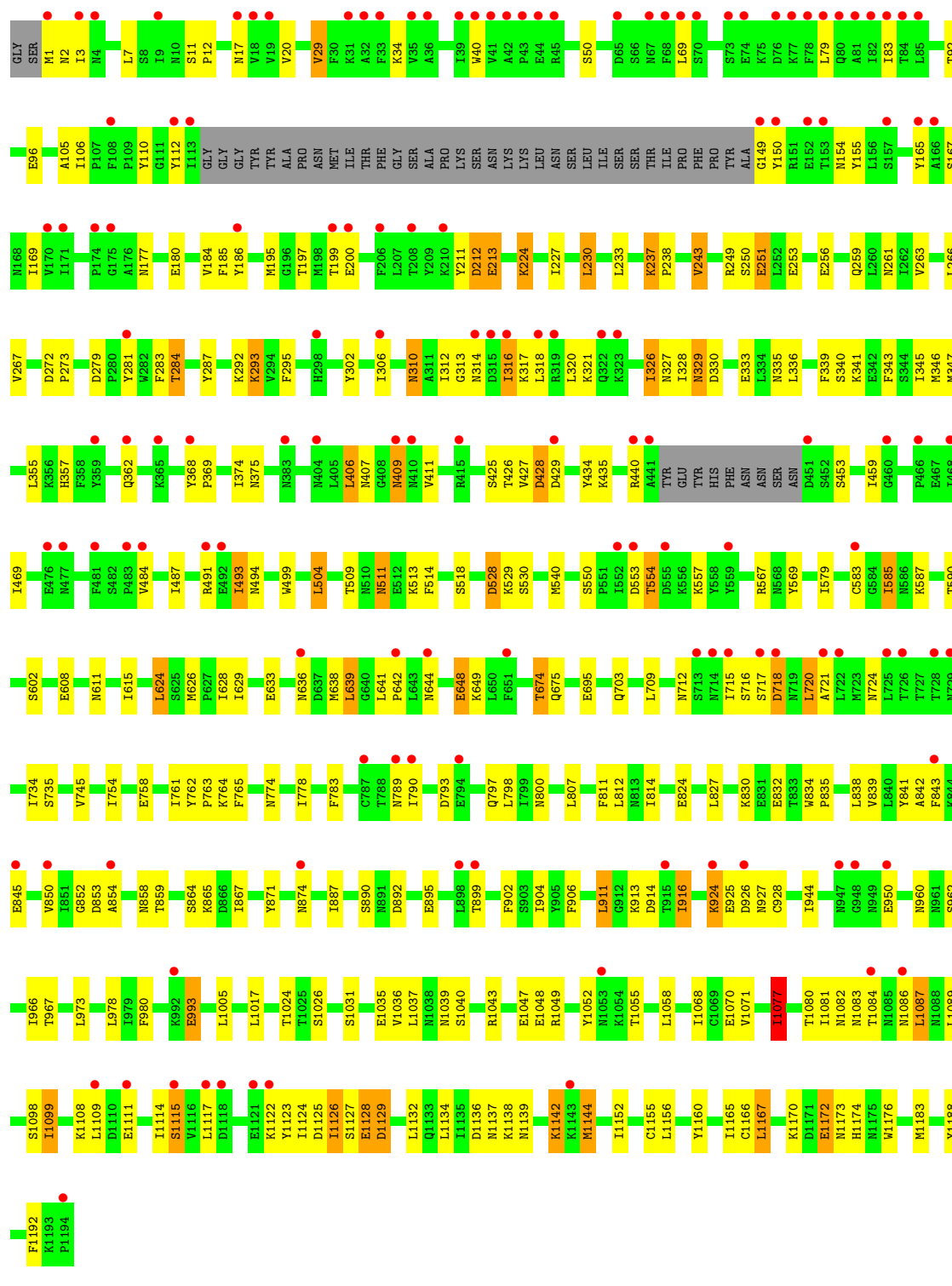
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: BoNT/A





• Molecule 2: NTNH



4 Data and refinement statistics

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, α , β , γ	282.23Å 282.23Å 374.82Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.47 – 3.90 48.47 – 3.90	Depositor EDS
% Data completeness (in resolution range)	92.1 (48.47-3.90) 92.1 (48.47-3.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.63 (at 3.88Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, R_{free}	0.252 , 0.280 0.251 , 0.277	Depositor DCC
R_{free} test set	3740 reflections (4.65%)	wwPDB-VP
Wilson B-factor (Å ²)	139.8	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 155.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	19830	wwPDB-VP
Average B, all atoms (Å ²)	179.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.10% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: CA, ZN

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	0.39	0/10639	0.77	5/14405 (0.0%)
2	B	0.39	0/9605	0.80	12/13015 (0.1%)
All	All	0.39	0/20244	0.78	17/27420 (0.1%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1172	GLU	N-CA-C	7.70	120.79	111.40
2	B	425	SER	N-CA-C	6.57	120.24	109.85
2	B	899	THR	N-CA-C	6.16	120.95	113.38
1	A	932	ILE	N-CA-C	5.84	118.62	112.83
1	A	235	ILE	N-CA-C	5.80	117.74	112.29
1	A	1041	ILE	N-CA-C	5.69	118.36	112.90
2	B	212	ASP	CB-CA-C	-5.59	109.63	117.23
1	A	938	TYR	N-CA-C	5.52	120.12	113.17
2	B	1037	LEU	CA-C-N	-5.48	114.66	122.77
2	B	1037	LEU	C-N-CA	-5.48	114.66	122.77
1	A	1285	ILE	N-CA-C	5.26	112.76	107.55
2	B	1087	LEU	N-CA-C	-5.23	106.87	113.20
2	B	284	THR	N-CA-C	5.21	115.17	108.34
2	B	428	ASP	N-CA-CB	5.12	119.20	110.50
2	B	237	LYS	CA-C-N	5.09	125.07	120.03
2	B	237	LYS	C-N-CA	5.09	125.07	120.03
2	B	1077	ILE	N-CA-C	5.05	115.18	108.11

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	10418	0	10297	201	30
2	B	9410	0	9202	220	31
3	A	1	0	0	0	0
4	A	1	0	0	0	0
All	All	19830	0	19499	399	32

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 10.

