



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2026 – 12:05 AM UTC

PDB ID : 4IH4 / pdb_00004ih4
Title : Crystal structure of Arabidopsis DWARF14 orthologue, AtD14
Authors : Zhou, X.E.; Zhao, L.-H.; Wu, Z.-S.; Yi, W.; Li, S.; Li, Y.; Xu, Y.; Xu, T.-H.; Liu, Y.; Chen, R.-Z.; Kovach, A.; Kang, Y.; Hou, L.; He, Y.; Zhang, C.; Melcher, K.; Xu, H.E.
Deposited on : 2012-12-18
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

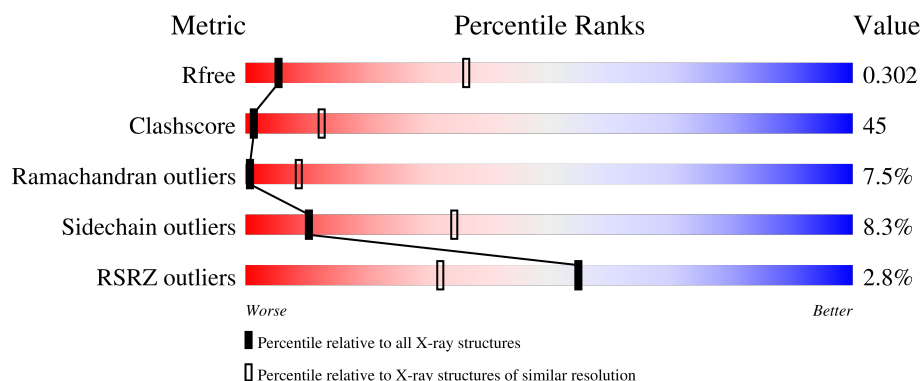
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	267	
1	B	267	
1	C	267	
1	D	267	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 8160 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.

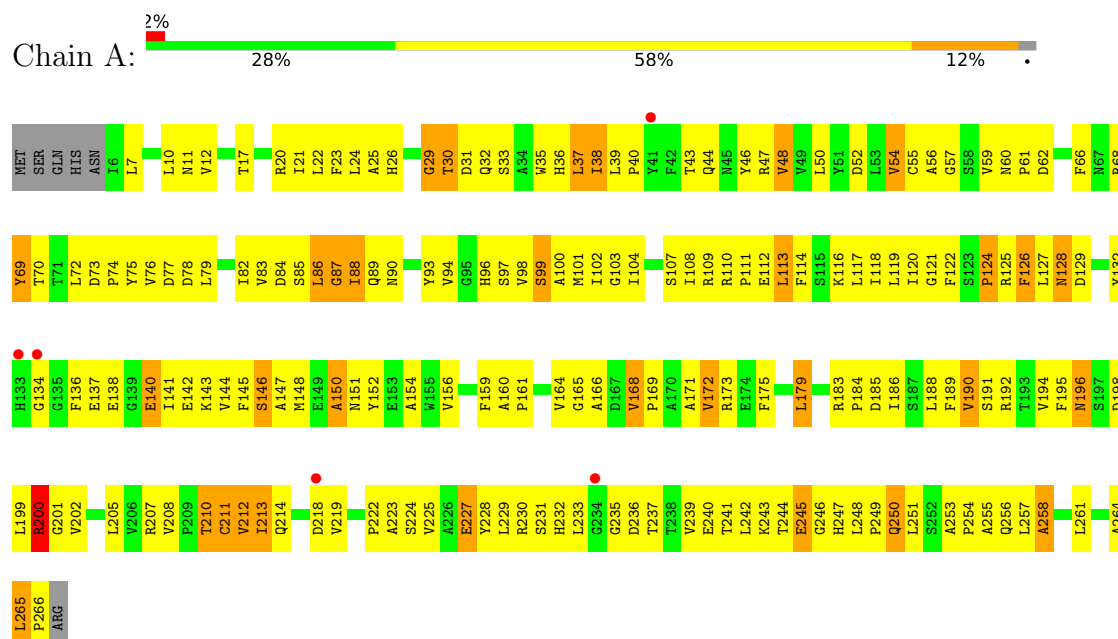
- Molecule 1 is a protein called AT3g03990/T11I18_10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	261	Total	C	N	O	S	0	0	0
			2040	1312	346	376	6			
1	B	261	Total	C	N	O	S	0	0	0
			2040	1312	346	376	6			
1	C	261	Total	C	N	O	S	0	0	0
			2040	1312	346	376	6			
1	D	261	Total	C	N	O	S	0	0	0
			2040	1312	346	376	6			

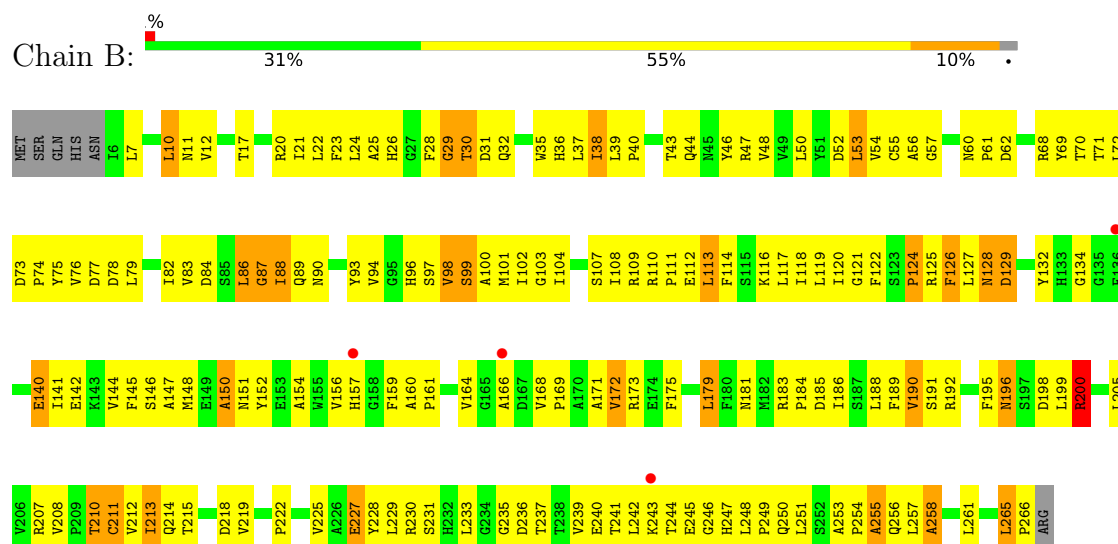
3 Residue-property plots

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.

