Full wwPDB X-ray Structure Validation Report (i)

Jan 28, 2024 – 02:02 PM EST

PDB ID	:	1EJ6
Title	:	Reovirus core
Authors	:	Reinisch, K.M.; Nibert, M.L.; Harrison, S.C.
Deposited on	:	2000-02-29
Resolution	:	3.60 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

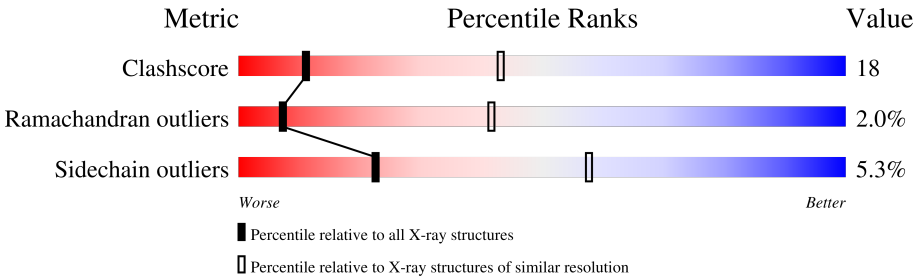
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1289	67% 29% .
2	B	1275	53% 25% . 19%
2	C	1275	61% 32% . .
3	D	418	64% 33% .
3	E	418	61% 34% .

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 34487 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 LAMBDA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1284	Total	C	N	O	S	0	0	0
			10126	6468	1699	1917	42			

- Molecule 2 is a protein called LAMBDA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1031	Total	C	N	O	S	0	0	0
			8143	5208	1375	1510	50			
2	C	1221	Total	C	N	O	S	0	0	0
			9591	6078	1649	1809	55			

- Molecule 3 is a protein called SIGMA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	417	Total	C	N	O	S	0	0	0
			3313	2092	600	604	17			
3	E	417	Total	C	N	O	S	0	0	0
			3313	2092	600	604	17			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total	Zn	0	0
			1	1		

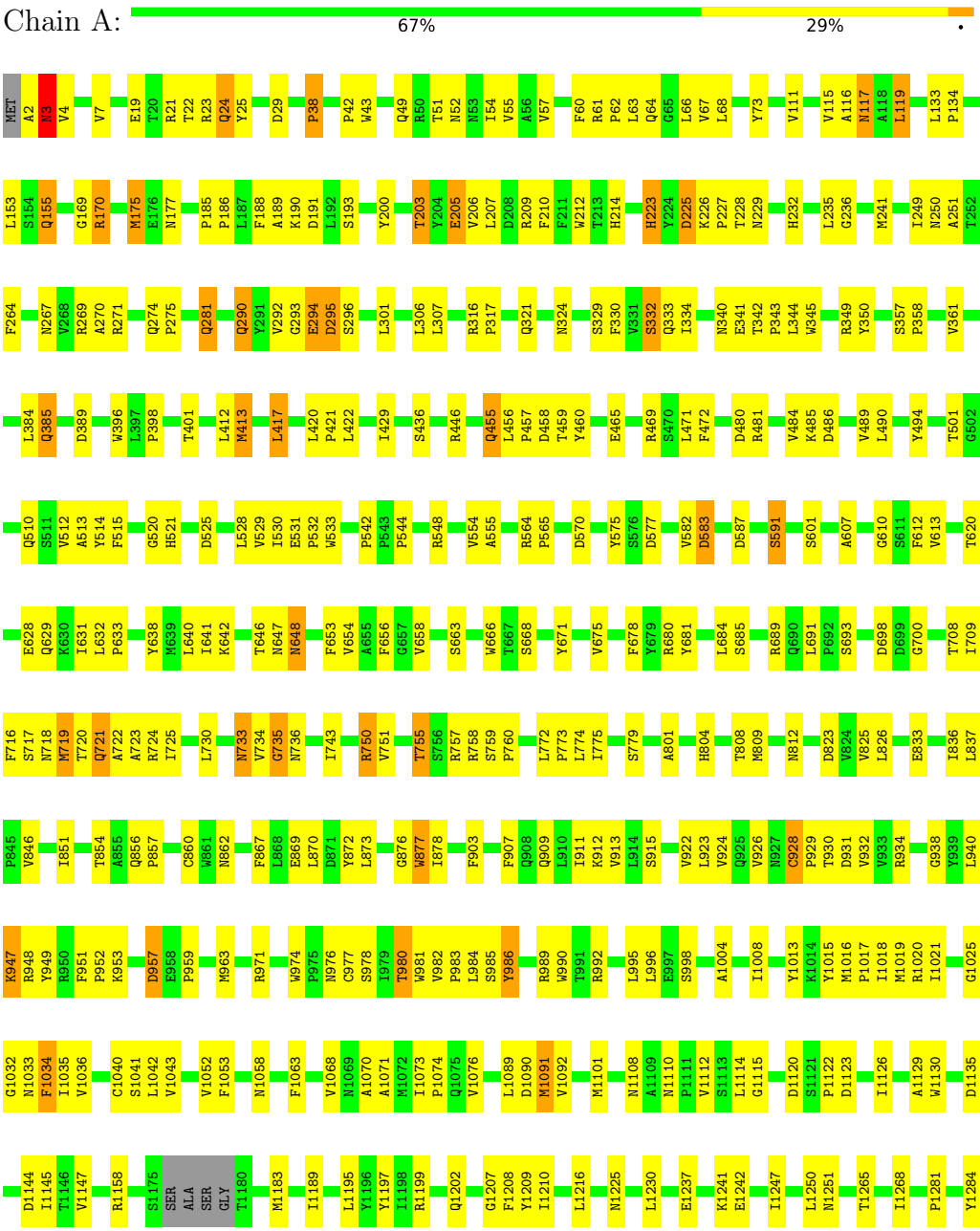
3 Residue-property plots (i)

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. 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

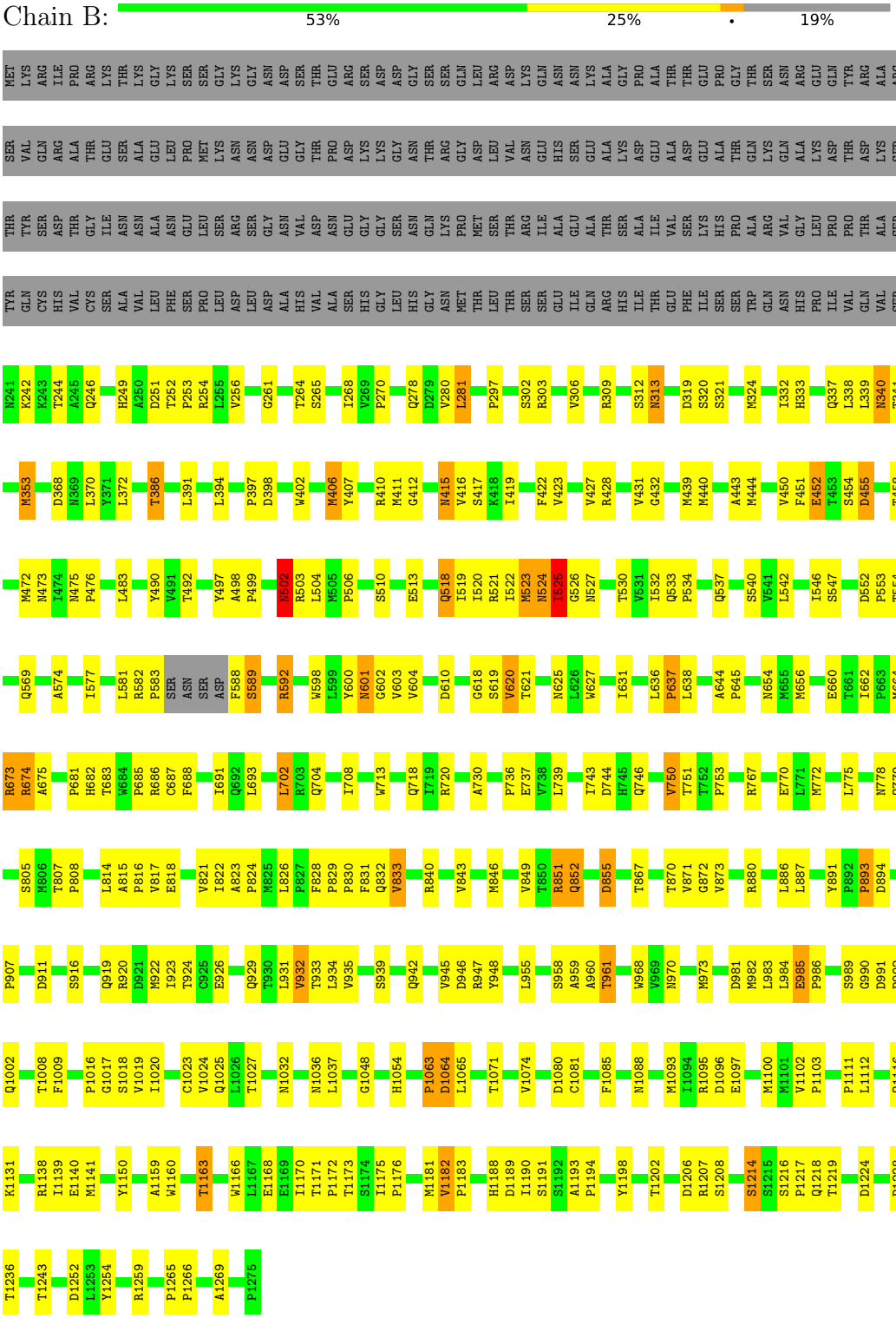
- Molecule 1: LAMBDA2

Chain A:



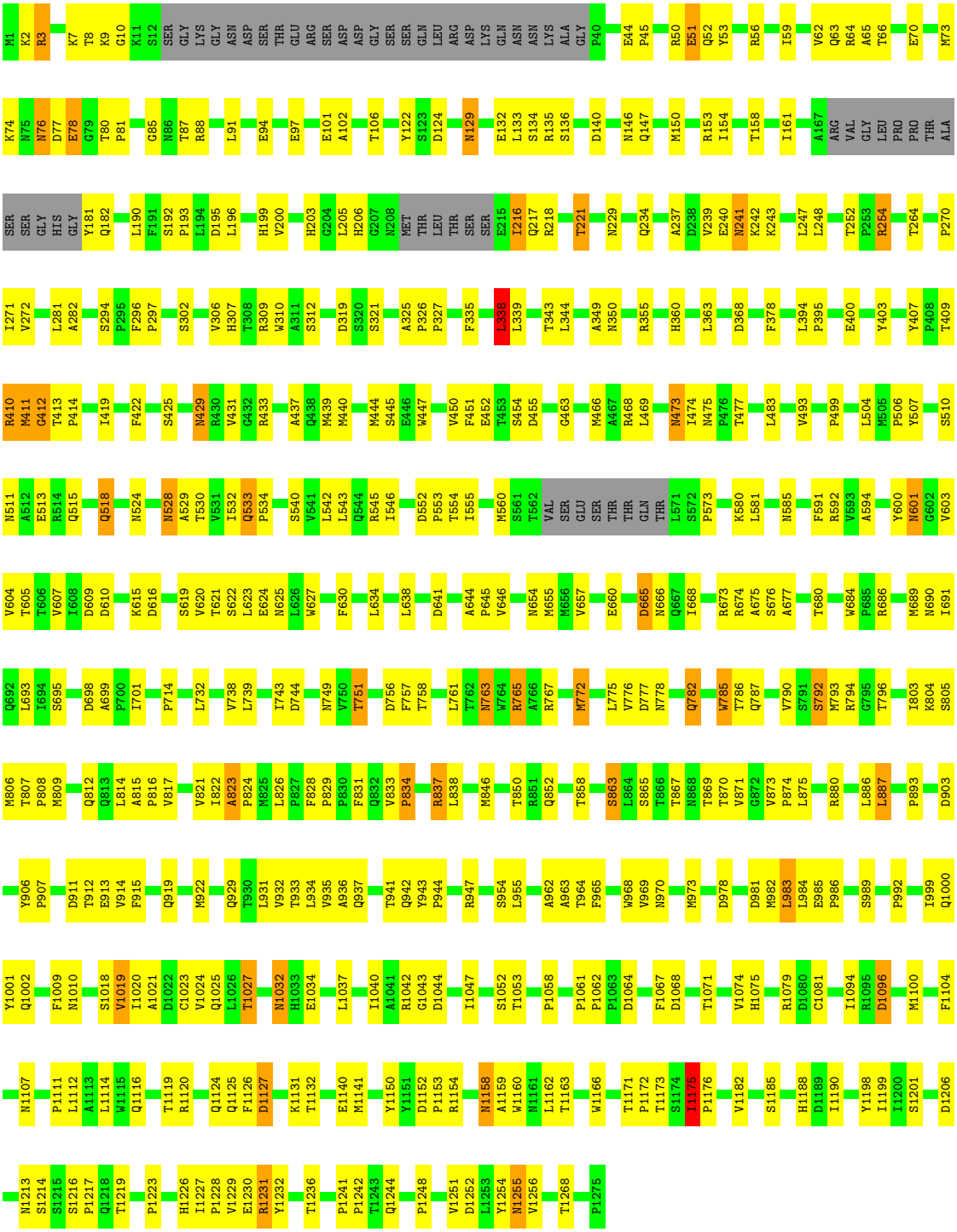
• Molecule 2: LAMBDA1

Chain B:



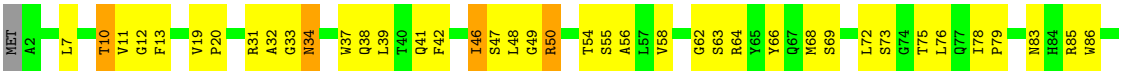
• Molecule 2: LAMBDA1

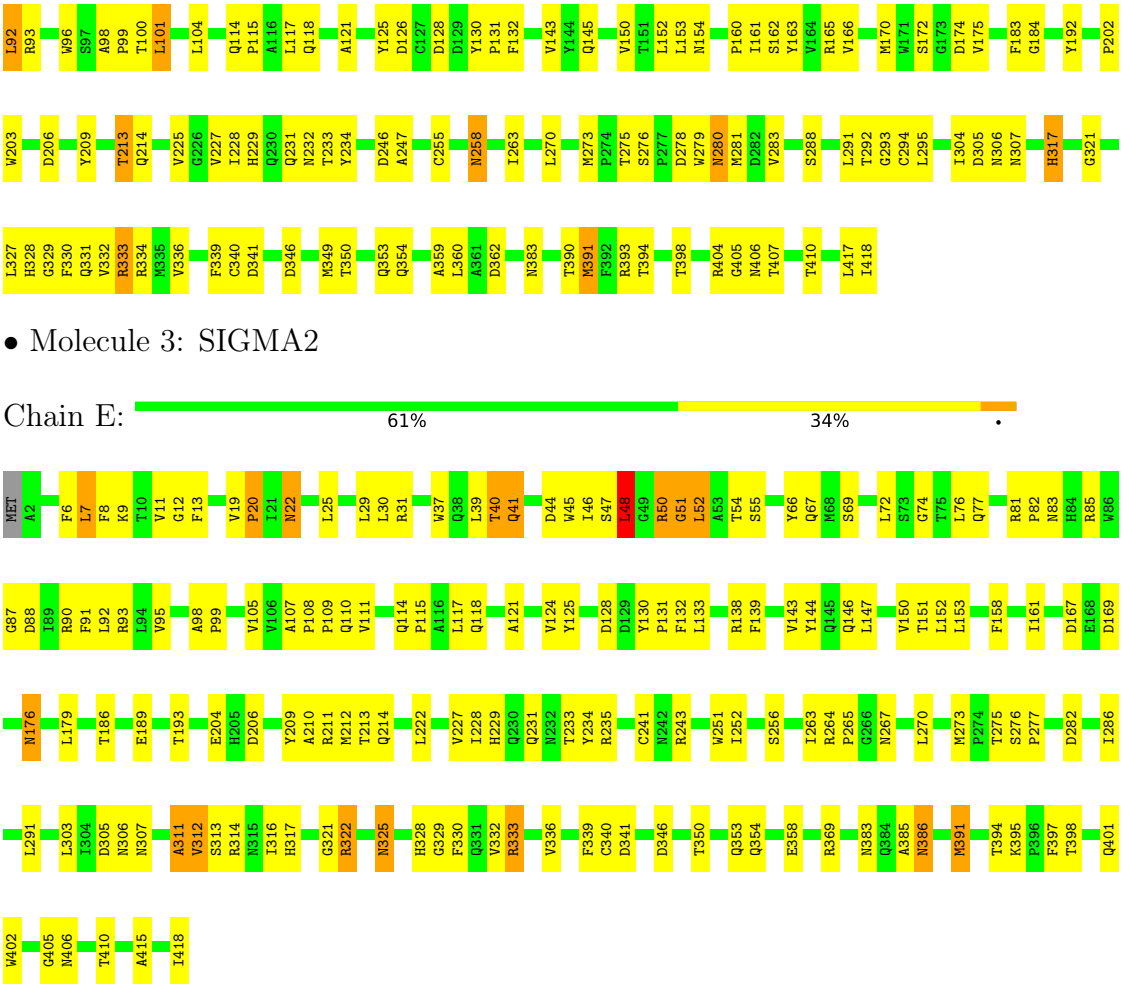
Chain C:



• Molecule 3: SIGMA2

Chain D:





- Molecule 3: SIGMA2

Chain E:

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	F 4 3 2	Depositor
Cell constants a, b, c, α, β, γ	1255.00Å 1255.00Å 1255.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.60	Depositor
% Data completeness (in resolution range)	88.5 (20.00-3.60)	Depositor
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.206 , 0.208	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	34487	wwPDB-VP
Average B, all atoms (Å^2)	14.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.42	0/10384	0.62	0/14170
2	B	0.47	0/8363	0.66	0/11454
2	C	0.46	0/9833	0.65	0/13437
3	D	0.45	0/3398	0.62	0/4626
3	E	0.44	0/3398	0.63	0/4626
All	All	0.45	0/35376	0.64	0/48313

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	10126	0	9906	315	0
2	B	8143	0	8063	302	0
2	C	9591	0	9453	358	0
3	D	3313	0	3215	139	0
3	E	3313	0	3215	143	0
4	C	1	0	0	0	0
All	All	34487	0	33852	1231	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 18.