All (399) 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:340:SER:HB2	2:B:347:MET:HE3	1.30	1.11
2:B:528:ASP:HB2	2:B:530:SER:H	1.07	1.09
2:B:336:LEU:HB3	2:B:347:MET:HE1	1.31	1.07
2:B:426:THR:HB	2:B:427:VAL:HA	1.02	1.02
2:B:528:ASP:HB2	2:B:530:SER:N	1.76	1.00
2:B:426:THR:HB	2:B:427:VAL:CA	1.91	0.99
2:B:426:THR:CB	2:B:427:VAL:HA	1.93	0.98
1:A:421:GLY:H	1:A:424:GLU:HG3	1.33	0.92
2:B:528:ASP:CB	2:B:530:SER:H	1.88	0.87
1:A:1265:ASN:ND2	2:B:845:GLU:HG2	1.93	0.83
2:B:314:ASN:HB3	2:B:318:LEU:HD12	1.60	0.82
2:B:1099:ILE:HD12	2:B:1099:ILE:H	1.44	0.81
1:A:10:TYR:CZ	1:A:84:LYS:HD3	2.16	0.81
1:A:80:THR:HG22	1:A:82:ASN:H	1.47	0.80
1:A:988:GLN:HG3	1:A:994:LYS:HB3	1.64	0.80
1:A:149:LEU:HD12	1:A:183:THR:CG2	2.12	0.80
2:B:715:ILE:HG22	2:B:720:LEU:HD22	1.61	0.80
2:B:426:THR:OG1	2:B:427:VAL:CG2	2.30	0.80
1:A:482:THR:HG22	1:A:484:ASP:H	1.46	0.79
1:A:525:ILE:HD12	1:A:525:ILE:H	1.47	0.78
1:A:52:THR:HG23	1:A:528:LEU:HD11	1.66	0.77
1:A:1265:ASN:HD22	2:B:845:GLU:HG2	1.48	0.77
1:A:487:ILE:HG23	1:A:704:GLU:OE2	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:602:SER:HB2	2:B:608:GLU:OE1	1.85	0.75
1:A:1271:ILE:HG13	2:B:854:ALA:HB1	1.67	0.75
2:B:426:THR:HG21	2:B:428:ASP:OD2	1.86	0.75
1:A:421:GLY:N	1:A:424:GLU:HG3	2.02	0.74
1:A:1271:ILE:HG13	2:B:854:ALA:CB	2.18	0.73
2:B:1031:SER:O	2:B:1035:GLU:HG2	1.89	0.73
2:B:1170:LYS:HE3	2:B:1173:ASN:HB3	1.69	0.73
1:A:1265:ASN:ND2	2:B:845:GLU:CG	2.51	0.73
1:A:1137:LYS:HG2	1:A:1138:GLY:H	1.53	0.73
2:B:426:THR:OG1	2:B:427:VAL:HG22	1.89	0.72
1:A:1275:SER:HA	2:B:827:LEU:HD21	1.70	0.72
2:B:251:GLU:HG2	2:B:357:HIS:HE1	1.54	0.71
2:B:243:VAL:HG13	2:B:259:GLN:HB2	1.72	0.71
1:A:149:LEU:HD12	1:A:183:THR:HG23	1.71	0.71
1:A:482:THR:HG22	1:A:484:ASP:N	2.07	0.70
1:A:1278:LEU:HD23	1:A:1281:SER:OG	1.92	0.70
1:A:1265:ASN:HD22	2:B:845:GLU:CG	2.03	0.69
2:B:834:TRP:HB2	2:B:835:PRO:HD2	1.74	0.69
2:B:96:GLU:HG2	2:B:459:ILE:HD13	1.75	0.68
2:B:243:VAL:CG1	2:B:259:GLN:HB2	2.22	0.68
2:B:1123:TYR:CE1	2:B:1138:LYS:HB2	2.28	0.68
1:A:870:ILE:O	1:A:874:ILE:HG13	1.93	0.67
1:A:1228:ASP:HB3	1:A:1232:THR:H	1.60	0.67
2:B:528:ASP:HB2	2:B:529:LYS:CA	2.25	0.67
2:B:715:ILE:CG2	2:B:720:LEU:HD22	2.24	0.67
2:B:426:THR:OG1	2:B:427:VAL:HG23	1.94	0.66
2:B:310:ASN:OD1	2:B:310:ASN:N	2.29	0.66
2:B:528:ASP:HB2	2:B:529:LYS:HA	1.76	0.66
1:A:1037:ASP:OD1	2:B:812:LEU:HD23	1.95	0.66
1:A:1170:LYS:H	1:A:1170:LYS:HD3	1.60	0.66
2:B:295:PHE:CD1	2:B:328:ILE:HD11	2.32	0.65
1:A:1269:ARG:HG2	2:B:841:TYR:CE1	2.32	0.65
1:A:1236:LYS:NZ	1:A:1280:CYS:SG	2.70	0.65
2:B:302:TYR:OH	2:B:321:LYS:HB2	1.98	0.64
1:A:149:LEU:HD12	1:A:183:THR:HG21	1.79	0.64
1:A:1170:LYS:HD3	1:A:1170:LYS:N	2.13	0.64
1:A:80:THR:HG22	1:A:82:ASN:N	2.12	0.64
2:B:493:ILE:HD11	2:B:499:TRP:CZ2	2.33	0.64
2:B:336:LEU:CB	2:B:347:MET:HE1	2.21	0.64
1:A:453:LEU:HD23	1:A:453:LEU:H	1.62	0.63
2:B:336:LEU:HB3	2:B:347:MET:CE	2.18	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1170:LYS:O	1:A:1170:LYS:HG2	1.99	0.63
2:B:251:GLU:HG2	2:B:357:HIS:CE1	2.34	0.63
2:B:409:ASN:OD1	2:B:409:ASN:N	2.31	0.63
1:A:149:LEU:CD1	1:A:183:THR:HG21	2.28	0.63
1:A:1:MET:N	1:A:2:PRO:HD3	2.14	0.62
2:B:1132:LEU:HD21	2:B:1165:ILE:HD13	1.79	0.62
1:A:135:ILE:HD13	1:A:149:LEU:CD2	2.30	0.62
1:A:117:PHE:HA	1:A:317:PHE:CE1	2.34	0.62
1:A:611:VAL:HG12	1:A:1024:LEU:HD11	1.81	0.62
1:A:1000:LYS:HE2	2:B:811:PHE:CE1	2.35	0.61
2:B:960:ASN:OD1	2:B:962:SER:HB3	2.00	0.61
2:B:1142:LYS:HD3	2:B:1160:TYR:CE1	2.36	0.61
1:A:681:LEU:HD23	1:A:694:THR:HG22	1.81	0.61
1:A:184:GLN:OE1	1:A:231:ARG:HD3	2.01	0.60
1:A:963:THR:HB	1:A:1058:ASP:HB3	1.84	0.60
2:B:715:ILE:HB	2:B:720:LEU:HD21	1.82	0.60
1:A:10:TYR:CZ	1:A:84:LYS:CD	2.84	0.60
1:A:482:THR:CG2	1:A:484:ASP:H	2.14	0.60
1:A:67:GLN:O	1:A:460:TRP:HZ2	1.85	0.59
2:B:1172:GLU:H	2:B:1174:HIS:H	1.50	0.59
1:A:52:THR:CG2	1:A:528:LEU:HD11	2.31	0.59
2:B:638:MET:HE3	2:B:649:LYS:HD3	1.84	0.59
2:B:639:LEU:HD12	2:B:783:PHE:HE1	1.67	0.59
1:A:53:ASN:OD1	1:A:55:GLU:HB2	2.01	0.59
1:A:1092:SER:O	1:A:1098:LYS:NZ	2.34	0.59
2:B:639:LEU:HD12	2:B:783:PHE:CE1	2.37	0.59
2:B:1082:ASN:ND2	2:B:1084:THR:O	2.36	0.59
1:A:706:TRP:CD2	1:A:808:LEU:HD13	2.37	0.59
1:A:149:LEU:CD1	1:A:183:THR:CG2	2.81	0.58
2:B:169:ILE:CD1	2:B:199:THR:HB	2.33	0.58
2:B:924:LYS:HG3	2:B:928:CYS:O	2.03	0.58
1:A:1128:VAL:HG11	1:A:1191:TYR:CE2	2.38	0.58
2:B:79:LEU:O	2:B:83:ILE:HG13	2.03	0.58
1:A:388:ASP:HB3	1:A:391:ASN:O	2.03	0.58
2:B:313:GLY:H	2:B:317:LYS:HZ2	1.50	0.58
2:B:1125:ASP:OD1	2:B:1126:ILE:N	2.36	0.58
2:B:110:TYR:O	2:B:150:TYR:HD1	1.87	0.58
1:A:687:ASN:ND2	1:A:690:LEU:HD22	2.19	0.58
1:A:568:LEU:HD12	1:A:594:VAL:HG11	1.85	0.57
1:A:1271:ILE:HD11	2:B:839:VAL:HG21	1.86	0.57
1:A:985:TRP:CD2	1:A:1019:ILE:HG21	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1228:ASP:OD2	1:A:1231:ILE:HB	2.05	0.57
2:B:674:THR:HG22	2:B:675:GLN:HG3	1.85	0.57
2:B:281:TYR:OH	2:B:440:ARG:O	2.23	0.56
2:B:238:PRO:HG3	2:B:287:TYR:CZ	2.40	0.56
1:A:1277:THR:O	1:A:1277:THR:HG23	2.05	0.56
1:A:1122:TYR:CZ	1:A:1156:ARG:NE	2.74	0.56
1:A:35:ALA:HB2	1:A:45:ILE:HG12	1.88	0.55
2:B:283:PHE:HA	2:B:434:TYR:OH	2.06	0.55
1:A:1117:TYR:CD1	1:A:1277:THR:OG1	2.55	0.55
2:B:1137:ASN:OD1	2:B:1139:ASN:HB2	2.07	0.55
1:A:80:THR:HB	1:A:83:GLU:HG3	1.88	0.55
1:A:869:TYR:HD1	1:A:870:ILE:HD12	1.72	0.55
2:B:112:TYR:CE1	2:B:149:GLY:HA3	2.42	0.55
1:A:996:ARG:HE	2:B:807:LEU:HD11	1.72	0.55
1:A:67:GLN:HG2	1:A:425:PHE:CE1	2.41	0.55
1:A:1137:LYS:HG2	1:A:1138:GLY:N	2.21	0.55
1:A:648:TYR:O	1:A:651:ASP:HB2	2.07	0.54
1:A:1134:MET:HE1	1:A:1193:LEU:HD13	1.88	0.54
1:A:49:ASP:OD1	1:A:52:THR:HB	2.06	0.54
1:A:1122:TYR:OH	1:A:1156:ARG:NE	2.40	0.54
2:B:169:ILE:HD13	2:B:199:THR:HB	1.88	0.54
1:A:553:TYR:CZ	1:A:572:VAL:HG21	2.43	0.54
1:A:565:ARG:HB2	1:A:749:TYR:CZ	2.43	0.54
1:A:1228:ASP:HB3	1:A:1232:THR:N	2.23	0.54
1:A:322:LEU:HD12	1:A:341:LEU:HB2	1.90	0.54
1:A:763:ASN:O	1:A:937:MET:HE1	2.07	0.54
2:B:762:TYR:HB3	2:B:763:PRO:HD3	1.89	0.54