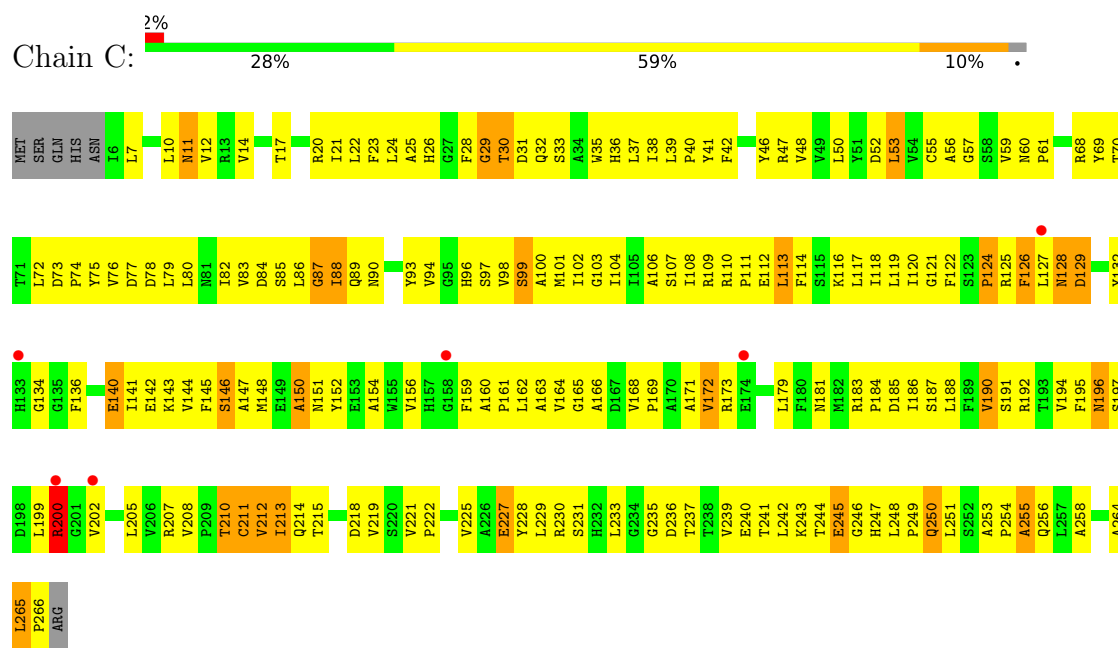
• Molecule 1: AT3g03990/T11I18_10



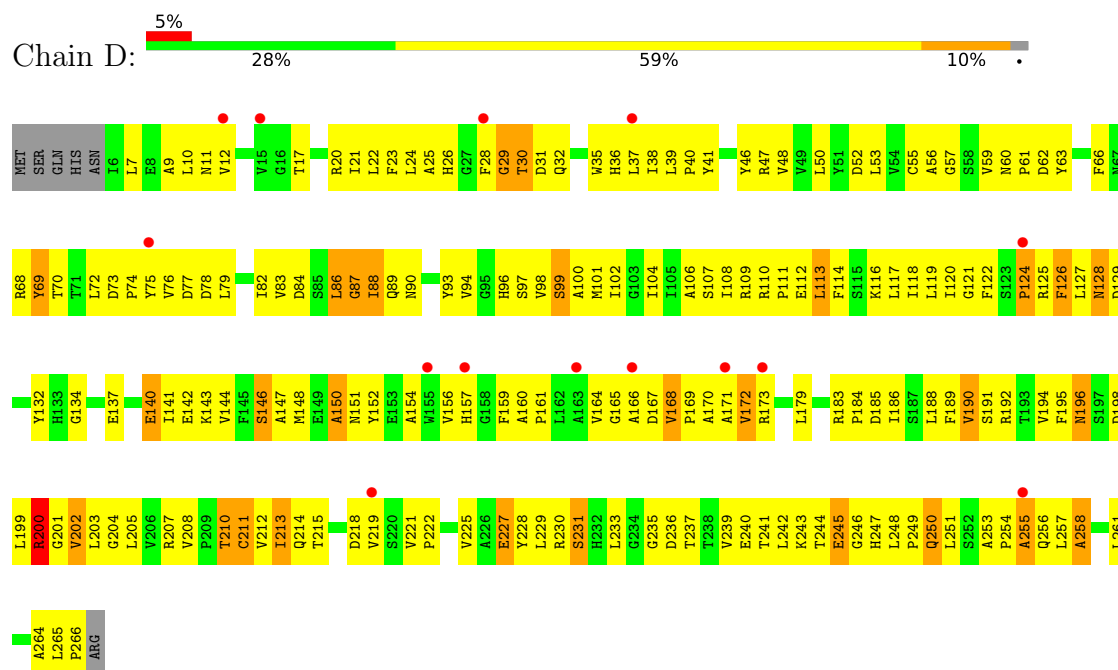
• Molecule 1: AT3g03990/T11I18_10



• Molecule 1: AT3g03990/T11I18_10



• Molecule 1: AT3g03990/T11I18_10



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	184.86Å 44.63Å 160.97Å 90.00° 121.07° 90.00°	Depositor
Resolution (Å)	30.00 – 3.50 30.00 – 3.50	Depositor EDS
% Data completeness (in resolution range)	64.3 (30.00-3.50) 77.6 (30.00-3.50)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 3.47Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.279 , 0.336 (Not available) , 0.302	Depositor DCC
R_{free} test set	871 reflections (6.98%)	wwPDB-VP
Wilson B-factor (Å ²)	51.5	Xtriage
Anisotropy	0.404	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 25.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.77	EDS
Total number of atoms	8160	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.85% 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](#)

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	0.67	0/2089	0.95	6/2847 (0.2%)
1	B	0.66	1/2089 (0.0%)	0.96	4/2847 (0.1%)
1	C	0.61	0/2089	0.95	2/2847 (0.1%)
1	D	0.61	0/2089	0.95	6/2847 (0.2%)
All	All	0.64	1/8356 (0.0%)	0.95	18/11388 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	98	VAL	CA-CB	-5.93	1.47	1.54

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	172	VAL	N-CA-C	-7.52	106.16	113.53
1	B	10	LEU	N-CA-C	-6.38	100.05	109.11
1	C	172	VAL	N-CA-C	-6.24	107.42	113.53
1	A	212	VAL	N-CA-C	6.16	117.53	109.58
1	A	172	VAL	N-CA-C	-6.16	107.49	113.53
1	D	172	VAL	N-CA-C	-5.86	107.79	113.53
1	C	212	VAL	N-CA-C	5.65	116.87	109.58
1	B	86	LEU	N-CA-C	-5.58	106.14	113.17
1	A	86	LEU	N-CA-C	-5.55	106.18	113.17
1	D	168	VAL	CA-C-N	5.49	125.84	119.47
1	D	168	VAL	C-N-CA	5.49	125.84	119.47
1	A	168	VAL	CA-C-N	5.30	125.61	119.47
1	A	168	VAL	C-N-CA	5.30	125.61	119.47
1	D	86	LEU	N-CA-C	-5.26	106.54	113.17
1	D	231	SER	N-CA-C	5.15	116.74	111.03
1	B	172	VAL	CB-CA-C	-5.14	105.61	110.65
1	A	48	VAL	N-CA-C	5.09	115.61	108.89
1	D	172	VAL	CB-CA-C	-5.08	105.67	110.65

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	2040	0	2014	189	0
1	B	2040	0	2014	191	0
1	C	2040	0	2014	181	0
1	D	2040	0	2014	197	0
All	All	8160	0	8056	737	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 45.

