Full wwPDB X-ray Structure Validation Report ⓘ

Oct 23, 2021 – 01:49 PM EDT

PDB ID	:	1KCT
Title	:	ALPHA1-ANTITRYPSIN
Authors	:	Song, H.K.; Suh, S.W.
Deposited on	:	1996-08-06
Resolution	:	3.46 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 following versions of software and data (see references ⓘ) were used in the production of this report:

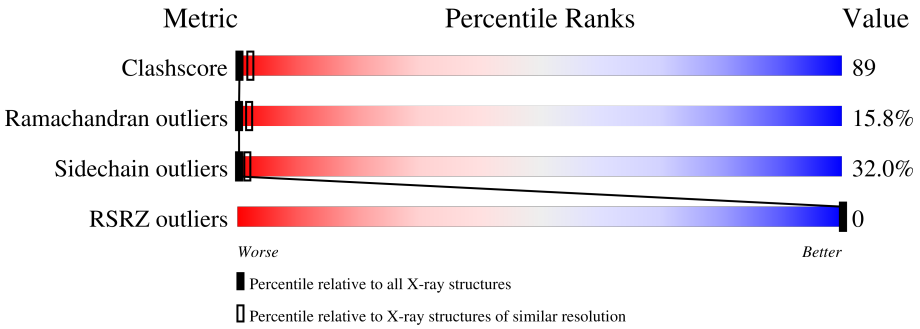
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 3.46 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	1372 (3.52-3.40)
Ramachandran outliers	138981	1337 (3.52-3.40)
Sidechain outliers	138945	1338 (3.52-3.40)
RSRZ outliers	127900	1205 (3.52-3.40)

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% 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	394	13% 48% 30% • 5%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2965 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 ALPHA1-ANTITRYPSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	375	2965	1910	484	561	10	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

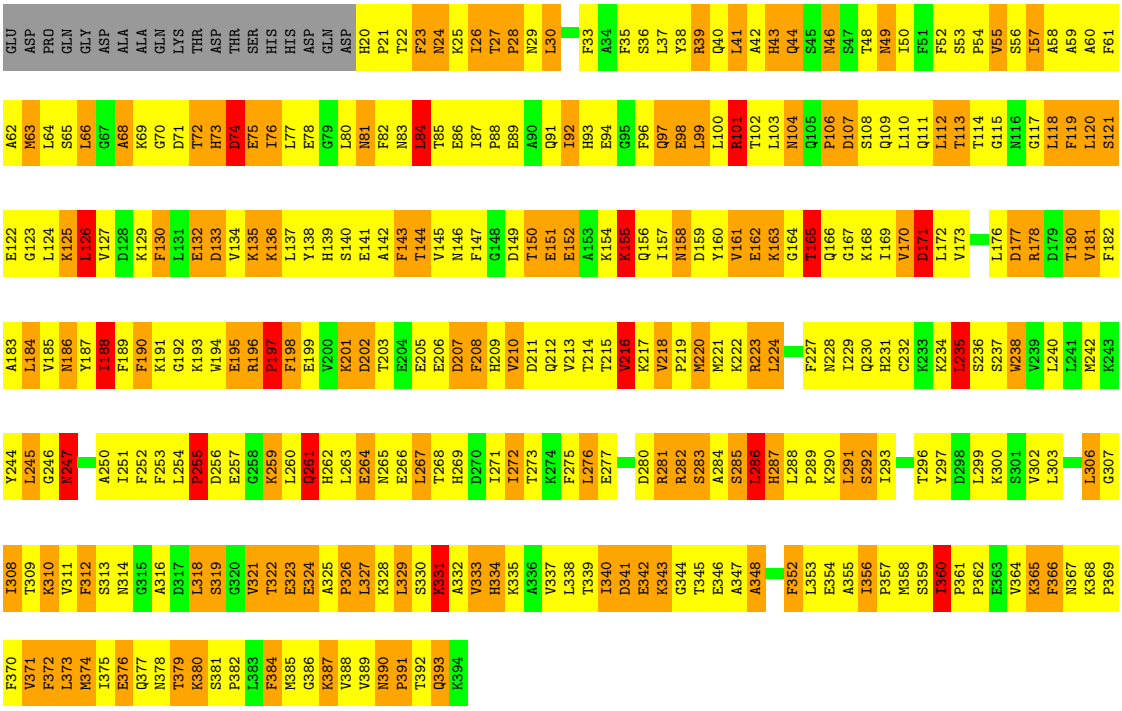
Chain	Residue	Modelled	Actual	Comment	Reference
A	59	ALA	THR	engineered mutation	UNP P01009
A	68	ALA	THR	engineered mutation	UNP P01009
A	70	GLY	ALA	engineered mutation	UNP P01009

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 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: ALPHA1-ANTITRYPSIN

Chain A: 13% 48% 30% • 5%



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	114.87Å 39.98Å 92.42Å 90.00° 102.82° 90.00°	Depositor
Resolution (Å)	8.00 – 3.46 33.86 – 3.46	Depositor EDS
% Data completeness (in resolution range)	81.2 (8.00-3.46) 81.2 (33.86-3.46)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.61 (at 3.47Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.184 , (Not available) 0.175 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	29.0	Xtriage
Anisotropy	0.436	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 377.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.32$, $< L^2 > = 0.15$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.80	EDS
Total number of atoms	2965	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.18% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

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	0.69	0/3027	1.07	11/4092 (0.3%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	360	ILE	N-CA-C	-8.26	88.69	111.00
1	A	126	LEU	CA-CB-CG	8.09	133.91	115.30
1	A	286	LEU	CA-CB-CG	6.18	129.51	115.30
1	A	74	ASP	N-CA-C	-5.65	95.74	111.00
1	A	197	PRO	N-CA-C	5.53	126.47	112.10
1	A	66	LEU	CA-CB-CG	5.52	128.00	115.30
1	A	98	GLU	N-CA-C	-5.44	96.32	111.00
1	A	235	LEU	CA-CB-CG	5.32	127.53	115.30
1	A	208	PHE	N-CA-C	-5.17	97.05	111.00
1	A	247	ASN	N-CA-C	5.09	124.75	111.00
1	A	216	VAL	N-CA-C	5.03	124.58	111.00

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	2965	0	2974	531	0
All	All	2965	0	2974	531	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 89.

