



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:29 AM UTC

PDB ID : 3HAI / pdb_00003hai
Title : Crystal structure of human PACSIN1 F-BAR domain (P21 lattice)
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Deposited on : 2009-05-01
Resolution : 2.88 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

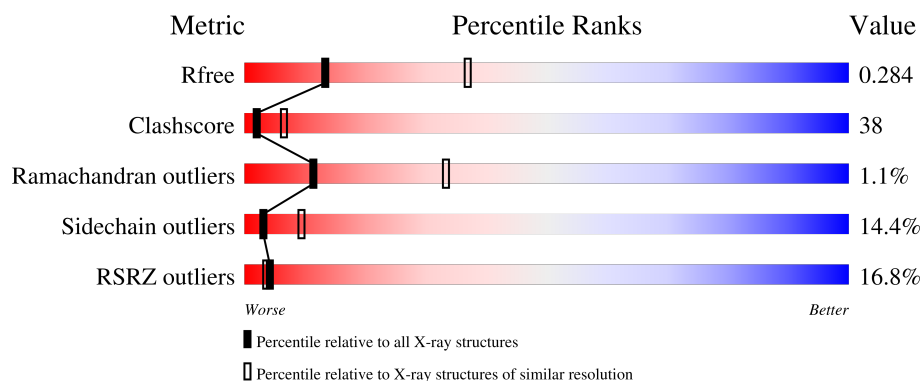
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.88 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3557 (2.90-2.86)
Clashscore	190562	3801 (2.90-2.86)
Ramachandran outliers	187476	3699 (2.90-2.86)
Sidechain outliers	187428	3702 (2.90-2.86)
RSRZ outliers	180081	3558 (2.90-2.86)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	308	21% 38% 45% 12% 5%
1	B	308	11% 37% 50% 8% 5%
1	C	308	12% 36% 49% 7% 7%
1	D	308	19% 39% 41% 10% 10%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9553 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 human PACSIN1 F-BAR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	294	Total	C	N	O	S	0	0	0
			2441	1529	432	465	15			
1	B	294	Total	C	N	O	S	0	0	0
			2438	1527	432	464	15			
1	C	285	Total	C	N	O	S	0	0	0
			2359	1477	420	447	15			
1	D	276	Total	C	N	O	S	0	0	0
			2294	1441	408	430	15			

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

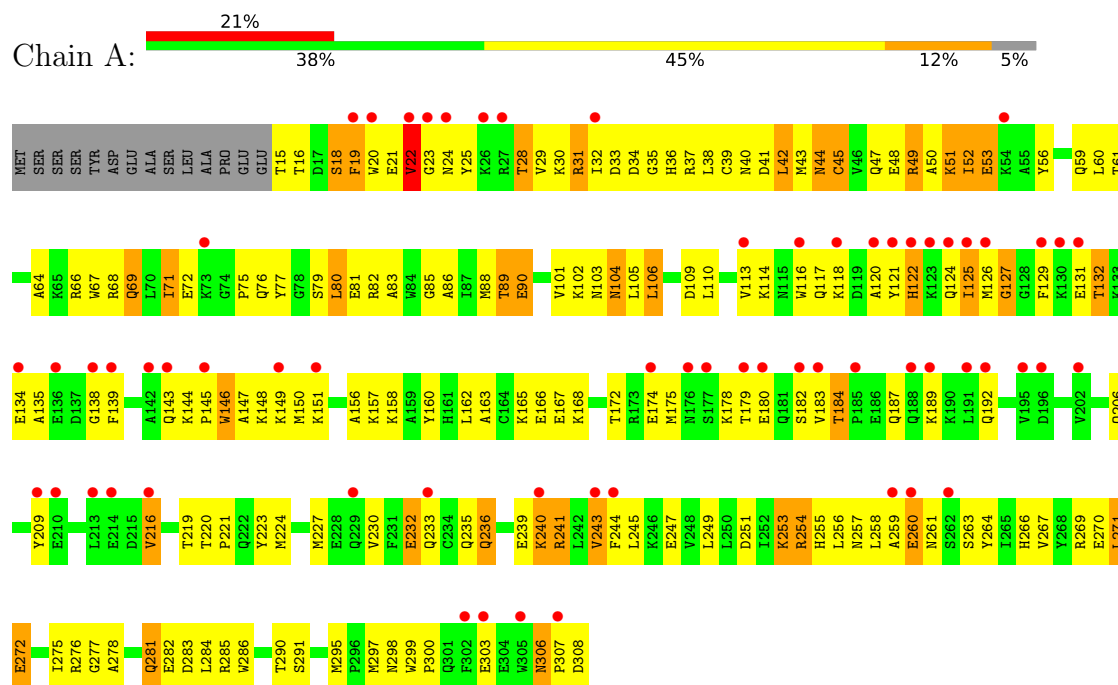
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	5	Total	O	0	0
			5	5		
3	B	10	Total	O	0	0
			10	10		
3	C	2	Total	O	0	0
			2	2		
3	D	3	Total	O	0	0
			3	3		

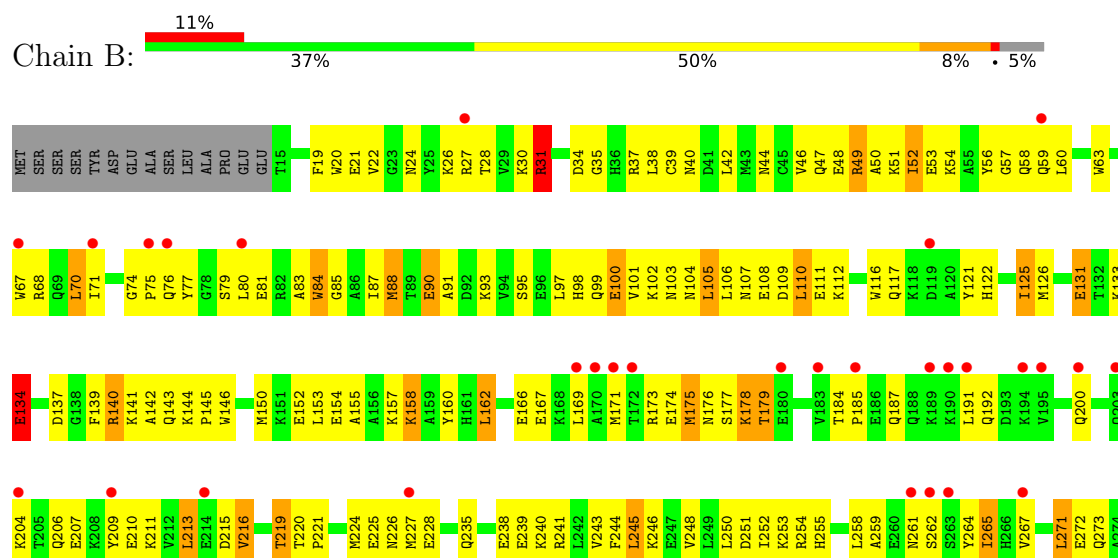
3 Residue-property plots

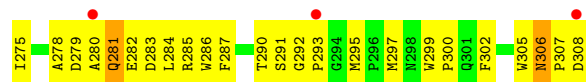
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: human PACSIN1 F-BAR

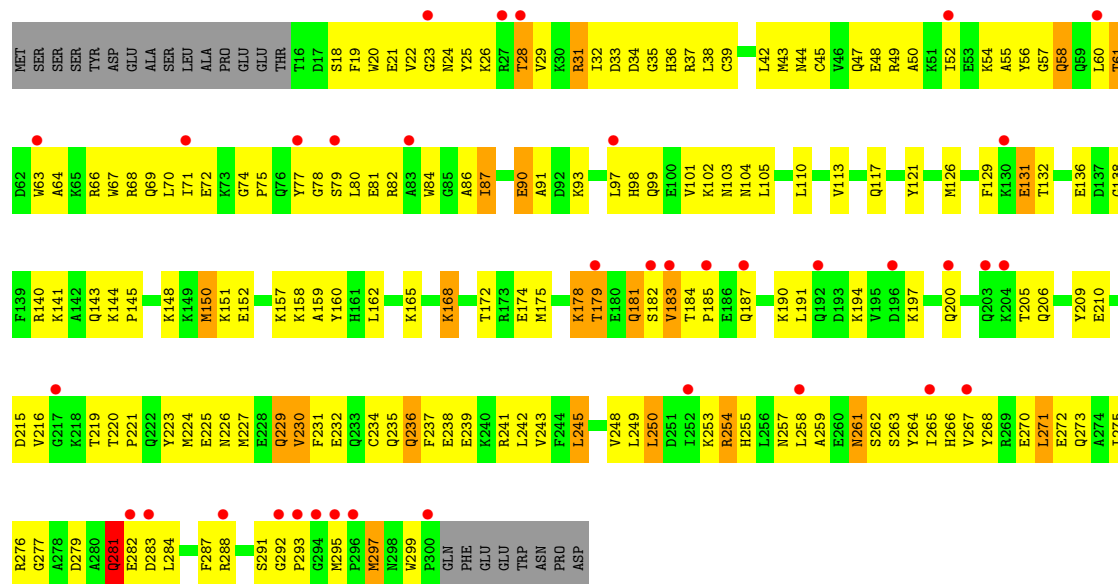


• Molecule 1: human PACSIN1 F-BAR

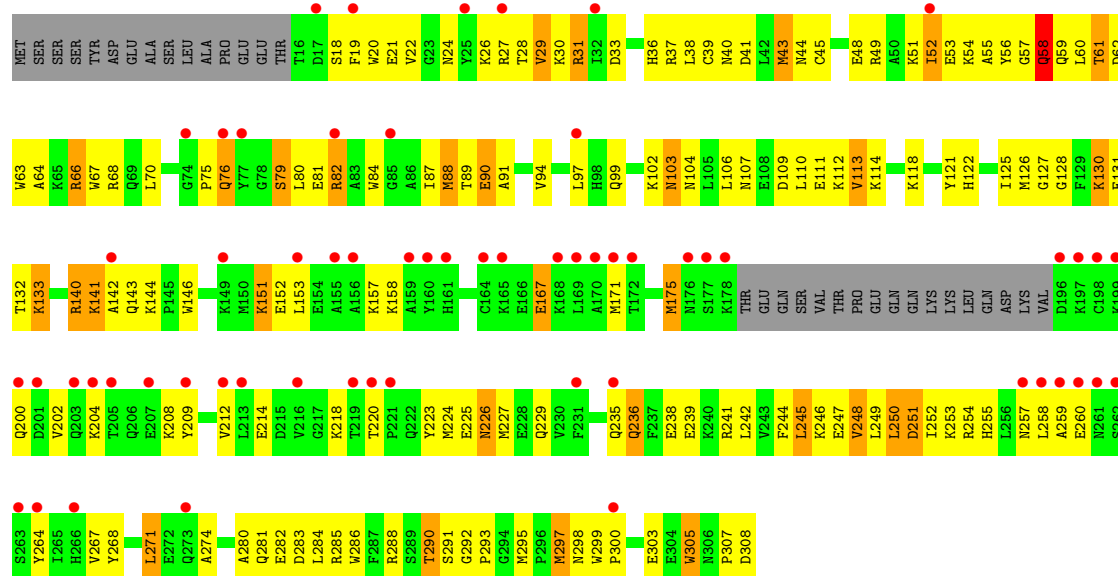




● Molecule 1: human PACSIN1 F-BAR



● Molecule 1: human PACSIN1 F-BAR



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	163.62Å 32.16Å 181.16Å 90.00° 111.23° 90.00°	Depositor
Resolution (Å)	48.52 – 2.88 48.52 – 2.88	Depositor EDS
% Data completeness (in resolution range)	98.8 (48.52-2.88) 97.8 (48.52-2.88)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.43 (at 2.86Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.282 , 0.319 0.277 , 0.284	Depositor DCC
R_{free} test set	2052 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	56.8	Xtriage
Anisotropy	0.657	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 57.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	9553	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.44% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section:
CA

