Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:15 PM GMT

PDB ID	:	1EQN
Title	:	E.COLI PRIMASE CATALYTIC CORE
Authors	:	Podobnik, M.; McInerney, P.; O'Donnell, M.; Kuriyan, J.
Deposited on	:	2000-04-05
Resolution	:	2.90 Å(reported)

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

The following versions of software and data (see references (1)) were used in the production of this report:

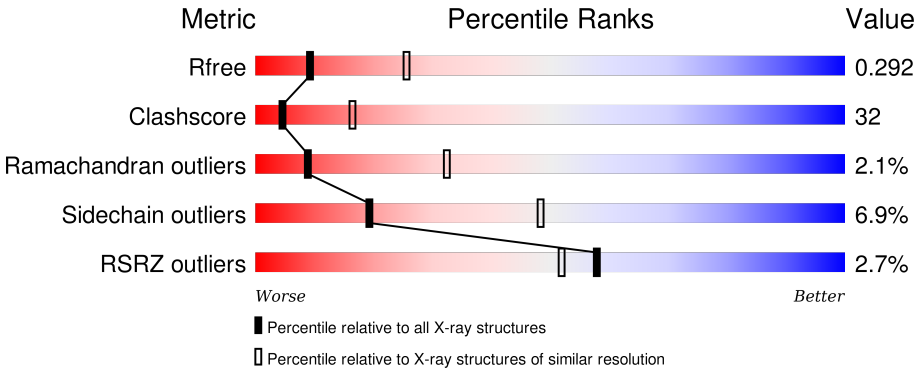
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	321	51% 42%
1	B	321	5% 50% 44%
1	C	321	4% 50% 42% 6%
1	D	321	53% 41%
1	E	321	2% 52% 37% 7%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 12156 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 DNA PRIMASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	315	Total	C	N	O	S	Se	0	0	0
			2462	1551	446	454	2	9			
1	B	313	Total	C	N	O	S	Se	0	0	0
			2435	1533	440	451	2	9			
1	C	315	Total	C	N	O	S	Se	0	0	0
			2446	1542	439	454	2	9			
1	D	314	Total	C	N	O	S	Se	0	0	0
			2430	1534	438	447	2	9			
1	E	308	Total	C	N	O	S	Se	0	0	0
			2383	1509	429	434	2	9			

There are 55 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	109	GLY	-	EXPRESSION TAG	UNP P0ABS5
A	110	ALA	-	EXPRESSION TAG	UNP P0ABS5
A	120	MSE	MET	MODIFIED RESIDUE	UNP P0ABS5
A	187	MSE	MET	MODIFIED RESIDUE	UNP P0ABS5
A	205	MSE	MET	MODIFIED RESIDUE	UNP P0ABS5
A	268	MSE	MET	MODIFIED RESIDUE	UNP P0ABS5
A	329	MSE	MET	MODIFIED RESIDUE	UNP P0ABS5
A	338	MSE	MET	MODIFIED RESIDUE	UNP P0ABS5
A	362	MSE	MET	MODIFIED RESIDUE	UNP P0ABS5
A	366	MSE	MET	MODIFIED RESIDUE	UNP P0ABS5
A	377	MSE	MET	MODIFIED RESIDUE	UNP P0ABS5
B	109	GLY	-	EXPRESSION TAG	UNP P0ABS5
B	110	ALA	-	EXPRESSION TAG	UNP P0ABS5
B	120	MSE	MET	MODIFIED RESIDUE	UNP P0ABS5
B	187	MSE	MET	MODIFIED RESIDUE	UNP P0ABS5
B	205	MSE	MET	MODIFIED RESIDUE	UNP P0ABS5
B	268	MSE	MET	MODIFIED RESIDUE	UNP P0ABS5
B	329	MSE	MET	MODIFIED RESIDUE	UNP P0ABS5
B	338	MSE	MET	MODIFIED RESIDUE	UNP P0ABS5

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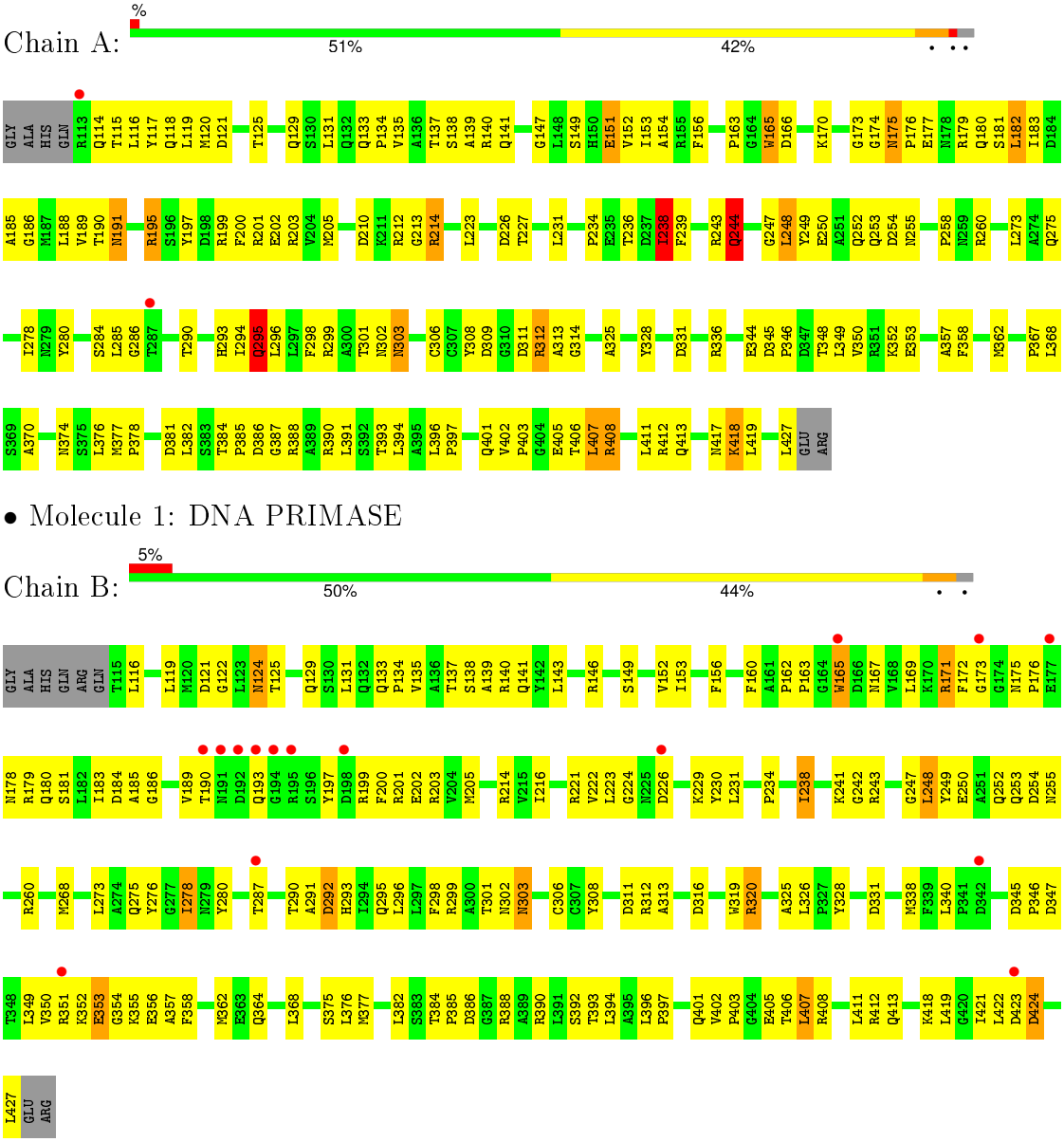
Chain	Residue	Modelled	Actual	Comment	Reference
B	362	MSE	MET	MODIFIED RESIDUE	UNP P0ABS5
B	366	MSE	MET	MODIFIED RESIDUE	UNP P0ABS5
B	377	MSE	MET	MODIFIED RESIDUE	UNP P0ABS5
C	109	GLY	-	EXPRESSION TAG	UNP P0ABS5
C	110	ALA	-	EXPRESSION TAG	UNP P0ABS5
C	120	MSE	MET	MODIFIED RESIDUE	UNP P0ABS5
C	187	MSE	MET	MODIFIED RESIDUE	UNP P0ABS5
C	205	MSE	MET	MODIFIED RESIDUE	UNP P0ABS5
C	268	MSE	MET	MODIFIED RESIDUE	UNP P0ABS5
C	329	MSE	MET	MODIFIED RESIDUE	UNP P0ABS5
C	338	MSE	MET	MODIFIED RESIDUE	UNP P0ABS5
C	362	MSE	MET	MODIFIED RESIDUE	UNP P0ABS5
C	366	MSE	MET	MODIFIED RESIDUE	UNP P0ABS5
C	377	MSE	MET	MODIFIED RESIDUE	UNP P0ABS5
D	109	GLY	-	EXPRESSION TAG	UNP P0ABS5
D	110	ALA	-	EXPRESSION TAG	UNP P0ABS5
D	120	MSE	MET	MODIFIED RESIDUE	UNP P0ABS5
D	187	MSE	MET	MODIFIED RESIDUE	UNP P0ABS5
D	205	MSE	MET	MODIFIED RESIDUE	UNP P0ABS5
D	268	MSE	MET	MODIFIED RESIDUE	UNP P0ABS5
D	329	MSE	MET	MODIFIED RESIDUE	UNP P0ABS5
D	338	MSE	MET	MODIFIED RESIDUE	UNP P0ABS5
D	362	MSE	MET	MODIFIED RESIDUE	UNP P0ABS5
D	366	MSE	MET	MODIFIED RESIDUE	UNP P0ABS5
D	377	MSE	MET	MODIFIED RESIDUE	UNP P0ABS5
E	109	GLY	-	EXPRESSION TAG	UNP P0ABS5
E	110	ALA	-	EXPRESSION TAG	UNP P0ABS5
E	120	MSE	MET	MODIFIED RESIDUE	UNP P0ABS5
E	187	MSE	MET	MODIFIED RESIDUE	UNP P0ABS5
E	205	MSE	MET	MODIFIED RESIDUE	UNP P0ABS5
E	268	MSE	MET	MODIFIED RESIDUE	UNP P0ABS5
E	329	MSE	MET	MODIFIED RESIDUE	UNP P0ABS5
E	338	MSE	MET	MODIFIED RESIDUE	UNP P0ABS5
E	362	MSE	MET	MODIFIED RESIDUE	UNP P0ABS5
E	366	MSE	MET	MODIFIED RESIDUE	UNP P0ABS5
E	377	MSE	MET	MODIFIED RESIDUE	UNP P0ABS5