2:B:341:LYS:HA	2:B:824:GLU:HG2	1.90	0.54
1:A:61:PRO:HB3	1:A:419:PHE:CZ	2.43	0.53
2:B:243:VAL:HG11	2:B:259:GLN:CD	2.33	0.53
1:A:1036:ILE:O	2:B:814:ILE:N	2.28	0.53
1:A:888:LEU:HB3	1:A:900:ILE:HD11	1.91	0.53
1:A:1271:ILE:O	1:A:1271:ILE:HG22	2.07	0.53
1:A:42:ILE:HD13	1:A:151:LEU:HB3	1.90	0.53
1:A:207:LEU:HD11	1:A:1076:ASP:HB3	1.91	0.53
1:A:1228:ASP:OD1	1:A:1234:LYS:HD2	2.09	0.53
2:B:513:LYS:HD2	2:B:514:PHE:H	1.74	0.53
1:A:67:GLN:O	1:A:460:TRP:CZ2	2.62	0.53
2:B:227:ILE:HD11	2:B:339:PHE:CE2	2.43	0.53
1:A:108:LEU:O	1:A:112:VAL:HG23	2.09	0.53
2:B:306:ILE:HG23	2:B:312:ILE:CD1	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:513:LYS:HD2	2:B:514:PHE:N	2.24	0.53
1:A:644:GLY:O	1:A:645:ASN:ND2	2.43	0.52
1:A:1241:ASP:HB3	1:A:1247:ILE:HD11	1.91	0.52
2:B:40:TRP:CD1	2:B:167:SER:HB2	2.45	0.52
2:B:887:ILE:HG23	2:B:1005:LEU:HB3	1.92	0.52
1:A:1122:TYR:OH	1:A:1137:LYS:HD2	2.09	0.52
2:B:329:ASN:O	2:B:333:GLU:HG2	2.10	0.52
2:B:112:TYR:HE1	2:B:149:GLY:HA3	1.75	0.52
2:B:227:ILE:HG22	2:B:267:VAL:HG22	1.92	0.52
2:B:266:LEU:O	2:B:335:ASN:HB3	2.10	0.52
2:B:1043:ARG:HB3	2:B:1047:GLU:HA	1.92	0.51
1:A:52:THR:HG22	1:A:53:ASN:N	2.25	0.51
1:A:1031:ILE:HG12	1:A:1036:ILE:HG13	1.92	0.51
1:A:864:SER:HA	1:A:867:THR:HB	1.93	0.51
1:A:599:GLU:HB2	1:A:602:MET:HE2	1.93	0.51
1:A:1209:LEU:CD1	1:A:1217:LEU:HD13	2.40	0.51
1:A:115:ILE:HD11	1:A:512:PRO:HB2	1.92	0.51
1:A:706:TRP:CE3	1:A:808:LEU:HD13	2.46	0.51
1:A:1037:ASP:HA	2:B:814:ILE:HD12	1.93	0.51
1:A:1278:LEU:HG	1:A:1280:CYS:SG	2.51	0.51
2:B:528:ASP:HB2	2:B:529:LYS:C	2.35	0.50
2:B:1058:LEU:HD23	2:B:1068:ILE:HG13	1.93	0.50
1:A:1003:GLN:HA	1:A:1011:ILE:HD11	1.92	0.50
1:A:729:ARG:HD2	1:A:785:ASN:OD1	2.11	0.50
1:A:1238:ASN:HB2	1:A:1249:PHE:CE1	2.46	0.50
1:A:699:LEU:HD22	1:A:844:THR:HG21	1.93	0.50
2:B:426:THR:CB	2:B:427:VAL:CA	2.69	0.50
1:A:504:LEU:O	2:B:1170:LYS:HB2	2.12	0.50
1:A:525:ILE:HD12	1:A:525:ILE:N	2.23	0.50
2:B:1172:GLU:H	2:B:1174:HIS:N	2.09	0.50
2:B:1:MET:HG2	2:B:2:ASN:H	1.76	0.50
2:B:227:ILE:O	2:B:230:LEU:HB2	2.12	0.50
1:A:688:LYS:HD3	1:A:833:GLN:NE2	2.27	0.50
1:A:172:VAL:HG23	1:A:173:LEU:N	2.26	0.49
1:A:1269:ARG:CZ	2:B:850:VAL:HG11	2.42	0.49
2:B:212:ASP:HB3	2:B:213:GLU:OE2	2.12	0.49
2:B:874:ASN:HB2	2:B:1036:VAL:HG13	1.94	0.49
1:A:179:GLY:O	1:A:321:TYR:OH	2.29	0.49
1:A:671:ILE:HG23	1:A:671:ILE:O	2.11	0.49
2:B:374:ILE:HD12	2:B:375:ASN:N	2.27	0.49
2:B:227:ILE:HD11	2:B:339:PHE:HE2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:864:SER:HB2	2:B:867:ILE:HG13	1.93	0.49
1:A:1096:ILE:O	1:A:1098:LYS:HE3	2.11	0.49
1:A:948:ARG:HB3	1:A:1068:TRP:HB2	1.95	0.49
2:B:326:ILE:HG23	2:B:327:ASN:N	2.28	0.49
2:B:1115:SER:HB2	2:B:1123:TYR:CD2	2.48	0.49
1:A:913:GLN:HG2	1:A:1070:LYS:HD3	1.94	0.49
1:A:172:VAL:HG23	1:A:173:LEU:H	1.77	0.49
1:A:634:ILE:HD12	1:A:634:ILE:N	2.27	0.49
1:A:954:ASN:OD1	1:A:956:ILE:HG12	2.13	0.49
2:B:633:GLU:OE1	2:B:633:GLU:HA	2.12	0.49
2:B:407:ASN:OD1	2:B:411:VAL:HG12	2.13	0.48
1:A:45:ILE:HB	1:A:154:ILE:HG22	1.94	0.48
2:B:259:GLN:OE1	2:B:426:THR:O	2.31	0.48
1:A:532:PRO:O	1:A:534:ILE:HD12	2.14	0.48
2:B:615:ILE:O	2:B:615:ILE:HG13	2.12	0.48
1:A:980:TYR:OH	1:A:1148:ILE:O	2.28	0.48
2:B:528:ASP:CB	2:B:530:SER:N	2.61	0.48
1:A:1164:LYS:NZ	1:A:1170:LYS:HA	2.29	0.48
2:B:944:ILE:HB	2:B:950:GLU:HG3	1.95	0.47
1:A:177:ARG:HD3	1:A:238:ASN:HA	1.95	0.47
2:B:1123:TYR:HE1	2:B:1138:LYS:HB2	1.77	0.47
2:B:238:PRO:HD2	2:B:263:VAL:CG2	2.45	0.47
2:B:902:PHE:HE1	2:B:904:ILE:HD11	1.80	0.47
2:B:1172:GLU:HB2	2:B:1173:ASN:C	2.39	0.47
1:A:1186:VAL:HB	1:A:1191:TYR:CE1	2.49	0.47
1:A:97:ARG:HA	1:A:386:ILE:HG23	1.97	0.47
2:B:316:ILE:HG22	2:B:317:LYS:N	2.29	0.47
2:B:914:ASP:OD2	2:B:916:ILE:HG23	2.14	0.47
2:B:1144:MET:HE2	2:B:1144:MET:HB2	1.61	0.47
1:A:179:GLY:CA	1:A:234:GLY:HA3	2.44	0.47
1:A:565:ARG:HB2	1:A:749:TYR:CE2	2.50	0.47
2:B:761:ILE:N	2:B:761:ILE:HD12	2.30	0.47
1:A:858:ASP:N	1:A:858:ASP:OD1	2.47	0.47
1:A:1:MET:H2	1:A:2:PRO:HD3	1.78	0.46
2:B:272:ASP:N	2:B:273:PRO:HD2	2.29	0.46
1:A:590:TYR:O	1:A:594:VAL:HG12	2.15	0.46
1:A:1014:TRP:CH2	1:A:1068:TRP:HB3	2.49	0.46
1:A:1122:TYR:CE2	1:A:1156:ARG:NE	2.83	0.46
2:B:1172:GLU:N	2:B:1173:ASN:HA	2.29	0.46
2:B:892:ASP:O	2:B:895:GLU:HG2	2.15	0.46
2:B:1166:CYS:HB3	2:B:1188:TYR:CD1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:17:ASN:HD22	2:B:34:LYS:HE3	1.81	0.46
2:B:426:THR:CG2	2:B:428:ASP:OD2	2.58	0.46
2:B:1039:ASN:O	2:B:1040:SER:CB	2.63	0.46
2:B:1129:ASP:OD1	2:B:1129:ASP:N	2.49	0.46
1:A:334:ASP:HB3	1:A:337:LYS:HB2	1.98	0.46
1:A:930:ASN:O	1:A:933:VAL:HG13	2.16	0.46
2:B:1115:SER:HB2	2:B:1123:TYR:CE2	2.50	0.46
2:B:435:LYS:HA	2:B:628:ILE:HG23	1.98	0.46
2:B:528:ASP:CB	2:B:529:LYS:HA	2.40	0.46
2:B:569:TYR:CE2	2:B:734:ILE:HG23	2.51	0.46
1:A:1125:VAL:HG22	1:A:1134:MET:HG2	1.98	0.46
2:B:636:ASN:HA	2:B:639:LEU:CD1	2.46	0.46
2:B:92:THR:HB	2:B:343:PHE:CZ	2.51	0.46
2:B:966:ILE:HD12	2:B:966:ILE:N	2.30	0.46
2:B:1070:GLU:CD	2:B:1077:ILE:HD11	2.40	0.46
1:A:1268:ASN:HB2	2:B:843:PHE:CE2	2.51	0.46
2:B:1123:TYR:HD1	2:B:1138:LYS:HA	1.80	0.46
2:B:842:ALA:HA	2:B:850:VAL:O	2.16	0.45
2:B:1167:LEU:HD12	2:B:1167:LEU:HA	1.81	0.45
2:B:261:ASN:OD1	2:B:263:VAL:HG23	2.16	0.45
1:A:421:GLY:H	1:A:424:GLU:CG	2.18	0.45
2:B:368:TYR:HA	2:B:369:PRO:HA	1.62	0.45
2:B:1080:THR:OG1	2:B:1081:ILE:N	2.49	0.45
1:A:125:THR:O	1:A:301:LYS:N	2.48	0.45
1:A:1209:LEU:HD11	1:A:1217:LEU:HD13	1.99	0.45
1:A:1271:ILE:HG13	2:B:854:ALA:HB3	1.94	0.45
1:A:230:HIS:CE1	1:A:264:ARG:HD3	2.51	0.45
2:B:774:ASN:O	2:B:778:ILE:HG12	2.16	0.45
1:A:135:ILE:HD13	1:A:149:LEU:HD23	1.99	0.45
1:A:162:GLN:HE21	1:A:164:GLU:CD	2.25	0.45
2:B:587:LYS:HB3	2:B:587:LYS:HE2	1.67	0.45
1:A:26:ASN:HD21	1:A:54:PRO:HD3	1.81	0.45
2:B:155:TYR:HA	2:B:165:TYR:O	2.16	0.45
1:A:49:ASP:HB2	1:A:154:ILE:HD12	1.98	0.44
2:B:314:ASN:O	2:B:318:LEU:HB2	2.16	0.44
2:B:1114:ILE:HB	2:B:1124:ILE:HD12	1.98	0.44
2:B:184:VAL:CG2	2:B:200:GLU:HB2	2.47	0.44
1:A:257:GLU:HG3	1:A:534:ILE:HG21	1.98	0.44