All (737) 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:B:128:ASN:HB3	1:B:134:GLY:H	1.21	1.01
1:C:128:ASN:HB3	1:C:134:GLY:H	1.24	0.99
1:D:128:ASN:HB3	1:D:134:GLY:H	1.23	0.99
1:A:128:ASN:HB3	1:A:134:GLY:H	1.23	0.98
1:A:104:ILE:HD11	1:A:119:LEU:HD11	1.49	0.95
1:B:98:VAL:HA	1:B:101:MET:HE2	1.48	0.94
1:C:233:LEU:HD13	1:C:237:THR:HG21	1.48	0.93
1:A:98:VAL:HA	1:A:101:MET:HE2	1.48	0.93
1:D:104:ILE:HD11	1:D:119:LEU:HD11	1.49	0.92
1:B:233:LEU:HD13	1:B:237:THR:HG21	1.48	0.92
1:C:104:ILE:HD11	1:C:119:LEU:HD11	1.50	0.91
1:C:98:VAL:HA	1:C:101:MET:HE2	1.50	0.90
1:D:233:LEU:HD13	1:D:237:THR:HG21	1.53	0.90
1:A:85:SER:HB3	1:B:157:HIS:NE2	1.89	0.87
1:A:218:ASP:OD1	1:A:247:HIS:ND1	2.07	0.87
1:D:98:VAL:HA	1:D:101:MET:HE2	1.56	0.86
1:C:218:ASP:OD1	1:C:247:HIS:ND1	2.05	0.86
1:C:86:LEU:HD23	1:D:169:PRO:HB3	1.55	0.86
1:B:60:ASN:HD22	1:B:61:PRO:HD2	1.38	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:110:ARG:HD2	1:D:113:LEU:HD22	1.57	0.86
1:A:233:LEU:HD13	1:A:237:THR:HG21	1.56	0.85
1:B:104:ILE:HD11	1:B:119:LEU:HD11	1.57	0.84
1:C:164:VAL:HG21	1:C:172:VAL:HA	1.61	0.82
1:C:214:GLN:HB3	1:C:241:THR:HG22	1.60	0.82
1:A:164:VAL:HG21	1:A:172:VAL:HA	1.60	0.82
1:A:110:ARG:HD2	1:A:113:LEU:HD22	1.62	0.82
1:B:121:GLY:H	1:B:213:ILE:HG22	1.45	0.82
1:D:99:SER:HA	1:D:102:ILE:HD12	1.61	0.82
1:B:110:ARG:HD2	1:B:113:LEU:HD22	1.60	0.81
1:B:164:VAL:HG21	1:B:172:VAL:HA	1.61	0.81
1:C:22:LEU:HD12	1:C:23:PHE:H	1.44	0.81
1:D:218:ASP:OD1	1:D:247:HIS:ND1	2.14	0.81
1:B:205:LEU:HD11	1:D:202:VAL:HG21	1.61	0.81
1:A:22:LEU:HD12	1:A:23:PHE:H	1.45	0.81
1:C:121:GLY:H	1:C:213:ILE:HG22	1.47	0.79
1:C:129:ASP:HB2	1:C:132:TYR:HB3	1.62	0.79
1:A:214:GLN:HB3	1:A:241:THR:HG22	1.64	0.79
1:B:218:ASP:OD1	1:B:247:HIS:ND1	2.15	0.79
1:B:99:SER:HA	1:B:102:ILE:HD12	1.63	0.79
1:A:60:ASN:HD22	1:A:61:PRO:HD2	1.45	0.79
1:D:32:GLN:HB2	1:D:50:LEU:HD12	1.63	0.78
1:B:214:GLN:HB3	1:B:241:THR:HG22	1.65	0.78
1:C:60:ASN:HD22	1:C:61:PRO:HD2	1.47	0.78
1:A:124:PRO:HG2	1:A:125:ARG:H	1.48	0.78
1:D:60:ASN:HD22	1:D:61:PRO:HD2	1.48	0.78
1:C:32:GLN:HB2	1:C:50:LEU:HD12	1.66	0.78
1:B:32:GLN:HB2	1:B:50:LEU:HD12	1.65	0.78
1:D:121:GLY:H	1:D:213:ILE:HG22	1.48	0.78
1:C:218:ASP:CG	1:C:247:HIS:HD1	1.92	0.77
1:A:121:GLY:H	1:A:213:ILE:HG22	1.49	0.77
1:B:129:ASP:HB2	1:B:132:TYR:HB3	1.67	0.76
1:B:7:LEU:O	1:B:12:VAL:HG22	1.86	0.76
1:D:214:GLN:HB3	1:D:241:THR:HG22	1.67	0.76
1:B:60:ASN:HD22	1:B:61:PRO:CD	1.99	0.76
1:B:205:LEU:HD11	1:D:202:VAL:CG2	2.15	0.76
1:B:124:PRO:HG2	1:B:125:ARG:H	1.52	0.75
1:C:212:VAL:HB	1:C:239:VAL:HG13	1.67	0.75
1:D:164:VAL:HG21	1:D:172:VAL:HA	1.67	0.74
1:B:212:VAL:HB	1:B:239:VAL:HG13	1.70	0.74
1:C:110:ARG:HD2	1:C:113:LEU:HD22	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:THR:HB	1:C:237:THR:HG23	1.70	0.73
1:D:218:ASP:CG	1:D:247:HIS:HD1	1.95	0.73
1:D:7:LEU:O	1:D:12:VAL:HG22	1.88	0.73
1:C:124:PRO:HG2	1:C:125:ARG:H	1.54	0.73
1:C:99:SER:HA	1:C:102:ILE:HD12	1.70	0.73
1:A:32:GLN:HB2	1:A:50:LEU:HD12	1.71	0.72
1:D:129:ASP:HB2	1:D:132:TYR:HB3	1.69	0.72
1:C:141:ILE:HD12	1:C:142:GLU:N	2.04	0.72
1:D:124:PRO:HG2	1:D:125:ARG:H	1.55	0.72
1:D:60:ASN:HD22	1:D:61:PRO:CD	2.03	0.72
1:A:129:ASP:HB2	1:A:132:TYR:HB3	1.70	0.72
1:A:218:ASP:CG	1:A:247:HIS:HD1	1.97	0.72
1:D:22:LEU:HD12	1:D:23:PHE:H	1.54	0.72
1:C:108:ILE:O	1:C:111:PRO:HD3	1.90	0.72
1:A:85:SER:HB3	1:B:157:HIS:CE1	2.24	0.71
1:D:25:ALA:HB1	1:D:99:SER:OG	1.90	0.71
1:A:212:VAL:HB	1:A:239:VAL:HG13	1.73	0.71
1:B:22:LEU:HD12	1:B:23:PHE:H	1.56	0.70
1:B:218:ASP:CG	1:B:247:HIS:HD1	1.98	0.70
1:B:112:GLU:HG2	1:B:113:LEU:H	1.55	0.70
1:B:119:LEU:HD13	1:B:122:PHE:CD2	2.27	0.70
1:B:109:ARG:O	1:B:110:ARG:HG2	1.91	0.70
1:B:210:THR:HB	1:B:237:THR:HG23	1.73	0.70
1:D:119:LEU:HD13	1:D:122:PHE:CD2	2.27	0.70
1:B:192:ARG:O	1:B:196:ASN:HB2	1.93	0.69
1:D:210:THR:HB	1:D:237:THR:HG23	1.75	0.69
1:A:25:ALA:HB1	1:A:99:SER:OG	1.92	0.69
1:A:60:ASN:HD22	1:A:61:PRO:CD	2.06	0.68
1:C:112:GLU:HG2	1:C:113:LEU:H	1.58	0.68
1:A:7:LEU:O	1:A:12:VAL:HG22	1.93	0.68
1:C:185:ASP:O	1:C:188:LEU:HB3	1.92	0.68
1:A:99:SER:HA	1:A:102:ILE:HD12	1.74	0.68
1:C:85:SER:HB3	1:D:157:HIS:NE2	2.09	0.68
1:C:148:MET:HE3	1:C:188:LEU:HA	1.76	0.68
1:B:108:ILE:O	1:B:111:PRO:HD3	1.94	0.68
1:D:108:ILE:O	1:D:111:PRO:HD3	1.93	0.68
1:C:25:ALA:HB1	1:C:99:SER:OG	1.94	0.68
1:C:7:LEU:O	1:C:12:VAL:HG22	1.93	0.68
1:A:117:LEU:HD23	1:A:208:VAL:HG11	1.75	0.67