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: DNA PRIMASE

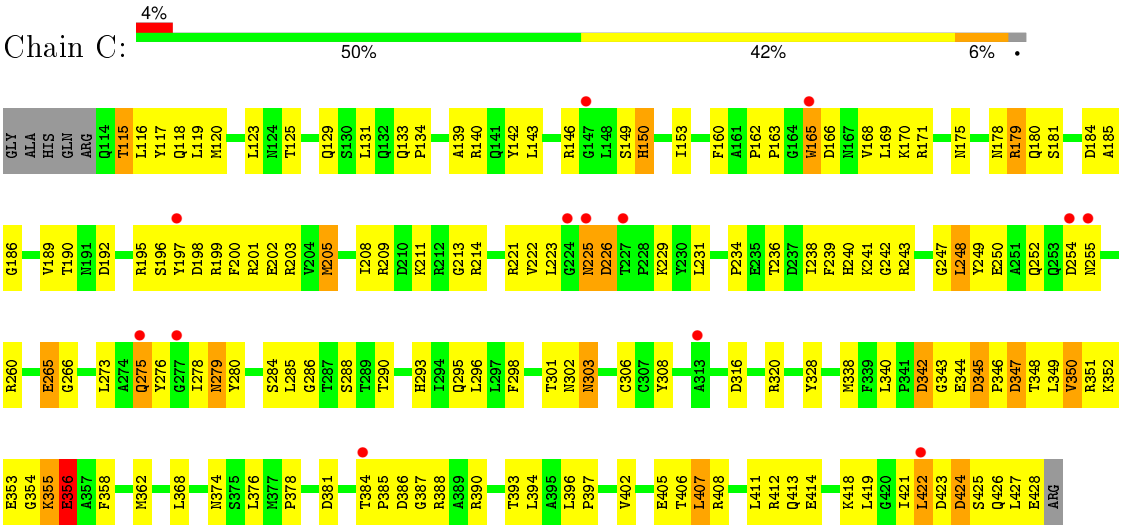
Chain A:



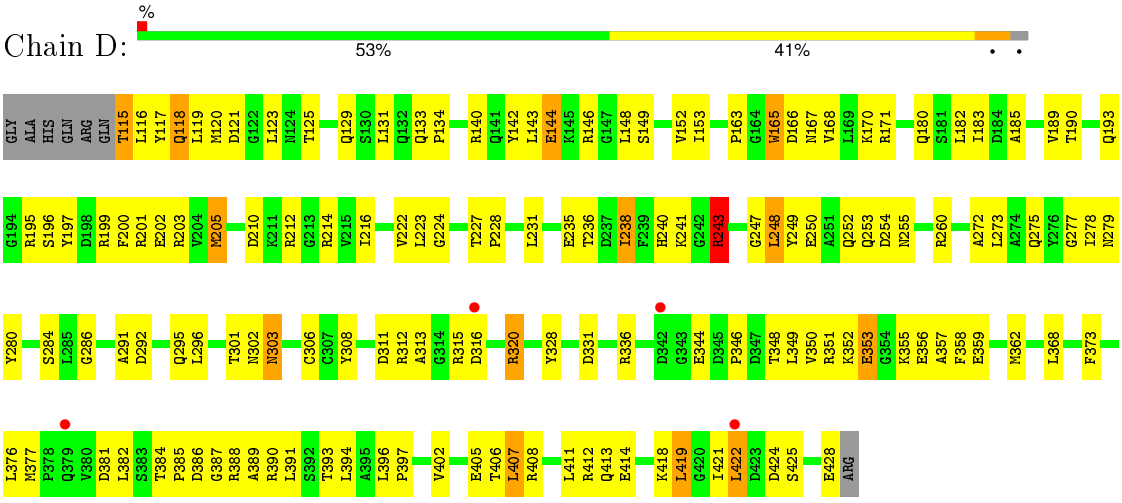
- Molecule 1: DNA PRIMASE

Chain B:

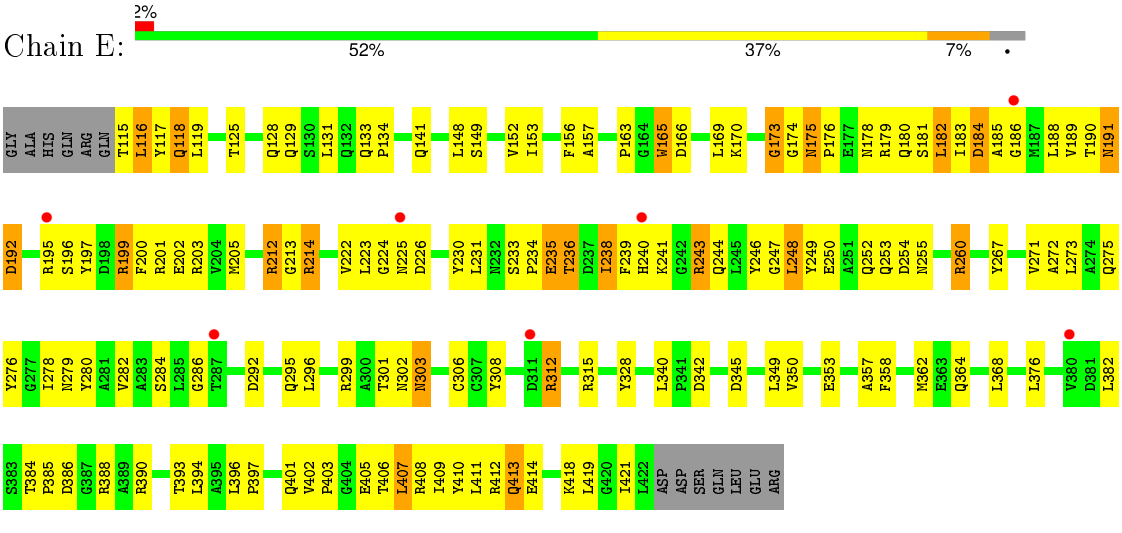
- Molecule 1: DNA PRIMASE



- Molecule 1: DNA PRIMASE



- Molecule 1: DNA PRIMASE



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	62.67Å 107.63Å 263.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	500.00 – 2.90 19.91 – 2.89	Depositor EDS
% Data completeness (in resolution range)	90.3 (500.00-2.90) 95.7 (19.91-2.89)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.05 (at 2.88Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.220 , 0.276 0.238 , 0.292	Depositor DCC
R_{free} test set	3929 reflections (11.38%)	DCC
Wilson B-factor (Å^2)	51.7	Xtriage
Anisotropy	0.330	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 57.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 75010 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	12156	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.76	5/2502 (0.2%)	0.71	1/3372 (0.0%)
1	B	0.64	3/2475 (0.1%)	0.81	5/3339 (0.1%)
1	C	0.56	3/2486 (0.1%)	0.72	4/3355 (0.1%)
1	D	0.58	2/2470 (0.1%)	0.70	1/3333 (0.0%)
1	E	0.55	1/2423 (0.0%)	0.66	0/3271
All	All	0.62	14/12356 (0.1%)	0.72	11/16670 (0.1%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	295	GLN	CD-OE1	-16.85	0.86	1.24
1	A	295	GLN	CD-NE2	-11.53	1.04	1.32
1	B	413	GLN	CG-CD	-10.70	1.26	1.51
1	E	413	GLN	CG-CD	-6.79	1.35	1.51
1	A	413	GLN	CG-CD	-6.30	1.36	1.51
1	B	413	GLN	CD-OE1	-6.08	1.10	1.24
1	C	413	GLN	CG-CD	-5.76	1.37	1.51
1	B	338	MSE	SE-CE	-5.73	1.61	1.95
1	C	205	MSE	CG-SE	-5.36	1.77	1.95
1	D	205	MSE	CG-SE	-5.31	1.77	1.95
1	D	413	GLN	CG-CD	-5.30	1.38	1.51
1	A	244	GLN	CD-OE1	-5.13	1.12	1.24
1	A	120	MSE	CG-SE	-5.11	1.78	1.95
1	C	338	MSE	SE-CE	-5.09	1.65	1.95

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	121	ASP	CB-CG-OD2	15.31	132.08	118.30
1	B	121	ASP	CB-CG-OD1	14.60	131.44	118.30
1	B	121	ASP	OD1-CG-OD2	-14.12	96.47	123.30
1	B	413	GLN	CG-CD-OE1	-6.39	108.81	121.60
1	A	121	ASP	CB-CG-OD1	5.54	123.28	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	121	ASP	CB-CG-OD1	5.52	123.27	118.30
1	C	226	ASP	N-CA-C	-5.46	96.25	111.00
1	C	422	LEU	N-CA-C	-5.46	96.25	111.00
1	C	422	LEU	CA-CB-CG	-5.15	103.46	115.30
1	B	413	GLN	CB-CG-CD	-5.07	98.42	111.60
1	C	422	LEU	CB-CA-C	5.04	119.78	110.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	2462	0	2407	146	0
1	B	2435	0	2366	148	0
1	C	2446	0	2383	195	0
1	D	2430	0	2368	155	0
1	E	2383	0	2327	179	0
All	All	12156	0	11851	772	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 32.