All (531) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:PRO:HB3	1:A:344:GLY:HA3	1.20	1.12
1:A:244:TYR:HE1	1:A:340:ILE:HG13	1.15	1.10
1:A:62:ALA:HB2	1:A:80:LEU:HD12	1.30	1.07
1:A:30:LEU:HD11	1:A:58:ALA:HB1	1.32	1.06
1:A:310:LYS:HA	1:A:313:SER:HB2	1.36	1.06
1:A:97:GLN:HA	1:A:100:LEU:HB2	1.31	1.06
1:A:276:LEU:HD13	1:A:375:ILE:HG21	1.39	1.02
1:A:360:ILE:HG23	1:A:362:PRO:HD2	1.42	1.01
1:A:178:ARG:HH11	1:A:178:ARG:H	1.03	1.00
1:A:352:PHE:HA	1:A:355:ALA:HB3	1.45	0.99
1:A:25:LYS:HD3	1:A:87:ILE:HD11	1.47	0.97
1:A:282:ARG:HG3	1:A:283:SER:H	1.30	0.96
1:A:114:THR:HA	1:A:187:TYR:O	1.68	0.94
1:A:168:LYS:HB3	1:A:337:VAL:HG11	1.52	0.92
1:A:348:ALA:HA	1:A:352:PHE:HD2	1.36	0.90
1:A:127:VAL:HB	1:A:130:PHE:HB3	1.54	0.89
1:A:232:CYS:O	1:A:236:SER:HA	1.74	0.88
1:A:234:LYS:HD3	1:A:271:ILE:HG23	1.55	0.88
1:A:244:TYR:CE1	1:A:340:ILE:HG13	2.07	0.87
1:A:356:ILE:HG13	1:A:357:PRO:HD3	1.56	0.86
1:A:121:SER:HB2	1:A:181:VAL:HG13	1.56	0.85
1:A:223:ARG:HA	1:A:356:ILE:HB	1.60	0.83
1:A:216:VAL:HG12	1:A:217:LYS:H	1.44	0.83
1:A:284:ALA:HB2	1:A:360:ILE:HG22	1.59	0.82
1:A:84:LEU:HD12	1:A:84:LEU:H	1.45	0.82
1:A:178:ARG:HD3	1:A:178:ARG:N	1.94	0.82
1:A:234:LYS:HD3	1:A:271:ILE:HD12	1.61	0.81
1:A:224:LEU:HB3	1:A:355:ALA:O	1.80	0.81
1:A:230:GLN:OE1	1:A:232:CYS:HB2	1.80	0.81
1:A:154:LYS:NZ	1:A:173:VAL:HG12	1.97	0.80
1:A:224:LEU:HB2	1:A:356:ILE:C	2.02	0.80
1:A:286:LEU:HA	1:A:364:VAL:HB	1.61	0.80
1:A:273:THR:HA	1:A:276:LEU:HD23	1.64	0.80
1:A:245:LEU:HD12	1:A:245:LEU:H	1.47	0.79
1:A:240:LEU:HB3	1:A:252:PHE:HB2	1.62	0.79
1:A:119:PHE:HE1	1:A:145:VAL:HG11	1.48	0.79
1:A:169:ILE:HA	1:A:335:LYS:HD2	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:ASP:HB3	1:A:222:LYS:HB2	1.65	0.78
1:A:291:LEU:HB2	1:A:340:ILE:O	1.83	0.78
1:A:97:GLN:HG3	1:A:137:LEU:O	1.83	0.78
1:A:158:ASN:HA	1:A:161:VAL:HG23	1.65	0.78
1:A:268:THR:HG22	1:A:269:HIS:H	1.49	0.77
1:A:68:ALA:HB1	1:A:72:THR:HG21	1.67	0.77
1:A:162:GLU:HG2	1:A:170:VAL:HG12	1.64	0.77
1:A:161:VAL:HG12	1:A:169:ILE:HB	1.67	0.77
1:A:291:LEU:HD22	1:A:340:ILE:HG22	1.66	0.77
1:A:115:GLY:O	1:A:186:ASN:HA	1.85	0.77
1:A:127:VAL:HG12	1:A:130:PHE:H	1.48	0.76
1:A:224:LEU:HB2	1:A:356:ILE:O	1.85	0.76
1:A:161:VAL:HG13	1:A:187:TYR:HB3	1.68	0.76
1:A:197:PRO:CB	1:A:344:GLY:HA3	2.11	0.76
1:A:169:ILE:HG12	1:A:335:LYS:HB3	1.67	0.76
1:A:291:LEU:HD13	1:A:341:ASP:HA	1.67	0.75
1:A:118:LEU:HD12	1:A:142:ALA:HA	1.67	0.75
1:A:76:ILE:O	1:A:80:LEU:HG	1.86	0.74
1:A:193:LYS:HG2	1:A:194:TRP:H	1.52	0.74
1:A:276:LEU:HD21	1:A:380:LYS:HD3	1.68	0.74
1:A:49:ASN:HD21	1:A:388:VAL:HA	1.52	0.74
1:A:119:PHE:CE1	1:A:145:VAL:HG11	2.22	0.74
1:A:113:THR:OG1	1:A:189:PHE:HB3	1.88	0.73
1:A:242:MET:HG3	1:A:252:PHE:HE2	1.52	0.73
1:A:119:PHE:HA	1:A:143:PHE:CE1	2.22	0.73
1:A:287:HIS:HB2	1:A:365:LYS:HA	1.70	0.73
1:A:302:VAL:O	1:A:306:LEU:HD23	1.88	0.73
1:A:125:LYS:HE3	1:A:324:GLU:HG2	1.71	0.72
1:A:199:GLU:HB3	1:A:201:LYS:HD2	1.70	0.72
1:A:358:MET:HG2	1:A:358:MET:O	1.87	0.72
1:A:182:PHE:HD2	1:A:329:LEU:HD13	1.54	0.72
1:A:365:LYS:HD3	1:A:367:ASN:HD22	1.54	0.72
1:A:247:ASN:O	1:A:377:GLN:HB2	1.89	0.72
1:A:24:ASN:O	1:A:28:PRO:HD3	1.90	0.72
1:A:322:THR:HG23	1:A:323:GLU:N	2.05	0.71
1:A:154:LYS:C	1:A:156:GLN:H	1.92	0.71
1:A:254:LEU:HD13	1:A:366:PHE:CD1	2.26	0.71
1:A:238:TRP:HB2	1:A:254:LEU:HB3	1.72	0.70
1:A:260:LEU:CD1	1:A:261:GLN:HE22	2.05	0.70
1:A:224:LEU:H	1:A:356:ILE:HG22	1.57	0.70
1:A:154:LYS:HZ1	1:A:173:VAL:HG12	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:SER:HB2	1:A:181:VAL:CG1	2.23	0.69
1:A:165:THR:HG23	1:A:188:ILE:H	1.58	0.69
1:A:267:LEU:CD2	1:A:272:ILE:HD11	2.23	0.69
1:A:190:PHE:HD2	1:A:339:THR:H	1.39	0.69
1:A:210:VAL:HG21	1:A:390:ASN:HB2	1.73	0.69
1:A:371:VAL:HA	1:A:387:LYS:HA	1.75	0.69
1:A:183:ALA:HA	1:A:330:SER:HB2	1.75	0.69
1:A:172:LEU:HD11	1:A:333:VAL:HB	1.73	0.69
1:A:375:ILE:HG22	1:A:376:GLU:H	1.57	0.68
1:A:39:ARG:O	1:A:43:HIS:HB2	1.94	0.68
1:A:151:GLU:HA	1:A:154:LYS:HG3	1.74	0.68
1:A:50:ILE:HG22	1:A:386:GLY:HA2	1.76	0.67
1:A:119:PHE:HA	1:A:143:PHE:HE1	1.59	0.67
1:A:299:LEU:HB3	1:A:303:LEU:HD12	1.74	0.67
1:A:172:LEU:HD23	1:A:173:VAL:HG23	1.75	0.67
1:A:322:THR:HG23	1:A:323:GLU:H	1.60	0.67
1:A:194:TRP:HB2	1:A:197:PRO:HA	1.77	0.67
1:A:224:LEU:HD22	1:A:285:SER:HA	1.77	0.67
1:A:65:SER:OG	1:A:77:LEU:HD22	1.94	0.67
1:A:282:ARG:HG3	1:A:283:SER:N	2.07	0.67
1:A:299:LEU:HD22	1:A:332:ALA:CB	2.25	0.66
1:A:254:LEU:HD12	1:A:370:PHE:HB3	1.77	0.66
1:A:374:MET:O	1:A:382:PRO:HA	1.94	0.66
1:A:135:LYS:O	1:A:139:HIS:HA	1.95	0.66
1:A:121:SER:CB	1:A:181:VAL:HG13	2.25	0.66
1:A:276:LEU:HD11	1:A:380:LYS:HG2	1.77	0.66
1:A:221:MET:HE3	1:A:288:LEU:HG	1.75	0.66
1:A:235:LEU:CD2	1:A:235:LEU:H	2.09	0.66
1:A:224:LEU:N	1:A:356:ILE:HA	2.11	0.66
1:A:282:ARG:CG	1:A:283:SER:H	2.07	0.66
1:A:77:LEU:HD11	1:A:89:GLU:HG3	1.76	0.65
1:A:120:LEU:HA	1:A:181:VAL:O	1.96	0.65
1:A:260:LEU:HD13	1:A:261:GLN:HE22	1.60	0.65
1:A:375:ILE:HG22	1:A:376:GLU:N	2.10	0.65
1:A:318:LEU:O	1:A:321:VAL:HG12	1.97	0.65
1:A:76:ILE:HD11	1:A:311:VAL:HG11	1.78	0.65
1:A:154:LYS:HA	1:A:157:ILE:HG22	1.79	0.65
1:A:299:LEU:HD22	1:A:332:ALA:HB3	1.77	0.65
1:A:49:ASN:ND2	1:A:389:VAL:H	1.95	0.65
1:A:157:ILE:HG23	1:A:158:ASN:H	1.61	0.65
1:A:267:LEU:HD21	1:A:272:ILE:HD11	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:TYR:HB2	1:A:334:HIS:CD2	2.32	0.64
1:A:73:HIS:HB2	1:A:77:LEU:HD23	1.78	0.64
1:A:111:GLN:OE1	1:A:191:LYS:HG3	1.98	0.64
1:A:119:PHE:CD2	1:A:143:PHE:HZ	2.16	0.64
1:A:390:ASN:HD22	1:A:392:THR:H	1.43	0.64
1:A:234:LYS:CD	1:A:271:ILE:HG23	2.27	0.64
1:A:100:LEU:HD13	1:A:137:LEU:O	1.98	0.63
1:A:160:TYR:HA	1:A:163:LYS:HB3	1.79	0.63
1:A:206:GLU:O	1:A:218:VAL:HG12	1.99	0.63
1:A:73:HIS:HA	1:A:76:ILE:HB	1.78	0.63
1:A:127:VAL:HG12	1:A:129:LYS:H	1.62	0.63
1:A:178:ARG:H	1:A:178:ARG:NH1	1.87	0.63