1:C:124:PRO:HD3	1:C:229:LEU:HD21	1.76	0.67
1:C:192:ARG:O	1:C:196:ASN:HB2	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:ASP:O	1:B:188:LEU:HB3	1.95	0.67
1:A:141:ILE:HD12	1:A:142:GLU:N	2.09	0.66
1:A:185:ASP:O	1:A:188:LEU:HB3	1.95	0.66
1:C:119:LEU:HD13	1:C:122:PHE:CD2	2.31	0.66
1:D:212:VAL:HB	1:D:239:VAL:HG13	1.78	0.66
1:A:210:THR:HB	1:A:237:THR:HG23	1.78	0.65
1:D:117:LEU:HD23	1:D:208:VAL:HG11	1.79	0.65
1:B:125:ARG:HB3	1:B:132:TYR:CE2	2.31	0.65
1:C:60:ASN:HD22	1:C:61:PRO:CD	2.09	0.65
1:B:141:ILE:HD12	1:B:142:GLU:N	2.12	0.65
1:A:119:LEU:HD13	1:A:122:PHE:CD2	2.32	0.64
1:D:148:MET:HE3	1:D:188:LEU:HA	1.78	0.64
1:D:21:ILE:HD13	1:D:90:ASN:O	1.96	0.64
1:B:124:PRO:HD3	1:B:229:LEU:HD21	1.79	0.64
1:C:233:LEU:CD1	1:C:237:THR:HG21	2.27	0.64
1:D:141:ILE:HD12	1:D:142:GLU:N	2.12	0.64
1:C:14:VAL:HG11	1:D:170:ALA:HB2	1.79	0.63
1:A:112:GLU:HG2	1:A:113:LEU:H	1.62	0.63
1:D:112:GLU:HG2	1:D:113:LEU:H	1.64	0.63
1:C:20:ARG:HB3	1:C:46:TYR:HD2	1.63	0.63
1:C:24:LEU:HD23	1:C:94:VAL:HB	1.80	0.63
1:D:192:ARG:O	1:D:196:ASN:HB2	1.99	0.62
1:C:96:HIS:CE1	1:C:97:SER:HB2	2.34	0.62
1:B:100:ALA:HB1	1:B:119:LEU:HD22	1.82	0.62
1:D:185:ASP:O	1:D:188:LEU:HB3	1.99	0.62
1:A:124:PRO:HD3	1:A:229:LEU:HD21	1.81	0.62
1:B:101:MET:O	1:B:104:ILE:N	2.33	0.62
1:B:148:MET:HE3	1:B:188:LEU:HA	1.82	0.62
1:D:124:PRO:HD3	1:D:229:LEU:HD21	1.81	0.62
1:D:253:ALA:HB1	1:D:256:GLN:HE21	1.64	0.62
1:A:26:HIS:O	1:A:99:SER:HB2	2.01	0.61
1:B:98:VAL:HA	1:B:101:MET:CE	2.28	0.61
1:B:116:LYS:O	1:B:118:ILE:HD12	1.99	0.61
1:A:148:MET:HE3	1:A:188:LEU:HA	1.80	0.61
1:D:101:MET:O	1:D:104:ILE:N	2.33	0.61
1:D:76:VAL:HG22	1:D:102:ILE:HG23	1.82	0.61
1:B:112:GLU:HG2	1:B:113:LEU:N	2.16	0.61
1:D:125:ARG:HB3	1:D:132:TYR:CE2	2.35	0.61
1:C:88:ILE:HA	1:D:167:ASP:OD2	2.01	0.61
1:D:247:HIS:HD2	1:D:248:LEU:HD11	1.65	0.61
1:A:20:ARG:HB3	1:A:46:TYR:HD2	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:ALA:HB1	1:B:99:SER:OG	2.01	0.60
1:B:84:ASP:O	1:B:87:GLY:N	2.31	0.60
1:D:17:THR:HA	1:D:47:ARG:NE	2.16	0.60
1:B:109:ARG:NH1	1:D:207:ARG:HH22	2.00	0.60
1:B:110:ARG:C	1:B:112:GLU:H	2.09	0.60
1:B:184:PRO:O	1:B:185:ASP:C	2.45	0.60
1:C:21:ILE:HD13	1:C:90:ASN:O	2.01	0.60
1:C:125:ARG:HB3	1:C:132:TYR:CE2	2.37	0.60
1:C:22:LEU:HD12	1:C:23:PHE:N	2.16	0.60
1:C:222:PRO:HB2	1:C:225:VAL:HG23	1.84	0.60
1:A:125:ARG:HB3	1:A:132:TYR:CE2	2.37	0.60
1:A:69:TYR:HB3	1:A:75:TYR:CE1	2.37	0.59
1:A:116:LYS:O	1:A:118:ILE:HD12	2.01	0.59
1:A:76:VAL:HG22	1:A:102:ILE:HG23	1.83	0.59
1:A:109:ARG:O	1:A:110:ARG:HG2	2.02	0.59
1:C:76:VAL:HG22	1:C:102:ILE:HG23	1.84	0.59
1:C:101:MET:O	1:C:104:ILE:N	2.36	0.59
1:D:184:PRO:O	1:D:185:ASP:C	2.46	0.59
1:A:46:TYR:OH	1:A:266:PRO:HD3	2.02	0.59
1:D:109:ARG:O	1:D:110:ARG:HG2	2.02	0.59
1:A:35:TRP:O	1:A:38:ILE:HG22	2.03	0.58
1:A:17:THR:HA	1:A:47:ARG:NE	2.18	0.58
1:B:35:TRP:O	1:B:38:ILE:HG22	2.04	0.58
1:C:247:HIS:HD2	1:C:248:LEU:HD11	1.68	0.58
1:A:110:ARG:C	1:A:112:GLU:H	2.12	0.58
1:B:69:TYR:HB3	1:B:75:TYR:CE1	2.38	0.58
1:B:222:PRO:HB2	1:B:225:VAL:HG23	1.84	0.58
1:A:192:ARG:O	1:A:196:ASN:HB2	2.04	0.58
1:D:128:ASN:HB3	1:D:134:GLY:N	2.07	0.58
1:A:50:LEU:O	1:A:50:LEU:HG	2.04	0.57
1:B:21:ILE:HD13	1:B:90:ASN:O	2.04	0.57
1:A:36:HIS:C	1:A:38:ILE:H	2.12	0.57
1:B:233:LEU:CD1	1:B:237:THR:HG21	2.28	0.57
1:B:76:VAL:HG22	1:B:102:ILE:HG23	1.85	0.57
1:D:50:LEU:O	1:D:50:LEU:HG	2.03	0.57
1:A:84:ASP:O	1:A:87:GLY:N	2.32	0.57
1:B:117:LEU:HD23	1:B:208:VAL:HG11	1.87	0.57
1:D:125:ARG:HG2	1:D:127:LEU:O	2.04	0.57
1:B:253:ALA:HB1	1:B:256:GLN:HE21	1.68	0.57
1:C:17:THR:HA	1:C:47:ARG:NE	2.19	0.57
1:A:85:SER:HB3	1:B:157:HIS:CD2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:35:TRP:O	1:C:38:ILE:HG22	2.04	0.57
1:D:126:PHE:HB3	1:D:195:PHE:CD1	2.40	0.57
1:D:110:ARG:C	1:D:112:GLU:H	2.12	0.57
1:D:98:VAL:HA	1:D:101:MET:CE	2.32	0.56
1:B:26:HIS:O	1:B:99:SER:HB2	2.04	0.56
1:A:183:ARG:O	1:A:186:ILE:HB	2.05	0.56
1:B:89:GLN:O	1:B:113:LEU:HA	2.05	0.56
1:A:108:ILE:O	1:A:111:PRO:HD3	2.05	0.56
1:B:20:ARG:HB3	1:B:46:TYR:HD2	1.70	0.56
1:B:39:LEU:N	1:B:40:PRO:HD2	2.20	0.56
1:C:20:ARG:HB3	1:C:46:TYR:CD2	2.41	0.56
1:C:26:HIS:O	1:C:99:SER:HB2	2.06	0.56
1:C:110:ARG:C	1:C:112:GLU:H	2.12	0.56
1:C:116:LYS:O	1:C:118:ILE:HD12	2.05	0.56
1:A:126:PHE:HB3	1:A:195:PHE:CD1	2.40	0.56
1:C:69:TYR:HB3	1:C:75:TYR:CE1	2.40	0.56
1:B:24:LEU:HD23	1:B:94:VAL:HB	1.88	0.55
1:B:183:ARG:O	1:B:186:ILE:HB	2.06	0.55