All (1231) 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:C:1171:THR:HG22	2:C:1173:THR:H	1.08	1.16
1:A:1138:ILE:HD12	1:A:1138:ILE:H	1.21	1.05
2:C:106:THR:HG22	2:C:122:TYR:H	1.15	1.04
1:A:149:THR:HG22	1:A:151:ALA:H	1.22	1.01
2:B:1171:THR:HG22	2:B:1173:THR:H	1.22	1.01
1:A:851:ILE:HD12	1:A:851:ILE:H	1.26	0.98
3:E:229:HIS:HD2	3:E:231:GLN:H	1.11	0.97
2:B:691:ILE:HD12	2:B:691:ILE:H	1.30	0.96
3:D:258:ASN:HD22	3:D:258:ASN:H	1.01	0.96
3:D:209:TYR:O	3:D:213:THR:HG22	1.65	0.96
1:A:750:ARG:HH11	1:A:750:ARG:HG2	1.26	0.96
1:A:825:VAL:HB	1:A:846:VAL:HG12	1.45	0.96
1:A:456:LEU:HD12	1:A:457:PRO:HD2	1.46	0.94
3:E:47:SER:HB2	3:E:50:ARG:HH22	1.33	0.94
1:A:263:GLN:HG2	1:A:281:GLN:HB2	1.47	0.94
2:C:691:ILE:HD12	2:C:691:ILE:H	1.32	0.93
3:E:41:GLN:HE21	3:E:41:GLN:HA	1.35	0.92
3:D:258:ASN:HD22	3:D:258:ASN:N	1.66	0.90
2:B:1112:LEU:HG	2:B:1116:GLN:HE21	1.38	0.89
3:E:306:ASN:HB3	3:E:314:ARG:HD3	1.55	0.89
2:C:1171:THR:HG22	2:C:1173:THR:N	1.89	0.87
2:C:601:ASN:ND2	2:C:833:VAL:H	1.73	0.86
1:A:306:LEU:HD23	1:A:344:LEU:HB3	1.57	0.86
2:B:1168:GLU:HB3	2:C:50:ARG:HG3	1.56	0.85
2:B:522:ILE:O	2:B:525:ILE:HG23	1.76	0.85
2:C:1171:THR:HG23	2:C:1172:PRO:HD2	1.58	0.85
2:C:533:GLN:HB3	2:C:534:PRO:HD3	1.59	0.84
2:C:2:LYS:HG2	2:C:3:ARG:H	1.44	0.83
2:B:1171:THR:HG22	2:B:1173:THR:N	1.93	0.83
3:D:258:ASN:H	3:D:258:ASN:ND2	1.76	0.83
2:B:1096:ASP:HB3	2:B:1100:MET:H	1.44	0.82
2:B:823:ALA:HA	2:B:826:LEU:HD23	1.60	0.82
1:A:153:LEU:HB3	1:A:155:GLN:HG2	1.60	0.82
2:B:532:ILE:HG12	2:B:604:VAL:HG21	1.61	0.81
3:E:325:ASN:N	3:E:325:ASN:HD22	1.78	0.81
2:B:339:LEU:HB2	2:B:353:MET:HG3	1.62	0.81
2:B:1229:VAL:HG13	2:B:1236:THR:HG21	1.61	0.80
2:B:527:ASN:HA	2:B:873:VAL:HG13	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:630:PHE:HB2	2:C:772:MET:HE1	1.63	0.79
1:A:1138:ILE:H	1:A:1138:ILE:CD1	1.96	0.79
2:C:106:THR:CG2	2:C:122:TYR:H	1.95	0.78
2:B:610:ASP:HB2	2:C:786:THR:HG21	1.66	0.78
1:A:455:GLN:HG2	1:A:621:ARG:HG3	1.65	0.77
3:E:37:TRP:CZ3	3:E:143:VAL:HG13	2.19	0.77
2:C:528:ASN:HD21	2:C:530:THR:HB	1.50	0.77
2:C:1023:CYS:O	2:C:1027:THR:HG23	1.85	0.77
2:C:1152:ASP:OD1	2:C:1154:ARG:HG2	1.84	0.77
3:D:7:LEU:HD11	3:D:317:HIS:HB3	1.66	0.77
2:B:265:SER:OG	2:B:458:THR:HG21	1.85	0.76
2:C:106:THR:HG22	2:C:122:TYR:N	1.96	0.76
3:D:50:ARG:HG3	3:D:50:ARG:HH11	1.49	0.75
2:B:603:VAL:HG23	2:B:604:VAL:HG23	1.69	0.75
3:E:229:HIS:CD2	3:E:231:GLN:H	2.01	0.75
2:B:510:SER:OG	2:B:513:GLU:HG3	1.86	0.75
1:A:708:THR:HB	1:A:755:THR:HG23	1.69	0.75
1:A:648:ASN:C	1:A:648:ASN:HD22	1.90	0.75
2:C:1079:ARG:HG2	2:C:1079:ARG:HH11	1.52	0.74
1:A:1068:VAL:HG11	1:A:1076:VAL:O	1.87	0.74
3:E:8:PHE:HA	3:E:151:THR:HG21	1.70	0.74
2:C:254:ARG:HH11	2:C:254:ARG:HB3	1.52	0.74
1:A:290:GLN:H	1:A:290:GLN:NE2	1.83	0.74
2:B:280:VAL:HG23	2:B:281:LEU:N	2.03	0.74
2:C:433:ARG:HA	2:C:450:VAL:HG12	1.70	0.74
3:E:81:ARG:HB3	3:E:82:PRO:HD2	1.69	0.74
1:A:721:GLN:O	1:A:725:ILE:HG12	1.87	0.74
3:D:328:HIS:HB3	3:D:410:THR:HB	1.70	0.74
3:E:383:ASN:HD21	3:E:391:MET:H	1.33	0.74
1:A:750:ARG:HG2	1:A:750:ARG:NH1	1.97	0.74
2:B:822:ILE:HG22	2:B:826:LEU:HD21	1.70	0.74
2:B:662:ILE:HG13	2:B:664:MET:HE3	1.70	0.73
3:E:51:GLY:O	3:E:52:LEU:HB2	1.88	0.73
1:A:24:GLN:H	1:A:24:GLN:CD	1.89	0.73
3:E:47:SER:CB	3:E:50:ARG:HH22	2.00	0.73
3:D:273:MET:CE	3:D:327:LEU:HD13	2.19	0.73
3:E:263:ILE:HD13	3:E:418:ILE:HG23	1.71	0.73
2:B:278:GLN:HE21	2:B:281:LEU:H	1.36	0.72
2:B:893:PRO:HG2	2:B:894:ASP:H	1.53	0.72
2:B:553:PRO:HB3	2:B:583:PRO:HB2	1.69	0.72
2:C:413:THR:N	2:C:414:PRO:HD3	2.04	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:815:ALA:HB3	2:C:816:PRO:HD3	1.69	0.72
1:A:878:ILE:HG13	1:A:913:VAL:HG12	1.72	0.72
2:B:340:ASN:N	2:B:340:ASN:HD22	1.86	0.72
2:C:528:ASN:C	2:C:528:ASN:HD22	1.90	0.72
1:A:1126:ILE:HG13	1:A:1147:VAL:CG2	2.20	0.72
1:A:149:THR:HG22	1:A:151:ALA:N	2.01	0.72
3:E:276:SER:HG	3:E:332:VAL:HG23	1.55	0.71
2:C:607:VAL:HG12	2:C:641:ASP:HB2	1.72	0.71
2:C:62:VAL:O	2:C:66:THR:HG23	1.89	0.71
2:C:601:ASN:HD21	2:C:833:VAL:H	1.35	0.71
2:B:278:GLN:HE21	2:B:280:VAL:HG22	1.55	0.71
2:C:644:ALA:HB3	2:C:645:PRO:HD3	1.71	0.71
3:D:46:ILE:HD11	3:D:283:VAL:HG13	1.72	0.70
2:C:870:THR:HG22	2:C:871:VAL:H	1.56	0.70
3:D:276:SER:OG	3:D:332:VAL:HG23	1.91	0.70
2:C:74:LYS:HD3	2:C:530:THR:HG22	1.71	0.70
1:A:720:THR:HG22	1:A:723:ALA:HB3	1.72	0.70
2:B:552:ASP:OD1	2:B:554:THR:HG23	1.92	0.70
2:C:912:THR:OG1	2:C:914:VAL:HG23	1.90	0.70
2:C:154:ILE:O	2:C:158:THR:HG23	1.92	0.70
1:A:963:MET:HG3	1:A:981:TRP:CZ2	2.27	0.70
1:A:642:LYS:NZ	1:A:648:ASN:HD21	1.90	0.70
2:B:278:GLN:HE21	2:B:280:VAL:CG2	2.05	0.69
2:B:320:SER:O	2:B:368:ASP:HB2	1.92	0.69
2:C:400:GLU:HA	2:C:403:TYR:CD2	2.26	0.69
2:C:528:ASN:ND2	2:C:530:THR:HB	2.06	0.69
1:A:292:VAL:HG13	1:A:296:SER:OG	1.92	0.69
2:B:674:ARG:H	2:B:674:ARG:HD3	1.56	0.69
3:E:22:ASN:C	3:E:22:ASN:HD22	1.95	0.69
2:B:468:ARG:HB2	2:B:1019:VAL:HG11	1.73	0.69
2:C:192:SER:HB3	2:C:195:ASP:HB2	1.75	0.69
1:A:632:LEU:N	1:A:633:PRO:HD2	2.08	0.69
2:B:339:LEU:HB2	2:B:353:MET:CG	2.21	0.69
2:B:1023:CYS:O	2:B:1027:THR:HG23	1.92	0.69
3:E:22:ASN:ND2	3:E:25:LEU:H	1.91	0.69
2:B:961:THR:HG22	2:C:893:PRO:O	1.92	0.68
2:B:1171:THR:HG23	2:B:1172:PRO:HD2	1.74	0.68
2:C:2:LYS:O	2:C:3:ARG:HB2	1.93	0.68
2:C:605:THR:HG21	2:C:870:THR:HG21	1.75	0.68
1:A:980:THR:HB	1:A:1115:GLY:HA2	1.73	0.68
2:B:280:VAL:HG23	2:B:281:LEU:H	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:22:ASN:HD21	3:E:25:LEU:H	1.41	0.68
2:C:218:ARG:HH21	2:C:239:VAL:HG21	1.56	0.68
2:B:242:LYS:H	2:B:242:LYS:HD2	1.57	0.68
2:B:278:GLN:NE2	2:B:280:VAL:HG22	2.07	0.68
1:A:385:GLN:HE21	1:A:385:GLN:HA	1.58	0.68
2:C:1171:THR:HG23	2:C:1172:PRO:CD	2.23	0.68
2:C:94:GLU:HB3	2:C:133:LEU:HD22	1.74	0.68
2:B:1188:HIS:O	2:B:1190:ILE:HG23	1.94	0.68
1:A:1063:PHE:HD2	1:A:1073:ILE:HD12	1.58	0.68
2:C:483:LEU:HB2	2:C:493:VAL:HG21	1.75	0.68
2:B:503:ARG:HD3	2:B:1265:PRO:HG3	1.76	0.68
2:B:1217:PRO:HG2	2:B:1218:GLN:OE1	1.94	0.68
2:C:666:ASN:OD1	2:C:668:ILE:HB	1.93	0.67
2:B:851:ARG:HA	2:B:996:GLN:O	1.94	0.67
2:C:237:ALA:HA	2:C:247:LEU:HD22	1.75	0.67
1:A:700:GLY:HA2	1:A:758:ARG:NH2	2.10	0.67
3:E:209:TYR:O	3:E:213:THR:HG23	1.95	0.67
1:A:1145:ILE:HG22	1:A:1147:VAL:HG23	1.77	0.67
2:C:218:ARG:HH21	2:C:239:VAL:CG2	2.07	0.67
2:C:763:ASN:ND2	2:C:767:ARG:HG2	2.10	0.67
3:E:386:ASN:N	3:E:386:ASN:HD22	1.93	0.67
2:B:851:ARG:HG3	2:B:851:ARG:HH11	1.58	0.67
3:D:114:GLN:HB3	3:D:115:PRO:HD2	1.77	0.67
3:E:276:SER:OG	3:E:332:VAL:HG23	1.95	0.67
1:A:494:TYR:CD2	1:A:542:PRO:HD2	2.30	0.67
1:A:413:MET:O	1:A:417:LEU:HD12	1.96	0.66
2:B:303:ARG:HH11	2:B:1208:SER:HB3	1.59	0.66
2:C:321:SER:HA	2:C:368:ASP:OD1	1.95	0.66
1:A:909:GLN:O	1:A:913:VAL:HG23	1.95	0.66
1:A:1108:ASN:HD21	1:A:1110:ASN:HD21	1.42	0.66
1:A:1242:GLU:HB2	1:A:1247:ILE:HD11	1.77	0.66
3:E:222:LEU:HB3	3:E:228:ILE:HG12	1.76	0.66
3:E:386:ASN:N	3:E:386:ASN:ND2	2.42	0.66
2:B:472:MET:HE2	2:B:506:PRO:HB2	1.78	0.66
2:B:867:THR:HG22	2:B:867:THR:O	1.96	0.66
2:C:271:ILE:HG22	2:C:272:VAL:HG23	1.78	0.66
3:E:210:ALA:O	3:E:214:GLN:HG3	1.96	0.66
1:A:506:LEU:HD22	1:A:510:GLN:HE22	1.61	0.66
3:E:9:LYS:H	3:E:151:THR:HG22	1.61	0.66
3:D:270:LEU:C	3:D:270:LEU:HD12	2.16	0.65
1:A:857:PRO:HB2	1:A:860:CYS:SG	2.37	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:THR:HG22	1:A:774:LEU:O	1.95	0.65
1:A:582:VAL:HG13	1:A:587:ASP:HB2	1.78	0.65
1:A:851:ILE:HD12	1:A:851:ILE:N	2.06	0.65
1:A:621:ARG:HB2	1:A:622:PRO:HD3	1.79	0.65
2:B:353:MET:SD	2:B:955:LEU:HD23	2.36	0.65
2:B:823:ALA:HB3	2:B:824:PRO:HD3	1.78	0.65
2:C:221:THR:HB	2:C:234:GLN:HB2	1.78	0.65
3:D:288:SER:O	3:D:292:THR:HG23	1.96	0.65
1:A:1063:PHE:CD2	1:A:1073:ILE:HD12	2.31	0.65
3:E:328:HIS:HB3	3:E:410:THR:HB	1.79	0.65
1:A:1108:ASN:HD21	1:A:1110:ASN:ND2	1.93	0.65
2:B:682:HIS:CD2	2:C:778:ASN:HB3	2.31	0.65
2:C:474:ILE:HD12	2:C:507:TYR:HB2	1.78	0.65
1:A:1068:VAL:HG13	1:A:1076:VAL:HB	1.78	0.65
2:B:252:THR:HG21	2:B:916:SER:HB3	1.78	0.65
2:B:532:ILE:HG12	2:B:604:VAL:CG2	2.26	0.65
3:D:383:ASN:HD21	3:D:391:MET:H	1.43	0.65
1:A:1138:ILE:HD12	1:A:1138:ILE:N	2.05	0.65
2:C:622:SER:HB3	2:C:625:ASN:HD22	1.61	0.65
2:B:1112:LEU:HG	2:B:1116:GLN:NE2	2.10	0.65
2:C:1124:GLN:HG3	2:C:1125:GLN:NE2	2.11	0.65
1:A:613:VAL:HG22	1:A:654:VAL:HG13	1.79	0.64
1:A:1019:MET:CE	1:A:1021:ILE:HD11	2.26	0.64
2:B:815:ALA:HB3	2:B:816:PRO:HD3	1.80	0.64
2:C:690:ASN:HB3	2:C:693:LEU:HD12	1.78	0.64
2:C:937:GLN:HA	2:C:947:ARG:HH21	1.61	0.64
1:A:290:GLN:H	1:A:290:GLN:HE21	1.42	0.64
1:A:374:GLN:CD	1:A:374:GLN:H	1.99	0.64
3:E:90:ARG:HD3	3:E:111:VAL:HG12	1.79	0.64
2:C:1112:LEU:HD22	2:C:1141:MET:HE3	1.79	0.64
3:E:227:VAL:HG21	3:E:415:ALA:HA	1.78	0.64
2:C:765:ARG:HG3	2:C:765:ARG:HH11	1.63	0.64
3:D:360:LEU:C	3:D:360:LEU:HD23	2.18	0.64
3:E:176:ASN:C	3:E:176:ASN:HD22	2.00	0.64
1:A:903:PHE:CE2	1:A:926:VAL:HG13	2.32	0.64
3:E:11:VAL:HG22	3:E:12:GLY:N	2.12	0.64
3:D:11:VAL:HG22	3:D:12:GLY:N	2.12	0.64
2:B:527:ASN:HA	2:B:873:VAL:CG1	2.27	0.64
1:A:62:PRO:O	1:A:63:LEU:HB2	1.98	0.64
2:B:468:ARG:HD2	2:B:468:ARG:O	1.98	0.64
3:D:165:ARG:HH11	3:D:214:GLN:HE22	1.44	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:258:ASN:N	3:D:258:ASN:ND2	2.39	0.64
3:D:406:ASN:O	3:D:410:THR:HG23	1.98	0.64
1:A:1074:PRO:HG2	1:A:1092:VAL:O	1.98	0.63
2:B:750:VAL:HG12	2:B:751:THR:H	1.64	0.63
2:B:982:MET:HB3	2:B:985:GLU:HG3	1.79	0.63
2:C:1158:ASN:C	2:C:1158:ASN:HD22	2.02	0.63
2:C:439:MET:HE3	3:E:193:THR:HB	1.79	0.63
2:B:840:ARG:HA	2:B:843:VAL:HG23	1.80	0.63
1:A:720:THR:CG2	1:A:723:ALA:HB3	2.28	0.63
2:C:122:TYR:CE2	2:C:875:LEU:HD13	2.34	0.63
3:D:334:ARG:HB3	3:D:407:THR:HG21	1.81	0.63
1:A:25:TYR:CZ	1:A:61:ARG:HD3	2.34	0.63
2:B:416:VAL:HG12	2:B:416:VAL:O	1.98	0.63
2:C:473:ASN:HD22	2:C:474:ILE:H	1.45	0.63
1:A:153:LEU:HB3	1:A:155:GLN:CG	2.28	0.63
1:A:642:LYS:HZ1	1:A:648:ASN:HD21	1.46	0.63
1:A:1126:ILE:HG13	1:A:1147:VAL:HG22	1.80	0.62
2:B:253:PRO:HD3	2:B:920:ARG:HD3	1.80	0.62
2:B:601:ASN:ND2	2:B:832:GLN:HA	2.13	0.62
2:B:1163:THR:HG21	2:B:1198:TYR:HB2	1.80	0.62
3:E:41:GLN:HA	3:E:41:GLN:NE2	2.12	0.62
1:A:429:ILE:HG23	1:A:995:LEU:HD22	1.80	0.62
1:A:907:PHE:O	1:A:911:ILE:HG12	1.99	0.62
2:C:7:LYS:HG2	2:C:978:ASP:OD2	2.00	0.62
2:C:451:PHE:CE2	2:C:1256:VAL:HG22	2.35	0.62
3:E:50:ARG:O	3:E:51:GLY:O	2.17	0.62
2:B:822:ILE:HG22	2:B:826:LEU:CD2	2.27	0.62
2:C:1000:GLN:HB3	2:C:1010:ASN:HA	1.82	0.62
3:E:270:LEU:HD12	3:E:270:LEU:C	2.20	0.62
1:A:214:HIS:HA	2:B:718:GLN:HE22	1.65	0.62
3:E:31:ARG:H	3:E:41:GLN:HE22	1.46	0.62
3:E:243:ARG:O	3:E:243:ARG:HG3	1.99	0.61
1:A:307:LEU:HD23	1:A:344:LEU:HD12	1.82	0.61
2:C:744:ASP:O	2:C:812:GLN:HG3	1.99	0.61
3:E:83:ASN:ND2	3:E:85:ARG:HB2	2.15	0.61
1:A:529:VAL:O	1:A:532:PRO:HD2	2.00	0.61
2:C:580:LYS:HE2	2:C:624:GLU:HG2	1.81	0.61
1:A:1073:ILE:HG23	1:A:1074:PRO:HD2	1.81	0.61
2:B:627:TRP:O	2:B:631:ILE:HG12	2.00	0.61
2:C:412:GLY:C	2:C:414:PRO:HD3	2.21	0.61
2:C:528:ASN:C	2:C:528:ASN:ND2	2.54	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:948:ARG:HH21	1:A:957:ASP:HB3	1.64	0.61
2:B:542:LEU:O	2:B:546:ILE:HG22	2.00	0.61
2:C:129:ASN:HD21	2:C:869:THR:H	1.47	0.61
2:C:1032:ASN:HD21	2:C:1042:ARG:NH2	1.98	0.61
2:B:451:PHE:O	2:B:452:GLU:HB3	1.99	0.61
2:C:70:GLU:OE2	2:C:911:ASP:OD1	2.17	0.61
2:C:499:PRO:HG3	3:E:45:TRP:CE2	2.36	0.61
2:C:622:SER:HB3	2:C:625:ASN:ND2	2.15	0.61
3:E:328:HIS:HB3	3:E:410:THR:CG2	2.31	0.61
1:A:55:VAL:HG12	1:A:177:ASN:HB2	1.83	0.61
2:C:504:LEU:HG	2:C:506:PRO:HD3	1.81	0.61
3:D:273:MET:HG3	3:D:273:MET:O	2.00	0.61
3:D:350:THR:OG1	3:D:353:GLN:HG3	2.00	0.61
3:E:114:GLN:HB3	3:E:115:PRO:HD2	1.83	0.61
2:C:937:GLN:HE22	2:C:1025:GLN:HE22	1.47	0.61
2:C:1216:SER:HB3	2:C:1217:PRO:HD2	1.81	0.61
2:C:912:THR:HG1	2:C:914:VAL:HG23	1.64	0.60
2:B:270:PRO:HG3	2:B:297:PRO:HB3	1.83	0.60
2:C:603:VAL:HG23	2:C:604:VAL:HG23	1.82	0.60
1:A:374:GLN:H	1:A:374:GLN:NE2	2.00	0.60
1:A:446:ARG:HD3	1:A:1071:ALA:O	2.02	0.60
1:A:1019:MET:HE3	1:A:1021:ILE:HD11	1.83	0.60
2:C:102:ALA:O	2:C:106:THR:HG23	2.01	0.60
1:A:401:THR:HG21	1:A:724:ARG:NH2	2.17	0.60
1:A:456:LEU:HD12	1:A:457:PRO:CD	2.26	0.60
2:B:313:ASN:C	2:B:313:ASN:HD22	2.04	0.60
3:E:39:LEU:C	3:E:41:GLN:H	2.05	0.60
1:A:68:LEU:O	1:A:170:ARG:NH2	2.35	0.60
1:A:983:PRO:C	1:A:984:LEU:HD12	2.21	0.60
2:B:321:SER:HA	2:B:368:ASP:OD1	2.02	0.60
2:C:8:THR:HG22	2:C:9:LYS:N	2.17	0.60
2:C:743:ILE:HG22	2:C:744:ASP:N	2.17	0.60
2:B:278:GLN:NE2	2:B:280:VAL:CG2	2.65	0.60
2:C:982:MET:HG2	2:C:983:LEU:N	2.17	0.60
3:D:117:LEU:HD12	3:D:118:GLN:H	1.67	0.60
2:C:248:LEU:HA	2:C:913:GLU:OE2	2.02	0.59
2:C:937:GLN:HE22	2:C:1025:GLN:NE2	2.00	0.59
3:D:340:CYS:HB3	3:D:349:MET:HE3	1.83	0.59
2:B:1095:ARG:NH1	3:E:50:ARG:HB3	2.18	0.59
2:C:2:LYS:HG2	2:C:3:ARG:N	2.15	0.59
3:E:91:PHE:O	3:E:92:LEU:HB2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:974:TRP:HB2	1:A:977:CYS:HB3	1.84	0.59
2:B:983:LEU:O	2:B:984:LEU:HB2	2.01	0.59
2:B:1171:THR:HG23	2:B:1172:PRO:CD	2.32	0.59
1:A:907:PHE:HZ	1:A:1019:MET:HE1	1.68	0.59
2:C:580:LYS:HE2	2:C:624:GLU:CG	2.32	0.59
2:B:502:ASN:HD22	2:B:502:ASN:N	2.00	0.59
3:E:147:LEU:O	3:E:151:THR:HG23	2.02	0.59
1:A:582:VAL:HG21	1:A:591:SER:HB2	1.84	0.59
1:A:646:THR:HG22	1:A:647:ASN:N	2.18	0.59
1:A:22:THR:HG23	1:A:226:LYS:HE3	1.84	0.59
2:B:601:ASN:HD21	2:B:832:GLN:HA	1.66	0.59
2:B:1131:LYS:HD2	2:B:1160:TRP:CE2	2.38	0.59
2:C:85:GLY:HA2	2:C:964:THR:HG22	1.85	0.58
2:C:473:ASN:ND2	2:C:474:ILE:H	2.01	0.58
1:A:620:THR:OG1	1:A:623:VAL:HG23	2.03	0.58
2:B:280:VAL:CG2	2:B:281:LEU:H	2.15	0.58
2:C:1079:ARG:HG2	2:C:1079:ARG:NH1	2.16	0.58
2:C:1034:GLU:HG3	2:C:1251:VAL:HG23	1.86	0.58
2:B:1096:ASP:HB2	2:B:1100:MET:O	2.03	0.58
2:C:242:LYS:O	2:C:242:LYS:HG2	2.04	0.58
1:A:759:SER:HB2	1:A:760:PRO:HD2	1.85	0.58
2:B:533:GLN:HE21	2:B:537:GLN:NE2	2.01	0.58