1:A:223:ARG:HD3	1:A:227:PHE:HZ	1.64	0.63
1:A:260:LEU:HB2	1:A:261:GLN:NE2	2.12	0.63
1:A:122:GLU:HA	1:A:144:THR:HG22	1.81	0.63
1:A:33:PHE:O	1:A:36:SER:HB2	1.97	0.63
1:A:41:LEU:C	1:A:43:HIS:H	2.00	0.63
1:A:255:PRO:HD2	1:A:370:PHE:HA	1.82	0.62
1:A:218:VAL:HG21	1:A:289:PRO:HB3	1.81	0.62
1:A:365:LYS:HD3	1:A:367:ASN:ND2	2.15	0.62
1:A:193:LYS:HE3	1:A:245:LEU:HD23	1.82	0.62
1:A:261:GLN:NE2	1:A:261:GLN:H	1.98	0.62
1:A:354:GLU:C	1:A:356:ILE:H	2.02	0.62
1:A:205:GLU:HA	1:A:219:PRO:HA	1.82	0.62
1:A:296:THR:HA	1:A:335:LYS:HA	1.82	0.61
1:A:161:VAL:CG1	1:A:169:ILE:HB	2.29	0.61
1:A:72:THR:C	1:A:74:ASP:H	2.03	0.61
1:A:135:LYS:HG2	1:A:139:HIS:O	1.99	0.61
1:A:115:GLY:HA3	1:A:187:TYR:CZ	2.35	0.61
1:A:224:LEU:HB2	1:A:356:ILE:CA	2.31	0.61
1:A:26:ILE:HA	1:A:82:PHE:HE1	1.66	0.61
1:A:285:SER:HB2	1:A:359:SER:OG	2.01	0.61
1:A:73:HIS:HB2	1:A:77:LEU:CD2	2.30	0.60
1:A:118:LEU:HD11	1:A:120:LEU:HD23	1.82	0.60
1:A:314:ASN:HA	1:A:328:LYS:NZ	2.15	0.60
1:A:348:ALA:HA	1:A:352:PHE:CD2	2.27	0.60
1:A:281:ARG:HE	1:A:281:ARG:HA	1.65	0.60
1:A:232:CYS:SG	1:A:234:LYS:CB	2.89	0.60
1:A:109:GLN:HG3	1:A:245:LEU:O	2.01	0.60
1:A:319:SER:HA	1:A:322:THR:HG22	1.82	0.60
1:A:84:LEU:H	1:A:84:LEU:CD1	2.14	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:GLU:HG2	1:A:244:TYR:O	2.02	0.59
1:A:49:ASN:H	1:A:393:GLN:NE2	1.99	0.59
1:A:127:VAL:CG1	1:A:130:PHE:H	2.14	0.59
1:A:356:ILE:CG1	1:A:357:PRO:HD3	2.31	0.59
1:A:199:GLU:HA	1:A:201:LYS:HZ1	1.68	0.59
1:A:224:LEU:HG	1:A:358:MET:HB3	1.84	0.59
1:A:291:LEU:N	1:A:291:LEU:HD12	2.18	0.59
1:A:359:SER:HB3	1:A:362:PRO:O	2.03	0.59
1:A:109:GLN:O	1:A:111:GLN:HG3	2.03	0.58
1:A:91:GLN:O	1:A:92:ILE:HG13	2.03	0.58
1:A:190:PHE:HD2	1:A:339:THR:N	2.00	0.58
1:A:234:LYS:HB3	1:A:235:LEU:HD22	1.85	0.58
1:A:244:TYR:CE2	1:A:250:ALA:HB2	2.38	0.58
1:A:66:LEU:HD23	1:A:134:VAL:HG12	1.85	0.58
1:A:172:LEU:HD21	1:A:333:VAL:HG21	1.85	0.58
1:A:247:ASN:ND2	1:A:377:GLN:HB3	2.18	0.58
1:A:360:ILE:CG2	1:A:362:PRO:HD2	2.24	0.58
1:A:296:THR:OG1	1:A:335:LYS:HG3	2.04	0.58
1:A:287:HIS:ND1	1:A:365:LYS:HG3	2.19	0.58
1:A:308:ILE:HG22	1:A:311:VAL:HB	1.86	0.58
1:A:136:LYS:HG3	1:A:137:LEU:H	1.68	0.58
1:A:37:LEU:N	1:A:37:LEU:HD12	2.18	0.58
1:A:208:PHE:HE1	1:A:368:LYS:C	2.06	0.58
1:A:376:GLU:OE1	1:A:378:ASN:HB2	2.03	0.58
1:A:169:ILE:HD12	1:A:187:TYR:HA	1.85	0.57
1:A:211:ASP:HB3	1:A:213:VAL:HG12	1.84	0.57
1:A:390:ASN:ND2	1:A:392:THR:H	2.02	0.57
1:A:100:LEU:C	1:A:104:ASN:HB3	2.23	0.57
1:A:235:LEU:HB2	1:A:263:LEU:HG	1.86	0.57
1:A:33:PHE:CD2	1:A:58:ALA:HB2	2.40	0.57
1:A:89:GLU:O	1:A:92:ILE:HB	2.04	0.57
1:A:117:GLY:HA3	1:A:185:VAL:CG1	2.33	0.57
1:A:178:ARG:HH11	1:A:178:ARG:N	1.87	0.57
1:A:218:VAL:HG11	1:A:289:PRO:HG3	1.87	0.57
1:A:229:ILE:HG12	1:A:238:TRP:CE3	2.40	0.57
1:A:96:PHE:HD2	1:A:138:TYR:HE2	1.51	0.57
1:A:126:LEU:HD23	1:A:127:VAL:O	2.03	0.57
1:A:28:PRO:HD2	1:A:29:ASN:H	1.70	0.57
1:A:155:LYS:HE2	1:A:155:LYS:O	2.04	0.57
1:A:372:PHE:O	1:A:373:LEU:HB2	2.04	0.56
1:A:75:GLU:N	1:A:78:GLU:HB3	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:LEU:H	1:A:356:ILE:HA	1.69	0.56
1:A:63:MET:O	1:A:66:LEU:HD23	2.05	0.56
1:A:154:LYS:HZ3	1:A:173:VAL:HG12	1.69	0.56
1:A:192:GLY:HA2	1:A:245:LEU:HD11	1.86	0.56
1:A:169:ILE:HG23	1:A:335:LYS:HE2	1.87	0.56
1:A:127:VAL:HG12	1:A:129:LYS:N	2.21	0.56
1:A:165:THR:OG1	1:A:187:TYR:HB2	2.06	0.56
1:A:38:TYR:CE1	1:A:50:ILE:HD12	2.40	0.56
1:A:49:ASN:HB2	1:A:393:GLN:CD	2.27	0.55
1:A:262:HIS:O	1:A:266:GLU:HB2	2.05	0.55
1:A:376:GLU:HB2	1:A:381:SER:HB3	1.87	0.55
1:A:237:SER:OG	1:A:255:PRO:HA	2.06	0.55
1:A:26:ILE:HD13	1:A:96:PHE:CE1	2.41	0.55
1:A:96:PHE:CD2	1:A:138:TYR:HE2	2.25	0.55
1:A:276:LEU:CD1	1:A:375:ILE:HG21	2.26	0.55
1:A:193:LYS:HG2	1:A:194:TRP:N	2.21	0.55
1:A:338:LEU:HD13	1:A:338:LEU:C	2.26	0.55
1:A:375:ILE:CG2	1:A:376:GLU:H	2.20	0.55
1:A:40:GLN:HG2	1:A:306:LEU:HD21	1.89	0.55
1:A:33:PHE:CE2	1:A:58:ALA:HB2	2.41	0.54
1:A:299:LEU:HB3	1:A:303:LEU:CD1	2.37	0.54
1:A:371:VAL:O	1:A:372:PHE:HB3	2.07	0.54
1:A:26:ILE:HD13	1:A:96:PHE:HE1	1.72	0.54
1:A:259:LYS:N	1:A:259:LYS:HD2	2.20	0.54
1:A:268:THR:H	1:A:271:ILE:CG1	2.20	0.54
1:A:193:LYS:HB3	1:A:245:LEU:CD2	2.37	0.54
1:A:339:THR:O	1:A:339:THR:HG22	2.08	0.54
1:A:126:LEU:HA	1:A:321:VAL:O	2.07	0.54
1:A:56:SER:HA	1:A:186:ASN:OD1	2.08	0.54
1:A:107:ASP:HB2	1:A:111:GLN:HA	1.89	0.53
1:A:235:LEU:HD12	1:A:253:PHE:HE2	1.73	0.53
1:A:261:GLN:C	1:A:263:LEU:H	2.12	0.53
1:A:296:THR:HG1	1:A:335:LYS:HZ3	1.55	0.53
1:A:232:CYS:SG	1:A:234:LYS:HB2	2.48	0.53
1:A:75:GLU:O	1:A:308:ILE:HG12	2.08	0.53
1:A:208:PHE:HB3	1:A:218:VAL:HB	1.90	0.53
1:A:221:MET:CE	1:A:290:LYS:HD3	2.38	0.53
1:A:263:LEU:O	1:A:265:ASN:N	2.42	0.53
1:A:208:PHE:HA	1:A:367:ASN:HA	1.90	0.53
1:A:224:LEU:CD2	1:A:285:SER:HA	2.38	0.53
1:A:203:THR:HA	1:A:221:MET:HA	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:GLN:HG2	1:A:231:HIS:H	1.74	0.53
1:A:330:SER:O	1:A:331:LYS:HB2	2.09	0.53
1:A:109:GLN:HB3	1:A:245:LEU:HD22	1.91	0.52
1:A:193:LYS:NZ	1:A:344:GLY:HA2	2.24	0.52
1:A:210:VAL:HG12	1:A:211:ASP:H	1.73	0.52
1:A:157:ILE:HG23	1:A:158:ASN:N	2.23	0.52
1:A:193:LYS:HG3	1:A:343:LYS:CB	2.39	0.52
1:A:193:LYS:HG3	1:A:343:LYS:HB2	1.90	0.52
1:A:49:ASN:H	1:A:393:GLN:HE22	1.57	0.52
1:A:322:THR:CG2	1:A:323:GLU:H	2.21	0.52
1:A:104:ASN:OD1	1:A:139:HIS:HE1	1.91	0.52
1:A:198:PHE:CE2	1:A:221:MET:HB3	2.44	0.52
1:A:359:SER:C	1:A:360:ILE:O	2.48	0.52
1:A:96:PHE:C	1:A:98:GLU:H	2.13	0.52
1:A:190:PHE:CD1	1:A:191:LYS:N	2.78	0.52
1:A:232:CYS:SG	1:A:234:LYS:HB3	2.48	0.52
1:A:310:LYS:CA	1:A:313:SER:HB2	2.26	0.52
1:A:314:ASN:HA	1:A:328:LYS:HZ2	1.73	0.52
1:A:88:PRO:HB2	1:A:91:GLN:HB3	1.92	0.52
1:A:224:LEU:HB2	1:A:356:ILE:HA	1.92	0.52
1:A:209:HIS:ND1	1:A:215:THR:HB	2.25	0.51
1:A:197:PRO:HG3	1:A:345:THR:N	2.25	0.51
1:A:206:GLU:HG2	1:A:207:ASP:H	1.74	0.51