All (772) 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:C:165:TRP:CZ2	1:E:413:GLN:HG3	1.24	1.64
1:C:165:TRP:CE2	1:E:413:GLN:HG3	1.71	1.26
1:C:165:TRP:CZ2	1:E:413:GLN:CG	2.19	1.23
1:C:229:LYS:HD2	1:D:240:HIS:CE1	1.76	1.19
1:C:165:TRP:CZ3	1:E:409:ILE:HG22	1.78	1.18
1:C:165:TRP:NE1	1:E:413:GLN:NE2	1.99	1.09
1:A:149:SER:H	1:A:275:GLN:NE2	1.55	1.05
1:D:422:LEU:N	1:D:422:LEU:HD22	1.68	1.04
1:C:423:ASP:O	1:C:425:SER:N	1.90	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:422:LEU:HD22	1:D:422:LEU:H	0.89	1.03
1:C:165:TRP:CZ3	1:E:409:ILE:CG2	2.42	1.02
1:E:191:ASN:ND2	1:E:192:ASP:H	1.58	1.01
1:D:422:LEU:H	1:D:422:LEU:CD2	1.74	0.99
1:E:191:ASN:HD22	1:E:192:ASP:N	1.59	0.98
1:E:212:ARG:HB3	1:E:214:ARG:HD2	1.44	0.98
1:B:377:MSE:HE1	1:B:418:LYS:HD2	1.45	0.97
1:E:301:THR:HG22	1:E:303:ASN:H	1.31	0.96
1:C:165:TRP:CE2	1:E:413:GLN:CG	2.46	0.94
1:C:301:THR:HG22	1:C:303:ASN:H	1.32	0.94
1:B:222:VAL:HG11	1:B:226:ASP:HB2	1.45	0.94
1:C:165:TRP:CH2	1:E:413:GLN:HG3	2.03	0.93
1:B:301:THR:HG22	1:B:303:ASN:H	1.31	0.93
1:A:301:THR:HG22	1:A:303:ASN:H	1.31	0.93
1:D:301:THR:HG22	1:D:303:ASN:H	1.32	0.93
1:C:279:ASN:H	1:C:279:ASN:HD22	1.11	0.91
1:E:230:TYR:HD2	1:E:267:TYR:OH	1.52	0.91
1:E:191:ASN:HD22	1:E:192:ASP:H	0.92	0.91
1:C:165:TRP:HE1	1:E:413:GLN:HE21	0.97	0.91
1:B:384:THR:HG22	1:B:386:ASP:H	1.39	0.88
1:E:353:GLU:HB3	1:E:357:ALA:HB3	1.56	0.88
1:D:377:MSE:HE1	1:D:418:LYS:HD3	1.55	0.87
1:C:421:ILE:HG22	1:C:422:LEU:H	1.40	0.86
1:C:421:ILE:HG22	1:C:422:LEU:N	1.91	0.85
1:B:412:ARG:NH2	1:B:427:LEU:CB	2.40	0.85
1:A:290:THR:OG1	1:A:293:HIS:HD2	1.58	0.85
1:A:116:LEU:HD12	1:A:238:ILE:HD12	1.58	0.83
1:E:384:THR:HG22	1:E:386:ASP:H	1.44	0.83
1:E:239:PHE:CZ	1:E:241:LYS:HG2	2.14	0.83
1:D:222:VAL:HG12	1:D:224:GLY:H	1.44	0.82
1:A:179:ARG:O	1:A:183:ILE:HG13	1.78	0.82
1:A:273:LEU:HD23	1:A:350:VAL:HG21	1.60	0.82
1:B:276:TYR:O	1:B:355:LYS:HD2	1.78	0.82
1:A:384:THR:HG22	1:A:386:ASP:H	1.44	0.82
1:C:165:TRP:HH2	1:E:410:TYR:HA	1.43	0.82
1:E:184:ASP:N	1:E:184:ASP:OD1	2.12	0.81
1:D:115:THR:HG22	1:D:118:GLN:H	1.45	0.81
1:C:117:TYR:HD2	1:C:214:ARG:HD2	1.45	0.81
1:B:242:GLY:HA2	1:B:293:HIS:CE1	2.15	0.81
1:C:384:THR:HG22	1:C:386:ASP:H	1.45	0.81
1:B:349:LEU:HD21	1:B:353:GLU:OE1	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:186:GLY:O	1:E:199:ARG:HD2	1.80	0.80
1:D:149:SER:H	1:D:275:GLN:HE22	1.27	0.80
1:A:149:SER:H	1:A:275:GLN:HE22	1.26	0.80
1:B:137:THR:HG22	1:B:141:GLN:NE2	1.96	0.79
1:D:384:THR:HG22	1:D:386:ASP:H	1.48	0.78
1:C:165:TRP:HZ3	1:E:409:ILE:CG2	1.97	0.78
1:D:117:TYR:HE2	1:D:216:ILE:HG22	1.46	0.78
1:B:137:THR:HG22	1:B:141:GLN:HE21	1.46	0.78
1:D:273:LEU:HD23	1:D:350:VAL:HG21	1.64	0.78
1:A:116:LEU:HD23	1:A:181:SER:HB3	1.67	0.77
1:B:260:ARG:HA	1:B:301:THR:HG21	1.66	0.77
1:D:167:ASN:O	1:D:171:ARG:HG3	1.83	0.77
1:D:346:PRO:O	1:D:350:VAL:HG23	1.85	0.77
1:A:346:PRO:O	1:A:350:VAL:HG23	1.85	0.76
1:A:149:SER:N	1:A:275:GLN:NE2	2.32	0.76
1:D:421:ILE:C	1:D:422:LEU:HD13	2.06	0.76
1:B:134:PRO:CG	1:D:425:SER:HA	2.15	0.76
1:C:208:ILE:HD13	1:C:285:LEU:HD11	1.66	0.76
1:A:139:ALA:HA	1:A:223:LEU:HD21	1.68	0.76
1:A:260:ARG:HA	1:A:301:THR:HG21	1.68	0.75
1:E:189:VAL:CG2	1:E:199:ARG:HG3	2.16	0.75
1:C:265:GLU:HG3	1:C:266:GLY:N	2.00	0.75
1:C:171:ARG:HH11	1:C:171:ARG:HG3	1.51	0.75
1:D:260:ARG:HA	1:D:301:THR:HG21	1.67	0.75
1:C:115:THR:HG22	1:C:118:GLN:H	1.51	0.75
1:E:260:ARG:HA	1:E:301:THR:HG21	1.68	0.74
1:A:180:GLN:O	1:A:183:ILE:N	2.21	0.74
1:C:240:HIS:HD2	1:C:243:ARG:NH2	1.85	0.74
1:C:260:ARG:HA	1:C:301:THR:HG21	1.69	0.74
1:C:208:ILE:CD1	1:C:285:LEU:HD11	2.17	0.74
1:C:139:ALA:HA	1:C:223:LEU:HD21	1.69	0.74
1:B:200:PHE:CD2	1:B:205:MSE:HE1	2.22	0.74
1:C:189:VAL:CG2	1:C:199:ARG:HD2	2.18	0.74
1:B:291:ALA:O	1:B:295:GLN:HG2	1.88	0.74
1:D:291:ALA:O	1:D:295:GLN:HG2	1.88	0.74
1:E:385:PRO:HA	1:E:388:ARG:NH1	2.04	0.73
1:E:176:PRO:HA	1:E:179:ARG:HB3	1.71	0.73
1:B:273:LEU:HD23	1:B:350:VAL:HG21	1.69	0.73
1:A:191:ASN:HD21	1:A:195:ARG:H	1.34	0.73
1:E:133:GLN:HB3	1:E:134:PRO:HD2	1.69	0.73
1:B:146:ARG:NH2	1:B:347:ASP:OD2	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:222:VAL:HG11	1:C:226:ASP:HB3	1.72	0.72
1:C:284:SER:C	1:C:286:GLY:H	1.91	0.71
1:D:316:ASP:O	1:D:320:ARG:HD3	1.89	0.71
1:C:115:THR:HG23	1:C:116:LEU:N	2.04	0.71
1:E:180:GLN:O	1:E:184:ASP:OD1	2.08	0.71
1:D:353:GLU:HB2	1:D:357:ALA:HB3	1.73	0.71
1:C:117:TYR:CD2	1:C:214:ARG:HD2	2.26	0.71
1:A:138:SER:H	1:C:428:GLU:CB	2.04	0.71
1:C:165:TRP:HE1	1:E:413:GLN:NE2	1.78	0.71
1:C:423:ASP:C	1:C:425:SER:H	1.91	0.71
1:B:385:PRO:HA	1:B:388:ARG:NH1	2.06	0.71
1:B:186:GLY:O	1:B:199:ARG:HD3	1.91	0.70
1:C:279:ASN:H	1:C:279:ASN:ND2	1.88	0.70
1:D:133:GLN:HB3	1:D:134:PRO:HD2	1.74	0.70
1:E:239:PHE:CE2	1:E:241:LYS:HG2	2.26	0.70
1:C:385:PRO:HA	1:C:388:ARG:NH1	2.07	0.70
1:A:273:LEU:CD2	1:A:350:VAL:HG21	2.21	0.70
1:E:388:ARG:HB3	1:E:419:LEU:CD2	2.22	0.70
1:C:115:THR:HG22	1:C:118:GLN:HG3	1.72	0.69
1:B:133:GLN:HB3	1:B:134:PRO:HD2	1.73	0.69
1:C:346:PRO:O	1:C:350:VAL:HG23	1.92	0.69
1:C:229:LYS:CD	1:D:240:HIS:CE1	2.66	0.69
1:D:385:PRO:HA	1:D:388:ARG:NH1	2.08	0.69
1:C:209:ARG:NH2	1:C:250:GLU:OE1	2.24	0.69
1:C:165:TRP:CZ3	1:E:409:ILE:O	2.46	0.69
1:E:273:LEU:HD23	1:E:350:VAL:HG21	1.73	0.69
1:D:422:LEU:N	1:D:422:LEU:CD2	2.39	0.69
1:B:175:ASN:HB3	1:B:178:ASN:ND2	2.07	0.69
1:A:213:GLY:HA2	1:A:249:TYR:CE1	2.28	0.69
1:C:142:TYR:OH	1:C:221:ARG:CZ	2.41	0.69
1:C:165:TRP:CZ3	1:E:409:ILE:HG23	2.28	0.69
1:E:236:THR:HG23	1:E:238:ILE:HG22	1.73	0.69
1:B:175:ASN:HB3	1:B:178:ASN:CG	2.14	0.68
1:B:377:MSE:CE	1:B:418:LYS:HD2	2.22	0.68
1:A:301:THR:HG22	1:A:302:ASN:N	2.08	0.68
1:B:171:ARG:HB3	1:B:172:PHE:CD1	2.27	0.68
1:A:201:ARG:O	1:A:203:ARG:HG3	1.93	0.68
1:A:133:GLN:HB3	1:A:134:PRO:HD2	1.76	0.68
1:D:301:THR:HG22	1:D:302:ASN:N	2.08	0.68
1:D:422:LEU:N	1:D:422:LEU:HD13	2.09	0.68
1:E:353:GLU:HB3	1:E:357:ALA:CB	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:PHE:HZ	1:A:285:LEU:CD2	2.07	0.68
1:E:301:THR:HG22	1:E:302:ASN:N	2.09	0.68
1:A:385:PRO:HA	1:A:388:ARG:NH1	2.09	0.68
1:B:301:THR:HG22	1:B:302:ASN:N	2.09	0.67
1:C:225:ASN:OD1	1:D:235:GLU:HB2	1.94	0.67
1:B:134:PRO:HG2	1:D:425:SER:HA	1.74	0.67
1:A:236:THR:OG1	1:A:238:ILE:CG2	2.42	0.67
1:D:166:ASP:O	1:D:170:LYS:HB2	1.94	0.67
1:B:180:GLN:HA	1:B:183:ILE:HD12	1.77	0.67
1:A:295:GLN:O	1:A:299:ARG:HG3	1.95	0.66
1:C:421:ILE:O	1:C:422:LEU:HD23	1.95	0.66
1:B:137:THR:O	1:B:141:GLN:HG3	1.95	0.66
1:E:388:ARG:HB3	1:E:419:LEU:HD22	1.76	0.66
1:E:190:THR:HA	1:E:195:ARG:O	1.95	0.66
1:C:301:THR:HG22	1:C:302:ASN:N	2.10	0.66
1:C:133:GLN:HB3	1:C:134:PRO:HD2	1.76	0.66
1:D:254:ASP:C	1:D:255:ASN:HD22	1.99	0.66
1:C:165:TRP:CE2	1:E:413:GLN:NE2	2.62	0.66
1:C:421:ILE:CG2	1:C:422:LEU:H	2.09	0.66
1:A:236:THR:OG1	1:A:238:ILE:HG23	1.96	0.66
1:E:273:LEU:CD2	1:E:350:VAL:HG21	2.26	0.66
1:A:149:SER:N	1:A:275:GLN:HE22	1.93	0.66
1:E:222:VAL:HG12	1:E:223:LEU:N	2.10	0.66
1:C:419:LEU:HB2	1:C:421:ILE:HG13	1.79	0.65
1:D:119:LEU:HD13	1:D:182:LEU:HG	1.78	0.65
1:E:254:ASP:C	1:E:255:ASN:HD22	2.00	0.65
1:D:149:SER:H	1:D:275:GLN:NE2	1.95	0.65
1:E:212:ARG:CB	1:E:214:ARG:HD2	2.25	0.65
1:A:390:ARG:O	1:A:394:LEU:HD13	1.97	0.65
1:A:391:LEU:HD23	1:A:419:LEU:HD11	1.79	0.65
1:D:180:GLN:O	1:D:183:ILE:N	2.30	0.64
1:E:312:ARG:HG2	1:E:315:ARG:NH2	2.12	0.64
1:B:390:ARG:O	1:B:394:LEU:HD13	1.97	0.64
1:A:200:PHE:CD2	1:A:205:MSE:HE1	2.32	0.64
1:A:405:GLU:HA	1:A:408:ARG:NH1	2.12	0.64
1:D:235:GLU:HG2	1:D:241:LYS:HG3	1.78	0.64
1:E:382:LEU:HD13	1:E:418:LYS:O	1.97	0.64
1:E:182:LEU:HB3	1:E:188:LEU:HD12	1.78	0.64
1:E:235:GLU:OE2	1:E:241:LYS:HG3	1.98	0.64
1:D:115:THR:CG2	1:D:118:GLN:H	2.10	0.64
1:B:377:MSE:HE1	1:B:418:LYS:CD	2.23	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:233:SER:O	1:E:241:LYS:NZ	2.31	0.64
1:C:190:THR:HG22	1:C:196:SER:OG	1.98	0.64
1:C:419:LEU:HD12	1:C:421:ILE:HD11	1.80	0.64
1:C:421:ILE:CG2	1:C:422:LEU:N	2.60	0.63
1:E:200:PHE:CD2	1:E:205:MSE:HE1	2.32	0.63
1:B:146:ARG:NH1	1:B:268:MSE:CE	2.61	0.63
1:D:301:THR:HG22	1:D:302:ASN:H	1.64	0.63
1:A:381:ASP:O	1:A:387:GLY:HA3	1.99	0.63
1:B:135:VAL:HG13	1:D:424:ASP:O	1.98	0.63
1:B:222:VAL:HG11	1:B:226:ASP:CB	2.24	0.63
1:C:254:ASP:C	1:C:255:ASN:HD22	2.03	0.62
1:E:201:ARG:O	1:E:203:ARG:HG3	1.99	0.62
1:D:117:TYR:CE2	1:D:216:ILE:HG22	2.31	0.62
1:D:200:PHE:CD2	1:D:205:MSE:HE1	2.35	0.62
1:D:143:LEU:HD13	1:D:153:ILE:HD12	1.79	0.62
1:B:254:ASP:C	1:B:255:ASN:HD22	2.03	0.62
1:C:200:PHE:CD2	1:C:205:MSE:HE1	2.34	0.62
1:B:346:PRO:O	1:B:350:VAL:HG23	2.00	0.62
1:D:149:SER:O	1:D:153:ILE:HG12	2.00	0.62
1:B:421:ILE:HG22	1:B:422:LEU:N	2.15	0.61
1:B:149:SER:O	1:B:153:ILE:HG12	2.00	0.61
1:B:152:VAL:HG21	1:B:275:GLN:HG2	1.82	0.61
1:A:344:GLU:OE1	1:A:348:THR:HG22	2.00	0.61
1:E:156:PHE:CE2	1:E:250:GLU:HG3	2.36	0.61
1:C:166:ASP:O	1:C:170:LYS:HB2	2.00	0.61
1:C:201:ARG:O	1:C:203:ARG:HG3	2.01	0.61
1:E:149:SER:O	1:E:153:ILE:HG12	2.00	0.61
1:D:189:VAL:O	1:D:196:SER:HA	2.00	0.61
1:A:254:ASP:C	1:A:255:ASN:HD22	2.04	0.61
1:B:201:ARG:O	1:B:203:ARG:HG3	1.99	0.61
1:A:170:LYS:HB2	1:A:170:LYS:NZ	2.16	0.61
1:D:390:ARG:O	1:D:394:LEU:HD13	2.00	0.61
1:A:191:ASN:ND2	1:A:195:ARG:H	1.99	0.61
1:C:165:TRP:CH2	1:E:409:ILE:O	2.53	0.61
1:B:276:TYR:OH	1:B:351:ARG:HB2	2.00	0.61
1:A:301:THR:HG22	1:A:302:ASN:H	1.65	0.61
1:A:391:LEU:HD23	1:A:419:LEU:CD1	2.31	0.61
1:D:414:GLU:HB3	1:D:418:LYS:HZ3	1.65	0.60
1:A:294:ILE:HD12	1:A:325:ALA:HB2	1.81	0.60
1:C:414:GLU:O	1:C:418:LYS:HD3	2.01	0.60
1:B:301:THR:HG22	1:B:302:ASN:H	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:GLY:HA2	1:B:293:HIS:NE2	2.15	0.60
1:E:384:THR:HG22	1:E:386:ASP:HB3	1.83	0.60
1:C:149:SER:O	1:C:153:ILE:HG12	2.01	0.60
1:E:301:THR:HG22	1:E:302:ASN:H	1.66	0.60
1:C:139:ALA:O	1:C:143:LEU:HG	2.00	0.60
1:A:135:VAL:HG12	1:C:426:GLN:O	2.02	0.60
1:B:171:ARG:CB	1:B:172:PHE:CD1	2.84	0.60
1:B:222:VAL:HG12	1:B:223:LEU:N	2.17	0.60
1:C:252:GLN:HA	1:C:255:ASN:O	2.01	0.59
1:D:240:HIS:HD2	1:D:243:ARG:HH21	1.48	0.59
1:B:169:LEU:HD22	1:B:173:GLY:HA3	1.84	0.59
1:C:165:TRP:CH2	1:E:413:GLN:CG	2.71	0.59
1:C:419:LEU:CD1	1:C:421:ILE:HD11	2.33	0.59
1:D:284:SER:C	1:D:286:GLY:H	2.06	0.59
1:D:201:ARG:O	1:D:203:ARG:HG3	2.03	0.59
1:E:243:ARG:HG2	1:E:243:ARG:O	2.02	0.59
1:C:119:LEU:O	1:C:123:LEU:HD13	2.03	0.59
1:E:384:THR:CG2	1:E:386:ASP:HB3	2.32	0.59
1:D:212:ARG:HB2	1:D:214:ARG:HG2	1.84	0.59
1:B:134:PRO:HG3	1:D:425:SER:HA	1.83	0.59
1:B:189:VAL:CG2	1:B:199:ARG:HD2	2.32	0.59
1:B:421:ILE:HG22	1:B:423:ASP:H	1.68	0.59
1:C:185:ALA:HA	1:C:236:THR:HG21	1.85	0.59
1:B:200:PHE:CG	1:B:205:MSE:HE1	2.38	0.58
1:E:235:GLU:OE1	1:E:241:LYS:N	2.36	0.58
1:E:179:ARG:O	1:E:183:ILE:HG13	2.02	0.58
1:C:350:VAL:O	1:C:354:GLY:N	2.36	0.58
1:A:115:THR:O	1:A:119:LEU:HB2	2.02	0.58
1:C:165:TRP:CH2	1:E:410:TYR:HA	2.32	0.58
1:D:414:GLU:O	1:D:418:LYS:HG3	2.03	0.58
1:C:273:LEU:HD23	1:C:350:VAL:HG21	1.85	0.58
1:C:279:ASN:HD22	1:C:279:ASN:N	1.85	0.58
1:C:390:ARG:O	1:C:394:LEU:HD13	2.04	0.58
1:C:171:ARG:NH1	1:C:171:ARG:HG3	2.18	0.58
1:B:146:ARG:NH1	1:B:268:MSE:HE2	2.17	0.58
1:E:213:GLY:HA2	1:E:249:TYR:CE1	2.39	0.58
1:E:254:ASP:OD2	1:E:279:ASN:ND2	2.36	0.58
1:D:252:GLN:HA	1:D:255:ASN:O	2.04	0.58
1:E:402:VAL:HG11	1:E:407:LEU:HD13	1.85	0.58
1:B:319:TRP:CZ3	1:B:375:SER:OG	2.54	0.58
1:E:230:TYR:HD2	1:E:267:TYR:HH	0.71	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:236:THR:CG2	1:E:238:ILE:HG22	2.34	0.57
1:D:349:LEU:HD23	1:D:349:LEU:O	2.04	0.57
1:E:349:LEU:O	1:E:349:LEU:HD23	2.04	0.57