2:C:931:LEU:O	2:C:935:VAL:HG12	2.04	0.58
3:E:7:LEU:HB3	3:E:125:TYR:O	2.04	0.58
3:E:91:PHE:CZ	3:E:92:LEU:HD12	2.38	0.58
2:C:1112:LEU:HD22	2:C:1141:MET:CE	2.33	0.58
3:E:74:GLY:HA3	3:E:91:PHE:CE2	2.39	0.58
1:A:24:GLN:H	1:A:24:GLN:NE2	2.01	0.58
2:C:528:ASN:HD21	2:C:530:THR:CB	2.15	0.58
3:D:214:GLN:CG	3:D:295:LEU:HD21	2.34	0.58
3:E:406:ASN:O	3:E:410:THR:HG23	2.04	0.58
2:B:610:ASP:CB	2:C:786:THR:HG21	2.32	0.58
2:C:507:TYR:CE2	2:C:915:PHE:HB3	2.39	0.58
2:C:776:VAL:HG21	2:C:793:MET:HG2	1.85	0.58
3:E:12:GLY:HA2	3:E:121:ALA:HB1	1.86	0.58
3:E:124:VAL:HG11	3:E:316:ILE:HG23	1.86	0.58
1:A:1129:ALA:HB3	1:A:1144:ASP:HB2	1.85	0.57
2:B:1166:TRP:CD1	2:B:1176:PRO:HG2	2.39	0.57
2:C:837:ARG:HG3	2:C:838:LEU:H	1.68	0.57
2:C:1162:LEU:H	2:C:1162:LEU:HD12	1.69	0.57
2:C:1162:LEU:HD12	2:C:1162:LEU:N	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:743:ILE:CG2	2:B:744:ASP:N	2.68	0.57
2:C:2:LYS:CG	2:C:3:ARG:H	2.13	0.57
3:D:163:TYR:H	3:D:292:THR:HG21	1.69	0.57
1:A:290:GLN:HE21	1:A:290:GLN:N	2.02	0.57
2:B:332:ILE:HD11	2:B:349:ALA:HB3	1.87	0.57
2:C:1229:VAL:HG13	2:C:1236:THR:HG21	1.86	0.57
1:A:1034:PHE:HA	1:A:1040:CYS:SG	2.45	0.57
2:C:654:ASN:O	2:C:657:VAL:HG23	2.04	0.57
3:E:153:LEU:HG	3:E:153:LEU:O	2.05	0.57
2:B:1112:LEU:HD13	2:B:1141:MET:HE3	1.87	0.57
2:C:983:LEU:O	2:C:984:LEU:HB2	2.03	0.57
3:D:50:ARG:HG3	3:D:50:ARG:NH1	2.15	0.57
1:A:54:ILE:HD12	1:A:54:ILE:N	2.19	0.57
1:A:412:LEU:C	1:A:412:LEU:HD23	2.24	0.57
2:B:1002:GLN:HG3	2:B:1008:THR:HG22	1.87	0.57
2:C:234:GLN:NE2	2:C:911:ASP:OD1	2.37	0.57
3:D:83:ASN:HD21	3:D:85:ARG:HB2	1.67	0.57
3:E:54:THR:HG22	3:E:55:SER:N	2.20	0.57
3:E:158:PHE:HB2	3:E:273:MET:HE3	1.86	0.57
1:A:836:ILE:HG23	1:A:837:LEU:N	2.20	0.57
2:B:280:VAL:CG2	2:B:281:LEU:N	2.67	0.57
2:B:620:VAL:HG11	2:B:656:MET:SD	2.45	0.57
2:B:851:ARG:HG3	2:B:851:ARG:NH1	2.19	0.57
3:D:130:TYR:CE2	3:D:132:PHE:HB2	2.40	0.57
3:E:46:ILE:C	3:E:48:LEU:H	2.08	0.57
2:B:574:ALA:O	2:B:577:ILE:HG22	2.04	0.56
2:C:1042:ARG:HG2	2:C:1043:GLY:N	2.20	0.56
3:D:246:ASP:HA	3:D:360:LEU:HD21	1.87	0.56
1:A:854:THR:HG21	1:A:867:PHE:CD2	2.41	0.56
1:A:985:SER:O	1:A:986:TYR:HB3	2.06	0.56
2:C:97:GLU:O	2:C:101:GLU:HG3	2.05	0.56
3:D:340:CYS:HA	3:D:349:MET:HE1	1.86	0.56
2:B:934:LEU:HD21	2:B:1024:VAL:HG11	1.87	0.56
2:B:983:LEU:H	2:B:985:GLU:HG2	1.70	0.56
1:A:1158:ARG:HG3	1:A:1158:ARG:HH11	1.71	0.56
2:B:432:GLY:O	2:B:450:VAL:HG23	2.05	0.56
2:B:455:ASP:OD2	2:B:458:THR:HG23	2.05	0.56
1:A:1216:LEU:HD12	1:A:1216:LEU:H	1.71	0.56
2:B:654:ASN:HD21	2:B:675:ALA:N	2.04	0.56
2:B:1159:ALA:O	2:B:1163:THR:HG23	2.05	0.56
2:C:205:LEU:HD22	2:C:205:LEU:H	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1032:ASN:O	2:C:1032:ASN:ND2	2.38	0.56
2:C:1175:ILE:HG23	2:C:1175:ILE:O	2.05	0.56
3:E:397:PHE:HB2	3:E:401:GLN:OE1	2.04	0.56
2:C:132:GLU:HA	2:C:867:THR:OG1	2.05	0.56
3:D:64:ARG:O	3:D:68:MET:HG3	2.05	0.56
2:B:1172:PRO:HG2	2:C:53:TYR:CE1	2.41	0.56
2:C:763:ASN:HD21	2:C:767:ARG:HG2	1.69	0.56
2:C:846:MET:O	2:C:1001:TYR:HA	2.05	0.56
3:D:276:SER:HG	3:D:332:VAL:HG23	1.69	0.56
1:A:851:ILE:H	1:A:851:ILE:CD1	2.02	0.55
2:C:673:ARG:HH11	2:C:673:ARG:HG2	1.71	0.55
1:A:62:PRO:O	1:A:63:LEU:CB	2.53	0.55
2:B:1229:VAL:HG13	2:B:1236:THR:CG2	2.35	0.55
2:C:129:ASN:ND2	2:C:869:THR:H	2.04	0.55
2:C:763:ASN:C	2:C:763:ASN:HD22	2.09	0.55
2:B:526:GLY:CA	2:B:871:VAL:HG13	2.36	0.55
2:B:720:ARG:HG3	2:B:737:GLU:HB3	1.89	0.55
2:C:468:ARG:HB2	2:C:1019:VAL:HG11	1.88	0.55
3:D:203:TRP:CZ3	3:D:213:THR:HG21	2.41	0.55
2:C:807:THR:N	2:C:808:PRO:HD2	2.21	0.55
2:C:837:ARG:CG	2:C:838:LEU:H	2.19	0.55
3:D:263:ILE:HD13	3:D:418:ILE:HG23	1.88	0.55
1:A:716:PHE:O	1:A:718:ASN:N	2.39	0.55
2:B:518:GLN:HG3	2:B:730:ALA:HB1	1.88	0.55
2:B:537:GLN:O	2:B:540:SER:HB3	2.06	0.55
2:C:59:ILE:O	2:C:63:GLN:HG3	2.06	0.55
1:A:531:GLU:HB3	1:A:532:PRO:HD3	1.86	0.55
2:B:338:LEU:HD11	2:B:968:TRP:CD2	2.42	0.55
2:B:562:THR:HG22	2:B:562:THR:O	2.07	0.55
2:B:691:ILE:HD12	2:B:691:ILE:N	2.12	0.55
2:B:871:VAL:HG12	2:B:872:GLY:N	2.20	0.55
2:C:192:SER:HB3	2:C:195:ASP:CB	2.36	0.55
3:E:146:GLN:O	3:E:150:VAL:HG23	2.07	0.55
3:E:305:ASP:OD2	3:E:307:ASN:HB2	2.07	0.55
2:C:1158:ASN:ND2	2:C:1160:TRP:H	2.04	0.55
1:A:60:PHE:O	1:A:64:GLN:HG3	2.06	0.55
2:C:349:ALA:O	2:C:1175:ILE:HG22	2.06	0.55
2:C:1188:HIS:O	2:C:1190:ILE:HG23	2.07	0.55
3:D:83:ASN:ND2	3:D:85:ARG:HB2	2.22	0.55
1:A:209:ARG:HG2	1:A:209:ARG:HH11	1.72	0.55
2:B:332:ILE:HG23	2:B:333:HIS:N	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1266:PRO:HG2	2:B:1269:ALA:HB2	1.89	0.55
2:B:303:ARG:NH1	2:B:1208:SER:HB3	2.22	0.54
3:D:58:VAL:HG11	3:D:64:ARG:HB2	1.89	0.54
3:D:117:LEU:HD12	3:D:118:GLN:N	2.22	0.54
3:E:39:LEU:O	3:E:41:GLN:N	2.40	0.54
1:A:554:VAL:HG22	1:A:555:ALA:N	2.22	0.54
1:A:625:HIS:O	1:A:628:GLU:HB3	2.08	0.54
2:B:340:ASN:N	2:B:340:ASN:ND2	2.53	0.54
2:C:743:ILE:HG22	2:C:744:ASP:O	2.08	0.54
2:C:1000:GLN:HB2	2:C:1009:PHE:O	2.07	0.54
3:D:304:ILE:HD13	3:D:327:LEU:HD21	1.89	0.54
3:E:311:ALA:HA	3:E:314:ARG:NH1	2.22	0.54
1:A:648:ASN:C	1:A:648:ASN:ND2	2.60	0.54
2:C:66:THR:HG22	2:C:542:LEU:CD1	2.37	0.54
1:A:730:LEU:C	1:A:730:LEU:HD23	2.27	0.54
1:A:841:PRO:HG2	1:A:844:SER:OG	2.07	0.54
2:C:1112:LEU:HG	2:C:1116:GLN:HE21	1.72	0.54
1:A:570:ASP:HB3	1:A:607:ALA:HB2	1.89	0.54
3:D:170:MET:HE1	3:D:214:GLN:CB	2.38	0.54
2:B:851:ARG:HH22	2:B:989:SER:CB	2.21	0.54
2:B:1036:ASN:HD22	2:B:1207:ARG:HB3	1.73	0.54
1:A:153:LEU:HD13	1:A:155:GLN:HG3	1.89	0.54
2:B:598:TRP:CH2	2:B:743:ILE:HD12	2.43	0.54
2:C:451:PHE:O	2:C:452:GLU:HB3	2.08	0.54
2:C:955:LEU:HD12	2:C:955:LEU:C	2.28	0.54
3:D:273:MET:HE1	3:D:327:LEU:HD13	1.90	0.54
2:C:66:THR:HG22	2:C:542:LEU:HD13	1.90	0.54
1:A:209:ARG:HA	1:A:212:TRP:CD1	2.43	0.54
2:C:627:TRP:HA	2:C:627:TRP:CE3	2.42	0.54
1:A:610:GLY:O	1:A:658:VAL:HG23	2.08	0.53
1:A:1013:TYR:CE1	1:A:1017:PRO:HA	2.43	0.53
2:B:386:THR:CG2	2:B:410:ARG:HG3	2.38	0.53
2:B:821:VAL:HG11	2:B:905:ILE:HD13	1.89	0.53
2:B:743:ILE:HG22	2:B:744:ASP:N	2.24	0.53
2:C:852:GLN:HG3	2:C:858:THR:HG21	1.89	0.53
3:D:231:GLN:HE21	3:D:231:GLN:HA	1.72	0.53
1:A:931:ASP:OD1	1:A:932:VAL:N	2.39	0.53
3:D:37:TRP:CZ3	3:D:143:VAL:HG13	2.43	0.53
2:C:10:GLY:HA3	2:C:319:ASP:OD1	2.08	0.53
2:C:474:ILE:CG2	2:C:475:ASN:N	2.70	0.53
2:C:518:GLN:OE1	2:C:829:PRO:HG2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:90:ARG:HG3	3:E:90:ARG:HH11	1.74	0.53
1:A:1216:LEU:HD12	1:A:1216:LEU:N	2.24	0.53
2:B:638:LEU:HD11	2:B:886:LEU:HD21	1.91	0.53
2:B:654:ASN:HD21	2:B:675:ALA:H	1.57	0.53
2:C:439:MET:CE	3:E:193:THR:HB	2.38	0.53
3:E:350:THR:HG23	3:E:353:GLN:OE1	2.09	0.53
2:C:294:SER:HB3	2:C:411:MET:HE1	1.91	0.53
2:C:339:LEU:HD21	2:C:964:THR:OG1	2.08	0.53
3:D:34:ASN:ND2	3:D:104:LEU:O	2.42	0.53
1:A:733:ASN:HD22	1:A:733:ASN:N	2.06	0.53
2:C:400:GLU:CD	2:C:400:GLU:H	2.11	0.53
2:C:775:LEU:HD23	2:C:775:LEU:C	2.28	0.53
3:D:33:GLY:HA3	3:D:41:GLN:NE2	2.23	0.53
1:A:992:ARG:O	1:A:996:LEU:HB2	2.08	0.53
2:B:592:ARG:HG3	2:B:592:ARG:HH11	1.72	0.53
1:A:775:ILE:O	1:A:775:ILE:HD12	2.09	0.53
2:C:264:THR:HB	2:C:454:SER:HA	1.91	0.53
2:C:646:VAL:HG21	2:C:684:TRP:CD1	2.43	0.53
2:C:985:GLU:N	2:C:986:PRO:HD2	2.23	0.53
3:E:152:LEU:HD22	3:E:161:ILE:HB	1.91	0.53
2:C:440:MET:HB2	2:C:444:MET:O	2.09	0.53
2:C:749:ASN:OD1	2:C:751:THR:HG23	2.09	0.53
2:C:823:ALA:HB3	2:C:824:PRO:CD	2.39	0.53
3:D:331:GLN:HE21	3:D:334:ARG:H	1.57	0.53
1:A:734:VAL:O	1:A:735:GLY:O	2.27	0.52
2:C:429:ASN:N	2:C:429:ASN:HD22	2.07	0.52
3:D:246:ASP:OD1	3:D:247:ALA:N	2.42	0.52
3:E:22:ASN:C	3:E:22:ASN:ND2	2.62	0.52
2:C:585:ASN:ND2	2:C:880:ARG:HH22	2.07	0.52
2:C:822:ILE:HG22	2:C:826:LEU:HG	1.91	0.52
2:C:941:THR:HG22	2:C:943:TYR:H	1.74	0.52
3:D:336:VAL:O	3:D:339:PHE:HB3	2.09	0.52
1:A:501:THR:HG22	1:A:503:LYS:HB2	1.90	0.52
2:C:817:VAL:O	2:C:821:VAL:HG23	2.08	0.52
1:A:907:PHE:CZ	1:A:1019:MET:HE1	2.44	0.52
1:A:971:ARG:HG3	1:A:971:ARG:HH11	1.75	0.52
2:C:439:MET:HE3	3:E:193:THR:CB	2.39	0.52
2:B:518:GLN:HG2	2:B:521:ARG:HH21	1.74	0.52
2:C:1171:THR:CG2	2:C:1172:PRO:N	2.72	0.52
3:D:328:HIS:HB3	3:D:410:THR:CB	2.39	0.52
1:A:203:THR:OG1	1:A:205:GLU:HG2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:PRO:O	1:A:229:ASN:N	2.43	0.52
2:C:50:ARG:O	2:C:52:GLN:N	2.42	0.52
2:C:440:MET:HB3	2:C:445:SER:HA	1.91	0.52
2:C:690:ASN:HB3	2:C:693:LEU:CD1	2.40	0.52
3:D:340:CYS:HB3	3:D:354:GLN:HG3	1.91	0.52
3:E:328:HIS:HB3	3:E:410:THR:CB	2.40	0.52
2:B:419:ILE:HG13	2:B:1214:SER:O	2.09	0.52
2:B:985:GLU:N	2:B:986:PRO:CD	2.73	0.52
3:D:231:GLN:HA	3:D:231:GLN:NE2	2.25	0.52
3:D:340:CYS:CB	3:D:349:MET:HE3	2.40	0.52
1:A:385:GLN:HA	1:A:385:GLN:NE2	2.25	0.52
1:A:456:LEU:HA	1:A:678:PHE:CE2	2.45	0.52
1:A:934:ARG:HD3	1:A:1208:PHE:O	2.10	0.52
2:B:644:ALA:HB3	2:B:645:PRO:HD3	1.92	0.52
2:C:1158:ASN:HD22	2:C:1159:ALA:N	2.07	0.52
3:E:340:CYS:HB3	3:E:354:GLN:OE1	2.10	0.52
2:B:533:GLN:N	2:B:534:PRO:HD2	2.25	0.51
1:A:1189:ILE:HD12	1:A:1230:LEU:HB2	1.91	0.51
2:B:526:GLY:O	2:B:527:ASN:HB2	2.10	0.51
2:C:929:GLN:O	2:C:932:VAL:HG22	2.10	0.51
3:D:7:LEU:HD23	3:D:126:ASP:HB2	1.92	0.51
3:D:279:TRP:C	3:D:281:MET:H	2.13	0.51
3:E:233:THR:HG21	3:E:256:SER:HB3	1.92	0.51
2:C:573:PRO:HG3	2:C:792:SER:HB2	1.92	0.51
2:B:513:GLU:HG2	2:B:1016:PRO:HG3	1.91	0.51
2:B:1193:ALA:HB1	2:B:1194:PRO:HD2	1.93	0.51
2:C:638:LEU:HD11	2:C:886:LEU:HD11	1.93	0.51
3:D:11:VAL:CG2	3:D:12:GLY:N	2.74	0.51
1:A:209:ARG:NH2	3:D:202:PRO:O	2.43	0.51
1:A:719:MET:CE	1:A:719:MET:HA	2.40	0.51
2:C:70:GLU:OE2	2:C:911:ASP:O	2.29	0.51
1:A:186:PRO:HG3	1:A:324:ASN:HD22	1.75	0.51
1:A:983:PRO:O	1:A:984:LEU:HD12	2.11	0.51
1:A:989:ARG:O	1:A:992:ARG:HG2	2.10	0.51
2:B:527:ASN:O	2:B:873:VAL:HG11	2.10	0.51
2:B:674:ARG:H	2:B:674:ARG:CD	2.24	0.51
3:D:54:THR:CG2	3:D:55:SER:N	2.73	0.51
2:C:560:MET:CE	2:C:796:THR:HG23	2.41	0.51
2:B:526:GLY:HA2	2:B:871:VAL:HG13	1.92	0.51
2:B:807:THR:N	2:B:808:PRO:HD2	2.25	0.51
1:A:1063:PHE:CD1	1:A:1063:PHE:C	2.84	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:775:LEU:HD12	2:B:775:LEU:O	2.10	0.51
2:C:80:THR:O	2:C:88:ARG:HG2	2.11	0.51
2:C:270:PRO:HG3	2:C:297:PRO:HB3	1.93	0.51
1:A:631:ILE:C	1:A:633:PRO:HD2	2.31	0.50
2:B:246:GLN:HE22	2:B:982:MET:H	1.57	0.50
2:B:970:ASN:OD1	2:B:984:LEU:HB2	2.12	0.50
2:B:1071:THR:HB	2:B:1074:VAL:HG21	1.92	0.50
2:B:1171:THR:C	2:B:1173:THR:H	2.14	0.50
2:C:70:GLU:OE2	2:C:913:GLU:OE2	2.28	0.50
2:C:309:ARG:HB3	2:C:312:SER:OG	2.12	0.50
2:C:510:SER:OG	2:C:513:GLU:HG3	2.12	0.50
3:E:158:PHE:HB2	3:E:273:MET:CE	2.41	0.50
2:B:440:MET:HB2	2:B:443:ALA:HB3	1.93	0.50
2:C:97:GLU:HG3	2:C:136:SER:HB2	1.93	0.50
2:C:934:LEU:HD11	2:C:1024:VAL:HG11	1.93	0.50
1:A:4:VAL:O	1:A:4:VAL:HG23	2.12	0.50
1:A:505:TYR:CD2	1:A:656:PHE:HB3	2.46	0.50
2:B:955:LEU:C	2:B:955:LEU:HD12	2.32	0.50
3:D:306:ASN:ND2	3:D:321:GLY:O	2.44	0.50
3:D:391:MET:SD	3:D:391:MET:C	2.90	0.50
2:B:370:LEU:HD22	2:B:465:TRP:CD2	2.47	0.50
2:C:122:TYR:OH	2:C:533:GLN:HA	2.10	0.50
1:A:251:ALA:O	1:A:255:MET:HG3	2.12	0.50
2:B:244:THR:CG2	2:B:534:PRO:HG3	2.41	0.50
2:B:524:ASN:N	2:B:524:ASN:HD22	2.09	0.50
2:C:463:GLY:O	2:C:466:MET:HB3	2.12	0.50
2:B:1171:THR:CG2	2:B:1172:PRO:N	2.74	0.50
2:C:8:THR:HG22	2:C:9:LYS:H	1.76	0.50
2:C:528:ASN:ND2	2:C:530:THR:H	2.09	0.50
3:D:228:ILE:HG23	3:D:232:ASN:O	2.11	0.50
3:D:275:THR:HG23	3:D:330:PHE:H	1.76	0.50
3:E:277:PRO:HD3	3:E:401:GLN:HB3	1.94	0.50
3:E:313:SER:HA	3:E:316:ILE:HD11	1.93	0.50
1:A:54:ILE:HD12	1:A:54:ILE:H	1.77	0.50
1:A:1041:SER:HA	1:A:1089:LEU:O	2.12	0.50
2:B:750:VAL:HG12	2:B:751:THR:N	2.25	0.50
2:B:871:VAL:CG1	2:B:872:GLY:N	2.74	0.50
2:C:158:THR:O	2:C:161:ILE:HG22	2.10	0.50
3:E:270:LEU:HD12	3:E:270:LEU:O	2.11	0.50
1:A:484:VAL:HG23	1:A:485:LYS:N	2.26	0.50
2:B:407:TYR:CD2	2:B:431:VAL:HG23	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:601:ASN:HD22	2:B:602:GLY:N	2.10	0.50
2:C:1166:TRP:CD1	2:C:1176:PRO:HG2	2.46	0.50
1:A:23:ARG:NH1	1:A:29:ASP:OD1	2.45	0.50
1:A:486:ASP:CB	1:A:529:VAL:HG21	2.41	0.50
2:C:394:LEU:HB3	2:C:395:PRO:HD2	1.94	0.50
3:D:92:LEU:O	3:D:93:ARG:HB2	2.11	0.50
3:E:336:VAL:O	3:E:339:PHE:HB3	2.12	0.50
2:B:264:THR:HB	2:B:454:SER:HA	1.94	0.49
1:A:417:LEU:CD2	1:A:711:ILE:HG13	2.42	0.49
2:C:555:ILE:HG22	2:C:803:ILE:HD11	1.94	0.49
2:C:603:VAL:HG13	2:C:831:PHE:HD2	1.77	0.49
2:C:675:ALA:O	2:C:677:ALA:N	2.45	0.49
2:C:743:ILE:CG2	2:C:744:ASP:N	2.74	0.49
2:C:941:THR:HG22	2:C:943:TYR:N	2.28	0.49
2:C:1034:GLU:OE2	2:C:1231:ARG:NH2	2.45	0.49
1:A:420:LEU:HD22	1:A:698:ASP:O	2.12	0.49
2:B:428:ARG:NH1	2:B:428:ARG:HG2	2.26	0.49
2:C:805:SER:HB2	2:C:887:LEU:O	2.12	0.49
3:D:46:ILE:HG23	3:D:192:TYR:OH	2.12	0.49
3:D:279:TRP:C	3:D:281:MET:N	2.65	0.49
3:D:305:ASP:OD2	3:D:307:ASN:HB2	2.11	0.49
3:E:72:LEU:O	3:E:76:LEU:HB2	2.12	0.49
1:A:2:ALA:O	1:A:3:ASN:HB2	2.11	0.49
2:B:490:TYR:CD2	2:B:901:TYR:HB3	2.48	0.49
2:B:1216:SER:HB3	2:B:1217:PRO:HD2	1.94	0.49
2:C:532:ILE:HD13	2:C:604:VAL:CG2	2.42	0.49
2:C:540:SER:HB2	2:C:592:ARG:CB	2.42	0.49
3:D:227:VAL:HG11	3:D:418:ILE:HD12	1.94	0.49
3:E:386:ASN:HD22	3:E:386:ASN:H	1.60	0.49
1:A:489:VAL:HG23	1:A:490:LEU:N	2.27	0.49
1:A:1008:ILE:HD12	1:A:1008:ILE:N	2.27	0.49
3:E:74:GLY:HA3	3:E:91:PHE:CZ	2.48	0.49
3:E:282:ASP:O	3:E:286:ILE:HG22	2.12	0.49
1:A:809:MET:HE3	1:A:990:TRP:HZ3	1.77	0.49
2:B:1150:TYR:HA	2:B:1182:VAL:O	2.13	0.49
2:C:468:ARG:HD2	2:C:468:ARG:O	2.12	0.49
3:D:96:TRP:CZ3	3:D:101:LEU:HB3	2.48	0.49
3:E:29:LEU:O	3:E:31:ARG:N	2.45	0.49
1:A:757:ARG:HG3	1:A:757:ARG:HH11	1.77	0.49
1:A:808:THR:HG22	1:A:812:ASN:ND2	2.27	0.49
2:B:674:ARG:HD3	2:B:674:ARG:N	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1116:GLN:HB3	2:B:1172:PRO:HA	1.95	0.49
2:C:306:VAL:HG23	2:C:1037:LEU:O	2.13	0.49
2:C:407:TYR:CD2	2:C:431:VAL:HG23	2.48	0.49
3:D:13:PHE:CD2	3:D:121:ALA:HB2	2.47	0.49