1:A:313:MET:HE1	1:A:515:ILE:HD13	1.99	0.44
1:A:22:ILE:HD11	1:A:45:ILE:HD11	1.99	0.44
2:B:406:LEU:HD11	2:B:494:ASN:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:773:LEU:O	1:A:777:ILE:HG13	2.17	0.44
2:B:798:LEU:HD23	2:B:798:LEU:HA	1.87	0.44
1:A:275:ASP:OD2	1:A:275:ASP:C	2.60	0.44
1:A:481:ILE:O	1:A:682:VAL:HG12	2.18	0.44
1:A:1097:LEU:HD12	1:A:1225:SER:HB3	2.00	0.44
2:B:293:LYS:HB2	2:B:293:LYS:NZ	2.32	0.44
1:A:749:TYR:CD1	1:A:749:TYR:C	2.95	0.44
1:A:1135:TYR:HB2	1:A:1259:ALA:O	2.18	0.44
1:A:1202:VAL:HG13	1:A:1203:GLU:OE2	2.18	0.44
2:B:426:THR:HB	2:B:428:ASP:HA	2.00	0.44
2:B:967:THR:HB	2:B:980:PHE:HB2	2.00	0.44
1:A:128:LYS:HG2	1:A:304:VAL:HB	1.99	0.44
2:B:841:TYR:CZ	2:B:852:GLY:HA3	2.53	0.43
2:B:1156:LEU:HD21	2:B:1192:PHE:CD2	2.53	0.43
2:B:306:ILE:HG23	2:B:312:ILE:HD12	1.99	0.43
2:B:762:TYR:O	2:B:765:PHE:HB3	2.18	0.43
1:A:43:TRP:CD1	1:A:149:LEU:HD22	2.53	0.43
1:A:1275:SER:CA	2:B:827:LEU:HD21	2.42	0.43
2:B:154:ASN:HB2	2:B:167:SER:O	2.18	0.43
2:B:1123:TYR:CD1	2:B:1138:LYS:HA	2.53	0.43
1:A:118:TRP:HB3	1:A:128:LYS:O	2.17	0.43
1:A:1122:TYR:CD1	1:A:1157:GLY:HA2	2.53	0.43
2:B:105:ALA:HB3	2:B:233:LEU:HD13	2.00	0.43
2:B:427:VAL:HA	2:B:428:ASP:HA	1.68	0.43
2:B:859:THR:HA	2:B:890:SER:O	2.18	0.43
2:B:1122:LYS:HB3	2:B:1134:LEU:HB3	2.00	0.43
2:B:34:LYS:HB2	2:B:40:TRP:CZ3	2.53	0.43
2:B:1084:THR:HB	2:B:1087:LEU:HB2	2.01	0.43
1:A:164:GLU:OE2	1:A:166:LYS:HE2	2.19	0.43
1:A:195:GLY:HA2	1:A:213:PHE:O	2.19	0.43
1:A:907:ASP:HB3	1:A:910:ASP:O	2.19	0.43
2:B:554:THR:OG1	2:B:557:LYS:HG3	2.19	0.43
2:B:110:TYR:CE1	2:B:195:MET:HE2	2.54	0.43
2:B:715:ILE:HB	2:B:720:LEU:CD2	2.49	0.43
1:A:10:TYR:CE1	1:A:84:LYS:HD3	2.53	0.43
1:A:149:LEU:HD11	1:A:183:THR:HG21	2.00	0.43
1:A:495:SER:OG	1:A:497:ASP:OD1	2.36	0.43
1:A:881:LEU:HD11	1:A:898:ILE:HG12	2.01	0.43
1:A:1277:THR:O	1:A:1277:THR:CG2	2.67	0.43
2:B:20:VAL:HG13	2:B:29:VAL:HG13	2.01	0.43
2:B:313:GLY:H	2:B:317:LYS:NZ	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:626:MET:HE1	2:B:764:LYS:HB3	2.00	0.43
1:A:322:LEU:HD23	1:A:322:LEU:HA	1.90	0.42
1:A:484:ASP:O	1:A:485:THR:C	2.61	0.42
2:B:40:TRP:HD1	2:B:167:SER:HB2	1.84	0.42
2:B:314:ASN:HB3	2:B:318:LEU:CD1	2.42	0.42
2:B:624:LEU:HD12	2:B:624:LEU:HA	1.76	0.42
2:B:993:GLU:H	2:B:993:GLU:HG3	1.45	0.42
1:A:600:ALA:HA	1:A:754:TYR:CZ	2.54	0.42
1:A:1265:ASN:ND2	2:B:845:GLU:HG3	2.33	0.42
2:B:185:PHE:HB2	2:B:197:THR:HG21	2.01	0.42
2:B:518:SER:HB3	2:B:540:MET:HE1	2.00	0.42
2:B:1071:VAL:CG1	2:B:1176:TRP:HZ3	2.33	0.42
1:A:178:ASN:OD1	1:A:180:TYR:HB2	2.19	0.42
1:A:1155:TYR:CD2	1:A:1293:GLU:HG3	2.53	0.42
1:A:1159:LYS:HB2	1:A:1185:VAL:HB	2.01	0.42
1:A:240:ASN:C	1:A:240:ASN:HD22	2.27	0.42
1:A:1030:TYR:O	1:A:1031:ILE:HD13	2.19	0.42
2:B:636:ASN:HA	2:B:639:LEU:HD13	2.01	0.42
2:B:871:TYR:CE2	2:B:1049:ARG:HD3	2.55	0.42
2:B:1173:ASN:O	2:B:1174:HIS:CD2	2.72	0.42
1:A:1293:GLU:O	1:A:1295:PRO:HD3	2.19	0.42
1:A:67:GLN:HA	1:A:425:PHE:CZ	2.54	0.42
1:A:135:ILE:CD1	1:A:149:LEU:HD23	2.49	0.42
1:A:1114:LEU:C	1:A:1114:LEU:HD23	2.44	0.42
2:B:638:MET:HE3	2:B:649:LYS:HB3	2.01	0.42
2:B:648:GLU:O	2:B:648:GLU:HG2	2.19	0.42
1:A:1169:ASN:HB3	2:B:1111:GLU:HG3	2.01	0.42
2:B:1052:TYR:CE1	2:B:1098:SER:HB2	2.55	0.42
1:A:1193:LEU:HD11	1:A:1206:LEU:HD13	2.00	0.42
2:B:1108:LYS:O	2:B:1109:LEU:HB2	2.19	0.42
1:A:97:ARG:HD2	1:A:386:ILE:O	2.20	0.42
1:A:1228:ASP:H	1:A:1232:THR:HA	1.85	0.42
2:B:426:THR:CB	2:B:427:VAL:CG2	2.98	0.42
2:B:639:LEU:CD1	2:B:783:PHE:HE1	2.32	0.42
1:A:987:LEU:HD23	1:A:987:LEU:HA	1.83	0.42
2:B:567:ARG:NH1	2:B:973:LEU:O	2.52	0.42
2:B:911:LEU:H	2:B:911:LEU:HG	1.68	0.42
1:A:242:VAL:HG13	1:A:258:VAL:O	2.20	0.41
2:B:249:ARG:NH1	2:B:256:GLU:OE2	2.52	0.41
2:B:504:LEU:HD12	2:B:504:LEU:HA	1.82	0.41
1:A:1023:ARG:NH1	1:A:1023:ARG:HB3	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:237:LYS:HA	2:B:238:PRO:HD3	1.87	0.41
2:B:184:VAL:HG22	2:B:200:GLU:HB2	2.01	0.41
2:B:224:LYS:HB2	2:B:336:LEU:HD11	2.03	0.41
2:B:674:THR:HG22	2:B:675:GLN:N	2.35	0.41
2:B:1183:MET:HE3	2:B:1183:MET:HB3	1.87	0.41
1:A:361:LEU:HD12	1:A:361:LEU:HA	1.95	0.41
1:A:471:PHE:CE2	1:A:720:LYS:HE3	2.54	0.41
1:A:711:LYS:HB3	1:A:711:LYS:HE2	1.80	0.41
1:A:964:ILE:HD13	1:A:978:LEU:HG	2.03	0.41
1:A:1241:ASP:OD1	1:A:1241:ASP:C	2.63	0.41
2:B:343:PHE:HB3	2:B:345:ILE:HG13	2.03	0.41
2:B:838:LEU:HD13	2:B:859:THR:HG21	2.01	0.41
2:B:1031:SER:O	2:B:1035:GLU:CG	2.64	0.41
1:A:788:LEU:HD23	1:A:788:LEU:HA	1.82	0.41
2:B:355:LEU:HD23	2:B:355:LEU:HA	1.85	0.41
2:B:638:MET:HA	2:B:641:LEU:HD13	2.01	0.41
2:B:754:ILE:O	2:B:758:GLU:HG3	2.21	0.41
1:A:688:LYS:HB2	1:A:688:LYS:HE3	1.79	0.41
2:B:330:ASP:HB3	2:B:453:SER:HB3	2.02	0.41
1:A:1023:ARG:NH2	1:A:1045:GLY:O	2.54	0.41
1:A:1271:ILE:HD11	2:B:839:VAL:HG11	2.03	0.41
2:B:11:SER:HA	2:B:12:PRO:HD3	1.96	0.41
2:B:177:ASN:ND2	2:B:180:GLU:HB2	2.36	0.41
2:B:211:TYR:O	2:B:212:ASP:HB2	2.21	0.41
2:B:528:ASP:OD1	2:B:528:ASP:N	2.54	0.41
2:B:579:ILE:O	2:B:585:ILE:HA	2.21	0.41
1:A:266:PHE:CE1	1:A:366:PHE:HB3	2.56	0.41
1:A:985:TRP:CE2	1:A:1019:ILE:HG21	2.55	0.41
1:A:1188:ASN:HD22	1:A:1188:ASN:C	2.25	0.41
2:B:514:PHE:CD1	2:B:514:PHE:C	2.99	0.41
2:B:853:ASP:OD1	2:B:859:THR:HB	2.22	0.40
2:B:906:PHE:HB3	2:B:1017:LEU:HA	2.02	0.40
1:A:179:GLY:HA2	1:A:234:GLY:HA3	2.02	0.40
1:A:1111:TYR:CG	1:A:1284:PHE:HB3	2.56	0.40
2:B:306:ILE:HG23	2:B:312:ILE:HD13	2.03	0.40
1:A:565:ARG:HD2	1:A:749:TYR:CE1	2.55	0.40
1:A:578:ASN:HA	1:A:579:PRO:HD3	1.80	0.40
2:B:511:ASN:HB3	2:B:513:LYS:O	2.21	0.40
2:B:1152:ILE:CG2	2:B:1155:CYS:HB2	2.52	0.40
1:A:48:ARG:HG2	1:A:78:LEU:HB3	2.04	0.40
2:B:105:ALA:O	2:B:106:ILE:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:346:MET:CE	2:B:832:GLU:HG3	2.52	0.40
2:B:1127:SER:OG	2:B:1128:GLU:N	2.54	0.40
1:A:688:LYS:O	1:A:692:VAL:HG23	2.21	0.40
1:A:1099:ASP:O	1:A:1233:ASN:OD1	2.39	0.40
2:B:328:ILE:HD13	2:B:328:ILE:HA	1.84	0.40
2:B:368:TYR:CD2	2:B:368:TYR:N	2.89	0.40
2:B:695:GLU:OE2	2:B:735:SER:HA	2.22	0.40