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	0.61	0/2489	0.95	4/3339 (0.1%)
1	B	0.68	0/2486	0.94	5/3336 (0.1%)
1	C	0.55	0/2403	0.91	6/3220 (0.2%)
1	D	0.53	0/2340	0.84	2/3136 (0.1%)
All	All	0.60	0/9718	0.91	17/13031 (0.1%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	68	ARG	N-CA-C	-7.41	102.89	110.97
1	A	269	ARG	N-CA-C	-6.93	103.81	111.36
1	B	74	GLY	CA-C-N	6.88	126.56	119.82
1	B	74	GLY	C-N-CA	6.88	126.56	119.82
1	C	74	GLY	CA-C-N	6.41	126.04	119.56
1	C	74	GLY	C-N-CA	6.41	126.04	119.56
1	A	135	ALA	N-CA-C	-6.38	103.85	111.69
1	D	58	GLN	N-CA-C	-5.87	104.24	111.40
1	B	105	LEU	N-CA-C	-5.79	104.33	111.33
1	C	84	TRP	N-CA-C	-5.72	104.49	112.45
1	C	230	VAL	CB-CA-C	-5.57	104.74	112.04
1	B	100	GLU	N-CA-C	-5.45	105.24	111.07
1	C	292	GLY	CA-C-N	5.39	125.10	119.82
1	C	292	GLY	C-N-CA	5.39	125.10	119.82
1	D	84	TRP	N-CA-C	-5.25	104.99	111.40
1	A	109	ASP	N-CA-C	5.25	116.68	111.07
1	A	233	GLN	N-CA-C	-5.22	105.76	111.82

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	2441	0	2395	252	0
1	B	2438	0	2388	209	0
1	C	2359	0	2332	203	0
1	D	2294	0	2241	196	0
2	A	1	0	0	0	0
3	A	5	0	0	1	0
3	B	10	0	0	0	0
3	C	2	0	0	0	0
3	D	3	0	0	0	0
All	All	9553	0	9356	721	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 38.