3:E:6:PHE:HB3	3:E:144:TYR:CE1	2.47	0.49
3:E:11:VAL:CG2	3:E:12:GLY:N	2.75	0.49
3:E:325:ASN:N	3:E:325:ASN:ND2	2.51	0.49
1:A:342:THR:HB	1:A:343:PRO:HD2	1.95	0.49
1:A:903:PHE:CZ	1:A:926:VAL:HG13	2.47	0.49
1:A:1135:ASP:OD2	1:A:1137:THR:HG23	2.12	0.49
1:A:1158:ARG:HG3	1:A:1158:ARG:NH1	2.28	0.49
2:B:782:GLN:N	2:B:783:PRO:CD	2.75	0.49
2:B:946:ASP:OD2	3:D:31:ARG:NE	2.38	0.49
2:C:552:ASP:OD1	2:C:554:THR:HG23	2.13	0.49
3:D:7:LEU:CD1	3:D:317:HIS:HB3	2.40	0.49
3:D:55:SER:OG	3:D:56:ALA:N	2.46	0.49
2:C:623:LEU:HD13	2:C:793:MET:HE2	1.93	0.49
2:C:1074:VAL:HG12	2:C:1075:HIS:N	2.28	0.49
3:D:228:ILE:HD13	3:D:234:TYR:HB2	1.95	0.49
3:E:229:HIS:HD2	3:E:231:GLN:N	1.94	0.49
1:A:51:THR:O	1:A:52:ASN:HB2	2.13	0.49
1:A:640:LEU:HD21	1:A:653:PHE:HD1	1.77	0.49
2:B:244:THR:HG23	2:B:534:PRO:HG3	1.94	0.49
2:B:340:ASN:HD22	2:B:340:ASN:H	1.58	0.49
2:B:332:ILE:HD11	2:B:349:ALA:CB	2.43	0.48
2:B:391:LEU:N	2:B:391:LEU:CD1	2.76	0.48
2:C:1104:PHE:CD1	2:C:1104:PHE:N	2.81	0.48
1:A:1004:ALA:O	1:A:1008:ILE:HD13	2.12	0.48
2:C:772:MET:O	2:C:776:VAL:HG12	2.12	0.48
3:D:162:SER:HA	3:D:292:THR:HG21	1.95	0.48
2:C:603:VAL:HG13	2:C:831:PHE:CD2	2.49	0.48
2:C:1229:VAL:HG13	2:C:1236:THR:CB	2.43	0.48
3:E:13:PHE:CE2	3:E:121:ALA:HB2	2.49	0.48
3:E:385:ALA:HB3	3:E:386:ASN:ND2	2.28	0.48
1:A:481:ARG:O	1:A:484:VAL:HG22	2.13	0.48
1:A:1016:MET:N	1:A:1017:PRO:CD	2.77	0.48
2:B:278:GLN:NE2	2:B:281:LEU:HB2	2.28	0.48
2:B:959:ALA:HB2	2:B:993:ARG:NH2	2.28	0.48
3:D:92:LEU:O	3:D:93:ARG:CB	2.62	0.48
3:D:214:GLN:HG3	3:D:295:LEU:HD21	1.94	0.48
1:A:149:THR:HG22	1:A:150:GLY:N	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:484:VAL:CG2	1:A:485:LYS:N	2.76	0.48
1:A:507:ARG:O	1:A:510:GLN:HG2	2.12	0.48
1:A:1130:TRP:CD1	1:A:1216:LEU:HD22	2.49	0.48
2:B:510:SER:HG	2:B:513:GLU:HG3	1.75	0.48
2:B:855:ASP:OD2	2:C:757:PHE:N	2.47	0.48
3:D:330:PHE:HB2	3:D:407:THR:HG23	1.96	0.48
3:E:98:ALA:HB1	3:E:99:PRO:HD2	1.94	0.48
2:C:307:HIS:ND1	2:C:310:TRP:HB3	2.29	0.48
3:D:54:THR:HG22	3:D:55:SER:N	2.28	0.48
3:D:55:SER:HB3	3:D:58:VAL:O	2.13	0.48
3:D:350:THR:HG23	3:D:353:GLN:HE21	1.78	0.48
1:A:720:THR:HG22	1:A:724:ARG:H	1.79	0.48
1:A:1241:LYS:O	1:A:1284:TYR:HA	2.13	0.48
2:C:203:HIS:HB2	2:C:205:LEU:HD23	1.96	0.48
2:C:850:THR:HG23	2:C:1000:GLN:HE22	1.79	0.48
1:A:49:GLN:NE2	1:A:321:GLN:HG2	2.29	0.48
1:A:175:MET:HA	1:A:175:MET:CE	2.43	0.48
1:A:1032:GLY:HA3	1:A:1040:CYS:HA	1.96	0.48
2:B:306:VAL:H	2:B:324:MET:HE2	1.78	0.48
2:B:439:MET:HE2	3:D:184:GLY:HA2	1.95	0.48
1:A:632:LEU:N	1:A:633:PRO:CD	2.74	0.48
2:B:415:ASN:HB3	2:B:417:SER:H	1.78	0.48
2:B:618:GLY:HA2	2:B:625:ASN:OD1	2.14	0.48
2:B:946:ASP:O	2:B:947:ARG:HG3	2.14	0.48
1:A:42:PRO:HD2	1:A:43:TRP:CZ3	2.49	0.47
1:A:582:VAL:HG13	1:A:587:ASP:CB	2.44	0.47
2:B:610:ASP:CG	2:C:786:THR:HG21	2.34	0.47
1:A:235:LEU:HD23	1:A:236:GLY:N	2.29	0.47
2:B:946:ASP:HB3	2:B:948:TYR:CE1	2.49	0.47
2:C:190:LEU:HD13	2:C:196:LEU:HA	1.96	0.47
2:C:1032:ASN:HD21	2:C:1042:ARG:HH21	1.62	0.47
2:C:1047:ILE:HA	2:C:1198:TYR:O	2.13	0.47
2:C:1096:ASP:HB2	2:C:1100:MET:O	2.14	0.47
3:D:13:PHE:CE2	3:D:121:ALA:HB2	2.50	0.47
1:A:133:LEU:N	1:A:134:PRO:HD2	2.30	0.47
1:A:647:ASN:OD1	1:A:681:TYR:HA	2.14	0.47
1:A:912:LYS:O	1:A:915:SER:HB2	2.14	0.47
1:A:942:ILE:HG12	1:A:949:TYR:CD2	2.49	0.47
2:B:687:CYS:HA	2:B:693:LEU:HD12	1.96	0.47
2:C:675:ALA:C	2:C:677:ALA:H	2.18	0.47
2:C:695:SER:HB3	2:C:698:ASP:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1067:PHE:CZ	2:C:1107:ASN:HB3	2.49	0.47
1:A:1019:MET:HE2	1:A:1021:ILE:HD11	1.96	0.47
2:B:619:SER:C	2:B:621:THR:H	2.18	0.47
2:C:1241:PRO:HG2	2:C:1244:GLN:HB2	1.95	0.47
3:D:66:TYR:O	3:D:69:SER:HB3	2.14	0.47
1:A:316:ARG:HH11	1:A:333:GLN:NE2	2.12	0.47
1:A:638:TYR:CD1	1:A:638:TYR:C	2.88	0.47
1:A:680:ARG:HG3	1:A:680:ARG:HH11	1.80	0.47
1:A:775:ILE:HD12	1:A:775:ILE:C	2.35	0.47
1:A:840:ILE:O	1:A:840:ILE:HD12	2.14	0.47
1:A:986:TYR:CD1	1:A:1058:ASN:HB3	2.50	0.47
2:B:402:TRP:O	2:B:406:MET:HB2	2.15	0.47
2:B:475:ASN:HB2	2:B:476:PRO:HD2	1.97	0.47
2:B:814:LEU:HD23	2:B:891:TYR:OH	2.15	0.47
2:B:929:GLN:HG2	3:D:32:ALA:O	2.14	0.47
2:B:982:MET:CB	2:B:985:GLU:HG3	2.43	0.47
2:B:1119:THR:HG22	2:B:1120:ARG:N	2.28	0.47
2:C:350:ASN:HA	2:C:1173:THR:O	2.15	0.47
2:C:822:ILE:O	2:C:823:ALA:C	2.53	0.47
2:C:943:TYR:CD1	2:C:944:PRO:HD2	2.48	0.47
3:D:153:LEU:HD13	3:D:160:PRO:HG3	1.96	0.47
3:E:29:LEU:HD11	3:E:67:GLN:HB3	1.95	0.47
3:E:176:ASN:C	3:E:176:ASN:ND2	2.68	0.47
1:A:646:THR:CG2	1:A:647:ASN:N	2.76	0.47
2:C:673:ARG:HG2	2:C:673:ARG:NH1	2.29	0.47
2:C:790:VAL:O	2:C:794:ARG:HG3	2.15	0.47
3:D:227:VAL:CG1	3:D:418:ILE:HD12	2.45	0.47
2:B:309:ARG:HB3	2:B:312:SER:HB2	1.96	0.47
2:B:490:TYR:CD2	2:B:901:TYR:CB	2.98	0.47
2:B:931:LEU:O	2:B:935:VAL:HG23	2.15	0.47
2:C:87:THR:HG21	2:C:140:ASP:HA	1.96	0.47
2:C:532:ILE:HD13	2:C:604:VAL:HG22	1.96	0.47
2:C:1104:PHE:N	2:C:1104:PHE:HD1	2.13	0.47
3:D:231:GLN:HE21	3:D:231:GLN:CA	2.28	0.47
3:D:328:HIS:HB3	3:D:410:THR:CG2	2.44	0.47
1:A:583:ASP:OD2	1:A:583:ASP:N	2.39	0.47
1:A:1250:LEU:O	1:A:1251:ASN:HB2	2.14	0.47
2:B:673:ARG:HE	2:B:674:ARG:NH2	2.12	0.47
2:C:65:ALA:HB2	2:C:545:ARG:HD2	1.96	0.47
2:C:419:ILE:O	2:C:422:PHE:HB3	2.15	0.47
2:C:560:MET:HE1	2:C:796:THR:HG23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:13:PHE:HE1	3:D:19:VAL:HG22	1.80	0.47
3:D:170:MET:HE1	3:D:214:GLN:HB3	1.96	0.47
1:A:641:ILE:HG22	1:A:642:LYS:N	2.30	0.46
2:C:475:ASN:OD1	2:C:477:THR:HB	2.15	0.46
3:E:273:MET:O	3:E:273:MET:HG3	2.15	0.46
1:A:203:THR:HG23	1:A:206:VAL:CG2	2.44	0.46
2:B:428:ARG:HG2	2:B:428:ARG:HH11	1.79	0.46
2:B:601:ASN:HD21	2:B:832:GLN:CA	2.28	0.46
2:C:757:PHE:N	2:C:757:PHE:CD1	2.82	0.46
3:E:391:MET:SD	3:E:391:MET:C	2.93	0.46
1:A:512:VAL:HG12	1:A:513:ALA:N	2.30	0.46
2:C:474:ILE:HG22	2:C:475:ASN:N	2.30	0.46
2:C:984:LEU:O	2:C:985:GLU:C	2.51	0.46
3:E:263:ILE:CD1	3:E:418:ILE:HG23	2.43	0.46
1:A:422:LEU:HD12	1:A:422:LEU:C	2.36	0.46
2:B:1138:ARG:NH2	2:B:1202:THR:HG21	2.30	0.46
2:C:94:GLU:HG3	2:C:134:SER:O	2.16	0.46
2:C:355:ARG:HB3	2:C:954:SER:HB2	1.97	0.46
2:C:540:SER:HB2	2:C:592:ARG:HB3	1.98	0.46
2:C:962:ALA:O	2:C:965:PHE:HB3	2.14	0.46
3:D:279:TRP:O	3:D:281:MET:N	2.48	0.46
1:A:188:PHE:HA	1:A:241:MET:SD	2.55	0.46
1:A:203:THR:HG23	1:A:206:VAL:HG23	1.98	0.46
1:A:713:ASN:ND2	1:A:750:ARG:H	2.13	0.46
1:A:930:THR:CG2	1:A:1017:PRO:HG3	2.46	0.46
2:B:268:ILE:HG22	2:B:297:PRO:HG2	1.98	0.46
2:C:181:TYR:OH	2:C:193:PRO:HD3	2.15	0.46
2:C:437:ALA:HB2	2:C:447:TRP:CD1	2.50	0.46
2:B:281:LEU:HD13	2:B:281:LEU:HA	1.76	0.46
2:B:386:THR:HG22	2:B:410:ARG:HG3	1.98	0.46
2:B:704:GLN:O	2:B:708:ILE:HG13	2.15	0.46
2:C:122:TYR:CD2	2:C:875:LEU:HD13	2.50	0.46
2:C:344:LEU:HD12	2:C:1171:THR:CG2	2.46	0.46
2:C:630:PHE:CZ	2:C:634:LEU:HD22	2.50	0.46
2:C:660:GLU:OE2	2:C:701:ILE:HB	2.16	0.46
3:E:90:ARG:HG3	3:E:90:ARG:NH1	2.31	0.46
1:A:64:GLN:H	1:A:117:ASN:ND2	2.13	0.46
1:A:396:TRP:CH2	1:A:398:PRO:HB3	2.51	0.46
2:B:524:ASN:C	2:B:525:ILE:HG22	2.36	0.46
2:B:601:ASN:HA	2:B:604:VAL:O	2.16	0.46
2:B:1009:PHE:CD1	2:B:1009:PHE:N	2.83	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1166:TRP:CZ3	2:B:1170:ILE:HD11	2.51	0.46
2:C:532:ILE:O	2:C:533:GLN:C	2.54	0.46
2:C:619:SER:C	2:C:621:THR:H	2.19	0.46
1:A:64:GLN:O	1:A:169:GLY:HA3	2.16	0.46
1:A:612:PHE:CD1	1:A:612:PHE:C	2.89	0.46
2:B:660:GLU:OE2	2:B:702:LEU:HB2	2.16	0.46
2:B:945:VAL:HG22	2:B:946:ASP:N	2.30	0.46
2:C:609:ASP:OD1	2:C:610:ASP:OD2	2.33	0.46
2:C:833:VAL:HG13	2:C:834:PRO:HD2	1.98	0.46
3:D:229:HIS:CD2	3:D:231:GLN:H	2.34	0.46
3:E:213:THR:HB	3:E:291:LEU:HD21	1.97	0.46
1:A:564:ARG:HB3	1:A:565:PRO:HD2	1.97	0.46
2:B:520:ILE:O	2:B:523:MET:HB2	2.16	0.46
2:B:990:GLY:HA3	2:C:804:LYS:HB2	1.97	0.46
1:A:1028:MET:HE3	1:A:1101:MET:HG3	1.97	0.46
1:A:1036:VAL:CG2	1:A:1122:PRO:HD3	2.46	0.46
2:C:413:THR:N	2:C:414:PRO:CD	2.72	0.46
2:C:660:GLU:HG2	2:C:699:ALA:HA	1.96	0.46
1:A:340:ASN:HB3	1:A:345:TRP:CH2	2.50	0.45
1:A:577:ASP:OD1	1:A:577:ASP:O	2.34	0.45
1:A:823:ASP:O	1:A:844:SER:HB3	2.16	0.45
2:B:439:MET:CE	3:D:184:GLY:HA2	2.47	0.45
2:C:468:ARG:HB2	2:C:1019:VAL:CG1	2.45	0.45
2:C:627:TRP:HA	2:C:627:TRP:HE3	1.81	0.45
2:C:732:LEU:HD13	2:C:999:ILE:HG21	1.97	0.45
3:E:186:THR:HG22	3:E:252:ILE:HG12	1.99	0.45
3:E:329:GLY:O	3:E:410:THR:HG21	2.16	0.45
2:B:654:ASN:ND2	2:B:675:ALA:H	2.14	0.45
2:B:691:ILE:H	2:B:691:ILE:CD1	2.03	0.45
2:B:1088:ASN:HB2	3:E:40:THR:HG21	1.98	0.45
2:C:422:PHE:O	2:C:425:SER:N	2.47	0.45
3:D:228:ILE:HG23	3:D:233:THR:HA	1.98	0.45
3:D:263:ILE:CD1	3:D:418:ILE:HG23	2.47	0.45
3:E:9:LYS:H	3:E:151:THR:CG2	2.28	0.45
2:B:411:MET:HG2	2:B:412:GLY:N	2.31	0.45
2:C:216:ILE:C	2:C:218:ARG:N	2.69	0.45
2:C:507:TYR:CD2	2:C:915:PHE:HB3	2.51	0.45
2:B:397:PRO:O	2:B:398:ASP:HB3	2.17	0.45
2:B:566:SER:HB3	2:B:569:GLN:HG2	1.99	0.45
2:C:981:ASP:HB3	2:C:982:MET:H	1.62	0.45
2:C:1061:PRO:HA	2:C:1062:PRO:HD3	1.71	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1150:TYR:CZ	2:C:1182:VAL:HG21	2.52	0.45
3:E:107:ALA:HA	3:E:108:PRO:HD3	1.86	0.45
1:A:525:ASP:O	1:A:555:ALA:HB3	2.16	0.45
1:A:582:VAL:CG2	1:A:591:SER:HB2	2.46	0.45
2:B:521:ARG:O	2:B:524:ASN:ND2	2.49	0.45
2:B:906:TYR:N	2:B:907:PRO:HD2	2.32	0.45
1:A:188:PHE:C	1:A:190:LYS:H	2.20	0.45
1:A:938:GLY:O	1:A:952:PRO:HG2	2.16	0.45
2:B:671:GLN:O	2:B:671:GLN:HG2	2.17	0.45
2:B:1175:ILE:O	2:B:1175:ILE:HG13	2.17	0.45
2:B:1188:HIS:O	2:B:1189:ASP:C	2.55	0.45
2:C:325:ALA:HB1	2:C:326:PRO:HD2	1.98	0.45
2:C:1162:LEU:H	2:C:1162:LEU:CD1	2.30	0.45
3:E:109:PRO:HG2	3:E:110:GLN:NE2	2.31	0.45
1:A:533:TRP:NE1	1:A:544:PRO:HD3	2.32	0.45
2:B:526:GLY:HA3	2:B:871:VAL:HG13	1.98	0.45
2:C:241:ASN:C	2:C:243:LYS:H	2.20	0.45
1:A:1145:ILE:HD11	1:A:1183:MET:HB2	1.99	0.45
2:C:641:ASP:OD2	2:C:641:ASP:C	2.55	0.45
2:C:906:TYR:HB3	2:C:907:PRO:CD	2.47	0.45
3:D:42:PHE:O	3:D:46:ILE:HG22	2.17	0.45
3:E:98:ALA:HB1	3:E:99:PRO:CD	2.46	0.45
3:E:333:ARG:O	3:E:333:ARG:HD3	2.17	0.45
3:E:340:CYS:O	3:E:341:ASP:C	2.55	0.45
3:E:369:ARG:HG3	3:E:402:TRP:CZ2	2.52	0.45
1:A:421:PRO:O	1:A:422:LEU:HB3	2.16	0.45
1:A:515:PHE:N	1:A:575:TYR:O	2.50	0.45
1:A:668:SER:O	1:A:671:TYR:HB3	2.17	0.45
2:C:94:GLU:CB	2:C:133:LEU:HD22	2.42	0.45
2:C:150:MET:O	2:C:154:ILE:HG13	2.17	0.45
2:C:782:GLN:HG3	2:C:785:TRP:CE3	2.51	0.45
3:D:7:LEU:HA	3:D:125:TYR:O	2.16	0.45
3:E:39:LEU:C	3:E:41:GLN:N	2.69	0.45
1:A:185:PRO:HA	1:A:186:PRO:HD3	1.82	0.45
1:A:554:VAL:HG22	1:A:555:ALA:H	1.80	0.45
1:A:743:ILE:N	1:A:743:ILE:HD12	2.31	0.45
1:A:1028:MET:CE	1:A:1042:LEU:HD13	2.47	0.45
2:B:372:LEU:HD23	2:B:372:LEU:HA	1.81	0.45
2:B:473:ASN:HD21	2:B:504:LEU:HA	1.80	0.45
2:C:623:LEU:HD13	2:C:793:MET:CE	2.47	0.45
3:D:10:THR:HB	3:D:73:SER:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:846:MET:SD	2:B:846:MET:C	2.96	0.44
3:E:117:LEU:HD12	3:E:118:GLN:N	2.32	0.44
3:E:241:CYS:HB2	3:E:251:TRP:CE3	2.51	0.44
1:A:1090:ASP:C	1:A:1091:MET:HG3	2.37	0.44
2:B:527:ASN:CA	2:B:873:VAL:HG13	2.40	0.44
2:B:670:THR:HG23	2:B:672:SER:H	1.82	0.44
2:C:757:PHE:N	2:C:757:PHE:HD1	2.16	0.44
3:D:33:GLY:HA3	3:D:41:GLN:CD	2.37	0.44
3:E:263:ILE:CD1	3:E:418:ILE:HD12	2.47	0.44
1:A:200:TYR:CD2	1:A:232:HIS:HB3	2.51	0.44
2:B:807:THR:HG21	2:B:886:LEU:HD23	1.99	0.44
2:C:190:LEU:HD11	2:C:199:HIS:CD2	2.52	0.44
2:C:814:LEU:O	2:C:815:ALA:C	2.55	0.44
2:C:1131:LYS:HG2	2:C:1132:THR:HG23	1.99	0.44
2:C:1158:ASN:C	2:C:1158:ASN:ND2	2.69	0.44
2:C:1226:HIS:O	2:C:1227:ILE:C	2.55	0.44
3:D:340:CYS:O	3:D:341:ASP:C	2.56	0.44
3:D:359:ALA:O	3:D:362:ASP:HB2	2.18	0.44
3:E:130:TYR:CE2	3:E:132:PHE:HB2	2.52	0.44
3:E:206:ASP:O	3:E:211:ARG:NH1	2.50	0.44
1:A:293:GLY:C	1:A:295:ASP:H	2.20	0.44
1:A:329:SER:O	1:A:332:SER:HB3	2.17	0.44
1:A:460:TYR:O	1:A:469:ARG:NH2	2.48	0.44
2:B:547:SER:HA	2:B:818:GLU:OE2	2.17	0.44
2:B:1017:GLY:HA3	3:D:41:GLN:HG2	1.98	0.44
2:B:1065:LEU:HD23	2:B:1065:LEU:HA	1.84	0.44
2:C:248:LEU:C	2:C:248:LEU:HD23	2.38	0.44
2:C:1171:THR:C	2:C:1173:THR:H	2.21	0.44
3:D:75:THR:HG21	3:D:104:LEU:HD11	1.99	0.44
3:D:228:ILE:HG22	3:D:229:HIS:N	2.31	0.44
3:D:340:CYS:HA	3:D:349:MET:CE	2.48	0.44
3:E:76:LEU:HD11	3:E:147:LEU:HD21	1.99	0.44
3:E:85:ARG:HH21	3:E:87:GLY:H	1.65	0.44
3:E:241:CYS:HB2	3:E:251:TRP:CD2	2.53	0.44
3:E:303:LEU:HD13	3:E:321:GLY:HA3	1.99	0.44
3:E:333:ARG:HH22	3:E:358:GLU:HB3	1.82	0.44
1:A:872:TYR:HA	1:A:877:TRP:CZ2	2.53	0.44
2:B:602:GLY:HA3	2:B:831:PHE:CD2	2.52	0.44
2:C:135:ARG:HD3	2:C:989:SER:HB2	1.99	0.44
3:D:7:LEU:HD23	3:D:126:ASP:HA	2.00	0.44
3:D:62:GLY:HA3	3:D:280:ASN:HA	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:150:VAL:HG12	3:D:154:ASN:ND2	2.32	0.44
3:D:383:ASN:ND2	3:D:390:THR:HA	2.32	0.44
1:A:1052:VAL:HG12	1:A:1053:PHE:N	2.33	0.44
2:B:955:LEU:HD12	2:B:955:LEU:O	2.17	0.44
2:C:378:PHE:N	2:C:378:PHE:CD1	2.86	0.44
2:C:499:PRO:HG3	3:E:45:TRP:CD2	2.53	0.44
2:C:821:VAL:HG12	2:C:821:VAL:O	2.17	0.44
2:C:1032:ASN:ND2	2:C:1042:ARG:HH21	2.15	0.44
2:C:1163:THR:HG22	2:C:1199:ILE:HD12	2.00	0.44
1:A:671:TYR:O	1:A:675:VAL:HG23	2.17	0.44
2:B:427:VAL:HG23	2:B:1235:LEU:O	2.18	0.44
2:B:673:ARG:HE	2:B:674:ARG:NH1	2.15	0.44
2:B:702:LEU:HD12	2:B:702:LEU:HA	1.74	0.44
2:C:511:ASN:O	2:C:515:GLN:HG3	2.18	0.44
2:C:738:VAL:HG12	2:C:739:LEU:N	2.33	0.44
2:C:1163:THR:HG21	2:C:1198:TYR:HB2	1.99	0.44
1:A:189:ALA:C	1:A:191:ASP:H	2.22	0.44
1:A:632:LEU:HD22	1:A:638:TYR:CD2	2.53	0.44
1:A:685:SER:O	1:A:689:ARG:HB2	2.17	0.44
2:B:1096:ASP:CB	2:B:1100:MET:O	2.64	0.44
2:C:74:LYS:NZ	2:C:530:THR:HG21	2.33	0.44
2:C:941:THR:HG22	2:C:942:GLN:N	2.31	0.44
1:A:666:TRP:HA	1:A:666:TRP:CE3	2.53	0.44
1:A:922:VAL:HG12	1:A:924:VAL:HG23	1.99	0.44
1:A:923:LEU:HD12	1:A:923:LEU:N	2.33	0.44
1:A:934:ARG:HD2	1:A:1209:TYR:HA	2.00	0.44
2:C:44:GLU:HG3	2:C:45:PRO:HD2	2.00	0.44
2:C:756:ASP:C	2:C:758:THR:H	2.19	0.44