All (32) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:832:GLY:CA	2:B:925:GLU:OE1[4_655]	1.34	0.86
1:A:832:GLY:C	2:B:925:GLU:OE1[4_655]	1.35	0.85
1:A:1187:LYS:N	2:B:793:ASP:OD1[10_555]	1.42	0.78
1:A:825:ASP:N	2:B:718:ASP:CB[4_655]	1.53	0.67
1:A:832:GLY:N	2:B:925:GLU:OE2[4_655]	1.53	0.67
1:A:825:ASP:CA	2:B:718:ASP:CA[4_655]	1.67	0.53
1:A:824:TYR:C	2:B:718:ASP:CB[4_655]	1.74	0.46
1:A:825:ASP:N	2:B:718:ASP:CA[4_655]	1.83	0.37
1:A:832:GLY:N	2:B:925:GLU:OE1[4_655]	1.84	0.36
1:A:832:GLY:N	2:B:925:GLU:CD[4_655]	1.86	0.34
1:A:1153:SER:CB	2:B:644:ASN:OD1[10_555]	1.87	0.33
1:A:825:ASP:O	2:B:721:ALA:CB[4_655]	1.88	0.32
1:A:1143:VAL:CG1	2:B:644:ASN:ND2[10_555]	1.89	0.31
1:A:825:ASP:OD2	2:B:717:SER:CB[4_655]	1.90	0.30
1:A:825:ASP:OD1	2:B:717:SER:O[4_655]	1.91	0.29
1:A:1153:SER:OG	2:B:644:ASN:OD1[10_555]	1.91	0.29
1:A:1186:VAL:C	2:B:793:ASP:OD1[10_555]	1.92	0.28
2:B:409:ASN:O	2:B:491:ARG:NE[12_545]	1.96	0.24
1:A:1156:ARG:NH2	2:B:789:ASN:ND2[10_555]	1.97	0.23
1:A:835:ASP:OD1	2:B:926:ASP:N[4_655]	2.01	0.19
1:A:1156:ARG:NH2	2:B:789:ASN:O[10_555]	2.03	0.17
1:A:1156:ARG:NH1	2:B:642:PRO:CB[10_555]	2.04	0.16
1:A:825:ASP:CB	2:B:717:SER:OG[4_655]	2.08	0.12
1:A:832:GLY:O	2:B:925:GLU:OE1[4_655]	2.09	0.11
1:A:832:GLY:CA	2:B:925:GLU:CD[4_655]	2.11	0.09
1:A:833:GLN:N	2:B:925:GLU:OE1[4_655]	2.11	0.09
1:A:956:ILE:CD1	1:A:1294:ARG:CD[10_555]	2.11	0.09
1:A:1156:ARG:NH2	2:B:789:ASN:CG[10_555]	2.11	0.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:825:ASP:OD2	2:B:717:SER:OG[4_655]	2.14	0.06
1:A:835:ASP:OD1	2:B:926:ASP:CA[4_655]	2.14	0.06
1:A:825:ASP:CA	2:B:718:ASP:N[4_655]	2.15	0.05
2:B:409:ASN:O	2:B:491:ARG:CZ[12_545]	2.17	0.03