1:C:46:TYR:OH	1:C:266:PRO:HD3	2.06	0.55
1:C:117:LEU:HD23	1:C:208:VAL:HG11	1.87	0.55
1:D:210:THR:HG22	1:D:211:CYS:H	1.71	0.55
1:B:125:ARG:HG2	1:B:127:LEU:O	2.06	0.55
1:C:112:GLU:HG2	1:C:113:LEU:N	2.20	0.55
1:D:60:ASN:ND2	1:D:62:ASP:H	2.05	0.55
1:C:109:ARG:O	1:C:110:ARG:HG2	2.06	0.55
1:D:69:TYR:HB3	1:D:75:TYR:CE1	2.42	0.55
1:A:39:LEU:N	1:A:40:PRO:HD2	2.22	0.55
1:D:222:PRO:HB2	1:D:225:VAL:HG23	1.87	0.55
1:B:50:LEU:N	1:B:50:LEU:HD23	2.22	0.55
1:A:210:THR:HG22	1:A:211:CYS:H	1.71	0.55
1:C:85:SER:HB3	1:D:157:HIS:CE1	2.42	0.54
1:B:126:PHE:HB3	1:B:195:PHE:CD1	2.42	0.54
1:C:72:LEU:O	1:C:76:VAL:HG23	2.08	0.54
1:D:247:HIS:HD2	1:D:248:LEU:CD1	2.20	0.54
1:D:117:LEU:HB3	1:D:210:THR:HG23	1.90	0.54
1:A:50:LEU:HD23	1:A:50:LEU:N	2.22	0.54
1:A:101:MET:O	1:A:104:ILE:N	2.41	0.54
1:A:247:HIS:HD2	1:A:248:LEU:HD11	1.72	0.54
1:D:38:ILE:HD11	1:D:258:ALA:N	2.23	0.54
1:B:148:MET:HE3	1:B:188:LEU:HD12	1.90	0.54
1:A:21:ILE:HD13	1:A:90:ASN:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:TYR:OH	1:B:266:PRO:HD3	2.08	0.54
1:C:210:THR:HG22	1:C:211:CYS:H	1.72	0.54
1:D:46:TYR:OH	1:D:266:PRO:HD3	2.08	0.54
1:D:100:ALA:HB1	1:D:119:LEU:HD22	1.88	0.54
1:C:100:ALA:HB1	1:C:119:LEU:HD22	1.90	0.54
1:C:184:PRO:O	1:C:185:ASP:C	2.49	0.54
1:D:112:GLU:HG2	1:D:113:LEU:HD13	1.89	0.54
1:D:244:THR:HB	1:D:256:GLN:OE1	2.08	0.54
1:C:205:LEU:O	1:C:207:ARG:HD2	2.08	0.54
1:A:36:HIS:O	1:A:38:ILE:N	2.41	0.53
1:B:228:TYR:O	1:B:231:SER:HB2	2.08	0.53
1:C:151:ASN:HB3	1:C:154:ALA:HB3	1.89	0.53
1:A:20:ARG:HB3	1:A:46:TYR:CD2	2.43	0.53
1:A:22:LEU:HD12	1:A:23:PHE:N	2.18	0.53
1:C:230:ARG:HG3	1:C:230:ARG:HH11	1.73	0.53
1:D:50:LEU:N	1:D:50:LEU:HD23	2.22	0.53
1:D:114:PHE:HB3	1:D:117:LEU:CD2	2.39	0.53
1:D:183:ARG:O	1:D:186:ILE:HB	2.08	0.53
1:A:72:LEU:O	1:A:76:VAL:HG23	2.09	0.53
1:A:186:ILE:O	1:A:190:VAL:HG23	2.07	0.53
1:C:93:TYR:HB2	1:C:114:PHE:HE1	1.74	0.53
1:C:183:ARG:O	1:C:186:ILE:HB	2.09	0.53
1:D:60:ASN:HD22	1:D:61:PRO:N	2.07	0.53
1:B:110:ARG:C	1:B:112:GLU:N	2.67	0.53
1:B:128:ASN:HB3	1:B:134:GLY:N	2.06	0.53
1:C:126:PHE:HB3	1:C:195:PHE:CD1	2.43	0.53
1:D:228:TYR:O	1:D:231:SER:HB2	2.09	0.53
1:C:186:ILE:O	1:C:190:VAL:HG23	2.08	0.53
1:B:38:ILE:HD11	1:B:258:ALA:N	2.24	0.53
1:B:124:PRO:HG2	1:B:132:TYR:OH	2.08	0.53
1:A:240:GLU:HG3	1:A:241:THR:N	2.24	0.53
1:B:17:THR:HA	1:B:47:ARG:NE	2.24	0.53
1:B:96:HIS:CE1	1:B:97:SER:HB2	2.44	0.53
1:D:10:LEU:HB3	1:D:52:ASP:O	2.09	0.53
1:D:24:LEU:HD23	1:D:94:VAL:HB	1.91	0.53
1:A:222:PRO:HB2	1:A:225:VAL:HG23	1.90	0.52
1:B:36:HIS:C	1:B:38:ILE:H	2.17	0.52
1:B:60:ASN:ND2	1:B:61:PRO:HD2	2.16	0.52
1:C:169:PRO:HA	1:C:172:VAL:CG1	2.39	0.52
1:D:112:GLU:HG2	1:D:113:LEU:N	2.24	0.52
1:A:143:LYS:O	1:A:146:SER:HB3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:PRO:O	1:A:185:ASP:C	2.50	0.52
1:A:200:ARG:HG2	1:A:200:ARG:HH11	1.74	0.52
1:B:205:LEU:O	1:B:207:ARG:HD2	2.08	0.52
1:B:207:ARG:CZ	1:D:73:ASP:OD1	2.57	0.52
1:D:20:ARG:HB3	1:D:46:TYR:HD2	1.75	0.52
1:C:210:THR:HB	1:C:237:THR:CG2	2.39	0.52
1:A:147:ALA:O	1:A:150:ALA:HB3	2.10	0.52
1:B:120:ILE:HG23	1:B:213:ILE:HG21	1.91	0.52
1:C:17:THR:HG22	1:C:47:ARG:NH2	2.25	0.52
1:B:207:ARG:NH2	1:D:73:ASP:OD1	2.43	0.52
1:C:140:GLU:O	1:C:144:VAL:HG23	2.10	0.52
1:D:22:LEU:HD23	1:D:48:VAL:HG22	1.92	0.52
1:D:186:ILE:O	1:D:190:VAL:HG23	2.10	0.52
1:A:117:LEU:HB3	1:A:210:THR:HG23	1.90	0.52
1:B:22:LEU:HD23	1:B:48:VAL:HG22	1.92	0.52
1:B:247:HIS:HD2	1:B:248:LEU:CD1	2.23	0.52
1:B:219:VAL:HG22	1:B:219:VAL:O	2.10	0.52
1:D:26:HIS:O	1:D:99:SER:HB2	2.10	0.52
1:B:230:ARG:HG3	1:B:230:ARG:HH11	1.74	0.51
1:D:36:HIS:C	1:D:38:ILE:H	2.18	0.51
1:D:116:LYS:O	1:D:118:ILE:HD12	2.10	0.51
1:A:205:LEU:O	1:A:207:ARG:HD2	2.09	0.51
1:D:35:TRP:O	1:D:38:ILE:HG22	2.10	0.51
1:D:39:LEU:N	1:D:40:PRO:HD2	2.25	0.51
1:D:159:PHE:O	1:D:160:ALA:C	2.54	0.51
1:D:205:LEU:O	1:D:207:ARG:HD2	2.09	0.51
1:C:79:LEU:O	1:C:83:VAL:HG23	2.09	0.51
1:C:93:TYR:CE2	1:C:103:GLY:HA3	2.45	0.51
1:C:152:TYR:O	1:C:156:VAL:HG23	2.10	0.51
1:C:248:LEU:N	1:C:248:LEU:HD12	2.26	0.51
1:D:126:PHE:HB3	1:D:195:PHE:HD1	1.75	0.51
1:D:240:GLU:HG3	1:D:241:THR:N	2.26	0.51
1:D:73:ASP:N	1:D:74:PRO:HD2	2.26	0.51
1:C:169:PRO:HA	1:C:172:VAL:HG12	1.92	0.51
1:D:96:HIS:CE1	1:D:97:SER:HB2	2.45	0.51
1:B:159:PHE:O	1:B:160:ALA:C	2.54	0.51
1:C:110:ARG:C	1:C:112:GLU:N	2.69	0.51
1:C:169:PRO:O	1:C:173:ARG:HB2	2.10	0.51
1:D:84:ASP:O	1:D:87:GLY:N	2.36	0.51