1:A:290:THR:OG1	1:A:293:HIS:CD2	2.49	0.57
1:E:396:LEU:HB2	1:E:397:PRO:HD3	1.86	0.57
1:D:273:LEU:HB3	1:D:278:ILE:HB	1.87	0.57
1:C:273:LEU:HB3	1:C:278:ILE:HB	1.86	0.57
1:B:175:ASN:CB	1:B:178:ASN:ND2	2.67	0.57
1:A:114:GLN:O	1:A:118:GLN:HG3	2.04	0.57
1:B:292:ASP:O	1:B:296:LEU:HB2	2.03	0.57
1:A:117:TYR:CE2	1:A:238:ILE:HG13	2.40	0.57
1:D:402:VAL:HG11	1:D:407:LEU:HD13	1.85	0.57
1:C:344:GLU:OE1	1:C:348:THR:HG22	2.04	0.57
1:C:301:THR:HG22	1:C:302:ASN:H	1.68	0.57
1:A:116:LEU:CD2	1:A:181:SER:HB3	2.34	0.57
1:D:117:TYR:CE2	1:D:238:ILE:HB	2.40	0.57
1:E:390:ARG:O	1:E:394:LEU:HD13	2.04	0.56
1:E:115:THR:O	1:E:118:GLN:N	2.37	0.56
1:C:402:VAL:HG11	1:C:407:LEU:HD13	1.87	0.56
1:A:116:LEU:O	1:A:116:LEU:HD13	2.05	0.56
1:E:189:VAL:HG21	1:E:199:ARG:HG3	1.86	0.56
1:E:178:ASN:O	1:E:181:SER:N	2.37	0.56
1:D:115:THR:HG23	1:D:117:TYR:H	1.71	0.56
1:C:284:SER:C	1:C:286:GLY:N	2.56	0.56
1:A:199:ARG:NH1	1:A:199:ARG:HG2	2.20	0.56
1:E:235:GLU:HA	1:E:235:GLU:OE2	2.05	0.56
1:D:193:GLN:O	1:D:193:GLN:HG2	2.05	0.56
1:C:229:LYS:HZ2	1:D:240:HIS:CE1	2.24	0.56
1:D:408:ARG:O	1:D:412:ARG:HG3	2.05	0.56
1:E:182:LEU:CB	1:E:188:LEU:HD12	2.34	0.56
1:D:421:ILE:HG22	1:D:422:LEU:N	2.21	0.56
1:E:241:LYS:C	1:E:243:ARG:H	2.10	0.56
1:D:115:THR:HG22	1:D:118:GLN:HB2	1.88	0.56
1:A:199:ARG:HH11	1:A:199:ARG:HG2	1.71	0.56
1:A:175:ASN:HD22	1:A:176:PRO:N	2.04	0.56
1:E:233:SER:O	1:E:241:LYS:HE3	2.07	0.55
1:A:149:SER:HB3	1:A:275:GLN:HE22	1.71	0.55
1:E:241:LYS:C	1:E:243:ARG:N	2.59	0.55
1:A:236:THR:C	1:A:238:ILE:H	2.10	0.55
1:D:148:LEU:HA	1:D:275:GLN:NE2	2.21	0.55
1:E:252:GLN:HA	1:E:255:ASN:O	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:407:LEU:HD22	1:D:411:LEU:HG	1.89	0.55
1:A:396:LEU:HB2	1:A:397:PRO:HD3	1.89	0.55
1:E:166:ASP:O	1:E:170:LYS:N	2.38	0.55
1:B:349:LEU:O	1:B:349:LEU:HD23	2.06	0.54
1:D:273:LEU:CD2	1:D:350:VAL:HG21	2.34	0.54
1:C:115:THR:CG2	1:C:118:GLN:H	2.20	0.54
1:D:350:VAL:C	1:D:352:LYS:H	2.10	0.54
1:A:417:ASN:O	1:A:419:LEU:N	2.40	0.54
1:C:186:GLY:O	1:C:199:ARG:HD3	2.06	0.54
1:E:169:LEU:O	1:E:173:GLY:HA3	2.07	0.54
1:C:349:LEU:HD23	1:C:349:LEU:O	2.08	0.54
1:B:306:CYS:HB3	1:B:308:TYR:CE1	2.42	0.54
1:A:182:LEU:HB3	1:A:188:LEU:HD12	1.87	0.54
1:E:408:ARG:O	1:E:412:ARG:HG3	2.07	0.54
1:D:422:LEU:CD1	1:D:422:LEU:N	2.68	0.54
1:D:382:LEU:HD13	1:D:418:LYS:O	2.08	0.54
1:B:252:GLN:HA	1:B:255:ASN:O	2.08	0.54
1:D:381:ASP:O	1:D:387:GLY:HA3	2.08	0.54
1:E:212:ARG:HG2	1:E:212:ARG:NH1	2.23	0.54
1:B:405:GLU:HA	1:B:408:ARG:NH1	2.22	0.54
1:E:235:GLU:OE2	1:E:241:LYS:HD2	2.07	0.54
1:D:405:GLU:HA	1:D:408:ARG:NH1	2.23	0.54
1:D:396:LEU:HB2	1:D:397:PRO:HD3	1.89	0.54
1:E:212:ARG:HG2	1:E:212:ARG:HH11	1.72	0.54
1:A:175:ASN:C	1:A:175:ASN:HD22	2.10	0.54
1:B:396:LEU:HB2	1:B:397:PRO:HD3	1.90	0.54
1:A:349:LEU:HD23	1:A:353:GLU:HG2	1.88	0.54
1:E:272:ALA:O	1:E:275:GLN:HB3	2.07	0.54
1:E:384:THR:HG22	1:E:386:ASP:N	2.20	0.53
1:E:273:LEU:HB3	1:E:278:ILE:HB	1.90	0.53
1:D:116:LEU:HD11	1:D:185:ALA:HB2	1.88	0.53
1:C:276:TYR:OH	1:C:351:ARG:HD3	2.07	0.53
1:A:273:LEU:HB3	1:A:278:ILE:HB	1.89	0.53
1:A:134:PRO:HD2	1:C:424:ASP:O	2.09	0.53
1:A:295:GLN:HE21	1:A:328:TYR:HE2	1.57	0.53
1:D:353:GLU:CB	1:D:357:ALA:HB3	2.37	0.53
1:A:402:VAL:HG11	1:A:407:LEU:HD13	1.91	0.53
1:E:421:ILE:O	1:E:421:ILE:HG23	2.08	0.53
1:C:285:LEU:HD23	1:C:285:LEU:O	2.09	0.53
1:B:242:GLY:CA	1:B:293:HIS:NE2	2.72	0.53
1:B:421:ILE:CG2	1:B:422:LEU:N	2.70	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:396:LEU:HB2	1:C:397:PRO:HD3	1.90	0.53
1:D:116:LEU:O	1:D:120:MSE:HG2	2.08	0.53
1:B:247:GLY:HA2	1:B:250:GLU:HG2	1.90	0.53
1:A:191:ASN:ND2	1:A:195:ARG:N	2.56	0.53
1:E:236:THR:CG2	1:E:239:PHE:HB3	2.39	0.52
1:E:152:VAL:CG1	1:E:271:VAL:HG13	2.39	0.52
1:E:233:SER:O	1:E:241:LYS:CE	2.58	0.52
1:C:390:ARG:O	1:C:393:THR:HB	2.10	0.52
1:A:349:LEU:HD23	1:A:349:LEU:O	2.09	0.52
1:E:152:VAL:HG11	1:E:271:VAL:HG13	1.92	0.52
1:A:149:SER:O	1:A:153:ILE:HG12	2.09	0.52
1:B:384:THR:HG22	1:B:386:ASP:N	2.17	0.52
1:C:116:LEU:HD23	1:C:120:MSE:HG2	1.91	0.52
1:E:247:GLY:HA2	1:E:250:GLU:HG2	1.92	0.52
1:C:115:THR:CG2	1:C:116:LEU:N	2.73	0.52
1:C:407:LEU:HD22	1:C:411:LEU:HG	1.91	0.52
1:A:353:GLU:O	1:A:357:ALA:HB3	2.10	0.52
1:B:241:LYS:C	1:B:243:ARG:H	2.13	0.52
1:B:229:LYS:HB3	1:B:230:TYR:CD1	2.44	0.52
1:E:349:LEU:HD21	1:E:353:GLU:CD	2.30	0.52
1:A:238:ILE:HG12	1:A:238:ILE:O	2.10	0.52
1:B:402:VAL:HG11	1:B:407:LEU:HD13	1.91	0.52
1:C:405:GLU:HA	1:C:408:ARG:NH1	2.25	0.52
1:B:276:TYR:CD2	1:B:350:VAL:HG12	2.45	0.52
1:C:247:GLY:HA2	1:C:250:GLU:HG2	1.92	0.52
1:E:166:ASP:HA	1:E:169:LEU:HB3	1.91	0.52
1:E:117:TYR:CZ	1:E:238:ILE:HG13	2.43	0.52
1:A:311:ASP:O	1:A:314:GLY:N	2.43	0.52
1:E:235:GLU:OE1	1:E:240:HIS:HA	2.10	0.52
1:B:169:LEU:HD13	1:B:169:LEU:C	2.30	0.52
1:E:407:LEU:HD22	1:E:411:LEU:HG	1.91	0.52
1:E:405:GLU:HA	1:E:408:ARG:NH1	2.24	0.52
1:A:401:GLN:O	1:A:403:PRO:HD3	2.10	0.52
1:B:171:ARG:HB2	1:B:172:PHE:HD1	1.75	0.52
1:C:320:ARG:HG3	1:C:320:ARG:NH1	2.24	0.52
1:C:229:LYS:HD2	1:D:240:HIS:NE2	2.21	0.51
1:A:247:GLY:HA2	1:A:250:GLU:HG2	1.92	0.51
1:C:189:VAL:HG22	1:C:199:ARG:HD2	1.91	0.51
1:B:152:VAL:CG2	1:B:275:GLN:HE21	2.23	0.51
1:A:252:GLN:HA	1:A:255:ASN:O	2.10	0.51
1:D:306:CYS:HB3	1:D:308:TYR:CE1	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:247:GLY:HA2	1:D:250:GLU:HG2	1.91	0.51
1:A:275:GLN:HA	1:A:275:GLN:OE1	2.11	0.51
1:D:391:LEU:HD23	1:D:419:LEU:CD1	2.40	0.51
1:E:119:LEU:HD21	1:E:178:ASN:HB3	1.93	0.51
1:D:222:VAL:HG12	1:D:223:LEU:N	2.26	0.51
1:E:222:VAL:HG12	1:E:223:LEU:H	1.76	0.51
1:C:418:LYS:N	1:C:418:LYS:HD2	2.26	0.51
1:A:331:ASP:OD1	1:A:406:THR:HB	2.10	0.51
1:A:175:ASN:HD22	1:A:176:PRO:CD	2.23	0.51
1:B:143:LEU:HD13	1:B:153:ILE:HD12	1.93	0.51
1:E:163:PRO:HB3	1:E:202:GLU:CG	2.41	0.51
1:E:240:HIS:O	1:E:243:ARG:HB3	2.11	0.51
1:C:352:LYS:HG2	1:C:352:LYS:O	2.11	0.51
1:D:272:ALA:O	1:D:275:GLN:HB3	2.11	0.50
1:D:189:VAL:HG12	1:D:190:THR:N	2.26	0.50
1:D:240:HIS:CD2	1:D:243:ARG:HH21	2.28	0.50
1:A:149:SER:CB	1:A:275:GLN:HE22	2.25	0.50
1:D:199:ARG:HH11	1:D:199:ARG:HG2	1.75	0.50
1:B:312:ARG:HG2	1:B:316:ASP:OD2	2.12	0.50
1:A:290:THR:O	1:A:294:ILE:HG12	2.11	0.50
1:B:171:ARG:CB	1:B:172:PHE:HD1	2.25	0.50
1:E:200:PHE:CG	1:E:205:MSE:HE1	2.47	0.50
1:E:148:LEU:HD22	1:E:271:VAL:HG12	1.94	0.50
1:C:408:ARG:O	1:C:412:ARG:HG3	2.11	0.50
1:E:240:HIS:O	1:E:244:GLN:HG2	2.12	0.50
1:E:119:LEU:HD11	1:E:178:ASN:OD1	2.12	0.50
1:B:306:CYS:HB3	1:B:308:TYR:HE1	1.75	0.50
1:D:185:ALA:HA	1:D:236:THR:CG2	2.41	0.50
1:B:407:LEU:HD22	1:B:411:LEU:HG	1.93	0.50
1:A:137:THR:HB	1:C:428:GLU:CB	2.42	0.50
1:D:279:ASN:H	1:D:279:ASN:ND2	2.10	0.50
1:B:139:ALA:HA	1:B:223:LEU:HD21	1.93	0.50
1:C:190:THR:HA	1:C:195:ARG:O	2.12	0.50
1:B:146:ARG:HH12	1:B:268:MSE:CE	2.24	0.50
1:E:306:CYS:HB3	1:E:308:TYR:CE1	2.46	0.50
1:C:165:TRP:CH2	1:E:409:ILE:HG22	2.42	0.50
1:E:349:LEU:HD22	1:E:358:PHE:HD1	1.77	0.50
1:C:306:CYS:HB3	1:C:308:TYR:CE1	2.47	0.50
1:B:408:ARG:O	1:B:412:ARG:HG3	2.11	0.50
1:A:236:THR:OG1	1:A:238:ILE:HG22	2.10	0.50
1:A:175:ASN:ND2	1:A:177:GLU:H	2.09	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:392:SER:HB3	1:B:419:LEU:HD11	1.94	0.49
1:E:116:LEU:H	1:E:116:LEU:HD12	1.77	0.49
1:A:407:LEU:HD22	1:A:411:LEU:HG	1.94	0.49
1:C:165:TRP:CE2	1:E:413:GLN:CD	2.86	0.49
1:E:181:SER:C	1:E:184:ASP:OD1	2.50	0.49
1:B:119:LEU:HD21	1:B:178:ASN:HB3	1.94	0.49
1:C:349:LEU:HD22	1:C:358:PHE:HD1	1.77	0.49
1:E:224:GLY:O	1:E:226:ASP:N	2.45	0.49
1:C:165:TRP:CD1	1:E:413:GLN:NE2	2.78	0.49
1:B:390:ARG:O	1:B:393:THR:HB	2.12	0.49
1:B:156:PHE:CE2	1:B:250:GLU:HG3	2.47	0.49
1:A:280:TYR:OH	1:A:362:MSE:HE1	2.12	0.49
1:D:368:LEU:C	1:D:368:LEU:HD23	2.32	0.49
1:B:368:LEU:HD23	1:B:368:LEU:C	2.33	0.49
1:A:408:ARG:O	1:A:412:ARG:HG3	2.13	0.49
1:A:367:PRO:HG2	1:A:370:ALA:CB	2.42	0.49
1:C:165:TRP:HZ3	1:E:409:ILE:O	1.95	0.49
1:C:115:THR:N	1:C:118:GLN:OE1	2.37	0.49
1:A:417:ASN:C	1:A:419:LEU:H	2.16	0.49
1:E:390:ARG:O	1:E:393:THR:HB	2.12	0.49
1:C:346:PRO:O	1:C:350:VAL:CG2	2.60	0.49
1:B:273:LEU:CD2	1:B:350:VAL:HG21	2.42	0.49
1:C:284:SER:O	1:C:285:LEU:HB3	2.12	0.49
1:B:172:PHE:CD1	1:B:172:PHE:N	2.80	0.49
1:A:200:PHE:CG	1:A:205:MSE:HE1	2.47	0.49
1:D:390:ARG:O	1:D:393:THR:HB	2.12	0.49
1:A:349:LEU:HD21	1:A:353:GLU:CD	2.33	0.49
1:B:273:LEU:HB3	1:B:278:ILE:HB	1.94	0.49
1:B:353:GLU:O	1:B:357:ALA:HB3	2.12	0.49
1:C:178:ASN:O	1:C:181:SER:HB3	2.12	0.48
1:C:115:THR:HB	1:C:118:GLN:OE1	2.12	0.48
1:B:163:PRO:HB3	1:B:202:GLU:CG	2.43	0.48
1:C:290:THR:O	1:C:293:HIS:HB2	2.13	0.48
1:B:242:GLY:O	1:B:292:ASP:HB2	2.13	0.48
1:E:280:TYR:OH	1:E:362:MSE:HE1	2.13	0.48
1:C:115:THR:HG23	1:C:117:TYR:N	2.27	0.48
1:B:180:GLN:OE1	1:B:184:ASP:OD1	2.31	0.48
1:A:344:GLU:OE1	1:A:348:THR:CG2	2.61	0.48
1:D:240:HIS:HD2	1:D:243:ARG:NH2	2.12	0.48
1:A:239:PHE:HZ	1:A:285:LEU:HD21	1.76	0.48
1:A:390:ARG:O	1:A:393:THR:HB	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:149:SER:HB3	1:E:275:GLN:HE22	1.78	0.48
1:A:377:MSE:HE1	1:A:418:LYS:HE2	1.95	0.48
1:C:384:THR:HG22	1:C:386:ASP:N	2.23	0.48
1:B:189:VAL:HG12	1:B:190:THR:N	2.29	0.48
1:C:288:SER:O	1:C:290:THR:HG23	2.14	0.48
1:C:419:LEU:HD12	1:C:421:ILE:CD1	2.44	0.48
1:E:186:GLY:HA2	1:E:199:ARG:NH1	2.28	0.48
1:A:412:ARG:NH2	1:A:427:LEU:O	2.46	0.48
1:A:382:LEU:HD13	1:A:418:LYS:O	2.14	0.48
1:E:235:GLU:CA	1:E:235:GLU:OE2	2.62	0.48
1:B:349:LEU:CD2	1:B:353:GLU:OE1	2.56	0.48
1:E:222:VAL:CG1	1:E:223:LEU:N	2.76	0.48
1:E:189:VAL:HG22	1:E:199:ARG:CZ	2.44	0.48
1:C:163:PRO:HB3	1:C:202:GLU:CG	2.44	0.48
1:E:301:THR:CG2	1:E:302:ASN:N	2.77	0.47
1:D:228:PRO:HG2	1:D:231:LEU:HD13	1.95	0.47
1:A:311:ASP:O	1:A:312:ARG:C	2.52	0.47
1:A:306:CYS:HB3	1:A:308:TYR:CE1	2.49	0.47
1:D:301:THR:CG2	1:D:302:ASN:N	2.76	0.47
1:E:236:THR:HG23	1:E:238:ILE:CG2	2.44	0.47
1:D:384:THR:HG22	1:D:386:ASP:HB2	1.96	0.47
1:A:135:VAL:O	1:C:428:GLU:HA	2.14	0.47
1:C:200:PHE:CG	1:C:205:MSE:HE1	2.49	0.47
1:C:376:LEU:HD22	1:C:394:LEU:HD23	1.96	0.47
1:D:193:GLN:O	1:D:193:GLN:CG	2.62	0.47
1:C:165:TRP:CE3	1:E:409:ILE:CG2	2.94	0.47
1:E:191:ASN:ND2	1:E:192:ASP:N	2.35	0.47
1:C:343:GLY:CA	1:D:212:ARG:NH2	2.77	0.47
1:C:190:THR:HG22	1:C:196:SER:CB	2.44	0.47
1:A:191:ASN:HD21	1:A:195:ARG:N	2.07	0.47
1:B:176:PRO:O	1:B:179:ARG:HB3	2.14	0.47
1:E:213:GLY:CA	1:E:249:TYR:CE1	2.97	0.47
1:A:368:LEU:C	1:A:368:LEU:HD23	2.34	0.47
1:C:165:TRP:HH2	1:E:410:TYR:CA	2.21	0.47
1:C:240:HIS:HD2	1:C:243:ARG:CZ	2.28	0.47
1:A:417:ASN:C	1:A:419:LEU:N	2.65	0.47
1:A:116:LEU:HD12	1:A:238:ILE:CD1	2.36	0.47
1:D:311:ASP:OD1	1:D:313:ALA:N	2.48	0.47
1:C:213:GLY:HA2	1:C:249:TYR:CD1	2.49	0.47
1:C:355:LYS:O	1:C:356:GLU:C	2.52	0.47
1:A:301:THR:CG2	1:A:302:ASN:N	2.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:115:THR:HG22	1:C:118:GLN:CG	2.41	0.47
1:B:248:LEU:HD11	1:B:296:LEU:HD22	1.97	0.47
1:E:189:VAL:HG22	1:E:199:ARG:NH1	2.30	0.47
1:D:152:VAL:HG21	1:D:275:GLN:NE2	2.29	0.47
1:A:166:ASP:CG	1:A:170:LYS:HE3	2.35	0.47
1:C:316:ASP:O	1:C:320:ARG:NH1	2.48	0.47
1:D:280:TYR:OH	1:D:362:MSE:HE1	2.15	0.47
1:B:160:PHE:HE1	1:B:223:LEU:HD11	1.79	0.47
1:E:276:TYR:CD2	1:E:350:VAL:HG12	2.50	0.47
1:D:189:VAL:HG21	1:D:199:ARG:HD3	1.96	0.47
1:D:414:GLU:HB3	1:D:418:LYS:NZ	2.29	0.47
1:E:125:THR:O	1:E:129:GLN:HG3	2.15	0.47
1:D:394:LEU:HD12	1:D:394:LEU:N	2.30	0.46
1:C:394:LEU:O	1:C:397:PRO:HD2	2.15	0.46
1:E:368:LEU:C	1:E:368:LEU:HD23	2.35	0.46
1:A:163:PRO:HB3	1:A:202:GLU:CG	2.46	0.46
1:B:388:ARG:HB3	1:B:419:LEU:CD2	2.45	0.46
1:E:284:SER:C	1:E:286:GLY:H	2.18	0.46