3:D:360:LEU:C	3:D:360:LEU:CD2	2.86	0.44
3:E:350:THR:OG1	3:E:353:GLN:HG3	2.18	0.44
1:A:43:TRP:HB2	1:A:57:VAL:CG1	2.47	0.43
1:A:274:GLN:HA	1:A:275:PRO:HD3	1.80	0.43
1:A:907:PHE:CZ	1:A:911:ILE:HD11	2.53	0.43
2:C:296:PHE:HE2	2:C:1232:TYR:HH	1.65	0.43
2:C:344:LEU:HD12	2:C:1171:THR:HG21	2.00	0.43
2:C:782:GLN:HE21	2:C:782:GLN:HB3	1.67	0.43
1:A:19:GLU:OE2	1:A:225:ASP:OD1	2.36	0.43
1:A:249:ILE:HG23	1:A:253:ASP:HB2	2.00	0.43
2:C:1081:CYS:HB2	2:C:1094:ILE:HD11	2.00	0.43
1:A:735:GLY:O	1:A:736:ASN:HB2	2.18	0.43
1:A:869:GLU:O	1:A:870:LEU:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1035:ILE:HG22	1:A:1036:VAL:N	2.33	0.43
2:B:636:LEU:N	2:B:637:PRO:HD2	2.32	0.43
2:B:1097:GLU:O	2:B:1097:GLU:HG2	2.16	0.43
2:B:1159:ALA:HB2	2:B:1181:MET:SD	2.57	0.43
2:C:44:GLU:HA	2:C:45:PRO:HD3	1.76	0.43
2:C:378:PHE:CE2	2:C:433:ARG:HB2	2.53	0.43
3:D:78:ILE:HB	3:D:79:PRO:CD	2.48	0.43
2:B:852:GLN:OE1	2:C:804:LYS:NZ	2.50	0.43
2:C:518:GLN:HE21	2:C:518:GLN:HB3	1.57	0.43
2:C:963:ALA:HA	2:C:992:PRO:HG3	1.99	0.43
3:D:333:ARG:C	3:D:333:ARG:CD	2.87	0.43
1:A:401:THR:HG21	1:A:724:ARG:HH21	1.81	0.43
1:A:459:THR:O	1:A:465:GLU:HG3	2.19	0.43
1:A:757:ARG:HG3	1:A:757:ARG:NH1	2.33	0.43
1:A:1195:LEU:HG	1:A:1197:TYR:CE1	2.52	0.43
2:B:244:THR:HG23	2:B:534:PRO:CG	2.48	0.43
2:B:391:LEU:N	2:B:391:LEU:HD12	2.34	0.43
2:B:522:ILE:O	2:B:523:MET:C	2.56	0.43
2:B:645:PRO:HG3	2:B:713:TRP:CE2	2.54	0.43
2:C:146:ASN:HA	2:C:153:ARG:HH21	1.83	0.43
2:C:1111:PRO:HG2	2:C:1114:LEU:HG	1.99	0.43
1:A:155:GLN:HA	2:B:746:GLN:HE21	1.84	0.43
1:A:270:ALA:O	1:A:271:ARG:NH1	2.51	0.43
1:A:1073:ILE:HG22	1:A:1074:PRO:N	2.33	0.43
1:A:1073:ILE:CG2	1:A:1074:PRO:HD2	2.47	0.43
2:B:261:GLY:O	2:B:1259:ARG:NH2	2.50	0.43
2:B:736:PRO:O	2:B:737:GLU:HB2	2.18	0.43
2:C:935:VAL:HG13	2:C:936:ALA:N	2.33	0.43
3:D:130:TYR:HE2	3:D:132:PHE:HB2	1.82	0.43
1:A:873:LEU:HD23	1:A:873:LEU:HA	1.89	0.43
1:A:1242:GLU:CB	1:A:1247:ILE:HD11	2.48	0.43
2:B:823:ALA:CA	2:B:826:LEU:HD23	2.40	0.43
2:B:991:ASP:HA	2:B:992:PRO:HD3	1.68	0.43
2:C:553:PRO:O	2:C:554:THR:C	2.57	0.43
2:C:1119:THR:HG22	2:C:1120:ARG:N	2.34	0.43
2:C:1126:PHE:O	2:C:1127:ASP:C	2.57	0.43
2:C:1152:ASP:HA	2:C:1153:PRO:HD3	1.80	0.43
3:D:7:LEU:CD2	3:D:126:ASP:HB2	2.48	0.43
3:D:38:GLN:HB2	3:D:68:MET:HE3	2.01	0.43
1:A:772:LEU:HD12	1:A:773:PRO:HD2	2.00	0.43
1:A:924:VAL:O	1:A:926:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:976:ASN:HA	1:A:1027:PRO:HG2	2.00	0.43
1:A:982:VAL:HG23	1:A:1018:ILE:O	2.18	0.43
2:B:432:GLY:C	2:B:450:VAL:HG23	2.39	0.43
2:B:932:VAL:CG2	2:B:933:THR:N	2.81	0.43
2:B:946:ASP:HB2	2:B:1025:GLN:OE1	2.19	0.43
2:C:619:SER:O	2:C:621:THR:N	2.52	0.43
3:D:275:THR:HG23	3:D:330:PHE:N	2.33	0.43
3:E:66:TYR:O	3:E:69:SER:HB3	2.18	0.43
1:A:316:ARG:HA	1:A:317:PRO:HD3	1.82	0.43
1:A:582:VAL:CG1	1:A:587:ASP:HB2	2.47	0.43
2:B:619:SER:O	2:B:621:THR:N	2.51	0.43
2:C:241:ASN:OD1	2:C:243:LYS:HB2	2.19	0.43
3:D:145:GLN:HG2	3:D:294:CYS:HA	2.01	0.43
2:B:518:GLN:HE22	2:B:828:PHE:HE1	1.62	0.43
2:B:664:MET:HG3	2:B:671:GLN:N	2.33	0.43
2:C:473:ASN:ND2	2:C:474:ILE:N	2.66	0.43
2:C:765:ARG:HG3	2:C:765:ARG:NH1	2.33	0.43
2:C:806:MET:O	2:C:809:MET:HB3	2.18	0.43
2:C:1068:ASP:O	2:C:1071:THR:HB	2.19	0.43
2:B:829:PRO:HA	2:B:830:PRO:HD3	1.89	0.42
2:B:947:ARG:HG2	2:B:947:ARG:HH11	1.84	0.42
2:B:1048:GLY:O	2:B:1198:TYR:HA	2.20	0.42
2:B:1096:ASP:CG	2:B:1097:GLU:H	2.22	0.42
2:C:591:PHE:O	2:C:594:ALA:HB3	2.19	0.42
2:C:969:VAL:O	2:C:973:MET:HG3	2.19	0.42
2:C:1019:VAL:HG23	2:C:1020:ILE:H	1.83	0.42
2:C:1052:SER:OG	2:C:1053:THR:N	2.52	0.42
3:E:8:PHE:CA	3:E:151:THR:HG21	2.46	0.42
1:A:709:ILE:HG12	1:A:730:LEU:HD12	2.00	0.42
1:A:947:LYS:O	1:A:959:PRO:HA	2.19	0.42
2:B:601:ASN:HD22	2:B:601:ASN:C	2.22	0.42
2:C:360:HIS:O	2:C:363:LEU:HB3	2.19	0.42
3:D:78:ILE:HB	3:D:79:PRO:HD3	2.01	0.42
3:E:85:ARG:NH2	3:E:87:GLY:H	2.17	0.42
3:E:92:LEU:O	3:E:93:ARG:HB2	2.19	0.42
3:E:270:LEU:C	3:E:270:LEU:CD1	2.88	0.42
1:A:67:VAL:HG12	1:A:169:GLY:HA2	2.01	0.42
1:A:458:ASP:OD2	1:A:458:ASP:N	2.52	0.42
2:C:1058:PRO:HD2	2:C:1182:VAL:HG12	2.02	0.42
3:D:7:LEU:HD23	3:D:126:ASP:CB	2.49	0.42
3:D:12:GLY:HA2	3:D:121:ALA:HB1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:273:MET:O	3:D:329:GLY:HA2	2.19	0.42
3:E:81:ARG:NH2	3:E:88:ASP:OD1	2.50	0.42
1:A:293:GLY:O	1:A:295:ASP:N	2.52	0.42
1:A:330:PHE:CE2	1:A:334:ILE:HD11	2.54	0.42
1:A:1015:TYR:CD1	1:A:1015:TYR:N	2.87	0.42
2:B:1096:ASP:HB3	2:B:1100:MET:N	2.23	0.42
2:B:1139:ILE:HG22	2:B:1141:MET:HG2	2.01	0.42
2:C:76:ASN:HB3	2:C:524:ASN:ND2	2.35	0.42
3:D:63:SER:HB3	3:D:393:ARG:O	2.19	0.42
3:D:291:LEU:C	3:D:293:GLY:N	2.72	0.42
3:E:158:PHE:CD2	3:E:275:THR:HB	2.54	0.42
1:A:1033:ASN:O	1:A:1035:ILE:N	2.52	0.42
1:A:1036:VAL:HG23	1:A:1120:ASP:O	2.19	0.42
1:A:1237:GLU:HA	1:A:1250:LEU:O	2.19	0.42
2:B:415:ASN:HD22	2:B:415:ASN:HA	1.50	0.42
2:B:473:ASN:ND2	2:B:504:LEU:HA	2.34	0.42
2:C:239:VAL:HG22	2:C:240:GLU:H	1.83	0.42
2:C:335:PHE:CE2	2:C:1040:ILE:HD11	2.54	0.42
3:E:153:LEU:O	3:E:395:LYS:NZ	2.52	0.42
1:A:3:ASN:C	1:A:3:ASN:HD22	2.22	0.42
1:A:494:TYR:HD2	1:A:542:PRO:HD2	1.79	0.42
1:A:721:GLN:O	1:A:722:ALA:C	2.58	0.42
1:A:934:ARG:CD	1:A:1209:TYR:HA	2.49	0.42
2:B:332:ILE:CG2	2:B:333:HIS:N	2.82	0.42
2:B:347:ARG:HG2	2:B:347:ARG:HH11	1.85	0.42
2:C:761:LEU:HD23	2:C:761:LEU:HA	1.88	0.42
3:D:38:GLN:O	3:D:39:LEU:C	2.58	0.42
3:E:234:TYR:CE2	3:E:235:ARG:HD2	2.55	0.42
1:A:263:GLN:HE22	1:A:267:ASN:ND2	2.17	0.42
1:A:471:LEU:HD21	1:A:691:LEU:HB2	2.01	0.42
1:A:480:ASP:OD2	1:A:528:LEU:HD12	2.19	0.42
1:A:501:THR:CG2	1:A:503:LYS:HB2	2.49	0.42
1:A:743:ILE:HA	1:A:751:VAL:O	2.20	0.42
1:A:940:LEU:HD22	1:A:1016:MET:HE2	2.01	0.42
2:B:422:PHE:O	2:B:423:VAL:C	2.58	0.42
2:B:523:MET:HG2	2:B:849:VAL:HG21	2.02	0.42
2:B:681:PRO:O	2:B:683:THR:N	2.52	0.42
2:C:338:LEU:HB3	2:C:339:LEU:H	1.54	0.42
2:C:407:TYR:HD2	2:C:431:VAL:HG23	1.84	0.42
2:C:581:LEU:O	2:C:880:ARG:HD2	2.20	0.42
2:C:828:PHE:HA	2:C:829:PRO:HD2	1.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1131:LYS:HD2	2:C:1160:TRP:CE2	2.55	0.42
1:A:472:PHE:HD2	1:A:646:THR:HG23	1.85	0.42
1:A:486:ASP:HB2	1:A:529:VAL:HG21	2.01	0.42
1:A:718:ASN:HB3	1:A:719:MET:H	1.57	0.42
1:A:1101:MET:HB3	1:A:1114:LEU:HD12	2.01	0.42
2:B:347:ARG:HG2	2:B:347:ARG:NH1	2.35	0.42
2:B:1173:THR:O	2:B:1173:THR:HG22	2.18	0.42
2:B:1182:VAL:HG23	2:B:1183:PRO:HD2	2.00	0.42
2:B:1229:VAL:HG13	2:B:1236:THR:CB	2.50	0.42
2:C:91:LEU:N	2:C:91:LEU:HD12	2.35	0.42
2:C:473:ASN:HD22	2:C:474:ILE:N	2.16	0.42
2:C:600:TYR:HE2	2:C:828:PHE:O	2.03	0.42
2:C:1018:SER:HB3	2:C:1021:ALA:HB3	2.02	0.42
3:E:13:PHE:CE1	3:E:19:VAL:N	2.88	0.42
1:A:1199:ARG:HA	1:A:1210:ILE:O	2.20	0.42
1:A:1199:ARG:HB3	1:A:1207:GLY:CA	2.50	0.42
2:B:601:ASN:HD21	2:B:833:VAL:H	1.66	0.42
2:B:880:ARG:HG2	2:B:880:ARG:HH11	1.84	0.42
2:B:1112:LEU:HD22	2:B:1141:MET:CE	2.49	0.42
3:D:72:LEU:O	3:D:76:LEU:HB2	2.20	0.42
1:A:24:GLN:CD	1:A:24:GLN:N	2.64	0.42
1:A:301:LEU:HD23	1:A:301:LEU:HA	1.81	0.42
1:A:625:HIS:CE1	1:A:629:GLN:HG3	2.55	0.42
2:B:581:LEU:O	2:B:582:ARG:C	2.57	0.42
2:C:281:LEU:O	2:C:282:ALA:HB2	2.19	0.42
2:C:1185:SER:OG	2:C:1223:PRO:HG2	2.19	0.42
3:D:47:SER:O	3:D:49:GLY:N	2.53	0.42
3:E:398:THR:O	3:E:401:GLN:HB2	2.20	0.42
1:A:684:LEU:HD23	1:A:684:LEU:HA	1.85	0.41
1:A:1112:VAL:O	1:A:1112:VAL:HG23	2.19	0.41
3:D:50:ARG:NH1	3:D:50:ARG:CG	2.80	0.41
3:D:166:VAL:HG21	3:D:417:LEU:HB3	2.02	0.41
3:D:172:SER:OG	3:D:175:VAL:HG23	2.20	0.41
1:A:494:TYR:CE1	1:A:506:LEU:HD13	2.54	0.41
1:A:548:ARG:HG3	1:A:548:ARG:HH11	1.85	0.41
1:A:856:GLN:HA	1:A:857:PRO:HD3	1.85	0.41
2:B:817:VAL:O	2:B:818:GLU:C	2.58	0.41
2:B:870:THR:HG22	2:B:871:VAL:N	2.35	0.41
2:B:981:ASP:HB2	2:B:982:MET:H	1.68	0.41
2:C:932:VAL:HG23	2:C:933:THR:N	2.35	0.41
2:C:1171:THR:CG2	2:C:1172:PRO:CD	2.96	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:7:LEU:HD23	3:D:126:ASP:CA	2.49	0.41
3:D:270:LEU:C	3:D:270:LEU:CD1	2.88	0.41
3:E:179:LEU:HD23	3:E:212:MET:CE	2.50	0.41
1:A:3:ASN:ND2	1:A:7:VAL:O	2.53	0.41
1:A:60:PHE:O	1:A:62:PRO:O	2.38	0.41
2:B:600:TYR:C	2:B:602:GLY:H	2.23	0.41
2:C:77:ASP:O	2:C:78:GLU:C	2.59	0.41
2:C:343:THR:HG22	2:C:1173:THR:CG2	2.50	0.41
2:C:983:LEU:H	2:C:985:GLU:HG2	1.86	0.41
2:C:1171:THR:C	2:C:1173:THR:N	2.73	0.41
3:E:41:GLN:HE21	3:E:41:GLN:CA	2.10	0.41
1:A:115:VAL:O	1:A:116:ALA:C	2.59	0.41
1:A:207:LEU:O	1:A:210:PHE:HB3	2.20	0.41
1:A:384:LEU:HD23	1:A:384:LEU:HA	1.80	0.41
1:A:446:ARG:NH1	1:A:1070:ALA:HA	2.35	0.41
1:A:1225:ASN:C	1:A:1281:PRO:HB3	2.41	0.41
2:B:394:LEU:HD12	2:B:402:TRP:CG	2.54	0.41
2:C:1255:ASN:OD1	2:C:1255:ASN:N	2.53	0.41
3:E:167:ASP:HB2	3:E:267:ASN:OD1	2.20	0.41
3:E:322:ARG:HH11	3:E:322:ARG:HG2	1.85	0.41
1:A:357:SER:HA	1:A:358:PRO:HD3	1.91	0.41
1:A:446:ARG:NH1	1:A:1070:ALA:C	2.74	0.41
1:A:489:VAL:CG2	1:A:490:LEU:N	2.83	0.41
1:A:928:CYS:HA	1:A:929:PRO:HD3	1.88	0.41
2:B:673:ARG:O	2:B:674:ARG:C	2.58	0.41
2:B:805:SER:HB2	2:B:887:LEU:O	2.21	0.41
2:B:1217:PRO:O	2:B:1218:GLN:HB3	2.21	0.41
2:C:616:ASP:HA	2:C:674:ARG:HH21	1.86	0.41
2:C:665:ASP:HB3	2:C:686:ARG:HD3	2.02	0.41
1:A:148:GLY:O	1:A:149:THR:O	2.39	0.41
1:A:377:LEU:O	1:A:379:MET:N	2.53	0.41
2:B:268:ILE:N	2:B:268:ILE:HD12	2.36	0.41
2:B:958:SER:O	2:B:960:ALA:N	2.54	0.41
2:B:991:ASP:OD2	2:B:991:ASP:C	2.59	0.41
2:C:161:ILE:HD12	2:C:161:ILE:HA	1.76	0.41
2:C:1061:PRO:HG3	2:C:1201:SER:O	2.21	0.41
2:C:1213:ASN:ND2	2:C:1219:THR:OG1	2.42	0.41
3:D:152:LEU:HD22	3:D:161:ILE:HB	2.02	0.41
3:E:114:GLN:CB	3:E:115:PRO:HD2	2.45	0.41
2:B:627:TRP:CE3	2:B:627:TRP:HA	2.55	0.41
2:B:638:LEU:HD23	2:B:638:LEU:HA	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:685:PRO:HG2	2:B:688:PHE:HB2	2.03	0.41
2:B:1102:VAL:HA	2:B:1103:PRO:HD3	1.86	0.41
2:C:543:LEU:HA	2:C:546:ILE:HG22	2.03	0.41
2:C:1034:GLU:HG3	2:C:1251:VAL:CG2	2.49	0.41
3:D:126:ASP:OD1	3:D:126:ASP:C	2.59	0.41
3:E:275:THR:HG23	3:E:330:PHE:H	1.86	0.41
1:A:1036:VAL:HG21	1:A:1122:PRO:HD3	2.02	0.41
2:B:519:ILE:O	2:B:520:ILE:C	2.59	0.41
2:B:880:ARG:HG2	2:B:880:ARG:NH1	2.36	0.41
2:B:923:ILE:O	2:B:924:THR:C	2.59	0.41
2:B:1063:PRO:O	2:B:1065:LEU:N	2.54	0.41
2:B:1111:PRO:HA	2:B:1140:GLU:HB2	2.03	0.41
2:C:919:GLN:O	2:C:922:MET:HB3	2.21	0.41
3:D:86:TRP:CZ3	3:D:98:ALA:HA	2.56	0.41
3:D:165:ARG:HD3	3:D:214:GLN:NE2	2.36	0.41
3:E:77:GLN:HG2	3:E:125:TYR:OH	2.20	0.41
3:E:133:LEU:HD23	3:E:139:PHE:CD2	2.56	0.41
3:E:241:CYS:HB2	3:E:251:TRP:CZ3	2.56	0.41
1:A:825:VAL:HG12	1:A:826:LEU:N	2.36	0.41
1:A:940:LEU:HD22	1:A:1016:MET:CE	2.50	0.41
2:B:499:PRO:HB3	3:D:183:PHE:CE2	2.56	0.41
2:B:502:ASN:N	2:B:502:ASN:ND2	2.68	0.41
2:C:691:ILE:H	2:C:691:ILE:CD1	2.09	0.41
2:C:929:GLN:HG2	2:C:1018:SER:HB2	2.03	0.41
2:C:941:THR:CG2	2:C:942:GLN:N	2.83	0.41
2:C:968:TRP:C	2:C:970:ASN:N	2.74	0.41
2:C:1150:TYR:CD2	2:C:1182:VAL:HG23	2.55	0.41
2:C:1241:PRO:HA	2:C:1242:PRO:HD3	1.86	0.41
3:D:98:ALA:HB1	3:D:99:PRO:CD	2.50	0.41
3:D:225:VAL:O	3:D:225:VAL:HG12	2.20	0.41
3:E:333:ARG:CD	3:E:333:ARG:C	2.88	0.41
1:A:951:PHE:HA	1:A:952:PRO:HD2	1.92	0.41
2:B:483:LEU:HA	2:B:483:LEU:HD23	1.84	0.41
2:B:926:GLU:OE2	2:B:1018:SER:HA	2.21	0.41
2:C:44:GLU:HG3	2:C:45:PRO:CD	2.51	0.41
2:C:81:PRO:HA	2:C:87:THR:HA	2.02	0.41
3:D:37:TRP:CZ3	3:D:143:VAL:CG1	3.04	0.41
3:E:92:LEU:O	3:E:93:ARG:CB	2.69	0.41
3:E:95:VAL:HG23	3:E:107:ALA:HB2	2.02	0.41
3:E:273:MET:O	3:E:329:GLY:HA2	2.21	0.41
1:A:3:ASN:O	1:A:341:GLU:HB2	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:LEU:HD22	1:A:73:TYR:CE2	2.56	0.40
1:A:976:ASN:HA	1:A:1027:PRO:CG	2.50	0.40
2:B:600:TYR:C	2:B:602:GLY:N	2.75	0.40
2:B:601:ASN:HD22	2:B:601:ASN:N	2.18	0.40
2:B:958:SER:C	2:B:960:ALA:N	2.74	0.40
2:B:1019:VAL:HG23	2:B:1020:ILE:N	2.36	0.40
2:C:528:ASN:HD22	2:C:529:ALA:N	2.19	0.40
1:A:250:ASN:O	1:A:251:ALA:C	2.59	0.40
1:A:750:ARG:NH1	1:A:750:ARG:CG	2.72	0.40
1:A:1029:GLU:HB3	1:A:1043:VAL:HB	2.03	0.40
2:B:919:GLN:O	2:B:922:MET:HB3	2.21	0.40
2:B:1173:THR:O	2:B:1173:THR:CG2	2.69	0.40
2:B:1219:THR:HB	2:B:1224:ASP:OD1	2.22	0.40
2:C:218:ARG:HH22	2:C:241:ASN:HB3	1.86	0.40
2:C:528:ASN:ND2	2:C:530:THR:N	2.69	0.40
2:C:625:ASN:HB3	2:C:655:MET:CE	2.52	0.40
2:C:1034:GLU:CD	2:C:1231:ARG:HH21	2.25	0.40
3:E:306:ASN:CB	3:E:314:ARG:HD3	2.36	0.40
1:A:836:ILE:CG2	1:A:837:LEU:N	2.84	0.40
2:B:313:ASN:C	2:B:313:ASN:ND2	2.73	0.40
2:B:497:TYR:O	2:B:498:ALA:HB2	2.21	0.40
2:B:588:PHE:O	2:B:589:SER:C	2.59	0.40
2:C:63:GLN:O	2:C:64:ARG:C	2.60	0.40
2:C:776:VAL:O	2:C:776:VAL:HG22	2.21	0.40
2:C:863:SER:HB2	2:C:865:SER:OG	2.21	0.40
2:C:1044:ASP:OD1	2:C:1140:GLU:HA	2.22	0.40
1:A:21:ARG:HG2	1:A:21:ARG:HH11	1.87	0.40
1:A:223:HIS:O	1:A:227:PRO:HG3	2.21	0.40
1:A:772:LEU:HA	1:A:773:PRO:HD2	1.97	0.40
1:A:938:GLY:O	1:A:953:LYS:HE2	2.21	0.40
1:A:978:SER:HB2	1:A:1025:GLY:HA3	2.03	0.40
2:B:306:VAL:HG23	2:B:1037:LEU:O	2.20	0.40
2:B:691:ILE:N	2:B:691:ILE:CD1	2.80	0.40
2:B:778:ASN:O	2:B:780:ARG:N	2.54	0.40
2:C:410:ARG:HH11	2:C:410:ARG:HG2	1.87	0.40
2:C:605:THR:CG2	2:C:870:THR:HG21	2.46	0.40
2:C:873:VAL:HA	2:C:874:PRO:HD3	1.78	0.40
3:D:170:MET:HE1	3:D:214:GLN:HB2	2.03	0.40
3:E:19:VAL:HA	3:E:20:PRO:HD3	1.80	0.40
3:E:264:ARG:HA	3:E:265:PRO:HD3	1.96	0.40
1:A:1135:ASP:O	1:A:1141:THR:HG22	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:601:ASN:ND2	2:B:601:ASN:C	2.74	0.40
2:C:469:LEU:HD23	2:C:469:LEU:HA	1.88	0.40
3:E:189:GLU:O	3:E:193:THR:HG23	2.22	0.40
3:E:312:VAL:HG23	3:E:313:SER:N	2.37	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	1280/1289 (99%)	1131 (88%)	125 (10%)	24 (2%)	8	42
2	B	1027/1275 (80%)	872 (85%)	135 (13%)	20 (2%)	8	42
2	C	1211/1275 (95%)	1063 (88%)	127 (10%)	21 (2%)	9	45
3	D	415/418 (99%)	359 (86%)	46 (11%)	10 (2%)	6	37
3	E	415/418 (99%)	361 (87%)	41 (10%)	13 (3%)	4	32
All	All	4348/4675 (93%)	3786 (87%)	474 (11%)	88 (2%)	7	41