1:A:373:LEU:HA	1:A:384:PHE:O	2.10	0.51
1:A:157:ILE:O	1:A:161:VAL:HG23	2.09	0.51
1:A:178:ARG:H	1:A:178:ARG:HD3	1.71	0.51
1:A:220:MET:HA	1:A:289:PRO:HA	1.92	0.51
1:A:287:HIS:CB	1:A:365:LYS:HA	2.40	0.51
1:A:261:GLN:O	1:A:262:HIS:HB3	2.10	0.51
1:A:64:LEU:O	1:A:76:ILE:HG21	2.10	0.51
1:A:111:GLN:O	1:A:112:LEU:HB2	2.09	0.51
1:A:195:GLU:O	1:A:197:PRO:HD3	2.10	0.51
1:A:154:LYS:C	1:A:156:GLN:N	2.62	0.51
1:A:232:CYS:HB3	1:A:235:LEU:CD2	2.40	0.51
1:A:152:GLU:HA	1:A:155:LYS:CB	2.41	0.51
1:A:190:PHE:CG	1:A:191:LYS:N	2.78	0.51
1:A:211:ASP:CG	1:A:212:GLN:H	2.14	0.51
1:A:224:LEU:CB	1:A:356:ILE:HA	2.41	0.51
1:A:61:PHE:CD2	1:A:299:LEU:HD23	2.46	0.51
1:A:150:THR:HG21	1:A:177:ASP:O	2.11	0.51
1:A:30:LEU:CD1	1:A:58:ALA:HB1	2.22	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:LEU:O	1:A:264:GLU:HB2	2.11	0.50
1:A:370:PHE:CD1	1:A:370:PHE:N	2.79	0.50
1:A:132:GLU:O	1:A:136:LYS:HE2	2.09	0.50
1:A:273:THR:O	1:A:277:GLU:HB2	2.11	0.50
1:A:23:PHE:HD1	1:A:24:ASN:HD22	1.58	0.50
1:A:35:PHE:O	1:A:39:ARG:HG2	2.11	0.50
1:A:197:PRO:HG3	1:A:345:THR:H	1.75	0.50
1:A:217:LYS:NZ	1:A:217:LYS:HB3	2.26	0.50
1:A:100:LEU:CD1	1:A:138:TYR:HA	2.42	0.50
1:A:109:GLN:HB2	1:A:246:GLY:HA3	1.94	0.50
1:A:221:MET:O	1:A:222:LYS:HG3	2.12	0.50
1:A:322:THR:CG2	1:A:323:GLU:N	2.72	0.50
1:A:198:PHE:HE2	1:A:221:MET:HB3	1.76	0.50
1:A:201:LYS:HD2	1:A:201:LYS:H	1.77	0.50
1:A:373:LEU:HD22	1:A:374:MET:H	1.77	0.50
1:A:284:ALA:HA	1:A:360:ILE:H	1.77	0.49
1:A:61:PHE:HD2	1:A:299:LEU:HD23	1.77	0.49
1:A:194:TRP:HD1	1:A:343:LYS:O	1.95	0.49
1:A:194:TRP:HE1	1:A:342:GLU:HA	1.76	0.49
1:A:208:PHE:O	1:A:216:VAL:HB	2.13	0.49
1:A:30:LEU:O	1:A:33:PHE:HB3	2.13	0.49
1:A:110:LEU:HG	1:A:112:LEU:HD12	1.93	0.49
1:A:181:VAL:HB	1:A:327:LEU:HD21	1.93	0.49
1:A:23:PHE:O	1:A:27:THR:HB	2.13	0.49
1:A:113:THR:O	1:A:187:TYR:CD2	2.65	0.49
1:A:197:PRO:HD2	1:A:346:GLU:HB2	1.95	0.49
1:A:69:LYS:HG2	1:A:70:GLY:N	2.27	0.49
1:A:291:LEU:C	1:A:338:LEU:HD12	2.33	0.48
1:A:154:LYS:NZ	1:A:154:LYS:HB3	2.28	0.48
1:A:193:LYS:NZ	1:A:194:TRP:O	2.46	0.48
1:A:345:THR:C	1:A:347:ALA:H	2.14	0.48
1:A:119:PHE:HB3	1:A:183:ALA:HB3	1.95	0.48
1:A:210:VAL:HG12	1:A:211:ASP:N	2.29	0.48
1:A:234:LYS:CD	1:A:271:ILE:HD12	2.39	0.48
1:A:235:LEU:H	1:A:235:LEU:HD23	1.79	0.48
1:A:291:LEU:HD13	1:A:341:ASP:CA	2.39	0.48
1:A:55:VAL:O	1:A:59:ALA:HB3	2.14	0.48
1:A:221:MET:CE	1:A:290:LYS:HA	2.43	0.48
1:A:165:THR:HG1	1:A:187:TYR:HB2	1.78	0.48
1:A:299:LEU:HD22	1:A:332:ALA:HB1	1.95	0.48
1:A:387:LYS:NZ	1:A:387:LYS:HB3	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:SER:HB2	1:A:334:HIS:ND1	2.28	0.48
1:A:152:GLU:HA	1:A:155:LYS:HB2	1.96	0.48
1:A:257:GLU:H	1:A:259:LYS:HD3	1.76	0.48
1:A:273:THR:HG23	1:A:380:LYS:NZ	2.29	0.48
1:A:161:VAL:HG12	1:A:165:THR:HG1	1.78	0.48
1:A:53:SER:C	1:A:55:VAL:H	2.16	0.48
1:A:194:TRP:CZ3	1:A:242:MET:HB3	2.48	0.48
1:A:276:LEU:HD21	1:A:380:LYS:CD	2.40	0.48
1:A:202:ASP:OD1	1:A:356:ILE:HD12	2.14	0.48
1:A:39:ARG:HA	1:A:42:ALA:HB3	1.96	0.48
1:A:300:LYS:HB2	1:A:331:LYS:HG3	1.95	0.48
1:A:122:GLU:HG3	1:A:123:GLY:N	2.29	0.47
1:A:322:THR:O	1:A:323:GLU:HB3	2.14	0.47
1:A:273:THR:CA	1:A:276:LEU:HD23	2.40	0.47
1:A:354:GLU:C	1:A:356:ILE:N	2.66	0.47
1:A:96:PHE:HD2	1:A:138:TYR:CE2	2.31	0.47
1:A:124:LEU:HD23	1:A:126:LEU:HB3	1.96	0.47
1:A:194:TRP:CD1	1:A:343:LYS:O	2.66	0.47
1:A:254:LEU:HD22	1:A:366:PHE:CD1	2.48	0.47
1:A:99:LEU:HA	1:A:103:LEU:HB3	1.96	0.47
1:A:371:VAL:HG23	1:A:372:PHE:N	2.30	0.47
1:A:100:LEU:HD13	1:A:138:TYR:HA	1.97	0.47
1:A:311:VAL:HG12	1:A:329:LEU:HD23	1.97	0.47
1:A:38:TYR:HE1	1:A:50:ILE:HD12	1.79	0.47
1:A:100:LEU:O	1:A:101:ARG:HG2	2.14	0.47
1:A:66:LEU:HD11	1:A:93:HIS:HD1	1.79	0.47
1:A:152:GLU:HG2	1:A:155:LYS:HB3	1.97	0.47
1:A:154:LYS:HZ3	1:A:173:VAL:CG1	2.28	0.47
1:A:224:LEU:HD23	1:A:358:MET:N	2.29	0.47
1:A:235:LEU:CD1	1:A:253:PHE:HE2	2.27	0.47
1:A:198:PHE:CD1	1:A:223:ARG:HD2	2.49	0.47
1:A:303:LEU:HA	1:A:306:LEU:HB2	1.96	0.47
1:A:58:ALA:HA	1:A:80:LEU:HD13	1.97	0.47
1:A:190:PHE:CD1	1:A:384:PHE:HZ	2.32	0.47
1:A:118:LEU:HD22	1:A:119:PHE:H	1.81	0.46
1:A:210:VAL:HG21	1:A:390:ASN:CB	2.44	0.46
1:A:217:LYS:NZ	1:A:217:LYS:CB	2.78	0.46
1:A:53:SER:OG	1:A:55:VAL:HB	2.15	0.46
1:A:224:LEU:HG	1:A:358:MET:O	2.15	0.46
1:A:41:LEU:HA	1:A:44:GLN:HG3	1.96	0.46
1:A:182:PHE:CD2	1:A:318:LEU:HD11	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:LEU:HD11	1:A:283:SER:C	2.36	0.46
1:A:373:LEU:HD21	1:A:382:PRO:HB3	1.98	0.46
1:A:238:TRP:HD1	1:A:254:LEU:HD23	1.81	0.46
1:A:206:GLU:N	1:A:218:VAL:O	2.48	0.46
1:A:238:TRP:O	1:A:253:PHE:HA	2.16	0.46
1:A:282:ARG:O	1:A:283:SER:HB3	2.14	0.46
1:A:284:ALA:HB2	1:A:360:ILE:CG2	2.40	0.46
1:A:370:PHE:H	1:A:370:PHE:HD1	1.58	0.46
1:A:292:SER:N	1:A:338:LEU:HD12	2.30	0.46
1:A:338:LEU:HD13	1:A:340:ILE:H	1.80	0.46
1:A:171:ASP:O	1:A:172:LEU:HB3	2.15	0.46
1:A:308:ILE:HG22	1:A:308:ILE:O	2.14	0.46
1:A:338:LEU:HD13	1:A:339:THR:N	2.31	0.46
1:A:375:ILE:CG2	1:A:376:GLU:N	2.76	0.46
1:A:231:HIS:HA	1:A:237:SER:O	2.16	0.46
1:A:104:ASN:ND2	1:A:104:ASN:O	2.49	0.46
1:A:300:LYS:O	1:A:300:LYS:HD3	2.16	0.46
1:A:291:LEU:HD12	1:A:291:LEU:H	1.79	0.45
1:A:387:LYS:NZ	1:A:389:VAL:CG2	2.79	0.45
1:A:136:LYS:HG3	1:A:137:LEU:N	2.31	0.45
1:A:291:LEU:HD22	1:A:340:ILE:CG2	2.41	0.45
1:A:229:ILE:HG12	1:A:238:TRP:CZ3	2.51	0.45
1:A:20:HIS:O	1:A:22:THR:N	2.48	0.45
1:A:83:ASN:O	1:A:86:GLU:N	2.45	0.45
1:A:221:MET:HE1	1:A:290:LYS:HD3	1.97	0.45
1:A:26:ILE:CD1	1:A:30:LEU:HD22	2.47	0.45
1:A:117:GLY:O	1:A:118:LEU:HB3	2.16	0.45
1:A:252:PHE:O	1:A:253:PHE:HB2	2.17	0.45
1:A:338:LEU:HD22	1:A:339:THR:H	1.81	0.45
1:A:353:LEU:HA	1:A:356:ILE:HD11	1.97	0.45
1:A:125:LYS:HG2	1:A:324:GLU:CG	2.46	0.45
1:A:194:TRP:HE1	1:A:342:GLU:CA	2.29	0.45
1:A:373:LEU:HD13	1:A:374:MET:N	2.32	0.45
1:A:150:THR:HG21	1:A:177:ASP:C	2.37	0.45