1:C:394:LEU:HD12	1:C:394:LEU:N	2.30	0.46
1:D:165:TRP:HB3	1:D:201:ARG:HD3	1.97	0.46
1:E:248:LEU:HD11	1:E:296:LEU:HD22	1.98	0.46
1:B:388:ARG:HB3	1:B:419:LEU:HD22	1.97	0.46
1:B:116:LEU:HD23	1:B:119:LEU:HD12	1.97	0.46
1:A:394:LEU:N	1:A:394:LEU:HD12	2.30	0.46
1:A:175:ASN:HD22	1:A:176:PRO:HD2	1.81	0.46
1:A:349:LEU:HD23	1:A:353:GLU:CG	2.45	0.46
1:D:311:ASP:OD1	1:D:313:ALA:HB3	2.15	0.46
1:C:248:LEU:HD11	1:C:296:LEU:HD22	1.96	0.46
1:B:349:LEU:HD22	1:B:358:PHE:HD1	1.81	0.46
1:D:349:LEU:HD22	1:D:358:PHE:HD1	1.81	0.46
1:C:347:ASP:O	1:C:350:VAL:HG23	2.15	0.46
1:E:165:TRP:HB2	1:E:197:TYR:HB2	1.98	0.46
1:E:247:GLY:HA2	1:E:250:GLU:CG	2.46	0.46
1:C:166:ASP:HB2	1:C:170:LYS:HG3	1.98	0.46
1:B:165:TRP:HB3	1:B:201:ARG:HD3	1.98	0.46
1:C:213:GLY:HA3	1:C:249:TYR:CE1	2.51	0.46
1:D:163:PRO:HB3	1:D:202:GLU:CG	2.46	0.46
1:C:247:GLY:HA2	1:C:250:GLU:CG	2.45	0.46
1:B:394:LEU:HD12	1:B:394:LEU:N	2.30	0.46
1:C:175:ASN:O	1:C:179:ARG:HB2	2.16	0.46
1:E:353:GLU:O	1:E:357:ALA:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:200:PHE:CG	1:D:205:MSE:HE1	2.50	0.46
1:D:331:ASP:OD1	1:D:406:THR:HB	2.16	0.46
1:C:165:TRP:CZ3	1:E:409:ILE:C	2.89	0.46
1:B:376:LEU:HD22	1:B:394:LEU:HD23	1.97	0.46
1:A:248:LEU:HD11	1:A:296:LEU:HD22	1.98	0.45
1:D:384:THR:CG2	1:D:386:ASP:HB2	2.47	0.45
1:B:197:TYR:HE1	1:B:201:ARG:HH21	1.64	0.45
1:A:248:LEU:CD1	1:A:296:LEU:HD22	2.46	0.45
1:B:179:ARG:O	1:B:183:ILE:HG13	2.16	0.45
1:D:203:ARG:NH2	1:D:231:LEU:HB2	2.31	0.45
1:E:394:LEU:N	1:E:394:LEU:HD12	2.31	0.45
1:B:247:GLY:HA2	1:B:250:GLU:CG	2.45	0.45
1:E:235:GLU:OE2	1:E:241:LYS:CG	2.64	0.45
1:C:368:LEU:C	1:C:368:LEU:HD23	2.37	0.45
1:A:243:ARG:O	1:A:244:GLN:OE1	2.35	0.45
1:E:175:ASN:HA	1:E:176:PRO:HD2	1.86	0.45
1:E:165:TRP:HB3	1:E:201:ARG:HD3	1.98	0.45
1:C:280:TYR:OH	1:C:362:MSE:HE1	2.16	0.45
1:A:165:TRP:HB2	1:A:197:TYR:HB2	1.97	0.45
1:E:306:CYS:HB3	1:E:308:TYR:HE1	1.80	0.45
1:D:243:ARG:O	1:D:296:LEU:HD12	2.17	0.45
1:A:236:THR:HG1	1:A:238:ILE:HG23	1.82	0.45
1:B:122:GLY:HA3	1:B:172:PHE:HE2	1.81	0.45
1:A:344:GLU:OE2	1:B:214:ARG:NH2	2.50	0.45
1:D:247:GLY:HA2	1:D:250:GLU:CG	2.46	0.45
1:D:125:THR:O	1:D:129:GLN:HG3	2.16	0.45
1:D:210:ASP:OD1	1:D:212:ARG:HB2	2.16	0.45
1:D:384:THR:O	1:D:388:ARG:HG3	2.17	0.45
1:C:260:ARG:CA	1:C:301:THR:HG21	2.45	0.45
1:B:222:VAL:HG12	1:B:223:LEU:H	1.80	0.45
1:C:356:GLU:HG3	1:C:356:GLU:H	1.62	0.45
1:B:384:THR:O	1:B:388:ARG:HG3	2.17	0.45
1:D:377:MSE:HE1	1:D:418:LYS:CD	2.37	0.45
1:B:133:GLN:O	1:B:140:ARG:NH2	2.49	0.45
1:D:348:THR:O	1:D:352:LYS:HG3	2.17	0.45
1:D:306:CYS:HB3	1:D:308:TYR:HE1	1.81	0.44
1:A:394:LEU:O	1:A:397:PRO:HD2	2.16	0.44
1:D:248:LEU:HD11	1:D:296:LEU:HD22	1.98	0.44
1:B:167:ASN:O	1:B:171:ARG:HD3	2.17	0.44
1:C:320:ARG:HG3	1:C:320:ARG:HH11	1.81	0.44
1:C:165:TRP:HB3	1:C:201:ARG:HD3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:PHE:CE2	1:B:162:PRO:HA	2.53	0.44
1:B:171:ARG:HG2	1:B:171:ARG:NH1	2.32	0.44
1:B:165:TRP:HB2	1:B:197:TYR:HB2	1.99	0.44
1:E:115:THR:O	1:E:116:LEU:C	2.56	0.44
1:E:118:GLN:HB2	1:E:118:GLN:HE21	1.59	0.44
1:E:376:LEU:HD22	1:E:394:LEU:HD23	1.99	0.44
1:C:275:GLN:O	1:C:275:GLN:OE1	2.36	0.44
1:D:292:ASP:O	1:D:296:LEU:HB2	2.18	0.44
1:C:189:VAL:O	1:C:196:SER:HA	2.18	0.44
1:A:210:ASP:OD1	1:A:214:ARG:HG2	2.18	0.44
1:B:278:ILE:HD11	1:B:355:LYS:HG3	2.00	0.44
1:C:343:GLY:N	1:D:212:ARG:HH22	2.16	0.44
1:C:115:THR:HG23	1:C:117:TYR:H	1.82	0.44
1:D:421:ILE:CG2	1:D:422:LEU:N	2.81	0.44
1:C:384:THR:O	1:C:388:ARG:HG3	2.18	0.44
1:E:188:LEU:O	1:E:199:ARG:NH1	2.51	0.44
1:E:189:VAL:HG23	1:E:199:ARG:HG3	1.94	0.44
1:C:119:LEU:O	1:C:123:LEU:CD1	2.66	0.44
1:A:175:ASN:ND2	1:A:175:ASN:C	2.71	0.44
1:A:186:GLY:O	1:A:199:ARG:NH1	2.50	0.44
1:D:168:VAL:C	1:D:170:LYS:N	2.71	0.43
1:E:197:TYR:HE1	1:E:201:ARG:HH21	1.65	0.43
1:B:152:VAL:HG21	1:B:275:GLN:HE21	1.83	0.43
1:A:303:ASN:HD21	1:A:336:ARG:HH21	1.66	0.43
1:E:235:GLU:O	1:E:236:THR:HB	2.17	0.43
1:C:142:TYR:OH	1:C:221:ARG:NH1	2.51	0.43
1:A:189:VAL:CG2	1:A:199:ARG:HD3	2.48	0.43
1:B:163:PRO:HB3	1:B:202:GLU:CD	2.39	0.43
1:C:180:GLN:HA	1:C:180:GLN:OE1	2.17	0.43
1:D:384:THR:HG22	1:D:386:ASP:N	2.24	0.43
1:C:275:GLN:O	1:C:275:GLN:CD	2.57	0.43
1:C:301:THR:CG2	1:C:302:ASN:N	2.78	0.43
1:C:342:ASP:OD1	1:D:212:ARG:NH2	2.52	0.43
1:D:199:ARG:NH1	1:D:199:ARG:HG2	2.33	0.43
1:E:394:LEU:O	1:E:397:PRO:HD2	2.19	0.43
1:E:295:GLN:O	1:E:299:ARG:HG3	2.19	0.43
1:E:182:LEU:HD22	1:E:188:LEU:HD11	2.01	0.43
1:A:182:LEU:HA	1:A:182:LEU:HD12	1.79	0.43
1:A:133:GLN:HB3	1:C:424:ASP:O	2.18	0.43
1:A:239:PHE:CZ	1:A:285:LEU:CD2	2.95	0.43
1:E:203:ARG:NH2	1:E:231:LEU:HB2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:405:GLU:O	1:D:406:THR:C	2.57	0.43
1:E:163:PRO:HB3	1:E:202:GLU:CD	2.39	0.43
1:D:195:ARG:HG3	1:D:195:ARG:HH11	1.83	0.43
1:A:258:PRO:O	1:A:301:THR:HG23	2.18	0.43
1:B:354:GLY:O	1:B:355:LYS:C	2.57	0.43
1:D:376:LEU:HD22	1:D:394:LEU:HD23	2.01	0.43
1:A:349:LEU:HD22	1:A:358:PHE:HD1	1.83	0.43
1:C:340:LEU:HD13	1:C:345:ASP:HA	2.01	0.43
1:A:147:GLY:O	1:A:275:GLN:HG2	2.19	0.43
1:C:342:ASP:CG	1:D:212:ARG:HH22	2.22	0.43
1:C:344:GLU:OE1	1:C:348:THR:CG2	2.66	0.43
1:E:115:THR:HA	1:E:118:GLN:NE2	2.34	0.43
1:C:163:PRO:HB3	1:C:202:GLU:CD	2.40	0.43
1:C:423:ASP:C	1:C:425:SER:N	2.58	0.43
1:E:384:THR:O	1:E:388:ARG:HG3	2.19	0.43
1:A:384:THR:O	1:A:388:ARG:HG3	2.19	0.43
1:C:240:HIS:O	1:C:242:GLY:N	2.51	0.43
1:D:119:LEU:O	1:D:123:LEU:HD13	2.19	0.43
1:B:352:LYS:HB2	1:B:352:LYS:HE3	1.76	0.43
1:D:214:ARG:O	1:D:216:ILE:HG23	2.18	0.42
1:B:356:GLU:O	1:B:357:ALA:C	2.57	0.42
1:E:174:GLY:O	1:E:175:ASN:O	2.37	0.42
1:A:197:TYR:HE1	1:A:201:ARG:HH21	1.67	0.42
1:E:249:TYR:O	1:E:253:GLN:HG2	2.19	0.42
1:A:151:GLU:O	1:A:152:VAL:C	2.57	0.42
1:E:236:THR:HG22	1:E:239:PHE:HB3	2.01	0.42
1:E:190:THR:HG22	1:E:196:SER:CB	2.48	0.42
1:E:186:GLY:C	1:E:199:ARG:NH1	2.72	0.42
1:B:134:PRO:O	1:B:137:THR:OG1	2.28	0.42
1:C:240:HIS:HB2	1:C:243:ARG:HE	1.84	0.42
1:B:203:ARG:NH2	1:B:231:LEU:HB2	2.34	0.42
1:D:197:TYR:HE1	1:D:201:ARG:HH21	1.65	0.42
1:A:156:PHE:CE2	1:A:250:GLU:HG3	2.53	0.42
1:A:247:GLY:HA2	1:A:250:GLU:CG	2.48	0.42
1:B:316:ASP:O	1:B:320:ARG:HG2	2.19	0.42
1:A:352:LYS:HB2	1:A:352:LYS:HE3	1.83	0.42
1:A:331:ASP:CG	1:A:406:THR:HB	2.39	0.42
1:C:238:ILE:HG13	1:C:239:PHE:N	2.34	0.42
1:A:125:THR:O	1:A:129:GLN:HG3	2.19	0.42
1:C:229:LYS:NZ	1:D:240:HIS:CE1	2.86	0.42
1:C:116:LEU:O	1:C:116:LEU:HD23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:ARG:HB3	1:B:172:PHE:CE1	2.54	0.42
1:A:376:LEU:HD22	1:A:394:LEU:HD23	2.01	0.42
1:D:249:TYR:O	1:D:253:GLN:HG2	2.20	0.42
1:B:311:ASP:OD2	1:B:313:ALA:HB3	2.19	0.42
1:C:203:ARG:NH2	1:C:231:LEU:HB2	2.35	0.42
1:B:298:PHE:HA	1:B:301:THR:O	2.19	0.42
1:D:301:THR:CG2	1:D:302:ASN:H	2.31	0.42
1:B:137:THR:C	1:B:141:GLN:HE21	2.22	0.42
1:B:421:ILE:CG2	1:B:422:LEU:H	2.32	0.42
1:B:382:LEU:HD13	1:B:418:LYS:O	2.19	0.42
1:B:301:THR:CG2	1:B:302:ASN:N	2.78	0.42
1:A:298:PHE:HA	1:A:301:THR:O	2.20	0.42
1:E:235:GLU:OE2	1:E:241:LYS:CD	2.67	0.42
1:C:185:ALA:O	1:C:234:PRO:HD2	2.20	0.42
1:C:316:ASP:C	1:C:320:ARG:HH12	2.22	0.42
1:C:248:LEU:CD1	1:C:296:LEU:HD22	2.50	0.42
1:C:295:GLN:OE1	1:C:328:TYR:CE2	2.72	0.42
1:C:125:THR:O	1:C:129:GLN:HG3	2.19	0.42
1:D:386:ASP:O	1:D:389:ALA:HB3	2.20	0.42
1:D:350:VAL:C	1:D:352:LYS:N	2.73	0.42
1:C:166:ASP:HA	1:C:169:LEU:HB3	2.02	0.42
1:B:221:ARG:HA	1:B:229:LYS:O	2.19	0.42
1:C:306:CYS:HB3	1:C:308:TYR:HE1	1.82	0.42
1:C:349:LEU:O	1:C:353:GLU:CB	2.67	0.42
1:C:405:GLU:O	1:C:406:THR:C	2.58	0.42
1:A:151:GLU:O	1:A:154:ALA:N	2.52	0.42
1:C:197:TYR:HE1	1:C:201:ARG:HH21	1.68	0.42
1:D:212:ARG:CB	1:D:214:ARG:HG2	2.49	0.42
1:C:208:ILE:HD13	1:C:285:LEU:CD1	2.42	0.42
1:A:133:GLN:O	1:A:140:ARG:NH2	2.52	0.42
1:B:125:THR:O	1:B:129:GLN:HG3	2.20	0.42
1:C:298:PHE:HA	1:C:301:THR:O	2.20	0.41
1:D:303:ASN:HD21	1:D:336:ARG:HH21	1.67	0.41
1:D:148:LEU:HA	1:D:275:GLN:HE21	1.84	0.41
1:A:405:GLU:O	1:A:406:THR:C	2.58	0.41
1:C:119:LEU:HD21	1:C:178:ASN:HD22	1.85	0.41
1:E:128:GLN:NE2	1:E:157:ALA:HA	2.35	0.41
1:C:160:PHE:CE2	1:C:162:PRO:HA	2.55	0.41
1:A:185:ALA:O	1:A:234:PRO:HD2	2.20	0.41
1:D:373:PHE:CB	1:D:418:LYS:HE2	2.50	0.41
1:D:140:ARG:O	1:D:144:GLU:HB2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:279:ASN:N	1:C:279:ASN:ND2	2.56	0.41
1:D:255:ASN:HD22	1:D:255:ASN:N	2.17	0.41
1:B:421:ILE:HG22	1:B:423:ASP:N	2.35	0.41
1:D:185:ALA:HA	1:D:236:THR:HG21	2.01	0.41
1:B:249:TYR:O	1:B:253:GLN:HG2	2.20	0.41
1:B:138:SER:OG	1:D:428:GLU:O	2.36	0.41
1:E:246:TYR:O	1:E:282:VAL:HA	2.21	0.41
1:B:325:ALA:O	1:B:326:LEU:C	2.58	0.41
1:C:133:GLN:O	1:C:140:ARG:NH2	2.51	0.41
1:E:405:GLU:O	1:E:406:THR:C	2.58	0.41
1:E:295:GLN:OE1	1:E:328:TYR:CE2	2.73	0.41
1:E:401:GLN:O	1:E:403:PRO:HD3	2.21	0.41
1:A:309:ASP:HB2	1:B:299:ARG:HH22	1.85	0.41
1:C:165:TRP:CE3	1:E:409:ILE:HG23	2.56	0.41
1:A:203:ARG:NH2	1:A:231:LEU:HB2	2.36	0.41
1:D:203:ARG:NH2	1:D:228:PRO:O	2.36	0.41
1:D:277:GLY:O	1:D:279:ASN:ND2	2.42	0.41
1:B:384:THR:HG23	1:B:385:PRO:HD2	2.01	0.41
1:B:295:GLN:OE1	1:B:328:TYR:CE2	2.74	0.41
1:B:394:LEU:CD1	1:B:394:LEU:N	2.84	0.41
1:B:340:LEU:HD13	1:B:345:ASP:HA	2.02	0.41
1:B:124:ASN:ND2	1:B:124:ASN:C	2.74	0.41
1:C:381:ASP:O	1:C:387:GLY:HA3	2.21	0.41
1:D:295:GLN:OE1	1:D:328:TYR:CE2	2.73	0.41
1:C:320:ARG:CG	1:C:320:ARG:HH11	2.34	0.41
1:B:216:ILE:HB	1:B:238:ILE:O	2.20	0.41
1:B:401:GLN:O	1:B:403:PRO:HD3	2.20	0.41
1:C:115:THR:CG2	1:C:118:GLN:HG3	2.44	0.41
1:B:134:PRO:HG2	1:D:425:SER:CA	2.47	0.41
1:D:349:LEU:HD21	1:D:353:GLU:CD	2.41	0.41
1:C:166:ASP:OD2	1:C:170:LYS:HE3	2.20	0.41
1:E:340:LEU:HD13	1:E:345:ASP:HA	2.02	0.41
1:A:374:ASN:O	1:A:378:PRO:HD3	2.21	0.41
1:B:280:TYR:OH	1:B:362:MSE:HE1	2.21	0.41
1:D:419:LEU:HB3	1:D:421:ILE:HG13	2.02	0.41
1:A:394:LEU:N	1:A:394:LEU:CD1	2.84	0.41
1:A:417:ASN:N	1:A:417:ASN:HD22	2.17	0.41
1:D:165:TRP:HB2	1:D:197:TYR:HB2	2.03	0.41
1:D:312:ARG:HA	1:D:315:ARG:NH2	2.36	0.41
1:B:185:ALA:O	1:B:234:PRO:HD2	2.21	0.41
1:C:168:VAL:HB	1:C:198:ASP:OD2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:165:TRP:HB2	1:C:197:TYR:HB2	2.02	0.41
1:B:405:GLU:O	1:B:406:THR:C	2.58	0.41
1:E:190:THR:HG22	1:E:196:SER:CA	2.51	0.41
1:A:313:ALA:HB3	1:B:299:ARG:HE	1.86	0.41
1:C:150:HIS:ND1	1:C:150:HIS:N	2.69	0.41
1:C:374:ASN:O	1:C:378:PRO:HD3	2.21	0.41
1:D:235:GLU:HG2	1:D:241:LYS:CG	2.48	0.40
1:A:284:SER:C	1:A:286:GLY:H	2.24	0.40
1:A:301:THR:CG2	1:A:302:ASN:H	2.32	0.40
1:E:178:ASN:HA	1:E:178:ASN:HD22	1.66	0.40
1:E:384:THR:HG23	1:E:385:PRO:HD2	2.04	0.40
1:E:189:VAL:HG12	1:E:190:THR:N	2.36	0.40
1:B:189:VAL:HG22	1:B:199:ARG:HD2	2.01	0.40
1:E:243:ARG:CG	1:E:243:ARG:O	2.69	0.40
1:C:240:HIS:CD2	1:C:243:ARG:CZ	3.05	0.40
1:A:249:TYR:O	1:A:253:GLN:HG2	2.21	0.40
1:A:165:TRP:N	1:A:165:TRP:CD1	2.90	0.40
1:E:414:GLU:O	1:E:418:LYS:HG2	2.22	0.40
1:D:394:LEU:N	1:D:394:LEU:CD1	2.84	0.40
1:C:394:LEU:CD1	1:C:394:LEU:N	2.84	0.40
1:D:381:ASP:C	1:D:381:ASP:OD1	2.60	0.40
1:A:173:GLY:O	1:A:174:GLY:C	2.59	0.40
1:D:355:LYS:HE3	1:D:359:GLU:OE1	2.21	0.40
1:D:142:TYR:O	1:D:146:ARG:HG2	2.22	0.40
1:E:185:ALA:O	1:E:234:PRO:HD2	2.20	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	313/321 (98%)	273 (87%)	37 (12%)	3 (1%)	19 54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	311/321 (97%)	272 (88%)	33 (11%)	6 (2%)	10 35
1	C	313/321 (98%)	264 (84%)	40 (13%)	9 (3%)	6 23
1	D	312/321 (97%)	259 (83%)	48 (15%)	5 (2%)	12 40
1	E	306/321 (95%)	261 (85%)	36 (12%)	9 (3%)	6 23
All	All	1555/1605 (97%)	1329 (86%)	194 (12%)	32 (2%)	9 32