All (721) 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:300:PRO:HG3	1:B:150:MET:HE1	1.24	1.13
1:A:43:MET:HE2	1:A:113:VAL:HG23	1.30	1.11
1:A:241:ARG:HH21	1:A:241:ARG:HG3	1.17	1.08
1:D:130:LYS:HD3	1:D:131:GLU:H	1.13	1.08
1:D:140:ARG:HG2	1:D:140:ARG:HH11	1.21	1.05
1:C:19:PHE:H	1:D:295:MET:HE2	1.25	1.00
1:C:297:MET:HG3	1:D:20:TRP:HB2	1.45	0.98
1:A:150:MET:HE1	1:B:300:PRO:HG2	1.48	0.96
1:B:142:ALA:HB1	1:B:226:ASN:HB3	1.46	0.96
1:B:144:LYS:HB3	1:B:145:PRO:HD3	1.47	0.96
1:B:116:TRP:CH2	1:B:241:ARG:HB3	2.01	0.96
1:D:82:ARG:HH11	1:D:82:ARG:HG2	1.31	0.95
1:A:261:ASN:ND2	1:A:263:SER:HB2	1.81	0.94
1:D:130:LYS:HD3	1:D:131:GLU:N	1.82	0.94
1:B:90:GLU:HG3	1:B:91:ALA:N	1.82	0.93
1:A:295:MET:HE1	1:B:27:ARG:HH11	1.33	0.93
1:A:183:VAL:HG13	1:A:184:THR:HG22	1.49	0.91
1:A:257:ASN:ND2	1:A:260:GLU:HB2	1.85	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:GLU:HG3	1:B:253:LYS:HZ2	1.35	0.91
1:B:291:SER:C	1:B:295:MET:HE2	1.94	0.91
1:A:291:SER:C	1:A:295:MET:HE2	1.98	0.89
1:B:143:GLN:HB2	1:B:227:MET:HE2	1.54	0.89
1:C:206:GLN:O	1:C:210:GLU:HG3	1.74	0.88
1:C:56:TYR:HD1	1:D:56:TYR:HB2	1.40	0.86
1:B:116:TRP:HH2	1:B:241:ARG:HB3	1.39	0.85
1:A:249:LEU:O	1:B:275:ILE:HD13	1.76	0.85
1:B:31:ARG:HH22	1:B:235:GLN:HE21	1.21	0.85
1:C:58:GLN:HA	1:C:58:GLN:HE21	1.44	0.83
1:B:258:LEU:O	1:B:261:ASN:HB3	1.79	0.83
1:A:241:ARG:HH21	1:A:241:ARG:CG	1.91	0.82
1:A:295:MET:HE3	1:B:19:PHE:HB2	1.61	0.82
1:A:175:MET:HE1	1:D:107:ASN:OD1	1.80	0.82
1:C:36:HIS:O	1:C:39:CYS:HB2	1.80	0.81
1:B:143:GLN:HB2	1:B:227:MET:CE	2.10	0.81
1:B:291:SER:O	1:B:295:MET:HE2	1.79	0.81
1:D:88:MET:HA	1:D:88:MET:HE2	1.61	0.81
1:A:272:GLU:HG3	1:B:253:LYS:NZ	1.94	0.81
1:D:82:ARG:HH11	1:D:82:ARG:CG	1.94	0.81
1:B:292:GLY:O	1:B:295:MET:HG2	1.80	0.80
1:A:19:PHE:HE1	1:B:293:PRO:HG3	1.46	0.80
1:A:241:ARG:HG3	1:A:241:ARG:NH2	1.89	0.80
1:C:250:LEU:HD12	1:C:254:ARG:HH12	1.46	0.80
1:A:182:SER:HB3	1:A:183:VAL:HB	1.63	0.79
1:A:261:ASN:HD21	1:A:263:SER:HB2	1.45	0.79
1:A:183:VAL:HG22	1:A:184:THR:HA	1.63	0.79
1:D:140:ARG:HH11	1:D:140:ARG:CG	1.94	0.79
1:A:69:GLN:HE21	1:A:69:GLN:HA	1.48	0.78
1:B:54:LYS:HB2	1:B:102:LYS:HD3	1.66	0.77
1:B:67:TRP:HB3	1:B:88:MET:HE2	1.66	0.77
1:B:160:TYR:HE2	1:B:206:GLN:HB2	1.48	0.77
1:B:58:GLN:HA	1:B:58:GLN:NE2	2.00	0.77
1:D:297:MET:HE2	1:D:298:ASN:H	1.47	0.77
1:A:264:TYR:CD2	1:B:259:ALA:HB2	2.20	0.77
1:A:28:THR:HG22	1:B:287:PHE:HE1	1.50	0.77
1:C:87:ILE:HD12	1:C:87:ILE:H	1.50	0.77
1:D:87:ILE:HD13	1:D:271:LEU:HD11	1.68	0.76
1:C:150:MET:HE1	1:D:300:PRO:HG3	1.66	0.76
1:A:44:ASN:N	1:A:44:ASN:HD22	1.84	0.76
1:A:264:TYR:HD2	1:B:259:ALA:HB2	1.51	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:SER:HB3	1:A:183:VAL:CB	2.17	0.75
1:C:258:LEU:HB2	1:D:264:TYR:OH	1.85	0.75
1:C:90:GLU:HG3	1:C:91:ALA:N	2.00	0.75
1:B:306:ASN:HB2	1:B:307:PRO:C	2.11	0.75
1:A:81:GLU:HG3	1:A:82:ARG:N	2.01	0.74
1:A:134:GLU:O	1:A:134:GLU:HG3	1.85	0.74
1:A:43:MET:HE1	1:A:114:LYS:HA	1.68	0.74
1:C:259:ALA:HB2	1:D:264:TYR:CD2	2.23	0.74
1:A:239:GLU:HB2	1:B:284:LEU:HD11	1.70	0.74
1:B:67:TRP:CB	1:B:88:MET:HE2	2.18	0.74
1:A:150:MET:HE1	1:B:300:PRO:CG	2.17	0.74
1:A:36:HIS:O	1:A:39:CYS:HB2	1.88	0.73
1:C:242:LEU:HD22	1:D:80:LEU:HD22	1.70	0.73
1:A:220:THR:OG1	1:A:221:PRO:HD3	1.88	0.73
1:A:300:PRO:CG	1:B:150:MET:HE1	2.11	0.73
1:C:56:TYR:CD1	1:D:56:TYR:CD2	2.77	0.73
1:B:174:GLU:HA	1:B:191:LEU:HD22	1.71	0.73
1:B:306:ASN:H	1:B:306:ASN:ND2	1.87	0.73
1:A:259:ALA:HB1	1:B:265:ILE:HD13	1.70	0.72
1:A:90:GLU:OE2	1:B:49:ARG:NH2	2.23	0.72
1:B:146:TRP:CZ3	1:B:220:THR:HG22	2.23	0.72
1:C:104:ASN:HB3	1:C:255:HIS:CD2	2.24	0.72
1:B:50:ALA:HB1	1:B:102:LYS:HG3	1.71	0.72
1:B:57:GLY:HA2	1:B:60:LEU:HD12	1.70	0.72
1:D:251:ASP:O	1:D:255:HIS:CD2	2.43	0.72
1:A:21:GLU:HG3	1:A:22:VAL:HG22	1.70	0.71
1:C:284:LEU:CD1	1:D:239:GLU:HG3	2.20	0.71
1:C:284:LEU:HD11	1:D:239:GLU:HG3	1.72	0.71
1:A:18:SER:O	1:A:24:ASN:ND2	2.22	0.71
1:C:224:MET:HE3	1:D:299:TRP:CZ2	2.26	0.71
1:B:31:ARG:NH2	1:B:235:GLN:HE21	1.89	0.70
1:B:49:ARG:NH1	1:B:53:GLU:OE2	2.23	0.70
1:A:68:ARG:HH21	1:A:89:THR:HG22	1.55	0.70
1:A:43:MET:CE	1:A:113:VAL:HG23	2.16	0.70
1:C:297:MET:CG	1:D:20:TRP:HB2	2.20	0.70
1:A:43:MET:HG2	1:A:113:VAL:HG21	1.73	0.70
1:A:257:ASN:HD22	1:A:260:GLU:HB2	1.55	0.70
1:D:31:ARG:HH22	1:D:235:GLN:HE21	1.38	0.70
1:C:239:GLU:HB2	1:D:284:LEU:HD11	1.74	0.70
1:D:33:ASP:OD2	1:D:132:THR:HG21	1.92	0.69
1:A:121:TYR:HB3	1:A:129:PHE:HE1	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:HIS:CE1	1:A:117:GLN:NE2	2.60	0.69
1:A:291:SER:O	1:A:295:MET:HE2	1.91	0.69
1:C:49:ARG:O	1:C:49:ARG:HG3	1.91	0.69
1:A:183:VAL:HG13	1:A:184:THR:CG2	2.22	0.69
1:C:44:ASN:O	1:C:48:GLU:HG3	1.93	0.69
1:A:31:ARG:CG	1:A:31:ARG:HH11	2.05	0.69
1:B:160:TYR:CE2	1:B:206:GLN:HB2	2.27	0.69
1:C:261:ASN:C	1:C:261:ASN:HD22	2.00	0.69
1:D:22:VAL:HA	1:D:143:GLN:NE2	2.08	0.69
1:A:163:ALA:O	1:A:167:GLU:HB2	1.93	0.69
1:D:280:ALA:O	1:D:283:ASP:HB2	1.91	0.69
1:D:82:ARG:HG2	1:D:82:ARG:NH1	2.08	0.68
1:A:31:ARG:NH2	1:A:235:GLN:HG2	2.08	0.68
1:C:19:PHE:N	1:D:295:MET:HE2	2.06	0.68
1:D:297:MET:HE2	1:D:298:ASN:N	2.08	0.68
1:D:79:SER:HB3	1:D:283:ASP:OD1	1.94	0.68
1:A:75:PRO:HG2	1:B:38:LEU:HD21	1.74	0.68
1:B:60:LEU:HB2	1:B:95:SER:HB2	1.74	0.68
1:D:297:MET:HE3	1:D:297:MET:HA	1.76	0.68
1:C:49:ARG:HB2	1:D:63:TRP:CZ2	2.28	0.68
1:D:26:LYS:HZ1	1:D:30:LYS:HE3	1.58	0.68
1:C:184:THR:OG1	1:C:187:GLN:HB2	1.94	0.67
1:A:284:LEU:HD11	1:B:239:GLU:HB2	1.77	0.67
1:A:36:HIS:HB2	1:A:121:TYR:HE1	1.60	0.67
1:B:58:GLN:HA	1:B:58:GLN:HE21	1.60	0.67
1:C:87:ILE:HD12	1:C:87:ILE:N	2.08	0.67
1:A:126:MET:HA	1:A:127:GLY:O	1.94	0.67
1:C:293:PRO:HG3	1:D:19:PHE:CE1	2.30	0.67
1:B:110:LEU:C	1:B:110:LEU:HD13	2.19	0.66
1:C:293:PRO:HG3	1:D:19:PHE:HE1	1.61	0.66
1:A:144:LYS:HB3	1:A:145:PRO:HD3	1.76	0.66
1:A:31:ARG:HH11	1:A:31:ARG:HG2	1.60	0.66
1:A:44:ASN:HD22	1:A:44:ASN:H	1.43	0.66
1:C:54:LYS:HA	1:C:99:GLN:HE22	1.60	0.66
1:B:95:SER:O	1:B:99:GLN:HG2	1.96	0.66
1:C:144:LYS:HB3	1:C:145:PRO:HD3	1.76	0.66
1:C:98:HIS:CD2	1:C:258:LEU:HD11	2.31	0.66
1:A:21:GLU:HG3	1:A:22:VAL:CG2	2.25	0.66
1:B:175:MET:SD	1:B:178:LYS:HD3	2.36	0.66
1:A:116:TRP:CE3	1:A:117:GLN:HA	2.31	0.66
1:B:106:LEU:HD13	1:C:178:LYS:HB3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:63:TRP:CH2	1:D:88:MET:HE1	2.31	0.65
1:B:116:TRP:CH2	1:B:241:ARG:CB	2.78	0.65
1:A:37:ARG:HH11	1:B:75:PRO:HD3	1.59	0.65
1:B:144:LYS:HB3	1:B:145:PRO:CD	2.23	0.65
1:C:297:MET:HE2	1:D:21:GLU:N	2.12	0.65
1:A:104:ASN:HB3	1:A:255:HIS:CD2	2.32	0.65
1:A:183:VAL:HG22	1:A:184:THR:HB	1.79	0.65
1:A:85:GLY:HA2	1:A:88:MET:HE2	1.79	0.65
1:A:253:LYS:HE3	1:B:272:GLU:HB2	1.79	0.65
1:C:56:TYR:HD1	1:D:56:TYR:CB	2.09	0.65
1:A:15:THR:HG22	1:A:16:THR:H	1.62	0.65
1:B:79:SER:HB2	1:B:278:ALA:HA	1.79	0.65
1:C:56:TYR:CD1	1:D:56:TYR:HB2	2.29	0.65
1:A:76:GLN:HG3	1:A:81:GLU:HB3	1.78	0.65
1:B:22:VAL:HA	1:B:143:GLN:NE2	2.12	0.65
1:C:220:THR:HB	1:C:221:PRO:HD3	1.79	0.64
1:C:254:ARG:NH2	1:C:254:ARG:HB2	2.13	0.64
1:D:282:GLU:HA	1:D:285:ARG:HD2	1.78	0.64
1:A:66:ARG:NH1	1:B:48:GLU:OE1	2.31	0.64
1:C:259:ALA:HB2	1:D:264:TYR:CE2	2.32	0.64
1:A:183:VAL:HG22	1:A:184:THR:CA	2.28	0.64
1:D:143:GLN:HB2	1:D:227:MET:HE1	1.79	0.63
1:B:273:GLN:OE1	1:B:273:GLN:HA	1.97	0.63
1:A:179:THR:HG23	1:D:106:LEU:HD11	1.80	0.63
1:C:291:SER:HA	1:C:295:MET:HE2	1.80	0.63
1:B:200:GLN:HB3	1:B:204:LYS:HE3	1.80	0.63
1:C:23:GLY:H	1:C:143:GLN:HE22	1.46	0.63
1:B:146:TRP:HZ3	1:B:220:THR:HG22	1.60	0.63
1:C:19:PHE:H	1:D:295:MET:CE	2.08	0.63
1:A:146:TRP:CZ2	1:A:150:MET:HE3	2.34	0.63
1:A:303:GLU:HG3	1:B:157:LYS:NZ	2.14	0.63
1:A:146:TRP:CD1	1:A:146:TRP:C	2.77	0.62
1:A:264:TYR:HE2	1:B:259:ALA:H	1.47	0.62
1:D:36:HIS:O	1:D:39:CYS:HB2	1.99	0.62
1:B:31:ARG:NH2	1:B:235:GLN:NE2	2.48	0.62
1:B:107:ASN:OD1	1:C:175:MET:HE1	1.99	0.62
1:A:209:TYR:HE1	1:B:302:PHE:HD2	1.45	0.62
1:D:122:HIS:H	1:D:130:LYS:HG3	1.64	0.62