1:A:235:LEU:H	1:A:235:LEU:HD22	1.81	0.45
1:A:68:ALA:HB1	1:A:72:THR:CG2	2.44	0.45
1:A:119:PHE:CE2	1:A:143:PHE:HZ	2.35	0.45
1:A:198:PHE:HB3	1:A:342:GLU:O	2.16	0.45
1:A:296:THR:HG23	1:A:335:LYS:HB2	1.99	0.45
1:A:158:ASN:HA	1:A:161:VAL:CG2	2.41	0.45
1:A:53:SER:O	1:A:57:ILE:HG12	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:ASN:HB3	1:A:86:GLU:HB2	1.98	0.44
1:A:117:GLY:HA3	1:A:185:VAL:HG12	1.99	0.44
1:A:122:GLU:HA	1:A:144:THR:CG2	2.45	0.44
1:A:145:VAL:HG13	1:A:147:PHE:CE1	2.52	0.44
1:A:194:TRP:CZ2	1:A:340:ILE:HD12	2.52	0.44
1:A:268:THR:H	1:A:271:ILE:HG12	1.82	0.44
1:A:53:SER:C	1:A:55:VAL:N	2.70	0.44
1:A:126:LEU:HA	1:A:322:THR:HA	1.99	0.44
1:A:273:THR:HA	1:A:276:LEU:CD2	2.41	0.44
1:A:325:ALA:HA	1:A:326:PRO:HD2	1.76	0.44
1:A:61:PHE:CZ	1:A:312:PHE:CE2	3.05	0.44
1:A:141:GLU:CD	1:A:141:GLU:H	2.21	0.44
1:A:64:LEU:HD21	1:A:182:PHE:HE2	1.82	0.44
1:A:224:LEU:HG	1:A:358:MET:C	2.38	0.44
1:A:41:LEU:C	1:A:43:HIS:N	2.70	0.44
1:A:387:LYS:HZ1	1:A:389:VAL:CG2	2.31	0.44
1:A:390:ASN:ND2	1:A:390:ASN:C	2.71	0.44
1:A:52:PHE:CE2	1:A:54:PRO:HG3	2.53	0.44
1:A:87:ILE:HA	1:A:88:PRO:HD3	1.77	0.44
1:A:165:THR:C	1:A:167:GLY:N	2.71	0.44
1:A:184:LEU:O	1:A:185:VAL:HG23	2.17	0.44
1:A:61:PHE:O	1:A:76:ILE:HG23	2.18	0.43
1:A:160:TYR:HD1	1:A:163:LYS:HB3	1.83	0.43
1:A:218:VAL:CG2	1:A:289:PRO:HB3	2.46	0.43
1:A:235:LEU:HD11	1:A:275:PHE:HE2	1.83	0.43
1:A:340:ILE:HD13	1:A:341:ASP:H	1.83	0.43
1:A:169:ILE:CG1	1:A:335:LYS:HB3	2.42	0.43
1:A:209:HIS:O	1:A:369:PRO:HD3	2.18	0.43
1:A:211:ASP:CG	1:A:212:GLN:N	2.72	0.43
1:A:285:SER:O	1:A:364:VAL:N	2.51	0.43
1:A:72:THR:O	1:A:75:GLU:HB2	2.18	0.43
1:A:87:ILE:CG1	1:A:92:ILE:HD11	2.49	0.43
1:A:189:PHE:O	1:A:189:PHE:CD1	2.71	0.43
1:A:209:HIS:HA	1:A:216:VAL:HG23	1.99	0.43
1:A:21:PRO:HA	1:A:23:PHE:CZ	2.54	0.43
1:A:169:ILE:HG23	1:A:335:LYS:CE	2.47	0.43
1:A:190:PHE:CD2	1:A:339:THR:HB	2.53	0.43
1:A:238:TRP:CD1	1:A:254:LEU:HD23	2.53	0.43
1:A:354:GLU:O	1:A:357:PRO:HD2	2.18	0.43
1:A:191:LYS:HD3	1:A:191:LYS:HA	1.82	0.43
1:A:254:LEU:HD13	1:A:366:PHE:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:THR:HG23	1:A:346:GLU:N	2.34	0.43
1:A:354:GLU:O	1:A:356:ILE:N	2.52	0.43
1:A:283:SER:O	1:A:360:ILE:HB	2.19	0.43
1:A:287:HIS:CE1	1:A:365:LYS:HG3	2.54	0.43
1:A:130:PHE:O	1:A:133:ASP:HB2	2.19	0.43
1:A:230:GLN:HG2	1:A:231:HIS:N	2.34	0.43
1:A:254:LEU:HB2	1:A:366:PHE:HE1	1.84	0.43
1:A:84:LEU:HD12	1:A:84:LEU:N	2.25	0.43
1:A:196:ARG:HA	1:A:346:GLU:HB2	2.00	0.43
1:A:164:GLY:C	1:A:166:GLN:H	2.22	0.43
1:A:343:LYS:HB2	1:A:343:LYS:HE3	1.89	0.43
1:A:371:VAL:O	1:A:372:PHE:HD1	2.01	0.43
1:A:381:SER:HA	1:A:382:PRO:HD3	1.66	0.43
1:A:184:LEU:HD11	1:A:329:LEU:HD11	2.01	0.42
1:A:371:VAL:O	1:A:372:PHE:CB	2.67	0.42
1:A:197:PRO:HG3	1:A:347:ALA:H	1.84	0.42
1:A:268:THR:HG22	1:A:269:HIS:N	2.26	0.42
1:A:373:LEU:HD23	1:A:385:MET:HA	2.01	0.42
1:A:38:TYR:HB2	1:A:385:MET:SD	2.60	0.42
1:A:235:LEU:CD2	1:A:235:LEU:N	2.79	0.42
1:A:340:ILE:CD1	1:A:341:ASP:H	2.33	0.42
1:A:343:LYS:H	1:A:343:LYS:HD3	1.84	0.42
1:A:360:ILE:HG12	1:A:361:PRO:CD	2.49	0.42
1:A:182:PHE:CD2	1:A:329:LEU:HD13	2.43	0.42
1:A:227:PHE:O	1:A:282:ARG:HB3	2.19	0.42
1:A:353:LEU:HA	1:A:356:ILE:CD1	2.49	0.42
1:A:189:PHE:O	1:A:189:PHE:HD1	2.03	0.42
1:A:193:LYS:HB3	1:A:245:LEU:HG	2.02	0.42
1:A:209:HIS:NE2	1:A:216:VAL:O	2.52	0.42
1:A:255:PRO:CD	1:A:370:PHE:HA	2.48	0.42
1:A:260:LEU:HD12	1:A:261:GLN:HE22	1.84	0.42
1:A:74:ASP:HA	1:A:78:GLU:HB2	2.00	0.42
1:A:125:LYS:O	1:A:126:LEU:O	2.38	0.42
1:A:345:THR:C	1:A:347:ALA:N	2.73	0.42
1:A:72:THR:O	1:A:74:ASP:N	2.42	0.42
1:A:28:PRO:CD	1:A:29:ASN:H	2.33	0.41
1:A:120:LEU:HA	1:A:120:LEU:HD13	1.84	0.41
1:A:157:ILE:C	1:A:159:ASP:H	2.21	0.41
1:A:76:ILE:HD11	1:A:311:VAL:CG1	2.48	0.41
1:A:127:VAL:HG12	1:A:130:PHE:N	2.24	0.41
1:A:72:THR:C	1:A:74:ASP:N	2.72	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:LEU:HD12	1:A:296:THR:HG23	2.01	0.41
1:A:223:ARG:HA	1:A:356:ILE:CB	2.42	0.41
1:A:253:PHE:O	1:A:254:LEU:HB2	2.19	0.41
1:A:338:LEU:CD1	1:A:340:ILE:H	2.32	0.41
1:A:348:ALA:CA	1:A:352:PHE:HD2	2.20	0.41
1:A:101:ARG:HA	1:A:101:ARG:HD3	1.66	0.41
1:A:143:PHE:HD1	1:A:143:PHE:C	2.24	0.41
1:A:165:THR:HG23	1:A:188:ILE:N	2.31	0.41
1:A:176:LEU:HD12	1:A:176:LEU:HA	1.83	0.41
1:A:64:LEU:HA	1:A:64:LEU:HD12	1.78	0.41
1:A:327:LEU:HD22	1:A:328:LYS:O	2.21	0.41
1:A:373:LEU:HD11	1:A:382:PRO:HB3	2.03	0.41
1:A:286:LEU:HD13	1:A:286:LEU:C	2.40	0.41
1:A:318:LEU:HB3	1:A:327:LEU:HB3	2.03	0.41
1:A:143:PHE:C	1:A:143:PHE:CD1	2.94	0.41
1:A:147:PHE:CD1	1:A:180:THR:O	2.74	0.41
1:A:293:ILE:O	1:A:293:ILE:HG13	2.21	0.41
1:A:308:ILE:HG23	1:A:311:VAL:HG21	2.01	0.41
1:A:113:THR:O	1:A:187:TYR:HD2	2.04	0.41
1:A:118:LEU:HB3	1:A:141:GLU:O	2.20	0.41
1:A:29:ASN:HA	1:A:81:ASN:OD1	2.21	0.41
1:A:119:PHE:CE2	1:A:157:ILE:HA	2.55	0.41
1:A:145:VAL:HG13	1:A:145:VAL:O	2.21	0.41
1:A:240:LEU:HD23	1:A:252:PHE:CD2	2.55	0.41
1:A:216:VAL:HG12	1:A:217:LYS:N	2.24	0.41
1:A:261:GLN:C	1:A:263:LEU:N	2.73	0.41
1:A:24:ASN:O	1:A:28:PRO:CD	2.65	0.40
1:A:60:ALA:HA	1:A:63:MET:HG2	2.03	0.40
1:A:109:GLN:HB2	1:A:246:GLY:CA	2.51	0.40
1:A:110:LEU:O	1:A:191:LYS:CB	2.69	0.40
1:A:154:LYS:NZ	1:A:173:VAL:CG1	2.75	0.40
1:A:172:LEU:HB2	1:A:335:LYS:HE2	2.03	0.40
1:A:224:LEU:HG	1:A:358:MET:CB	2.50	0.40
1:A:371:VAL:O	1:A:372:PHE:CD1	2.73	0.40
1:A:57:ILE:HG22	1:A:299:LEU:HG	2.03	0.40
1:A:112:LEU:HG	1:A:190:PHE:HA	2.04	0.40
1:A:125:LYS:HG2	1:A:324:GLU:HG3	2.03	0.40
1:A:227:PHE:O	1:A:229:ILE:N	2.46	0.40
1:A:50:ILE:CG2	1:A:386:GLY:HA2	2.50	0.40
1:A:119:PHE:HE2	1:A:157:ILE:HA	1.86	0.40
1:A:26:ILE:O	1:A:30:LEU:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:HIS:CE1	1:A:215:THR:HB	2.57	0.40
1:A:379:THR:CG2	1:A:380:LYS:H	2.35	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	373/394 (95%)	195 (52%)	119 (32%)	59 (16%)	0 2