All (88) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	149	THR
1	A	193	SER
1	A	717	SER
1	A	735	GLY
1	A	945	THR
1	A	947	LYS
1	A	986	TYR
2	B	855	ASP
2	C	51	GLU
2	C	983	LEU

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Mol	Chain	Res	Type
3	D	317	HIS
3	E	48	LEU
3	E	51	GLY
3	E	317	HIS
3	E	322	ARG
3	E	405	GLY
1	A	38	PRO
1	A	228	THR
1	A	520	GLY
1	A	719	MET
1	A	877	TRP
1	A	1034	PHE
2	B	319	ASP
2	B	589	SER
2	B	779	GLN
2	B	1214	SER
2	C	3	ARG
2	C	676	SER
3	D	48	LEU
3	D	404	ARG
3	D	405	GLY
3	E	40	THR
3	E	312	VAL
1	A	119	LEU
1	A	152	SER
1	A	294	GLU
1	A	1202	GLN
2	B	502	ASN
2	B	1254	TYR
2	C	78	GLU
2	C	412	GLY
2	C	837	ARG
2	C	1096	ASP
2	C	1214	SER
3	D	128	ASP
3	E	30	LEU
1	A	225	ASP
1	A	349	ARG
1	A	721	GLN
2	B	525	ILE
2	B	530	THR
2	B	620	VAL