1:B:107:ASN:CG	1:C:175:MET:HE1	2.24	0.62
1:C:136:GLU:HG2	1:C:140:ARG:HD2	1.81	0.62
1:A:43:MET:HG2	1:A:113:VAL:CG2	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:GLU:CD	1:B:131:GLU:H	2.07	0.61
1:C:49:ARG:HB2	1:D:63:TRP:CE2	2.36	0.61
1:D:142:ALA:HB1	1:D:226:ASN:HB3	1.81	0.61
1:A:28:THR:O	1:A:32:ILE:HD13	2.01	0.61
1:A:31:ARG:HG2	1:A:31:ARG:NH1	2.15	0.61
1:A:104:ASN:HB3	1:A:255:HIS:CG	2.36	0.61
1:D:236:GLN:HA	1:D:236:GLN:HE21	1.66	0.61
1:C:254:ARG:HH21	1:C:254:ARG:HG3	1.65	0.61
1:D:26:LYS:O	1:D:29:VAL:HG12	2.00	0.61
1:D:90:GLU:O	1:D:94:VAL:HG23	2.01	0.60
1:B:245:LEU:HD22	1:B:245:LEU:O	2.01	0.60
1:C:31:ARG:HE	1:C:238:GLU:HG2	1.66	0.60
1:D:76:GLN:HE21	1:D:76:GLN:CA	2.14	0.60
1:A:106:LEU:HD13	1:A:110:LEU:HD22	1.82	0.60
1:C:264:TYR:OH	1:D:258:LEU:HB2	2.01	0.60
1:A:124:GLN:C	1:A:125:ILE:HD12	2.27	0.60
1:B:90:GLU:HG3	1:B:91:ALA:H	1.64	0.60
1:A:28:THR:HG22	1:B:287:PHE:CE1	2.35	0.60
1:A:36:HIS:HB2	1:A:121:TYR:CE1	2.36	0.60
1:D:141:LYS:N	1:D:141:LYS:HD2	2.17	0.60
1:C:57:GLY:O	1:C:61:THR:OG1	2.19	0.59
1:A:34:ASP:O	1:A:38:LEU:HD23	2.02	0.59
1:C:90:GLU:OE2	1:D:49:ARG:NH2	2.35	0.59
1:A:40:ASN:O	1:A:43:MET:HB2	2.03	0.59
1:C:297:MET:HG3	1:D:20:TRP:CB	2.27	0.59
1:A:110:LEU:HG	1:A:110:LEU:O	2.02	0.59
1:D:57:GLY:O	1:D:61:THR:HG23	2.02	0.59
1:B:251:ASP:HA	1:B:254:ARG:NH1	2.17	0.59
1:A:253:LYS:HG3	1:A:254:ARG:N	2.17	0.59
1:C:293:PRO:HB3	1:D:20:TRP:CZ2	2.37	0.59
1:B:83:ALA:C	1:B:85:GLY:H	2.10	0.59
1:B:169:LEU:O	1:B:173:ARG:HB2	2.03	0.58
1:C:165:LYS:HG3	1:D:305:TRP:CZ3	2.37	0.58
1:B:206:GLN:O	1:B:210:GLU:HB2	2.03	0.58
1:B:306:ASN:H	1:B:306:ASN:HD22	1.50	0.58
1:D:26:LYS:NZ	1:D:30:LYS:HE3	2.17	0.58
1:B:71:ILE:HD11	1:B:84:TRP:CH2	2.38	0.58
1:C:165:LYS:HG3	1:D:305:TRP:CH2	2.38	0.58
1:B:110:LEU:C	1:B:110:LEU:CD1	2.77	0.58
1:A:31:ARG:HH11	1:A:31:ARG:HB3	1.68	0.58
1:A:101:VAL:O	1:A:105:LEU:HG	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:88:MET:HE2	1:D:88:MET:CA	2.32	0.58
1:B:184:THR:N	1:B:185:PRO:HD3	2.19	0.58
1:C:254:ARG:HH21	1:C:254:ARG:CG	2.17	0.58
1:A:21:GLU:CG	1:A:22:VAL:HG22	2.34	0.57
1:A:75:PRO:HG2	1:B:38:LEU:CD2	2.33	0.57
1:A:79:SER:H	1:A:283:ASP:CG	2.12	0.57
1:C:18:SER:HA	1:D:295:MET:CE	2.35	0.57
1:C:216:VAL:HG11	1:D:300:PRO:HG2	1.86	0.57
1:A:19:PHE:CE1	1:B:293:PRO:HG3	2.33	0.57
1:D:56:TYR:HE1	1:D:60:LEU:HD21	1.69	0.57
1:A:243:VAL:CG1	1:A:244:PHE:N	2.66	0.57
1:C:55:ALA:O	1:C:56:TYR:C	2.46	0.57
1:A:259:ALA:HB2	1:B:264:TYR:CD2	2.39	0.57
1:D:76:GLN:HE21	1:D:76:GLN:HA	1.69	0.57
1:D:66:ARG:HH11	1:D:70:LEU:HD11	1.69	0.57
1:D:171:MET:O	1:D:175:MET:HB3	2.04	0.57
1:C:267:VAL:HG13	1:C:268:TYR:CD2	2.40	0.57
1:A:45:CYS:HA	1:B:67:TRP:CE2	2.40	0.56
1:A:69:GLN:O	1:A:72:GLU:HB3	2.04	0.56
1:A:138:GLY:O	1:A:230:VAL:HG21	2.05	0.56
1:C:138:GLY:C	1:C:230:VAL:HG21	2.30	0.56
1:C:75:PRO:HD2	1:D:38:LEU:HD21	1.86	0.56
1:C:168:LYS:O	1:C:172:THR:HG23	2.05	0.56
1:A:35:GLY:HA3	1:A:241:ARG:HE	1.69	0.56
1:A:53:GLU:OE2	1:A:53:GLU:HA	2.04	0.56
1:D:76:GLN:HG3	1:D:76:GLN:O	2.05	0.56
1:B:83:ALA:C	1:B:85:GLY:N	2.61	0.56
1:C:143:GLN:HB2	1:C:227:MET:HE1	1.87	0.56
1:A:81:GLU:HG3	1:A:82:ARG:H	1.71	0.56
1:B:44:ASN:O	1:B:48:GLU:HG3	2.05	0.56
1:B:177:SER:OG	1:B:191:LEU:HD11	2.05	0.56
1:B:184:THR:HB	1:B:187:GLN:HB3	1.88	0.56
1:D:281:GLN:O	1:D:284:LEU:HB2	2.05	0.56
1:A:43:MET:CE	1:A:114:LYS:HA	2.35	0.56
1:A:168:LYS:HE2	1:A:172:THR:HG21	1.88	0.56
1:C:197:LYS:O	1:C:200:GLN:HB3	2.06	0.56
1:D:113:VAL:HG23	1:D:244:PHE:HE1	1.70	0.56
1:C:254:ARG:HB2	1:C:254:ARG:CZ	2.36	0.56
1:D:286:TRP:CH2	1:D:290:THR:HG21	2.41	0.56
1:A:81:GLU:CG	1:A:82:ARG:N	2.69	0.55
1:C:54:LYS:HA	1:C:99:GLN:NE2	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:ASN:O	1:B:179:THR:HG22	2.07	0.55
1:D:250:LEU:HD13	1:D:250:LEU:O	2.06	0.55
1:A:32:ILE:HG22	1:A:132:THR:HG23	1.89	0.55
1:C:36:HIS:CE1	1:C:117:GLN:NE2	2.74	0.55
1:D:76:GLN:HE21	1:D:76:GLN:C	2.14	0.55
1:B:143:GLN:CB	1:B:227:MET:HE2	2.32	0.55
1:A:21:GLU:CD	1:A:22:VAL:HG22	2.32	0.55
1:B:80:LEU:HD22	1:B:278:ALA:HB1	1.89	0.55
1:C:261:ASN:C	1:C:261:ASN:ND2	2.64	0.55
1:A:67:TRP:O	1:A:68:ARG:C	2.49	0.55
1:D:76:GLN:O	1:D:81:GLU:HB2	2.07	0.55
1:A:49:ARG:HB2	1:B:63:TRP:CE2	2.42	0.55
1:B:51:LYS:HG2	1:C:179:THR:OG1	2.07	0.55
1:B:228:GLU:HG3	1:B:228:GLU:O	2.06	0.55
1:A:36:HIS:CE1	1:A:117:GLN:HE21	2.24	0.55
1:A:44:ASN:N	1:A:44:ASN:ND2	2.55	0.55
1:D:292:GLY:O	1:D:295:MET:HG3	2.07	0.55
1:D:43:MET:SD	1:D:113:VAL:CG1	2.95	0.55
1:D:110:LEU:C	1:D:110:LEU:HD23	2.32	0.55
1:C:33:ASP:OD1	1:C:132:THR:HG21	2.06	0.54
1:A:33:ASP:CG	1:A:132:THR:HG21	2.32	0.54
1:A:120:ALA:O	1:A:121:TYR:CD2	2.60	0.54
1:A:143:GLN:HB3	1:A:227:MET:HE1	1.88	0.54
1:A:15:THR:HG22	1:A:16:THR:N	2.21	0.54
1:A:80:LEU:HD11	1:B:246:LYS:HB2	1.89	0.54
1:C:60:LEU:HD22	1:D:52:ILE:HG21	1.88	0.54
1:A:31:ARG:HH11	1:A:31:ARG:CB	2.19	0.54
1:D:43:MET:HG3	1:D:113:VAL:HG11	1.89	0.54
1:A:35:GLY:CA	1:A:241:ARG:HE	2.21	0.54
1:B:157:LYS:HB2	1:B:209:TYR:HE1	1.72	0.54
1:A:257:ASN:HD21	1:A:260:GLU:HB2	1.71	0.54
1:A:286:TRP:CE2	1:A:290:THR:HG21	2.42	0.54
1:C:261:ASN:ND2	1:C:263:SER:H	2.06	0.54
1:C:297:MET:CE	1:D:21:GLU:HG2	2.38	0.54
1:C:56:TYR:O	1:C:60:LEU:HD23	2.08	0.53
1:A:138:GLY:C	1:A:230:VAL:HG21	2.32	0.53
1:B:50:ALA:O	1:B:51:LYS:C	2.50	0.53
1:C:87:ILE:H	1:C:87:ILE:CD1	2.20	0.53
1:C:239:GLU:O	1:C:243:VAL:HG23	2.08	0.53
1:D:37:ARG:O	1:D:40:ASN:N	2.42	0.53
1:C:38:LEU:HD21	1:D:75:PRO:HD2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:268:TYR:CE1	1:D:257:ASN:HA	2.43	0.53
1:D:82:ARG:CG	1:D:82:ARG:NH1	2.65	0.53
1:A:122:HIS:HD2	1:A:131:GLU:OE2	1.92	0.53
1:C:131:GLU:CD	1:C:131:GLU:H	2.15	0.53
1:A:56:TYR:CD1	1:B:56:TYR:HB2	2.42	0.53
1:A:266:HIS:CE1	1:A:270:GLU:HG3	2.44	0.53
1:C:150:MET:HE1	1:D:300:PRO:CG	2.35	0.53
1:C:288:ARG:HH11	1:C:288:ARG:HG2	1.72	0.53
1:A:182:SER:HB3	1:A:183:VAL:CG2	2.38	0.53
1:C:19:PHE:CD1	1:D:293:PRO:HA	2.44	0.53
1:C:143:GLN:HG3	1:C:223:TYR:OH	2.09	0.53
1:C:56:TYR:CD1	1:D:56:TYR:CG	2.97	0.53
1:D:56:TYR:CE1	1:D:60:LEU:HD21	2.43	0.53
1:A:146:TRP:CD1	1:A:146:TRP:O	2.62	0.52
1:D:140:ARG:HG2	1:D:140:ARG:NH1	2.02	0.52
1:A:183:VAL:HG22	1:A:184:THR:CB	2.39	0.52
1:A:37:ARG:NH1	1:B:75:PRO:HD3	2.24	0.52
1:C:261:ASN:O	1:C:262:SER:C	2.53	0.52
1:A:53:GLU:OE2	1:B:56:TYR:OH	2.27	0.52
1:A:156:ALA:O	1:A:209:TYR:HB2	2.09	0.52
1:C:236:GLN:HA	1:C:236:GLN:HE21	1.74	0.52
1:A:42:LEU:O	1:A:43:MET:C	2.52	0.52
1:B:261:ASN:O	1:B:262:SER:C	2.53	0.52
1:C:284:LEU:HD12	1:D:239:GLU:HG3	1.92	0.52
1:C:288:ARG:HG2	1:C:288:ARG:NH1	2.23	0.52
1:A:216:VAL:O	1:A:220:THR:HG23	2.09	0.52
1:A:236:GLN:HE21	1:A:236:GLN:HA	1.74	0.52
1:C:183:VAL:HG13	1:C:187:GLN:HB3	1.91	0.52
1:D:245:LEU:HD22	1:D:249:LEU:HD12	1.92	0.52
1:A:59:GLN:OE1	1:B:52:ILE:HG13	2.10	0.52
1:A:303:GLU:HG3	1:B:157:LYS:HZ2	1.74	0.52
1:B:31:ARG:HH22	1:B:235:GLN:NE2	1.97	0.52
1:B:259:ALA:C	1:B:261:ASN:H	2.17	0.52
1:D:43:MET:HG3	1:D:113:VAL:CG1	2.40	0.52
1:D:157:LYS:HB2	1:D:209:TYR:CE2	2.45	0.52
1:A:39:CYS:SG	1:A:116:TRP:CZ3	3.03	0.52
1:B:281:GLN:O	1:B:284:LEU:N	2.42	0.51
1:C:93:LYS:HD2	1:C:267:VAL:HG23	1.92	0.51
1:C:238:GLU:OE1	1:C:241:ARG:NH2	2.43	0.51
1:D:109:ASP:OD1	1:D:255:HIS:CD2	2.63	0.51
1:D:158:LYS:NZ	1:D:158:LYS:HB3	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:SER:N	1:A:283:ASP:OD2	2.43	0.51
1:B:133:LYS:HG3	1:B:137:ASP:OD2	2.10	0.51
1:A:271:LEU:HD22	1:A:275:ILE:CD1	2.41	0.51
1:B:38:LEU:HD12	1:B:241:ARG:NH1	2.25	0.51
1:C:261:ASN:HD22	1:C:263:SER:N	2.08	0.51
1:D:104:ASN:OD1	1:D:255:HIS:ND1	2.43	0.51
1:C:136:GLU:O	1:C:140:ARG:HG3	2.10	0.51
1:B:259:ALA:C	1:B:261:ASN:N	2.68	0.51
1:C:42:LEU:HD12	1:C:113:VAL:HG21	1.91	0.51
1:B:56:TYR:HD2	1:B:98:HIS:CE1	2.28	0.51
1:B:71:ILE:HD11	1:B:84:TRP:CZ2	2.45	0.51
1:B:157:LYS:HB2	1:B:209:TYR:CE1	2.45	0.51
1:C:78:GLY:O	1:C:81:GLU:HG2	2.11	0.51
1:D:151:LYS:HG3	1:D:152:GLU:N	2.25	0.51