All (59) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	30	LEU
1	A	46	ASN
1	A	99	LEU
1	A	126	LEU
1	A	180	THR
1	A	190	PHE
1	A	210	VAL
1	A	220	MET
1	A	247	ASN
1	A	255	PRO
1	A	283	SER
1	A	292	SER
1	A	309	THR
1	A	323	GLU
1	A	326	PRO
1	A	331	LYS
1	A	372	PHE
1	A	380	LYS
1	A	387	LYS

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Mol	Chain	Res	Type
1	A	68	ALA
1	A	75	GLU
1	A	84	LEU
1	A	92	ILE
1	A	104	ASN
1	A	107	ASP
1	A	140	SER
1	A	197	PRO
1	A	261	GLN
1	A	264	GLU
1	A	282	ARG
1	A	310	LYS
1	A	341	ASP
1	A	342	GLU
1	A	360	ILE
1	A	365	LYS
1	A	379	THR
1	A	391	PRO
1	A	101	ARG
1	A	106	PRO
1	A	165	THR
1	A	207	ASP
1	A	316	ALA
1	A	155	LYS
1	A	321	VAL
1	A	322	THR
1	A	348	ALA
1	A	28	PRO
1	A	171	ASP
1	A	73	HIS
1	A	118	LEU
1	A	125	LYS
1	A	371	VAL
1	A	373	LEU
1	A	76	ILE
1	A	170	VAL
1	A	55	VAL
1	A	188	ILE
1	A	307	GLY
1	A	308	ILE