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Mol	Chain	Res	Type
2	B	1191	SER
2	C	338	LEU
2	C	620	VAL
2	C	823	ALA
2	C	1254	TYR
3	E	52	LEU
3	E	128	ASP
1	A	3	ASN
1	A	801	ALA
2	B	523	MET
2	B	1063	PRO
2	C	200	VAL
2	C	1127	ASP
3	D	20	PRO
2	B	452	GLU
2	B	893	PRO
2	B	1054	HIS
2	B	1064	ASP
2	B	1228	PRO
2	C	327	PRO
2	C	533	GLN
2	C	714	PRO
2	C	1228	PRO
3	D	131	PRO
3	D	278	ASP
3	D	280	ASN
3	E	311	ALA
1	A	530	ILE
2	B	637	PRO
3	D	46	ILE
1	A	876	GLY
2	B	753	PRO
2	C	1175	ILE
3	E	20	PRO
3	E	131	PRO
2	C	834	PRO

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	1118/1121 (100%)	1062 (95%)	56 (5%)	24	59
2	B	911/1115 (82%)	857 (94%)	54 (6%)	19	55
2	C	1070/1115 (96%)	1013 (95%)	57 (5%)	22	58
3	D	352/353 (100%)	336 (96%)	16 (4%)	27	62
3	E	352/353 (100%)	335 (95%)	17 (5%)	25	60
All	All	3803/4057 (94%)	3603 (95%)	200 (5%)	22	58