1:A:184:THR:HG23	1:A:187:GLN:HB2	1.93	0.51
1:C:63:TRP:CZ2	1:D:49:ARG:HB2	2.45	0.51
1:C:66:ARG:O	1:C:70:LEU:HG	2.11	0.51
1:B:281:GLN:O	1:B:282:GLU:C	2.53	0.51
1:C:21:GLU:HB2	1:C:24:ASN:ND2	2.25	0.51
1:A:36:HIS:CE1	1:A:129:PHE:CZ	2.99	0.51
1:A:253:LYS:HB2	1:B:271:LEU:HD13	1.92	0.51
1:B:177:SER:CB	1:B:191:LEU:HD11	2.41	0.51
1:C:58:GLN:HA	1:C:58:GLN:NE2	2.21	0.51
1:A:182:SER:HB3	1:A:183:VAL:HG23	1.92	0.51
1:A:69:GLN:HE21	1:A:69:GLN:CA	2.23	0.50
1:B:107:ASN:ND2	1:C:175:MET:HE1	2.26	0.50
1:C:67:TRP:C	1:C:69:GLN:N	2.67	0.50
1:C:78:GLY:C	1:C:80:LEU:H	2.19	0.50
1:C:267:VAL:HG13	1:C:268:TYR:N	2.26	0.50
1:D:29:VAL:CG1	1:D:30:LYS:N	2.75	0.50
1:D:89:THR:O	1:D:90:GLU:C	2.54	0.50
1:A:160:TYR:CE1	1:A:206:GLN:HB2	2.47	0.50
1:C:25:TYR:O	1:C:28:THR:CG2	2.60	0.50
1:C:215:ASP:O	1:C:219:THR:HG23	2.12	0.50
1:A:66:ARG:HH12	1:B:48:GLU:CD	2.19	0.50
1:A:241:ARG:C	1:A:243:VAL:N	2.68	0.50
1:B:67:TRP:HB2	1:B:88:MET:HE2	1.93	0.50
1:B:104:ASN:O	1:B:105:LEU:C	2.51	0.50
1:B:252:ILE:O	1:B:253:LYS:C	2.52	0.50
1:A:45:CYS:HB2	1:B:67:TRP:CD2	2.45	0.50
1:A:221:PRO:HA	1:A:224:MET:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:GLN:HB3	1:B:81:GLU:HG3	1.93	0.50
1:A:105:LEU:HD11	1:A:256:LEU:HD11	1.92	0.50
1:B:39:CYS:O	1:B:40:ASN:C	2.54	0.50
1:C:113:VAL:HG12	1:C:113:VAL:O	2.11	0.50
1:B:238:GLU:OE2	1:B:238:GLU:HA	2.11	0.50
1:C:287:PHE:CE2	1:D:28:THR:HG22	2.46	0.50
1:A:19:PHE:CB	1:B:295:MET:HE3	2.42	0.50
1:A:76:GLN:HG3	1:A:77:TYR:N	2.27	0.50
1:B:306:ASN:HB2	1:B:308:ASP:N	2.27	0.50
1:A:247:GLU:HG3	3:A:313:HOH:O	2.12	0.49
1:C:63:TRP:CE2	1:D:49:ARG:HB2	2.47	0.49
1:C:157:LYS:O	1:C:158:LYS:C	2.53	0.49
1:C:160:TYR:CE1	1:C:206:GLN:HB2	2.47	0.49
1:C:224:MET:HE3	1:D:299:TRP:HZ2	1.75	0.49
1:D:90:GLU:HG3	1:D:91:ALA:N	2.25	0.49
1:A:64:ALA:HA	1:A:88:MET:HG3	1.93	0.49
1:C:253:LYS:HB2	1:D:271:LEU:HD13	1.94	0.49
1:D:307:PRO:O	1:D:308:ASP:C	2.54	0.49
1:B:24:ASN:C	1:B:26:LYS:N	2.69	0.49
1:B:110:LEU:HD13	1:B:110:LEU:O	2.13	0.49
1:A:291:SER:CA	1:A:295:MET:HE2	2.42	0.49
1:D:113:VAL:CG1	1:D:114:LYS:N	2.74	0.49
1:D:291:SER:HA	1:D:295:MET:SD	2.51	0.49
1:C:253:LYS:HD3	1:C:254:ARG:N	2.28	0.49
1:D:223:TYR:CE1	1:D:227:MET:HE2	2.47	0.49
1:A:126:MET:N	1:A:127:GLY:HA3	2.27	0.49
1:A:291:SER:HA	1:A:295:MET:HE2	1.95	0.49
1:B:101:VAL:O	1:B:102:LYS:C	2.53	0.49
1:D:214:GLU:O	1:D:218:LYS:HG3	2.13	0.49
1:A:66:ARG:NH1	1:B:48:GLU:CD	2.71	0.49
1:A:121:TYR:HD1	1:A:129:PHE:CE1	2.31	0.49
1:A:47:GLN:O	1:A:51:LYS:HB2	2.13	0.49
1:A:76:GLN:HE21	1:A:77:TYR:H	1.59	0.49
1:B:146:TRP:CH2	1:B:220:THR:HG22	2.47	0.49
1:B:152:GLU:O	1:B:155:ALA:HB3	2.13	0.49
1:C:47:GLN:O	1:C:50:ALA:HB3	2.12	0.49
1:D:62:ASP:O	1:D:66:ARG:HB2	2.12	0.49
1:A:271:LEU:HD13	1:B:253:LYS:HB2	1.95	0.49
1:B:215:ASP:O	1:B:219:THR:HG22	2.13	0.49
1:C:275:ILE:C	1:C:277:GLY:N	2.70	0.49
1:A:102:LYS:O	1:A:103:ASN:C	2.56	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:64:ALA:HB2	1:D:91:ALA:HB3	1.95	0.49
1:D:110:LEU:HD23	1:D:111:GLU:N	2.28	0.49
1:C:242:LEU:O	1:C:243:VAL:C	2.55	0.48
1:A:125:ILE:C	1:A:127:GLY:HA3	2.38	0.48
1:A:175:MET:HE1	1:D:107:ASN:CG	2.37	0.48
1:D:297:MET:HA	1:D:297:MET:CE	2.42	0.48
1:A:36:HIS:CE1	1:A:129:PHE:HZ	2.31	0.48
1:C:257:ASN:OD1	1:D:268:TYR:CD2	2.66	0.48
1:B:109:ASP:O	1:B:110:LEU:C	2.55	0.48
1:B:112:LYS:NZ	1:B:251:ASP:OD2	2.35	0.48
1:D:76:GLN:HA	1:D:76:GLN:NE2	2.28	0.48
1:D:126:MET:HB2	1:D:127:GLY:HA2	1.96	0.48
1:A:31:ARG:HD3	1:B:287:PHE:CE2	2.48	0.48
1:B:279:ASP:OD2	1:B:281:GLN:HB2	2.14	0.48
1:D:146:TRP:HZ3	1:D:220:THR:HA	1.78	0.48
1:C:245:LEU:HD22	1:C:249:LEU:HG	1.96	0.48
1:C:275:ILE:C	1:C:277:GLY:H	2.21	0.48
1:D:245:LEU:O	1:D:249:LEU:HB2	2.13	0.48
1:A:81:GLU:CG	1:A:82:ARG:H	2.25	0.48
1:B:109:ASP:CG	1:B:255:HIS:HD1	2.21	0.48
1:B:154:GLU:O	1:B:158:LYS:HB2	2.13	0.48
1:D:128:GLY:HA3	1:D:133:LYS:HE2	1.95	0.48
1:B:258:LEU:O	1:B:261:ASN:CB	2.58	0.48
1:D:252:ILE:O	1:D:253:LYS:C	2.56	0.48
1:B:20:TRP:CZ3	1:B:224:MET:HA	2.49	0.47
1:C:245:LEU:HD12	1:D:80:LEU:HD23	1.95	0.47
1:D:121:TYR:HA	1:D:130:LYS:CG	2.44	0.47
1:B:49:ARG:O	1:B:50:ALA:C	2.57	0.47
1:B:160:TYR:C	1:B:160:TYR:CD1	2.92	0.47
1:C:131:GLU:CD	1:C:131:GLU:N	2.71	0.47
1:C:266:HIS:C	1:C:266:HIS:CD2	2.92	0.47
1:A:209:TYR:CE1	1:B:302:PHE:HD2	2.28	0.47
1:B:20:TRP:CZ3	1:B:224:MET:HG2	2.49	0.47
1:C:36:HIS:HB2	1:C:121:TYR:CE1	2.50	0.47
1:C:291:SER:HA	1:C:295:MET:CE	2.44	0.47
1:A:71:ILE:C	1:A:71:ILE:HD13	2.39	0.47
1:A:39:CYS:O	1:A:43:MET:HG3	2.14	0.47
1:B:177:SER:HB3	1:B:191:LEU:HD11	1.96	0.47
1:D:20:TRP:CZ3	1:D:224:MET:HA	2.49	0.47
1:A:45:CYS:HA	1:B:67:TRP:CZ2	2.49	0.47
1:B:285:ARG:O	1:B:286:TRP:C	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:306:ASN:ND2	1:B:306:ASN:N	2.61	0.47
1:C:43:MET:HG2	1:C:110:LEU:HD12	1.97	0.47
1:C:148:LYS:HE3	1:C:152:GLU:OE2	2.15	0.47
1:D:26:LYS:HZ3	1:D:30:LYS:HG3	1.80	0.47
1:D:54:LYS:O	1:D:58:GLN:HB2	2.15	0.47
1:C:31:ARG:NE	1:C:238:GLU:HG2	2.29	0.47
1:C:56:TYR:CD1	1:D:56:TYR:CB	2.94	0.47
1:C:291:SER:CA	1:C:295:MET:HE2	2.44	0.47
1:D:238:GLU:OE1	1:D:241:ARG:NH1	2.48	0.47
1:A:31:ARG:HH21	1:A:235:GLN:HG2	1.78	0.47
1:A:241:ARG:CG	1:A:241:ARG:NH2	2.61	0.47
1:A:295:MET:HE3	1:B:19:PHE:CB	2.38	0.47
1:C:257:ASN:HA	1:D:268:TYR:CZ	2.48	0.47
1:D:87:ILE:HG22	1:D:88:MET:HE3	1.97	0.47
1:D:208:LYS:O	1:D:212:VAL:HG23	2.15	0.47
1:A:286:TRP:NE1	1:A:290:THR:HG21	2.30	0.47
1:A:295:MET:HE1	1:B:27:ARG:NH1	2.15	0.47
1:B:125:ILE:HG13	1:B:126:MET:N	2.24	0.47
1:D:44:ASN:O	1:D:45:CYS:C	2.58	0.47
1:D:113:VAL:HG12	1:D:114:LYS:N	2.29	0.47
1:D:200:GLN:HG2	1:D:204:LYS:HE3	1.97	0.47
1:A:45:CYS:O	1:B:63:TRP:HZ2	1.98	0.46
1:A:102:LYS:HG2	1:A:103:ASN:N	2.27	0.46
1:B:265:ILE:H	1:B:265:ILE:HG12	1.58	0.46
1:C:104:ASN:CB	1:C:255:HIS:CD2	2.98	0.46
1:C:272:GLU:HG3	1:D:250:LEU:HD21	1.97	0.46
1:A:52:ILE:HG12	1:B:59:GLN:NE2	2.31	0.46
1:A:143:GLN:O	1:A:147:ALA:N	2.49	0.46
1:B:245:LEU:HD22	1:B:245:LEU:C	2.40	0.46
1:C:49:ARG:HD3	1:D:63:TRP:CZ3	2.51	0.46
1:A:69:GLN:HA	1:A:69:GLN:NE2	2.24	0.46
1:A:165:LYS:HG3	1:B:305:TRP:HZ2	1.80	0.46
1:A:307:PRO:O	1:A:308:ASP:C	2.58	0.46
1:C:56:TYR:HD1	1:D:56:TYR:CG	2.33	0.46
1:C:184:THR:OG1	1:C:187:GLN:CB	2.63	0.46
1:D:167:GLU:HB2	1:D:202:VAL:HG21	1.96	0.46
1:C:25:TYR:OH	1:C:140:ARG:HG2	2.16	0.46
1:A:143:GLN:HA	1:A:223:TYR:HE1	1.80	0.46
1:C:190:LYS:HE2	1:C:194:LYS:HE3	1.98	0.46
1:C:229:GLN:HE21	1:C:229:GLN:HB3	1.55	0.46
1:D:111:GLU:O	1:D:112:LYS:C	2.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:174:GLU:HA	1:C:191:LEU:HD23	1.98	0.45
1:C:265:ILE:HD13	1:D:259:ALA:HB2	1.98	0.45
1:D:236:GLN:HA	1:D:236:GLN:NE2	2.30	0.45
1:B:51:LYS:HB3	1:B:51:LYS:HE2	1.72	0.45
1:C:31:ARG:NH2	1:C:235:GLN:NE2	2.64	0.45
1:C:80:LEU:HD13	1:D:245:LEU:CD1	2.46	0.45
1:D:113:VAL:HG23	1:D:244:PHE:CE1	2.51	0.45
1:D:88:MET:CA	1:D:88:MET:CE	2.94	0.45
1:A:22:VAL:HB	1:A:23:GLY:H	1.20	0.45
1:A:116:TRP:CE3	1:A:117:GLN:CA	2.99	0.45
1:A:232:GLU:O	1:A:236:GLN:HB2	2.17	0.45
1:A:253:LYS:HB2	1:B:271:LEU:CD1	2.46	0.45
1:C:25:TYR:O	1:C:28:THR:HG23	2.17	0.45
1:C:56:TYR:CE1	1:D:56:TYR:CD2	3.05	0.45
1:C:66:ARG:O	1:C:69:GLN:HB3	2.16	0.45
1:C:184:THR:HB	1:C:185:PRO:HD2	1.97	0.45
1:D:51:LYS:O	1:D:52:ILE:C	2.60	0.45
1:A:264:TYR:OH	1:B:258:LEU:HB2	2.17	0.45
1:A:116:TRP:HE3	1:A:117:GLN:N	2.14	0.45
1:A:297:MET:SD	1:A:298:ASN:N	2.89	0.45
1:C:54:LYS:HB2	1:C:102:LYS:HD3	1.98	0.45
1:C:68:ARG:O	1:C:72:GLU:HB2	2.17	0.45
1:C:295:MET:HE1	1:D:27:ARG:HH11	1.80	0.45
1:D:43:MET:SD	1:D:113:VAL:HG13	2.57	0.45
1:D:55:ALA:O	1:D:56:TYR:C	2.59	0.45
1:D:238:GLU:O	1:D:241:ARG:N	2.47	0.45
1:A:21:GLU:O	1:A:22:VAL:C	2.59	0.45
1:A:79:SER:HB2	1:A:278:ALA:HA	1.99	0.45
1:C:276:ARG:HA	1:D:246:LYS:HE2	1.99	0.45
1:C:287:PHE:HE2	1:D:28:THR:HG22	1.81	0.45
1:D:238:GLU:HA	1:D:238:GLU:OE2	2.17	0.45
1:D:248:VAL:O	1:D:251:ASP:HB2	2.17	0.45
1:A:251:ASP:OD1	1:A:254:ARG:NH1	2.47	0.45
1:D:49:ARG:NH1	1:D:53:GLU:OE2	2.48	0.45