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1276/1296 (98%)	1242 (97%)	34 (3%)	0	100	100
2	B	1144/1196 (96%)	1105 (97%)	38 (3%)	1 (0%)	48	80
All	All	2420/2492 (97%)	2347 (97%)	72 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	429	ASP

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1162/1176 (99%)	1114 (96%)	48 (4%)	27	51
2	B	1076/1114 (97%)	992 (92%)	84 (8%)	11	36
All	All	2238/2290 (98%)	2106 (94%)	132 (6%)	18	44

All (132) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	ILE
1	A	52	THR
1	A	55	GLU
1	A	58	ASP
1	A	240	ASN
1	A	434	ILE
1	A	482	THR
1	A	484	ASP
1	A	485	THR
1	A	507	ASN
1	A	510	ASN
1	A	513	GLU
1	A	520	LEU
1	A	525	ILE
1	A	541	LYS
1	A	546	ASP
1	A	572	VAL
1	A	608	GLU
1	A	645	ASN
1	A	682	VAL
1	A	690	LEU
1	A	733	LYS
1	A	757	GLU
1	A	770	SER
1	A	806	LYS
1	A	819	LEU
1	A	858	ASP
1	A	871	LYS
1	A	909	ILE
1	A	933	VAL
1	A	948	ARG
1	A	958	LEU
1	A	988	GLN
1	A	1013	ARG
1	A	1027	SER
1	A	1087	LEU
1	A	1146	THR
1	A	1169	ASN
1	A	1170	LYS
1	A	1188	ASN
1	A	1214	VAL
1	A	1226	LYS