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	328/346 (95%)	223 (68%)	105 (32%)	0 1

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	PHE
1	A	24	ASN
1	A	26	ILE
1	A	27	THR
1	A	39	ARG
1	A	41	LEU
1	A	43	HIS
1	A	44	GLN
1	A	46	ASN
1	A	48	THR
1	A	49	ASN
1	A	57	ILE
1	A	63	MET
1	A	71	ASP
1	A	72	THR
1	A	74	ASP
1	A	81	ASN
1	A	84	LEU
1	A	85	THR
1	A	94	GLU
1	A	97	GLN
1	A	101	ARG
1	A	102	THR
1	A	106	PRO
1	A	108	SER
1	A	112	LEU
1	A	113	THR
1	A	119	PHE
1	A	120	LEU
1	A	121	SER

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Mol	Chain	Res	Type
1	A	126	LEU
1	A	130	PHE
1	A	132	GLU
1	A	133	ASP
1	A	135	LYS
1	A	136	LYS
1	A	143	PHE
1	A	144	THR
1	A	146	ASN
1	A	149	ASP
1	A	150	THR
1	A	151	GLU
1	A	152	GLU
1	A	155	LYS
1	A	158	ASN
1	A	161	VAL
1	A	162	GLU
1	A	163	LYS
1	A	165	THR
1	A	171	ASP
1	A	177	ASP
1	A	178	ARG
1	A	181	VAL
1	A	184	LEU
1	A	186	ASN
1	A	188	ILE
1	A	195	GLU
1	A	196	ARG
1	A	198	PHE
1	A	201	LYS
1	A	202	ASP
1	A	214	THR
1	A	216	VAL
1	A	218	VAL
1	A	223	ARG
1	A	224	LEU
1	A	228	ASN
1	A	235	LEU
1	A	238	TRP
1	A	245	LEU
1	A	251	ILE
1	A	255	PRO