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	287	THR
1	B	424	ASP
1	C	342	ASP
1	C	356	GLU
1	C	424	ASP
1	E	192	ASP
1	E	238	ILE
1	C	225	ASN
1	C	355	LYS
1	D	238	ILE
1	E	175	ASN
1	E	225	ASN
1	A	312	ARG
1	A	418	LYS
1	C	241	LYS
1	C	427	LEU
1	D	243	ARG
1	D	344	GLU
1	D	356	GLU
1	B	193	GLN
1	C	265	GLU
1	C	347	ASP
1	D	351	ARG
1	E	342	ASP
1	E	116	LEU
1	E	260	ARG
1	B	353	GLU
1	E	236	THR
1	B	224	GLY
1	A	238	ILE
1	E	173	GLY
1	B	238	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	251/258 (97%)	230 (92%)	21 (8%)	14	37
1	B	248/258 (96%)	233 (94%)	15 (6%)	24	57
1	C	250/258 (97%)	233 (93%)	17 (7%)	20	49
1	D	246/258 (95%)	232 (94%)	14 (6%)	25	59
1	E	240/258 (93%)	222 (92%)	18 (8%)	17	44
All	All	1235/1290 (96%)	1150 (93%)	85 (7%)	19	48

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	131	LEU
1	A	141	GLN
1	A	151	GLU
1	A	165	TRP
1	A	175	ASN
1	A	182	LEU
1	A	190	THR
1	A	191	ASN
1	A	195	ARG
1	A	212	ARG
1	A	214	ARG
1	A	226	ASP
1	A	227	THR
1	A	238	ILE
1	A	244	GLN
1	A	248	LEU
1	A	295	GLN
1	A	303	ASN
1	A	345	ASP
1	A	407	LEU
1	A	408	ARG
1	B	124	ASN
1	B	131	LEU