1:D:190:VAL:O	1:D:194:VAL:HG23	2.11	0.51
1:A:125:ARG:HG2	1:A:127:LEU:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:GLU:HG2	1:A:113:LEU:N	2.25	0.51
1:A:159:PHE:O	1:A:160:ALA:C	2.53	0.51
1:B:117:LEU:HB3	1:B:210:THR:HG23	1.92	0.51
1:B:210:THR:HG22	1:B:211:CYS:H	1.76	0.51
1:C:242:LEU:HB3	1:C:244:THR:HG22	1.93	0.51
1:C:77:ASP:O	1:C:78:ASP:C	2.54	0.51
1:C:128:ASN:HB3	1:C:134:GLY:N	2.09	0.51
1:C:228:TYR:O	1:C:231:SER:HB2	2.11	0.51
1:B:20:ARG:HB3	1:B:46:TYR:CD2	2.45	0.51
1:A:77:ASP:O	1:A:78:ASP:C	2.53	0.50
1:B:31:ASP:OD2	1:B:31:ASP:C	2.53	0.50
1:B:169:PRO:O	1:B:173:ARG:HB2	2.11	0.50
1:C:143:LYS:O	1:C:146:SER:HB3	2.10	0.50
1:D:23:PHE:O	1:D:24:LEU:HD23	2.11	0.50
1:A:39:LEU:CD1	1:A:48:VAL:HG11	2.41	0.50
1:A:128:ASN:HB3	1:A:134:GLY:N	2.07	0.50
1:B:79:LEU:O	1:B:83:VAL:HG23	2.11	0.50
1:C:169:PRO:C	1:C:172:VAL:HG12	2.36	0.50
1:A:233:LEU:CD1	1:A:237:THR:HG21	2.33	0.50
1:C:38:ILE:HD11	1:C:258:ALA:N	2.27	0.50
1:D:110:ARG:C	1:D:112:GLU:N	2.67	0.50
1:D:230:ARG:HG3	1:D:230:ARG:HH11	1.75	0.50
1:A:38:ILE:HG12	1:A:38:ILE:O	2.11	0.50
1:B:79:LEU:HD11	1:B:93:TYR:CE1	2.45	0.50
1:C:36:HIS:C	1:C:38:ILE:H	2.20	0.50
1:A:248:LEU:N	1:A:248:LEU:HD12	2.27	0.50
1:B:74:PRO:O	1:B:77:ASP:HB2	2.12	0.50
1:B:147:ALA:O	1:B:150:ALA:HB3	2.11	0.50
1:C:21:ILE:HD12	1:C:21:ILE:N	2.27	0.50
1:B:82:ILE:O	1:B:86:LEU:HD13	2.12	0.50
1:D:31:ASP:OD2	1:D:31:ASP:C	2.53	0.50
1:D:248:LEU:HD12	1:D:248:LEU:N	2.27	0.50
1:B:50:LEU:O	1:B:50:LEU:HG	2.11	0.49
1:C:31:ASP:C	1:C:31:ASP:OD2	2.55	0.49
1:C:112:GLU:HG2	1:C:113:LEU:HD13	1.94	0.49
1:C:126:PHE:HE2	1:C:221:VAL:HG22	1.76	0.49
1:D:110:ARG:CD	1:D:113:LEU:HD22	2.36	0.49
1:D:242:LEU:HB3	1:D:244:THR:HG22	1.94	0.49
1:A:89:GLN:O	1:A:113:LEU:HA	2.12	0.49
1:A:230:ARG:HG3	1:A:230:ARG:HH11	1.76	0.49
1:A:253:ALA:HB1	1:A:256:GLN:HE21	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:GLU:HG2	1:B:113:LEU:HD13	1.94	0.49
1:B:198:ASP:OD1	1:B:200:ARG:HD3	2.11	0.49
1:A:100:ALA:HB1	1:A:119:LEU:HD22	1.95	0.49
1:A:242:LEU:HB3	1:A:244:THR:HG22	1.94	0.49
1:D:168:VAL:HG12	1:D:171:ALA:H	1.76	0.49
1:B:38:ILE:HG12	1:B:38:ILE:O	2.12	0.49
1:D:198:ASP:OD1	1:D:200:ARG:HD3	2.13	0.49
1:A:124:PRO:HG2	1:A:125:ARG:N	2.24	0.49
1:B:160:ALA:N	1:B:161:PRO:HD2	2.28	0.49
1:C:22:LEU:HD23	1:C:48:VAL:HG22	1.95	0.49
1:C:100:ALA:O	1:C:104:ILE:HG12	2.12	0.49
1:D:212:VAL:HG11	1:D:229:LEU:HD12	1.93	0.49
1:D:219:VAL:O	1:D:219:VAL:HG22	2.12	0.49
1:B:55:CYS:O	1:B:186:ILE:HG21	2.13	0.49
1:B:126:PHE:HB3	1:B:195:PHE:HD1	1.77	0.49
1:B:240:GLU:HG3	1:B:241:THR:N	2.27	0.49
1:C:125:ARG:HG2	1:C:127:LEU:O	2.12	0.49
1:A:110:ARG:C	1:A:112:GLU:N	2.69	0.49
1:C:50:LEU:HG	1:C:50:LEU:O	2.11	0.49
1:C:55:CYS:O	1:C:186:ILE:HG21	2.13	0.49
1:B:125:ARG:HD3	1:B:129:ASP:OD1	2.13	0.49
1:A:32:GLN:HG2	1:A:52:ASP:OD1	2.13	0.49
1:C:235:GLY:O	1:C:237:THR:N	2.46	0.49
1:A:10:LEU:HB3	1:A:52:ASP:O	2.12	0.48
1:A:240:GLU:HG3	1:A:241:THR:H	1.78	0.48
1:A:140:GLU:O	1:A:144:VAL:HG23	2.12	0.48
1:C:39:LEU:N	1:C:40:PRO:HD2	2.28	0.48
1:C:98:VAL:HA	1:C:101:MET:CE	2.34	0.48
1:C:79:LEU:C	1:C:79:LEU:HD23	2.37	0.48
1:C:212:VAL:HG11	1:C:229:LEU:HD12	1.95	0.48
1:C:219:VAL:HG22	1:C:219:VAL:O	2.13	0.48
1:D:21:ILE:N	1:D:21:ILE:HD12	2.28	0.48
1:D:77:ASP:O	1:D:78:ASP:C	2.54	0.48
1:A:160:ALA:N	1:A:161:PRO:HD2	2.27	0.48
1:B:60:ASN:HD22	1:B:61:PRO:N	2.11	0.48
1:B:55:CYS:HB2	1:B:190:VAL:HG21	1.95	0.48
1:B:72:LEU:O	1:B:76:VAL:HG23	2.14	0.48
1:C:253:ALA:HB1	1:C:256:GLN:HE21	1.78	0.48
1:D:143:LYS:O	1:D:146:SER:HB3	2.14	0.48
1:A:36:HIS:C	1:A:38:ILE:N	2.71	0.48
1:A:126:PHE:HB3	1:A:195:PHE:HD1	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:249:PRO:O	1:D:251:LEU:N	2.47	0.48
1:B:93:TYR:CE2	1:B:103:GLY:HA3	2.48	0.48
1:D:151:ASN:HB3	1:D:154:ALA:HB3	1.94	0.48
1:C:247:HIS:HB3	1:C:248:LEU:HD12	1.95	0.48
1:D:169:PRO:O	1:D:173:ARG:HB2	2.13	0.48
1:D:249:PRO:C	1:D:251:LEU:N	2.71	0.48
1:A:24:LEU:HD23	1:A:94:VAL:HB	1.96	0.48
1:A:169:PRO:C	1:A:172:VAL:HG12	2.39	0.48
1:B:200:ARG:HG2	1:B:200:ARG:HH11	1.78	0.48
1:C:128:ASN:ND2	1:C:136:PHE:N	2.62	0.48
1:B:242:LEU:HB3	1:B:244:THR:HG22	1.95	0.47
1:B:257:LEU:O	1:B:258:ALA:C	2.57	0.47
1:D:210:THR:HB	1:D:237:THR:CG2	2.43	0.47
1:B:140:GLU:O	1:B:144:VAL:HG23	2.14	0.47
1:B:186:ILE:O	1:B:190:VAL:HG23	2.14	0.47
1:C:244:THR:HB	1:C:256:GLN:OE1	2.14	0.47
1:D:86:LEU:O	1:D:87:GLY:O	2.32	0.47
1:A:228:TYR:O	1:A:231:SER:HB2	2.14	0.47
1:A:235:GLY:O	1:A:237:THR:N	2.48	0.47