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Mol	Chain	Res	Type
1	A	1234	LYS
1	A	1262	VAL
1	A	1271	ILE
1	A	1272	GLU
1	A	1274	SER
1	A	1278	LEU
2	B	3	ILE
2	B	7	LEU
2	B	29	VAL
2	B	50	SER
2	B	69	LEU
2	B	186	TYR
2	B	213	GLU
2	B	224	LYS
2	B	230	LEU
2	B	243	VAL
2	B	250	SER
2	B	251	GLU
2	B	253	GLU
2	B	279	ASP
2	B	284	THR
2	B	292	LYS
2	B	293	LYS
2	B	310	ASN
2	B	316	ILE
2	B	320	LEU
2	B	326	ILE
2	B	329	ASN
2	B	362	GLN
2	B	406	LEU
2	B	409	ASN
2	B	469	ILE
2	B	484	VAL
2	B	487	ILE
2	B	493	ILE
2	B	504	LEU
2	B	509	THR
2	B	511	ASN
2	B	528	ASP
2	B	550	SER
2	B	553	ASP
2	B	554	THR

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Mol	Chain	Res	Type
2	B	583	CYS
2	B	585	ILE
2	B	590	THR
2	B	611	ASN
2	B	624	LEU
2	B	629	ILE
2	B	639	LEU
2	B	648	GLU
2	B	674	THR
2	B	703	GLN
2	B	709	LEU
2	B	712	ASN
2	B	716	SER
2	B	718	ASP
2	B	720	LEU
2	B	724	ASN
2	B	745	VAL
2	B	790	ILE
2	B	797	GLN
2	B	800	ASN
2	B	830	LYS
2	B	858	ASN
2	B	865	LYS
2	B	911	LEU
2	B	913	LYS
2	B	916	ILE
2	B	924	LYS
2	B	927	ASN
2	B	978	LEU
2	B	993	GLU
2	B	1024	THR
2	B	1026	SER
2	B	1048	GLU
2	B	1055	THR
2	B	1077	ILE
2	B	1083	ASN
2	B	1086	ASN
2	B	1089	LEU
2	B	1099	ILE
2	B	1115	SER
2	B	1117	LEU
2	B	1126	ILE

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Mol	Chain	Res	Type
2	B	1128	GLU
2	B	1129	ASP
2	B	1136	ASP
2	B	1142	LYS
2	B	1144	MET
2	B	1167	LEU

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

Mol	Chain	Res	Type
1	A	162	GLN
1	A	205	ASN
1	A	400	ASN
1	A	500	GLN
1	A	573	ASN
1	A	578	ASN
1	A	748	ASN
1	A	753	GLN
1	A	765	ASN
1	A	859	ASN
1	A	905	ASN
1	A	913	GLN
1	A	915	GLN
1	A	970	ASN
1	A	1038	GLN
1	A	1046	ASN
1	A	1265	ASN
2	B	2	ASN
2	B	17	ASN
2	B	322	GLN
2	B	375	ASN
2	B	410	ASN
2	B	417	ASN
2	B	675	GLN
2	B	694	GLN
2	B	961	ASN
2	B	1057	GLN

5.3.3 RNA ⓘ

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 oligosaccharides 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	1280/1296 (98%)	0.46	100 (7%)	19 18	101, 183, 267, 448	10 (0%)
2	B	1150/1196 (96%)	0.71	139 (12%)	8 12	84, 158, 249, 587	14 (1%)
All	All	2430/2492 (97%)	0.58	239 (9%)	13 15	84, 172, 262, 587	24 (0%)