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Mol	Chain	Res	Type
1	B	165	TRP
1	B	171	ARG
1	B	181	SER
1	B	248	LEU
1	B	278	ILE
1	B	290	THR
1	B	292	ASP
1	B	303	ASN
1	B	320	ARG
1	B	331	ASP
1	B	364	GLN
1	B	407	LEU
1	B	424	ASP
1	C	115	THR
1	C	131	LEU
1	C	146	ARG
1	C	150	HIS
1	C	165	TRP
1	C	179	ARG
1	C	184	ASP
1	C	192	ASP
1	C	211	LYS
1	C	248	LEU
1	C	275	GLN
1	C	279	ASN
1	C	303	ASN
1	C	345	ASP
1	C	350	VAL
1	C	356	GLU
1	C	407	LEU
1	D	115	THR
1	D	118	GLN
1	D	131	LEU
1	D	144	GLU
1	D	165	TRP
1	D	227	THR
1	D	243	ARG
1	D	248	LEU
1	D	303	ASN
1	D	320	ARG
1	D	353	GLU
1	D	407	LEU

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Mol	Chain	Res	Type
1	D	419	LEU
1	D	422	LEU
1	E	118	GLN
1	E	131	LEU
1	E	141	GLN
1	E	165	TRP
1	E	182	LEU
1	E	184	ASP
1	E	191	ASN
1	E	199	ARG
1	E	212	ARG
1	E	214	ARG
1	E	235	GLU
1	E	243	ARG
1	E	248	LEU
1	E	292	ASP
1	E	303	ASN
1	E	312	ARG
1	E	364	GLN
1	E	407	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	GLN
1	A	175	ASN
1	A	178	ASN
1	A	180	GLN
1	A	191	ASN
1	A	255	ASN
1	A	275	GLN
1	A	293	HIS
1	A	295	GLN
1	A	303	ASN
1	A	374	ASN
1	A	417	ASN
1	B	133	GLN
1	B	141	GLN
1	B	180	GLN
1	B	255	ASN
1	B	275	GLN
1	B	295	GLN