1:A:244:THR:HB	1:A:256:GLN:NE2	2.30	0.47
1:B:175:PHE:CZ	1:B:179:LEU:HD23	2.49	0.47
1:D:200:ARG:HG2	1:D:200:ARG:HH11	1.79	0.47
1:D:233:LEU:CD1	1:D:237:THR:HG21	2.35	0.47
1:C:120:ILE:HG23	1:C:213:ILE:HG21	1.96	0.47
1:C:159:PHE:O	1:C:160:ALA:C	2.57	0.47
1:C:240:GLU:HG3	1:C:241:THR:N	2.29	0.47
1:D:22:LEU:HD12	1:D:23:PHE:N	2.26	0.47
1:A:198:ASP:OD1	1:A:200:ARG:HD3	2.15	0.47
1:A:35:TRP:O	1:A:36:HIS:C	2.56	0.47
1:A:114:PHE:HB3	1:A:117:LEU:CD2	2.44	0.47
1:B:60:ASN:ND2	1:B:62:ASP:H	2.12	0.47
1:B:79:LEU:HD23	1:B:79:LEU:C	2.39	0.47
1:B:249:PRO:C	1:B:251:LEU:N	2.72	0.47
1:C:14:VAL:CG1	1:D:170:ALA:HB2	2.43	0.47
1:D:25:ALA:CB	1:D:99:SER:OG	2.62	0.47
1:D:38:ILE:HG12	1:D:38:ILE:O	2.15	0.47
1:D:60:ASN:ND2	1:D:61:PRO:HD2	2.25	0.47
1:D:74:PRO:O	1:D:77:ASP:HB2	2.14	0.47
1:D:160:ALA:N	1:D:161:PRO:HD2	2.29	0.47
1:B:148:MET:CE	1:B:188:LEU:HD12	2.44	0.47
1:D:110:ARG:HD3	1:D:112:GLU:OE1	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:ASN:HB3	1:A:154:ALA:HB3	1.95	0.47
1:B:152:TYR:O	1:B:156:VAL:HG23	2.15	0.47
1:B:244:THR:HB	1:B:256:GLN:OE1	2.14	0.47
1:C:35:TRP:O	1:C:36:HIS:C	2.58	0.47
1:D:126:PHE:HE2	1:D:221:VAL:HG22	1.80	0.47
1:D:169:PRO:HA	1:D:172:VAL:HG12	1.97	0.47
1:A:93:TYR:HB2	1:A:114:PHE:HE1	1.80	0.46
1:B:120:ILE:O	1:B:121:GLY:C	2.56	0.46
1:B:169:PRO:HA	1:B:172:VAL:HG12	1.97	0.46
1:B:212:VAL:HG11	1:B:229:LEU:HD12	1.97	0.46
1:C:110:ARG:HD3	1:C:112:GLU:OE1	2.15	0.46
1:A:128:ASN:ND2	1:A:136:PHE:N	2.63	0.46
1:B:77:ASP:O	1:B:78:ASP:C	2.57	0.46
1:B:248:LEU:HD12	1:B:248:LEU:N	2.30	0.46
1:D:72:LEU:O	1:D:76:VAL:HG23	2.15	0.46
1:D:120:ILE:HG23	1:D:213:ILE:HG21	1.96	0.46
1:D:147:ALA:O	1:D:150:ALA:HB3	2.16	0.46
1:D:235:GLY:O	1:D:237:THR:N	2.48	0.46
1:A:47:ARG:NH1	1:B:168:VAL:HG13	2.30	0.46
1:A:79:LEU:HD11	1:A:93:TYR:CE1	2.50	0.46
1:A:125:ARG:HD2	1:A:198:ASP:CG	2.40	0.46
1:A:128:ASN:HD21	1:A:136:PHE:C	2.22	0.46
1:B:39:LEU:CD1	1:B:48:VAL:HG11	2.45	0.46
1:B:247:HIS:HD2	1:B:248:LEU:HD11	1.79	0.46
1:C:50:LEU:N	1:C:50:LEU:HD23	2.30	0.46
1:B:38:ILE:HD11	1:B:258:ALA:CA	2.44	0.46
1:B:70:THR:OG1	1:B:71:THR:HG23	2.16	0.46
1:A:21:ILE:N	1:A:21:ILE:HD12	2.30	0.46
1:A:110:ARG:CD	1:A:113:LEU:HD22	2.40	0.46
1:B:112:GLU:CG	1:B:113:LEU:HD13	2.46	0.46
1:B:114:PHE:HB3	1:B:117:LEU:CD2	2.46	0.46
1:A:219:VAL:O	1:A:219:VAL:HG22	2.15	0.46
1:C:10:LEU:HB3	1:C:52:ASP:O	2.15	0.46
1:D:38:ILE:HD11	1:D:258:ALA:CA	2.46	0.46
1:A:96:HIS:CE1	1:A:97:SER:HB2	2.51	0.46
1:B:53:LEU:HD13	1:B:53:LEU:HA	1.81	0.46
1:C:194:VAL:O	1:C:197:SER:OG	2.23	0.46
1:A:74:PRO:O	1:A:77:ASP:HB2	2.16	0.46
1:A:93:TYR:CE2	1:A:103:GLY:HA3	2.50	0.46
1:A:244:THR:HB	1:A:256:GLN:OE1	2.15	0.46
1:C:147:ALA:O	1:C:150:ALA:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:THR:HA	1:A:47:ARG:HE	1.81	0.46
1:A:57:GLY:C	1:A:59:VAL:H	2.23	0.46
1:B:73:ASP:O	1:B:74:PRO:C	2.57	0.46
1:B:230:ARG:HB2	1:B:239:VAL:HG21	1.98	0.46
1:C:39:LEU:O	1:C:40:PRO:C	2.57	0.46
1:D:20:ARG:HB3	1:D:46:TYR:CD2	2.51	0.46
1:D:140:GLU:O	1:D:144:VAL:HG23	2.16	0.46
1:A:169:PRO:O	1:A:173:ARG:HB2	2.16	0.46
1:C:160:ALA:N	1:C:161:PRO:HD2	2.30	0.46
1:D:55:CYS:HB2	1:D:190:VAL:HG21	1.98	0.46
1:A:39:LEU:O	1:A:40:PRO:C	2.56	0.45
1:B:10:LEU:HB3	1:B:52:ASP:O	2.15	0.45
1:B:74:PRO:O	1:B:77:ASP:N	2.49	0.45
1:A:86:LEU:HD23	1:B:169:PRO:HB3	1.99	0.45
1:A:190:VAL:O	1:A:194:VAL:HG23	2.16	0.45
1:C:112:GLU:CG	1:C:113:LEU:HD13	2.46	0.45
1:D:244:THR:HB	1:D:256:GLN:CD	2.42	0.45
1:A:73:ASP:N	1:A:74:PRO:HD2	2.31	0.45
1:A:83:VAL:O	1:A:88:ILE:HG13	2.16	0.45
1:A:228:TYR:HE2	1:A:232:HIS:CE1	2.34	0.45
1:B:235:GLY:O	1:B:237:THR:N	2.49	0.45
1:C:77:ASP:O	1:C:80:LEU:N	2.49	0.45
1:C:169:PRO:CA	1:C:172:VAL:HG12	2.47	0.45
1:D:29:GLY:O	1:D:30:THR:O	2.34	0.45
1:A:38:ILE:HD11	1:A:258:ALA:N	2.32	0.45
1:C:84:ASP:O	1:C:87:GLY:N	2.37	0.45
1:D:79:LEU:C	1:D:79:LEU:HD23	2.42	0.45
1:A:148:MET:HE3	1:A:188:LEU:HD12	1.97	0.45
1:B:110:ARG:HD3	1:B:112:GLU:OE1	2.16	0.45
1:C:38:ILE:HG12	1:C:38:ILE:O	2.17	0.45
1:C:47:ARG:NH1	1:D:168:VAL:HG13	2.32	0.45
1:C:68:ARG:O	1:C:70:THR:HG23	2.16	0.45
1:C:82:ILE:O	1:C:86:LEU:HD13	2.17	0.45
1:C:200:ARG:HH11	1:C:200:ARG:HG2	1.82	0.45
1:C:245:GLU:CD	1:C:246:GLY:H	2.25	0.45
1:D:112:GLU:CG	1:D:113:LEU:HD13	2.47	0.45
1:A:229:LEU:C	1:A:231:SER:N	2.74	0.45
1:B:22:LEU:HD12	1:B:23:PHE:N	2.28	0.45
1:C:114:PHE:HB3	1:C:117:LEU:CD2	2.46	0.45
1:C:117:LEU:HB3	1:C:210:THR:HG23	1.97	0.45