1:A:83:ALA:O	1:A:86:ALA:HB3	2.17	0.45
1:C:80:LEU:HD12	1:D:242:LEU:HD22	1.98	0.44
1:D:153:LEU:C	1:D:153:LEU:HD23	2.42	0.44
1:D:284:LEU:HD23	1:D:284:LEU:HA	1.70	0.44
1:B:139:PHE:HD1	1:B:227:MET:SD	2.40	0.44
1:B:37:ARG:O	1:B:40:ASN:HB2	2.17	0.44
1:A:41:ASP:O	1:A:42:LEU:C	2.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:HIS:CD2	1:A:131:GLU:OE2	2.70	0.44
1:B:174:GLU:HG3	1:B:191:LEU:HB3	2.00	0.44
1:A:165:LYS:C	1:A:167:GLU:H	2.24	0.44
1:C:261:ASN:HD22	1:C:263:SER:H	1.65	0.44
1:A:43:MET:HE1	1:A:114:LYS:HG3	2.00	0.44
1:A:165:LYS:C	1:A:167:GLU:N	2.74	0.44
1:B:83:ALA:O	1:B:85:GLY:N	2.51	0.44
1:B:153:LEU:HD11	1:B:213:LEU:HD23	1.99	0.44
1:C:181:GLN:HA	1:C:182:SER:HA	1.58	0.44
1:D:24:ASN:C	1:D:26:LYS:H	2.25	0.44
1:A:36:HIS:ND1	1:A:121:TYR:CD1	2.85	0.44
1:A:189:LYS:HD2	1:A:189:LYS:HA	1.71	0.44
1:B:107:ASN:O	1:B:111:GLU:HB2	2.17	0.44
1:C:56:TYR:CE1	1:D:56:TYR:HD2	2.35	0.44
1:C:235:GLN:HG3	1:D:288:ARG:NH2	2.33	0.44
1:D:140:ARG:CG	1:D:140:ARG:NH1	2.63	0.44
1:A:25:TYR:CD1	1:A:139:PHE:HB3	2.53	0.44
1:A:281:GLN:NE2	1:B:239:GLU:OE1	2.51	0.44
1:B:291:SER:O	1:B:295:MET:CE	2.60	0.44
1:C:34:ASP:O	1:C:35:GLY:C	2.60	0.44
1:C:237:PHE:O	1:C:238:GLU:C	2.60	0.44
1:A:253:LYS:O	1:A:254:ARG:C	2.59	0.43
1:B:220:THR:O	1:B:221:PRO:C	2.59	0.43
1:C:295:MET:HE1	1:D:27:ARG:NH1	2.33	0.43
1:A:19:PHE:HA	1:A:24:ASN:CB	2.48	0.43
1:A:157:LYS:CB	1:A:209:TYR:CE2	3.01	0.43
1:C:231:PHE:O	1:C:234:CYS:HB2	2.18	0.43
1:C:238:GLU:OE1	1:C:242:LEU:HD21	2.18	0.43
1:A:165:LYS:HG3	1:B:305:TRP:CZ2	2.54	0.43
1:B:280:ALA:O	1:B:283:ASP:HB2	2.17	0.43
1:D:143:GLN:O	1:D:144:LYS:C	2.62	0.43
1:A:300:PRO:HB3	1:B:153:LEU:HD21	2.01	0.43
1:C:98:HIS:CD2	1:C:258:LEU:CD1	2.99	0.43
1:C:272:GLU:HB2	1:D:253:LYS:HE3	2.00	0.43
1:A:116:TRP:CE3	1:A:116:TRP:C	2.97	0.43
1:B:47:GLN:HA	1:B:106:LEU:HD21	2.00	0.43
1:B:97:LEU:O	1:B:100:GLU:N	2.50	0.43
1:B:299:TRP:O	1:B:300:PRO:C	2.61	0.43
1:B:31:ARG:O	1:B:34:ASP:HB2	2.18	0.43
1:B:207:GLU:O	1:B:211:LYS:HB2	2.19	0.43
1:B:224:MET:O	1:B:225:GLU:C	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:279:ASP:C	1:C:279:ASP:OD1	2.61	0.43
1:D:67:TRP:HB3	1:D:88:MET:SD	2.59	0.43
1:C:20:TRP:CZ3	1:C:224:MET:HA	2.54	0.43
1:A:275:ILE:O	1:A:276:ARG:C	2.61	0.43
1:A:281:GLN:O	1:A:282:GLU:C	2.61	0.43
1:C:21:GLU:O	1:C:22:VAL:C	2.62	0.43
1:A:116:TRP:CE3	1:A:117:GLN:N	2.87	0.43
1:A:258:LEU:O	1:A:261:ASN:N	2.47	0.43
1:B:90:GLU:O	1:B:91:ALA:C	2.62	0.43
1:C:157:LYS:O	1:C:160:TYR:N	2.52	0.43
1:C:232:GLU:O	1:C:236:GLN:HG2	2.19	0.43
1:A:183:VAL:CG2	1:A:184:THR:HB	2.48	0.42
1:B:139:PHE:O	1:B:140:ARG:C	2.59	0.42
1:C:98:HIS:NE2	1:C:258:LEU:CD1	2.82	0.42
1:C:220:THR:O	1:C:221:PRO:C	2.60	0.42
1:C:270:GLU:HA	1:C:273:GLN:HB3	2.01	0.42
1:A:50:ALA:HB2	1:A:105:LEU:HB3	2.00	0.42
1:A:183:VAL:HG13	1:A:184:THR:CB	2.48	0.42
1:B:133:LYS:O	1:B:134:GLU:C	2.61	0.42
1:B:143:GLN:HB2	1:B:227:MET:HE1	1.96	0.42
1:C:32:ILE:CG2	1:C:132:THR:HG22	2.49	0.42
1:B:102:LYS:O	1:B:103:ASN:C	2.62	0.42
1:B:187:GLN:O	1:B:191:LEU:HG	2.19	0.42
1:B:213:LEU:O	1:B:216:VAL:HG12	2.20	0.42
1:C:238:GLU:O	1:C:239:GLU:C	2.62	0.42
1:D:48:GLU:O	1:D:49:ARG:C	2.62	0.42
1:D:305:TRP:O	1:D:305:TRP:CD1	2.72	0.42
1:A:44:ASN:HA	1:A:47:GLN:HB2	2.01	0.42
1:A:297:MET:HB3	1:A:299:TRP:NE1	2.35	0.42
1:D:76:GLN:CA	1:D:76:GLN:NE2	2.77	0.42
1:A:19:PHE:CE1	1:B:293:PRO:HD3	2.53	0.42
1:C:245:LEU:CD1	1:D:80:LEU:HD23	2.49	0.42
1:D:88:MET:H	1:D:88:MET:HG2	1.63	0.42
1:A:25:TYR:C	1:A:25:TYR:CD2	2.98	0.42
1:A:143:GLN:O	1:A:144:LYS:C	2.62	0.42
1:B:243:VAL:O	1:B:244:PHE:C	2.62	0.42
1:C:245:LEU:O	1:C:249:LEU:HG	2.19	0.42
1:D:81:GLU:O	1:D:82:ARG:C	2.61	0.42
1:A:76:GLN:HB2	1:B:38:LEU:HD13	2.02	0.42
1:A:209:TYR:HE1	1:B:302:PHE:CD2	2.33	0.42
1:A:264:TYR:CE2	1:B:259:ALA:HB2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:ASN:HA	1:A:307:PRO:HD3	1.91	0.42
1:C:52:ILE:HD13	1:D:59:GLN:HB3	2.02	0.42
1:C:102:LYS:HE2	1:C:102:LYS:HB3	1.71	0.42
1:C:254:ARG:NH2	1:C:254:ARG:CB	2.83	0.42
1:D:118:LYS:HD2	1:D:118:LYS:HA	1.83	0.42
1:A:143:GLN:HA	1:A:223:TYR:CE1	2.54	0.42
1:A:271:LEU:HD22	1:A:275:ILE:HD11	2.02	0.42
1:A:283:ASP:O	1:A:284:LEU:C	2.60	0.42
1:A:284:LEU:O	1:A:285:ARG:C	2.60	0.42
1:B:24:ASN:C	1:B:26:LYS:H	2.27	0.42
1:B:46:VAL:HG13	1:B:105:LEU:HB3	2.02	0.42
1:C:75:PRO:O	1:C:77:TYR:HD1	2.02	0.42
1:C:254:ARG:NH2	1:C:254:ARG:CG	2.78	0.42
1:D:52:ILE:O	1:D:53:GLU:C	2.62	0.42
1:A:43:MET:HE1	1:A:114:LYS:CA	2.45	0.42
1:A:116:TRP:HE3	1:A:117:GLN:CA	2.33	0.42
1:B:157:LYS:N	1:B:209:TYR:CD1	2.88	0.42
1:C:102:LYS:O	1:C:103:ASN:C	2.61	0.42
1:A:157:LYS:HA	1:A:209:TYR:CD2	2.55	0.42
1:B:35:GLY:HA3	1:B:121:TYR:OH	2.20	0.42
1:B:280:ALA:HA	1:B:283:ASP:HB2	2.01	0.42
1:C:281:GLN:H	1:C:281:GLN:HG2	1.62	0.42
1:A:31:ARG:HH22	1:A:235:GLN:HG2	1.84	0.41
1:A:80:LEU:HD12	1:B:245:LEU:CD1	2.50	0.41
1:A:157:LYS:HG3	1:A:158:LYS:N	2.35	0.41
1:C:157:LYS:HG2	1:C:209:TYR:CZ	2.55	0.41
1:D:151:LYS:HE2	1:D:151:LYS:HB2	1.94	0.41
1:B:167:GLU:O	1:B:171:MET:HB2	2.20	0.41
1:C:26:LYS:HA	1:C:29:VAL:HB	2.02	0.41
1:A:183:VAL:CG2	1:A:184:THR:HA	2.44	0.41
1:C:81:GLU:HG3	1:C:82:ARG:N	2.35	0.41
1:A:174:GLU:O	1:A:178:LYS:HG3	2.21	0.41
1:A:277:GLY:O	1:A:278:ALA:C	2.64	0.41
1:B:250:LEU:HD23	1:B:250:LEU:HA	1.76	0.41
1:C:101:VAL:O	1:C:105:LEU:HG	2.20	0.41
1:C:287:PHE:CD2	1:C:287:PHE:C	2.97	0.41
1:D:37:ARG:HD3	1:D:41:ASP:OD2	2.21	0.41
1:A:60:LEU:HA	1:A:60:LEU:HD23	1.82	0.41
1:A:122:HIS:CD2	1:A:122:HIS:H	2.37	0.41
1:C:87:ILE:HG22	1:C:87:ILE:O	2.21	0.41
1:D:59:GLN:O	1:D:60:LEU:C	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:THR:CG2	1:A:16:THR:H	2.30	0.41
1:A:284:LEU:CD1	1:B:239:GLU:HB2	2.49	0.41
1:C:25:TYR:O	1:C:28:THR:HG22	2.21	0.41
1:D:18:SER:O	1:D:21:GLU:HB2	2.20	0.41
1:D:102:LYS:O	1:D:103:ASN:C	2.64	0.41
1:A:20:TRP:HD1	1:B:297:MET:HB2	1.85	0.41
1:B:21:GLU:HB2	1:B:24:ASN:ND2	2.36	0.41
1:C:64:ALA:HB2	1:C:91:ALA:HB3	2.03	0.41
1:C:79:SER:H	1:C:283:ASP:CG	2.29	0.41
1:D:57:GLY:O	1:D:61:THR:CG2	2.69	0.41
1:A:50:ALA:HB2	1:A:105:LEU:CD1	2.51	0.41
1:C:86:ALA:HB1	1:C:271:LEU:HD22	2.02	0.41
1:B:67:TRP:CZ3	1:B:70:LEU:HD12	2.56	0.41
1:B:93:LYS:HD3	1:B:267:VAL:HG22	2.02	0.41
1:C:22:VAL:HA	1:C:143:GLN:NE2	2.36	0.41
1:C:245:LEU:HD23	1:C:245:LEU:HA	1.73	0.41
1:C:250:LEU:CD1	1:C:254:ARG:HH12	2.24	0.41
1:C:284:LEU:HD23	1:C:284:LEU:HA	1.80	0.41
1:D:67:TRP:O	1:D:68:ARG:C	2.63	0.41
1:D:122:HIS:HD2	1:D:130:LYS:HG2	1.86	0.41
1:A:80:LEU:HD12	1:B:245:LEU:HD13	2.03	0.41
1:A:106:LEU:N	1:A:106:LEU:CD2	2.84	0.41
1:B:162:LEU:O	1:B:166:GLU:HG2	2.21	0.41
1:B:192:GLN:O	1:B:192:GLN:HG2	2.21	0.41
1:C:272:GLU:O	1:C:272:GLU:HG2	2.19	0.41
1:D:146:TRP:O	1:D:146:TRP:CD1	2.74	0.41
1:B:248:VAL:O	1:B:251:ASP:HB2	2.20	0.40
1:C:129:PHE:HB2	1:C:132:THR:HG23	2.03	0.40
1:A:20:TRP:CZ3	1:A:224:MET:HA	2.56	0.40
1:A:90:GLU:CD	1:A:90:GLU:C	2.88	0.40
1:A:149:LYS:HE3	1:A:219:THR:HG21	2.02	0.40
1:C:45:CYS:HA	1:D:67:TRP:CZ2	2.56	0.40
1:C:239:GLU:CB	1:D:284:LEU:HD11	2.48	0.40
1:D:253:LYS:HD3	1:D:254:ARG:N	2.36	0.40
1:C:159:ALA:C	1:C:205:THR:HG21	2.46	0.40
1:D:24:ASN:C	1:D:26:LYS:N	2.80	0.40
1:D:260:GLU:O	1:D:260:GLU:HG3	2.22	0.40
1:D:271:LEU:O	1:D:274:ALA:N	2.54	0.40
1:A:148:LYS:HA	1:A:148:LYS:HD2	1.84	0.40
1:A:241:ARG:C	1:A:243:VAL:H	2.30	0.40
1:B:30:LYS:O	1:B:31:ARG:C	2.63	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:121:TYR:HA	1:D:130:LYS:HG2	2.03	0.40
1:A:31:ARG:HD2	1:B:77:TYR:OH	2.22	0.40
1:A:168:LYS:HE2	1:A:172:THR:CG2	2.50	0.40
1:A:240:LYS:HA	1:A:240:LYS:HE2	2.02	0.40
1:B:117:GLN:O	1:B:117:GLN:HG2	2.20	0.40
1:C:93:LYS:O	1:C:97:LEU:HD23	2.21	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	292/308 (95%)	254 (87%)	31 (11%)	7 (2%)	4	16
1	B	292/308 (95%)	256 (88%)	32 (11%)	4 (1%)	9	28
1	C	283/308 (92%)	259 (92%)	23 (8%)	1 (0%)	30	56
1	D	272/308 (88%)	246 (90%)	25 (9%)	1 (0%)	30	56
All	All	1139/1232 (92%)	1015 (89%)	111 (10%)	13 (1%)	11	33