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Mol	Chain	Res	Type
1	A	256	ASP
1	A	259	LYS
1	A	261	GLN
1	A	267	LEU
1	A	272	ILE
1	A	276	LEU
1	A	280	ASP
1	A	281	ARG
1	A	285	SER
1	A	286	LEU
1	A	287	HIS
1	A	291	LEU
1	A	306	LEU
1	A	312	PHE
1	A	318	LEU
1	A	319	SER
1	A	324	GLU
1	A	327	LEU
1	A	329	LEU
1	A	331	LYS
1	A	333	VAL
1	A	334	HIS
1	A	340	ILE
1	A	343	LYS
1	A	352	PHE
1	A	356	ILE
1	A	366	PHE
1	A	374	MET
1	A	376	GLU
1	A	384	PHE
1	A	390	ASN
1	A	391	PRO
1	A	393	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	44	GLN
1	A	46	ASN
1	A	49	ASN
1	A	97	GLN

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Mol	Chain	Res	Type
1	A	105	GLN
1	A	139	HIS
1	A	166	GLN
1	A	186	ASN
1	A	247	ASN
1	A	261	GLN
1	A	278	ASN
1	A	287	HIS
1	A	390	ASN
1	A	393	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	375/394 (95%)	-0.46	0 100 100	20, 20, 20, 20	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.