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Mol	Chain	Res	Type
1	B	303	ASN
1	B	374	ASN
1	B	426	GLN
1	C	128	GLN
1	C	191	ASN
1	C	240	HIS
1	C	255	ASN
1	C	279	ASN
1	C	295	GLN
1	C	303	ASN
1	C	374	ASN
1	D	128	GLN
1	D	141	GLN
1	D	255	ASN
1	D	275	GLN
1	D	295	GLN
1	D	303	ASN
1	D	374	ASN
1	E	118	GLN
1	E	128	GLN
1	E	178	ASN
1	E	191	ASN
1	E	193	GLN
1	E	255	ASN
1	E	295	GLN
1	E	303	ASN
1	E	374	ASN

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 carbohydrates 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	306/321 (95%)	-0.20	2 (0%) 89 88	13, 40, 70, 87	0
1	B	304/321 (94%)	0.13	15 (4%) 33 27	17, 49, 88, 100	0
1	C	306/321 (95%)	0.16	13 (4%) 40 33	20, 50, 81, 98	0
1	D	305/321 (95%)	-0.15	4 (1%) 79 78	10, 40, 67, 88	0
1	E	299/321 (93%)	0.11	7 (2%) 64 59	21, 55, 85, 100	0
All	All	1520/1605 (94%)	0.01	41 (2%) 58 52	10, 47, 81, 100	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	422	LEU	5.2
1	B	194	GLY	4.9
1	B	192	ASP	4.1
1	B	195	ARG	3.7
1	E	195	ARG	3.7
1	C	422	LEU	3.5
1	C	165	TRP	3.4
1	A	287	THR	3.0
1	E	240	HIS	3.0
1	B	193	GLN	2.9
1	C	254	ASP	2.9
1	B	351	ARG	2.7
1	C	384	THR	2.6
1	C	227	THR	2.6
1	B	423	ASP	2.6
1	A	113	ARG	2.5
1	C	197	TYR	2.5
1	C	225	ASN	2.5
1	E	287	THR	2.4
1	B	287	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	379	GLN	2.4
1	C	224	GLY	2.4
1	E	380	VAL	2.3
1	C	277	GLY	2.3
1	B	198	ASP	2.3
1	B	191	ASN	2.3
1	E	225	ASN	2.3
1	C	313	ALA	2.3
1	B	173	GLY	2.2
1	B	226	ASP	2.2
1	C	275	GLN	2.2
1	D	316	ASP	2.1
1	E	311	ASP	2.1
1	B	342	ASP	2.1
1	D	342	ASP	2.1
1	B	177	GLU	2.1
1	C	255	ASN	2.1
1	E	186	GLY	2.1
1	B	165	TRP	2.1
1	C	147	GLY	2.0
1	B	190	THR	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.