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	22	VAL
1	D	52	ILE
1	A	104	ASN
1	A	281	GLN
1	B	31	ARG
1	B	281	GLN
1	B	84	TRP
1	B	134	GLU
1	C	281	GLN

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Mol	Chain	Res	Type
1	A	18	SER
1	A	48	GLU
1	A	254	ARG
1	A	127	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	261/274 (95%)	217 (83%)	44 (17%)	2	6
1	B	260/274 (95%)	229 (88%)	31 (12%)	5	15
1	C	252/274 (92%)	219 (87%)	33 (13%)	4	11
1	D	241/274 (88%)	203 (84%)	38 (16%)	2	7
All	All	1014/1096 (92%)	868 (86%)	146 (14%)	3	9

All (146) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	PHE
1	A	22	VAL
1	A	28	THR
1	A	29	VAL
1	A	30	LYS
1	A	31	ARG
1	A	42	LEU
1	A	44	ASN
1	A	45	CYS
1	A	49	ARG
1	A	51	LYS
1	A	52	ILE
1	A	53	GLU
1	A	61	THR
1	A	69	GLN
1	A	71	ILE
1	A	80	LEU

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Mol	Chain	Res	Type
1	A	89	THR
1	A	90	GLU
1	A	106	LEU
1	A	118	LYS
1	A	122	HIS
1	A	125	ILE
1	A	132	THR
1	A	146	TRP
1	A	151	LYS
1	A	162	LEU
1	A	166	GLU
1	A	180	GLU
1	A	184	THR
1	A	192	GLN
1	A	216	VAL
1	A	232	GLU
1	A	236	GLN
1	A	240	LYS
1	A	241	ARG
1	A	243	VAL
1	A	245	LEU
1	A	253	LYS
1	A	260	GLU
1	A	267	VAL
1	A	271	LEU
1	A	272	GLU
1	A	306	ASN
1	B	28	THR
1	B	31	ARG
1	B	42	LEU
1	B	49	ARG
1	B	52	ILE
1	B	70	LEU
1	B	87	ILE
1	B	88	MET
1	B	90	GLU
1	B	108	GLU
1	B	110	LEU
1	B	122	HIS
1	B	125	ILE
1	B	131	GLU
1	B	134	GLU