All (239) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	721	ALA	7.8
1	A	1295	PRO	7.5
2	B	166	ALA	7.5
1	A	698	ALA	7.1
2	B	17	ASN	6.5
1	A	650	ASP	6.0
2	B	43	PRO	5.8
1	A	834	VAL	5.5
2	B	18	VAL	5.4
2	B	552	ILE	5.1
1	A	1232	THR	5.0
2	B	41	VAL	5.0
2	B	150	TYR	4.9
2	B	789	ASN	4.8
1	A	825	ASP	4.6
2	B	80	GLN	4.5
2	B	3	ILE	4.4
1	A	828	GLY	4.4
2	B	84	THR	4.3
1	A	649	LYS	4.3
1	A	491	GLU	4.3
2	B	165	TYR	4.3
1	A	1175	ARG	4.3
1	A	1276	ARG	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	1156	ARG	4.2
1	A	1277	THR	4.1
1	A	1278	LEU	4.1
2	B	152	GLU	4.1
2	B	76	ASP	4.1
2	B	33	PHE	4.0
2	B	81	ALA	4.0
1	A	1294	ARG	4.0
1	A	827	ARG	4.0
2	B	65	ASP	4.0
2	B	1118	ASP	4.0
2	B	322	GLN	3.9
1	A	490	ALA	3.9
2	B	40	TRP	3.9
2	B	926	ASP	3.8
1	A	1293	GLU	3.8
1	A	1146	THR	3.8
1	A	685	ILE	3.8
2	B	35	VAL	3.8
2	B	722	LEU	3.7
2	B	39	ILE	3.7
2	B	451	ASP	3.6
2	B	477	ASN	3.5
2	B	555	ASP	3.5
1	A	646	MET	3.5
2	B	850	VAL	3.5
2	B	44	GLU	3.5
2	B	83	ILE	3.5
2	B	644	ASN	3.5
1	A	681	LEU	3.4
2	B	492	GLU	3.4
2	B	19	VAL	3.4
1	A	254	SER	3.4
1	A	628	ALA	3.3
1	A	1227	ASN	3.3
2	B	583	CYS	3.3
2	B	947	ASN	3.3
2	B	170	VAL	3.3
2	B	415	ARG	3.3
2	B	491	ARG	3.3
2	B	32	ALA	3.2
1	A	1292	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
2	B	948	GLY	3.2
2	B	409	ASN	3.2
2	B	281	TYR	3.2
1	A	1139	PRO	3.2
2	B	466	PRO	3.1
2	B	636	ASN	3.1
1	A	489	ALA	3.1
1	A	1228	ASP	3.1
1	A	1226	LYS	3.1
1	A	132	THR	3.1
1	A	434	ILE	3.1
2	B	410	ASN	3.0
2	B	175	GLY	3.0
1	A	870	ILE	3.0
1	A	168	PHE	3.0
2	B	1122	LYS	3.0
1	A	66	LYS	3.0
2	B	713	SER	3.0
1	A	564	SER	2.9
2	B	9	ILE	2.9
2	B	31	LYS	2.9
2	B	4	ASN	2.9
2	B	383	ASN	2.9
2	B	726	THR	2.9
1	A	627	ILE	2.9
2	B	315	ASP	2.9
1	A	630	ILE	2.9
2	B	362	GLN	2.8
1	A	109	THR	2.8
1	A	833	GLN	2.8
1	A	956	ILE	2.8
1	A	183	THR	2.8
2	B	651	PHE	2.8
2	B	77	LYS	2.8
2	B	82	ILE	2.8
2	B	365	LYS	2.8
1	A	169	GLY	2.8
1	A	1157	GLY	2.8
2	B	208	THR	2.8
2	B	113	ILE	2.8
2	B	112	TYR	2.8
2	B	298	HIS	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	319	ARG	2.7
2	B	1	MET	2.7
2	B	36	ALA	2.7
1	A	1275	SER	2.7
2	B	718	ASP	2.7
2	B	368	TYR	2.7
1	A	692	VAL	2.7
2	B	1111	GLU	2.7
1	A	1257	ASN	2.7
2	B	85	LEU	2.7
2	B	68	PHE	2.6
2	B	725	LEU	2.6
2	B	441	ALA	2.6
1	A	185	TYR	2.6
2	B	843	PHE	2.6
2	B	67	ASN	2.6
1	A	818	ALA	2.6
2	B	790	ILE	2.5
2	B	210	LYS	2.5
2	B	314	ASN	2.5
2	B	79	LEU	2.5
1	A	1230	GLY	2.5
2	B	715	ILE	2.5
2	B	899	THR	2.5
1	A	1233	ASN	2.5
1	A	1158	ALA	2.5
2	B	108	PHE	2.5
2	B	316	ILE	2.5
1	A	957	SER	2.5
2	B	559	TYR	2.5
2	B	484	VAL	2.5
2	B	78	PHE	2.5
1	A	690	LEU	2.5
1	A	1116	LEU	2.5
2	B	199	THR	2.5
2	B	186	TYR	2.5
2	B	874	ASN	2.4
2	B	717	SER	2.4
2	B	206	PHE	2.4
1	A	657	ILE	2.4
1	A	422	LEU	2.4
1	A	1004	MET	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	647	LEU	2.4
1	A	830	LEU	2.4
1	A	514	ASN	2.4
1	A	1153	SER	2.4
2	B	1109	LEU	2.4
2	B	70	SER	2.4
1	A	585	PHE	2.4
2	B	481	PHE	2.4
2	B	728	THR	2.4
2	B	1086	ASN	2.4
1	A	648	TYR	2.4
1	A	1118	ASP	2.4
2	B	45	ARG	2.4
2	B	42	ALA	2.4
2	B	854	ALA	2.4
1	A	1147	ASN	2.3
2	B	553	ASP	2.3
1	A	831	ILE	2.3
2	B	69	LEU	2.3
1	A	1196	ASN	2.3
2	B	787	CYS	2.3
2	B	898	LEU	2.3
2	B	404	ASN	2.3
1	A	626	LYS	2.3
1	A	686	ALA	2.3
2	B	153	THR	2.3
2	B	323	LYS	2.3
2	B	440	ARG	2.3
1	A	1092	SER	2.3
1	A	17	VAL	2.3
1	A	1143	VAL	2.3
2	B	483	PRO	2.3
1	A	480	GLU	2.3
2	B	74	GLU	2.3
2	B	950	GLU	2.3
2	B	157	SER	2.2
2	B	1115	SER	2.2
1	A	1058	ASP	2.2
2	B	429	ASP	2.2
2	B	1053	ASN	2.2
1	A	1211	ILE	2.2
2	B	359	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	476	GLU	2.2
1	A	826	ASN	2.2
2	B	468	ILE	2.2
1	A	688	LYS	2.2
1	A	1187	LYS	2.2
2	B	642	PRO	2.2
2	B	1194	PRO	2.2
1	A	131	ASP	2.2
1	A	891	LEU	2.2
1	A	832	GLY	2.2
2	B	1121	GLU	2.2
2	B	171	ILE	2.2
1	A	541	LYS	2.2
1	A	1188	ASN	2.2
2	B	149	GLY	2.2
1	A	691	THR	2.2
1	A	1268	ASN	2.2
1	A	276	SER	2.1
1	A	1203	GLU	2.1
2	B	794	GLU	2.1
2	B	1143	LYS	2.1
1	A	262	GLU	2.1
2	B	306	ILE	2.1
1	A	855	LYS	2.1
2	B	992	LYS	2.1
2	B	915	THR	2.1
2	B	1084	THR	2.1
1	A	1236	LYS	2.1
2	B	924	LYS	2.1
1	A	629	ASP	2.1
2	B	845	GLU	2.1
1	A	228	ALA	2.1
1	A	417	LYS	2.1
2	B	729	ASN	2.1
2	B	1117	LEU	2.1
1	A	1138	GLY	2.1
2	B	73	SER	2.1
2	B	714	ASN	2.1
2	B	460	GLY	2.0
2	B	318	LEU	2.0
1	A	763	ASN	2.0
1	A	765	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	996	ARG	2.0
2	B	174	PRO	2.0
2	B	200	GLU	2.0
1	A	1102	GLY	2.0
1	A	764	PHE	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 oligosaccharides 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. 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	B-factors($\text{\AA}^2$)	Q<0.9
3	ZN	A	1297	1/1	0.84	0.48	550,550,550,550	0
4	CA	A	1298	1/1	0.89	0.07	169,169,169,169	1

6.5 Other polymers [i](#)

There are no such residues in this entry.