All (200) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	24	GLN
1	A	38	PRO
1	A	111	VAL
1	A	117	ASN
1	A	119	LEU
1	A	155	GLN
1	A	170	ARG
1	A	175	MET
1	A	203	THR
1	A	205	GLU
1	A	223	HIS
1	A	264	PHE
1	A	269	ARG
1	A	281	GLN
1	A	290	GLN
1	A	294	GLU
1	A	295	ASP
1	A	332	SER
1	A	350	TYR
1	A	361	VAL
1	A	374	GLN
1	A	377	LEU
1	A	385	GLN
1	A	389	ASP
1	A	413	MET
1	A	417	LEU
1	A	436	SER

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Mol	Chain	Res	Type
1	A	455	GLN
1	A	514	TYR
1	A	521	HIS
1	A	583	ASP
1	A	591	SER
1	A	601	SER
1	A	648	ASN
1	A	663	SER
1	A	693	SER
1	A	733	ASN
1	A	750	ARG
1	A	755	THR
1	A	779	SER
1	A	804	HIS
1	A	833	GLU
1	A	862	ASN
1	A	928	CYS
1	A	946	ASN
1	A	957	ASP
1	A	980	THR
1	A	998	SER
1	A	1020	ARG
1	A	1091	MET
1	A	1123	ASP
1	A	1138	ILE
1	A	1141	THR
1	A	1265	THR
1	A	1268	ILE
2	B	249	HIS
2	B	251	ASP
2	B	254	ARG
2	B	256	VAL
2	B	281	LEU
2	B	302	SER
2	B	313	ASN
2	B	337	GLN
2	B	340	ASN
2	B	341	THR
2	B	353	MET
2	B	386	THR
2	B	406	MET
2	B	415	ASN

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Mol	Chain	Res	Type
2	B	444	MET
2	B	455	ASP
2	B	492	THR
2	B	502	ASN
2	B	518	GLN
2	B	524	ASN
2	B	525	ILE
2	B	592	ARG
2	B	601	ASN
2	B	673	ARG
2	B	674	ARG
2	B	686	ARG
2	B	702	LEU
2	B	739	LEU
2	B	750	VAL
2	B	767	ARG
2	B	770	GLU
2	B	772	MET
2	B	833	VAL
2	B	851	ARG
2	B	852	GLN
2	B	911	ASP
2	B	932	VAL
2	B	939	SER
2	B	942	GLN
2	B	961	THR
2	B	973	MET
2	B	985	GLU
2	B	1032	ASN
2	B	1064	ASP
2	B	1080	ASP
2	B	1081	CYS
2	B	1085	PHE
2	B	1093	MET
2	B	1163	THR
2	B	1182	VAL
2	B	1206	ASP
2	B	1230	GLU
2	B	1243	THR
2	B	1252	ASP
2	C	51	GLU
2	C	56	ARG

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Mol	Chain	Res	Type
2	C	73	MET
2	C	76	ASN
2	C	124	ASP
2	C	129	ASN
2	C	147	GLN
2	C	182	GLN
2	C	206	HIS
2	C	216	ILE
2	C	217	GLN
2	C	221	THR
2	C	229	ASN
2	C	241	ASN
2	C	252	THR
2	C	254	ARG
2	C	302	SER
2	C	338	LEU
2	C	409	THR
2	C	410	ARG
2	C	411	MET
2	C	429	ASN
2	C	455	ASP
2	C	473	ASN
2	C	518	GLN
2	C	528	ASN
2	C	601	ASN
2	C	615	LYS
2	C	665	ASP
2	C	680	THR
2	C	689	MET
2	C	751	THR
2	C	763	ASN
2	C	765	ARG
2	C	772	MET
2	C	777	ASP
2	C	782	GLN
2	C	785	TRP
2	C	787	GLN
2	C	792	SER
2	C	863	SER
2	C	887	LEU
2	C	903	ASP
2	C	1002	GLN

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Mol	Chain	Res	Type
2	C	1019	VAL
2	C	1027	THR
2	C	1032	ASN
2	C	1064	ASP
2	C	1158	ASN
2	C	1175	ILE
2	C	1206	ASP
2	C	1230	GLU
2	C	1231	ARG
2	C	1248	PRO
2	C	1252	ASP
2	C	1255	ASN
2	C	1268	THR
3	D	10	THR
3	D	34	ASN
3	D	50	ARG
3	D	92	LEU
3	D	100	THR
3	D	101	LEU
3	D	174	ASP
3	D	206	ASP
3	D	213	THR
3	D	255	CYS
3	D	258	ASN
3	D	333	ARG
3	D	346	ASP
3	D	391	MET
3	D	394	THR
3	D	398	THR
3	E	7	LEU
3	E	22	ASN
3	E	41	GLN
3	E	44	ASP
3	E	48	LEU
3	E	50	ARG
3	E	105	VAL
3	E	138	ARG
3	E	169	ASP
3	E	176	ASN
3	E	204	GLU
3	E	325	ASN
3	E	333	ARG

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Mol	Chain	Res	Type
3	E	346	ASP
3	E	386	ASN
3	E	391	MET
3	E	394	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (120) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	24	GLN
1	A	37	ASN
1	A	49	GLN
1	A	58	GLN
1	A	71	GLN
1	A	117	ASN
1	A	139	ASN
1	A	155	GLN
1	A	263	GLN
1	A	267	ASN
1	A	281	GLN
1	A	290	GLN
1	A	333	GLN
1	A	352	GLN
1	A	374	GLN
1	A	385	GLN
1	A	466	GLN
1	A	510	GLN
1	A	526	GLN
1	A	625	HIS
1	A	648	ASN
1	A	713	ASN
1	A	733	ASN
1	A	812	ASN
1	A	862	ASN
1	A	1079	GLN
1	A	1110	ASN
1	A	1251	ASN
1	A	1253	GLN
2	B	246	GLN
2	B	278	GLN
2	B	293	GLN
2	B	313	ASN

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Mol	Chain	Res	Type
2	B	415	ASN
2	B	421	ASN
2	B	475	ASN
2	B	502	ASN
2	B	524	ASN
2	B	527	ASN
2	B	537	GLN
2	B	601	ASN
2	B	654	ASN
2	B	692	GLN
2	B	710	HIS
2	B	745	HIS
2	B	746	GLN
2	B	774	ASN
2	B	778	ASN
2	B	782	GLN
2	B	996	GLN
2	B	1032	ASN
2	B	1036	ASN
2	B	1051	GLN
2	B	1116	GLN
2	B	1149	HIS
2	B	1188	HIS
2	B	1213	ASN
2	C	76	ASN
2	C	93	ASN
2	C	129	ASN
2	C	138	ASN
2	C	147	GLN
2	C	199	HIS
2	C	229	ASN
2	C	337	GLN
2	C	375	HIS
2	C	390	ASN
2	C	429	ASN
2	C	438	GLN
2	C	473	ASN
2	C	518	GLN
2	C	524	ASN
2	C	528	ASN
2	C	585	ASN
2	C	601	ASN

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Mol	Chain	Res	Type
2	C	625	ASN
2	C	654	ASN
2	C	671	GLN
2	C	682	HIS
2	C	704	GLN
2	C	710	HIS
2	C	763	ASN
2	C	774	ASN
2	C	782	GLN
2	C	1000	GLN
2	C	1002	GLN
2	C	1025	GLN
2	C	1032	ASN
2	C	1116	GLN
2	C	1125	GLN
2	C	1149	HIS
2	C	1158	ASN
2	C	1213	ASN
3	D	17	GLN
3	D	18	ASN
3	D	114	GLN
3	D	181	ASN
3	D	214	GLN
3	D	229	HIS
3	D	231	GLN
3	D	258	ASN
3	D	331	GLN
3	D	353	GLN
3	D	383	ASN
3	E	22	ASN
3	E	41	GLN
3	E	110	GLN
3	E	141	HIS
3	E	154	ASN
3	E	176	ASN
3	E	181	ASN
3	E	185	HIS
3	E	200	ASN
3	E	229	HIS
3	E	242	ASN
3	E	325	ASN
3	E	365	GLN

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Mol	Chain	Res	Type
3	E	383	ASN
3	E	386	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 1 ligands modelled in this entry, 1 is 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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.