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Mol	Chain	Res	Type
1	B	140	ARG
1	B	141	LYS
1	B	158	LYS
1	B	162	LEU
1	B	175	MET
1	B	178	LYS
1	B	179	THR
1	B	213	LEU
1	B	216	VAL
1	B	219	THR
1	B	240	LYS
1	B	245	LEU
1	B	265	ILE
1	B	271	LEU
1	B	290	THR
1	B	306	ASN
1	C	28	THR
1	C	31	ARG
1	C	37	ARG
1	C	58	GLN
1	C	61	THR
1	C	71	ILE
1	C	87	ILE
1	C	90	GLU
1	C	126	MET
1	C	131	GLU
1	C	141	LYS
1	C	150	MET
1	C	151	LYS
1	C	162	LEU
1	C	168	LYS
1	C	178	LYS
1	C	179	THR
1	C	181	GLN
1	C	183	VAL
1	C	225	GLU
1	C	226	ASN
1	C	229	GLN
1	C	236	GLN
1	C	245	LEU
1	C	248	VAL
1	C	250	LEU

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Mol	Chain	Res	Type
1	C	254	ARG
1	C	261	ASN
1	C	271	LEU
1	C	281	GLN
1	C	282	GLU
1	C	297	MET
1	C	299	TRP
1	D	29	VAL
1	D	31	ARG
1	D	43	MET
1	D	58	GLN
1	D	61	THR
1	D	66	ARG
1	D	76	GLN
1	D	79	SER
1	D	82	ARG
1	D	88	MET
1	D	90	GLU
1	D	97	LEU
1	D	99	GLN
1	D	103	ASN
1	D	113	VAL
1	D	125	ILE
1	D	130	LYS
1	D	133	LYS
1	D	140	ARG
1	D	141	LYS
1	D	151	LYS
1	D	167	GLU
1	D	175	MET
1	D	225	GLU
1	D	226	ASN
1	D	229	GLN
1	D	236	GLN
1	D	245	LEU
1	D	247	GLU
1	D	248	VAL
1	D	250	LEU
1	D	251	ASP
1	D	267	VAL
1	D	271	LEU
1	D	290	THR

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Mol	Chain	Res	Type
1	D	297	MET
1	D	303	GLU
1	D	305	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	69	GLN
1	A	76	GLN
1	A	104	ASN
1	A	117	GLN
1	A	122	HIS
1	A	206	GLN
1	A	222	GLN
1	A	236	GLN
1	A	257	ASN
1	A	266	HIS
1	B	44	ASN
1	B	58	GLN
1	B	69	GLN
1	B	103	ASN
1	B	206	GLN
1	B	222	GLN
1	B	235	GLN
1	B	236	GLN
1	B	306	ASN
1	C	36	HIS
1	C	44	ASN
1	C	58	GLN
1	C	99	GLN
1	C	103	ASN
1	C	117	GLN
1	C	124	GLN
1	C	143	GLN
1	C	181	GLN
1	C	200	GLN
1	C	206	GLN
1	C	222	GLN
1	C	226	ASN
1	C	229	GLN
1	C	235	GLN

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Mol	Chain	Res	Type
1	C	236	GLN
1	C	255	HIS
1	C	261	ASN
1	C	266	HIS
1	D	36	HIS
1	D	69	GLN
1	D	76	GLN
1	D	122	HIS
1	D	124	GLN
1	D	143	GLN
1	D	222	GLN
1	D	226	ASN
1	D	229	GLN
1	D	235	GLN
1	D	236	GLN
1	D	281	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	294/308 (95%)	1.30	64 (21%) 2 2	43, 74, 116, 166	0
1	B	294/308 (95%)	0.98	33 (11%) 10 9	35, 66, 137, 168	0
1	C	285/308 (92%)	1.18	36 (12%) 8 7	55, 80, 118, 153	0
1	D	276/308 (89%)	1.46	60 (21%) 2 2	60, 85, 202, 232	0
All	All	1149/1232 (93%)	1.23	193 (16%) 4 3	35, 78, 151, 232	0

All (193) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	260	GLU	5.6
1	D	209	TYR	5.5
1	A	125	ILE	5.3
1	D	27	ARG	5.3
1	D	77	TYR	5.0
1	A	183	VAL	5.0
1	B	75	PRO	5.0
1	B	227	MET	4.7
1	A	27	ARG	4.7
1	D	196	ASP	4.6
1	B	191	LEU	4.5
1	A	124	GLN	4.4
1	C	27	ARG	4.4
1	D	200	GLN	4.2
1	D	213	LEU	4.2
1	D	212	VAL	3.9
1	A	32	ILE	3.7
1	B	189	LYS	3.7
1	B	204	LYS	3.7
1	A	233	GLN	3.7
1	D	161	HIS	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	60	LEU	3.7
1	A	262	SER	3.7
1	D	205	THR	3.6
1	A	213	LEU	3.6
1	D	97	LEU	3.6
1	A	113	VAL	3.5
1	C	265	ILE	3.5
1	D	259	ALA	3.5
1	A	196	ASP	3.4
1	D	85	GLY	3.4
1	D	216	VAL	3.4
1	D	262	SER	3.3
1	B	308	ASP	3.3
1	A	229	GLN	3.3
1	C	196	ASP	3.3
1	B	214	GLU	3.3
1	D	258	LEU	3.3
1	C	192	GLN	3.2
1	B	27	ARG	3.2
1	A	120	ALA	3.2
1	A	188	GLN	3.2
1	D	176	ASN	3.1
1	B	183	VAL	3.1
1	D	178	LYS	3.1
1	C	204	LYS	3.1
1	C	77	TYR	3.1
1	B	180	GLU	3.0
1	A	209	TYR	3.0
1	C	258	LEU	3.0
1	A	216	VAL	3.0
1	C	203	GLN	2.9
1	C	185	PRO	2.9
1	C	79	SER	2.9
1	D	199	LYS	2.9
1	D	76	GLN	2.9
1	D	160	TYR	2.9
1	A	131	GLU	2.9
1	C	288	ARG	2.9
1	D	177	SER	2.9
1	B	185	PRO	2.8
1	A	240	LYS	2.8
1	D	207	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	118	LYS	2.8
1	A	179	THR	2.8
1	B	262	SER	2.8
1	C	52	ILE	2.7
1	C	217	GLY	2.7
1	A	185	PRO	2.7
1	D	142	ALA	2.7
1	A	189	LYS	2.7
1	D	204	LYS	2.7
1	C	294	GLY	2.7
1	B	119	ASP	2.7
1	A	54	LYS	2.6
1	A	20	TRP	2.6
1	A	305	TRP	2.6
1	B	67	TRP	2.6
1	A	130	LYS	2.6
1	D	300	PRO	2.6
1	A	136	GLU	2.6
1	D	155	ALA	2.6
1	A	126	MET	2.6
1	A	143	GLN	2.6
1	B	203	GLN	2.6
1	A	19	PHE	2.6
1	D	149	LYS	2.6
1	D	231	PHE	2.6
1	D	153	LEU	2.5
1	D	264	TYR	2.5
1	B	200	GLN	2.5
1	D	261	ASN	2.5
1	D	82	ARG	2.5
1	A	122	HIS	2.5
1	A	23	GLY	2.5
1	C	130	LYS	2.5
1	D	201	ASP	2.5
1	B	293	PRO	2.5
1	C	292	GLY	2.5
1	A	26	LYS	2.5
1	C	182	SER	2.5
1	A	22	VAL	2.5
1	A	195	VAL	2.5
1	A	244	PHE	2.4
1	C	282	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	73	LYS	2.4
1	A	151	LYS	2.4
1	A	260	GLU	2.4
1	B	170	ALA	2.4
1	D	169	LEU	2.4
1	A	202	VAL	2.4
1	D	74	GLY	2.4
1	A	174	GLU	2.4
1	A	307	PRO	2.4
1	B	194	LYS	2.4
1	D	159	ALA	2.4
1	A	121	TYR	2.4
1	A	192	GLN	2.3
1	C	200	GLN	2.3
1	A	191	LEU	2.3
1	A	123	LYS	2.3
1	D	221	PRO	2.3
1	B	195	VAL	2.3
1	C	267	VAL	2.3
1	D	19	PHE	2.3
1	B	59	GLN	2.3
1	B	171	MET	2.3
1	C	187	GLN	2.3
1	D	171	MET	2.3
1	C	97	LEU	2.3
1	C	283	ASP	2.3
1	B	169	LEU	2.3
1	B	261	ASN	2.3
1	B	280	ALA	2.3
1	A	182	SER	2.3
1	B	172	THR	2.3
1	C	63	TRP	2.3
1	C	179	THR	2.3
1	D	219	THR	2.3
1	C	296	PRO	2.3
1	C	23	GLY	2.3
1	A	180	GLU	2.2
1	D	235	GLN	2.2
1	A	243	VAL	2.2
1	D	25	TYR	2.2
1	D	263	SER	2.2
1	D	170	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	165	LYS	2.2
1	A	116	TRP	2.2
1	C	300	PRO	2.2
1	A	138	GLY	2.2
1	B	190	LYS	2.2
1	A	214	GLU	2.2
1	C	83	ALA	2.2
1	A	176	ASN	2.2
1	D	17	ASP	2.2
1	C	293	PRO	2.2
1	A	134	GLU	2.2
1	D	156	ALA	2.2
1	A	24	ASN	2.2
1	B	71	ILE	2.1
1	B	76	GLN	2.1
1	D	266	HIS	2.1
1	A	139	PHE	2.1
1	D	198	CYS	2.1
1	D	257	ASN	2.1
1	B	209	TYR	2.1
1	A	210	GLU	2.1
1	D	52	ILE	2.1
1	D	203	GLN	2.1
1	D	273	GLN	2.1
1	A	259	ALA	2.1
1	C	71	ILE	2.1
1	D	168	LYS	2.1
1	A	145	PRO	2.1
1	C	28	THR	2.1
1	D	220	THR	2.1
1	D	32	ILE	2.1
1	A	177	SER	2.0
1	D	164	CYS	2.0
1	D	197	LYS	2.0
1	B	267	VAL	2.0
1	B	80	LEU	2.0
1	A	302	PHE	2.0
1	C	252	ILE	2.0
1	D	172	THR	2.0
1	A	303	GLU	2.0
1	C	295	MET	2.0
1	B	263	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	183	VAL	2.0
1	A	129	PHE	2.0
1	A	142	ALA	2.0
1	A	149	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CA	A	310	1/1	0.60	0.23	102,102,102,102	0

6.5 Other polymers [i](#)

There are no such residues in this entry.