1:C:249:PRO:C	1:C:251:LEU:N	2.72	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:36:HIS:O	1:D:38:ILE:N	2.50	0.45
1:D:86:LEU:O	1:D:87:GLY:C	2.59	0.45
1:D:93:TYR:HB2	1:D:114:PHE:HE1	1.81	0.45
1:A:249:PRO:C	1:A:251:LEU:N	2.72	0.45
1:C:76:VAL:HG13	1:C:106:ALA:HB2	1.98	0.45
1:B:21:ILE:N	1:B:21:ILE:HD12	2.31	0.45
1:C:126:PHE:HB3	1:C:195:PHE:HD1	1.82	0.45
1:D:35:TRP:O	1:D:36:HIS:C	2.59	0.45
1:D:60:ASN:HD22	1:D:60:ASN:C	2.25	0.45
1:A:112:GLU:HG2	1:A:113:LEU:HD13	1.99	0.45
1:A:225:VAL:C	1:A:227:GLU:N	2.75	0.45
1:C:97:SER:O	1:C:100:ALA:HB3	2.17	0.45
1:A:200:ARG:HG2	1:A:200:ARG:NH1	2.32	0.44
1:B:39:LEU:H	1:B:40:PRO:HD2	1.82	0.44
1:B:93:TYR:HB2	1:B:114:PHE:HE1	1.82	0.44
1:B:23:PHE:O	1:B:24:LEU:HD23	2.16	0.44
1:B:83:VAL:O	1:B:88:ILE:HG13	2.16	0.44
1:A:79:LEU:C	1:A:79:LEU:HD23	2.42	0.44
1:A:265:LEU:HD12	1:A:265:LEU:O	2.17	0.44
1:B:225:VAL:C	1:B:227:GLU:N	2.75	0.44
1:B:249:PRO:O	1:B:251:LEU:N	2.50	0.44
1:C:244:THR:HB	1:C:256:GLN:NE2	2.32	0.44
1:D:89:GLN:O	1:D:113:LEU:HA	2.17	0.44
1:A:79:LEU:O	1:A:83:VAL:HG23	2.17	0.44
1:A:250:GLN:HA	1:A:257:LEU:HD23	1.99	0.44
1:B:229:LEU:C	1:B:231:SER:N	2.74	0.44
1:C:31:ASP:OD2	1:C:33:SER:OG	2.26	0.44
1:C:89:GLN:O	1:C:113:LEU:HA	2.18	0.44
1:C:93:TYR:HB2	1:C:114:PHE:CE1	2.50	0.44
1:D:55:CYS:O	1:D:186:ILE:HG21	2.17	0.44
1:A:25:ALA:CB	1:A:99:SER:OG	2.64	0.44
1:A:86:LEU:O	1:A:87:GLY:C	2.61	0.44
1:A:112:GLU:C	1:A:114:PHE:H	2.26	0.44
1:A:120:ILE:HG23	1:A:213:ILE:HG21	1.99	0.44
1:B:36:HIS:O	1:B:38:ILE:N	2.51	0.44
1:B:52:ASP:O	1:B:53:LEU:C	2.61	0.44
1:C:120:ILE:HG21	1:C:250:GLN:HE22	1.83	0.44
1:D:68:ARG:O	1:D:70:THR:HG23	2.16	0.44
1:B:28:PHE:O	1:B:30:THR:N	2.51	0.44
1:B:35:TRP:O	1:B:36:HIS:C	2.61	0.44
1:C:168:VAL:HG12	1:C:171:ALA:H	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:83:VAL:O	1:D:88:ILE:HG13	2.16	0.44
1:A:124:PRO:CG	1:A:125:ARG:H	2.24	0.44
1:B:57:GLY:HA3	1:B:181:ASN:HB3	1.99	0.44
1:B:110:ARG:CD	1:B:113:LEU:HD22	2.41	0.44
1:D:82:ILE:O	1:D:86:LEU:HD13	2.18	0.44
1:D:215:THR:HG21	1:D:246:GLY:O	2.18	0.44
1:B:54:VAL:HG13	1:B:55:CYS:N	2.33	0.44
1:B:109:ARG:NH1	1:D:207:ARG:NH2	2.66	0.44
1:A:60:ASN:ND2	1:A:62:ASP:H	2.16	0.44
1:A:244:THR:HB	1:A:256:GLN:CD	2.43	0.44
1:B:254:PRO:O	1:B:255:ALA:C	2.59	0.44
1:D:79:LEU:O	1:D:83:VAL:HG23	2.17	0.44
1:D:124:PRO:CG	1:D:125:ARG:H	2.28	0.44
1:A:169:PRO:HA	1:A:172:VAL:HG12	2.00	0.43
1:B:109:ARG:C	1:B:110:ARG:HG2	2.42	0.43
1:C:36:HIS:O	1:C:38:ILE:N	2.51	0.43
1:A:124:PRO:HG2	1:A:132:TYR:OH	2.18	0.43
1:B:215:THR:HG21	1:B:246:GLY:O	2.18	0.43
1:C:125:ARG:HD3	1:C:129:ASP:OD1	2.19	0.43
1:A:116:LYS:HE2	1:A:264:ALA:HB1	2.01	0.43
1:B:169:PRO:C	1:B:172:VAL:HG12	2.43	0.43
1:C:141:ILE:CD1	1:C:142:GLU:N	2.80	0.43
1:D:104:ILE:HG13	1:D:122:PHE:CZ	2.53	0.43
1:A:68:ARG:O	1:A:70:THR:HG23	2.18	0.43
1:C:249:PRO:O	1:C:251:LEU:N	2.51	0.43
1:D:17:THR:HA	1:D:47:ARG:HE	1.84	0.43
1:D:169:PRO:C	1:D:172:VAL:HG12	2.44	0.43
1:A:254:PRO:O	1:A:255:ALA:C	2.61	0.43
1:B:38:ILE:HD11	1:B:258:ALA:HA	2.00	0.43
1:B:168:VAL:HG12	1:B:171:ALA:H	1.83	0.43
1:C:83:VAL:O	1:C:88:ILE:HG13	2.18	0.43
1:D:124:PRO:HG2	1:D:132:TYR:OH	2.18	0.43
1:A:31:ASP:OD2	1:A:33:SER:OG	2.32	0.43
1:B:86:LEU:O	1:B:87:GLY:C	2.60	0.43
1:B:257:LEU:HG	1:B:261:LEU:HD12	2.00	0.43
1:C:73:ASP:N	1:C:74:PRO:HD2	2.33	0.43
1:A:100:ALA:O	1:A:104:ILE:HG12	2.19	0.43
1:A:148:MET:CE	1:A:188:LEU:HD12	2.49	0.43
1:D:53:LEU:HD13	1:D:53:LEU:HA	1.84	0.43
1:D:148:MET:HE3	1:D:188:LEU:HD12	2.00	0.43
1:A:22:LEU:HD23	1:A:48:VAL:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:VAL:C	1:B:227:GLU:H	2.26	0.43
1:A:73:ASP:O	1:A:74:PRO:C	2.62	0.42
1:A:210:THR:HB	1:A:237:THR:CG2	2.46	0.42
1:C:244:THR:HB	1:C:256:GLN:CD	2.44	0.42
1:D:148:MET:CE	1:D:188:LEU:HD12	2.49	0.42
1:A:55:CYS:O	1:A:186:ILE:HG21	2.18	0.42
1:A:121:GLY:H	1:A:213:ILE:CG2	2.26	0.42
1:B:175:PHE:O	1:B:179:LEU:HB2	2.19	0.42
1:B:240:GLU:HG3	1:B:241:THR:H	1.84	0.42
1:A:32:GLN:HG2	1:A:52:ASP:OD2	2.19	0.42
1:A:245:GLU:CD	1:A:246:GLY:H	2.27	0.42
1:D:17:THR:HG22	1:D:47:ARG:NH2	2.34	0.42
1:D:121:GLY:H	1:D:213:ILE:CG2	2.26	0.42
1:C:57:GLY:HA3	1:C:181:ASN:HB3	2.01	0.42
1:C:145:PHE:CZ	1:C:192:ARG:HA	2.54	0.42
1:C:145:PHE:HZ	1:C:192:ARG:HA	1.84	0.42
1:D:60:ASN:ND2	1:D:60:ASN:C	2.77	0.42
1:B:124:PRO:CG	1:B:125:ARG:H	2.26	0.42
1:C:86:LEU:O	1:D:172:VAL:HG11	2.20	0.42
1:A:29:GLY:O	1:A:30:THR:O	2.37	0.42
1:A:39:LEU:H	1:A:40:PRO:HD2	1.84	0.42
1:B:151:ASN:HB3	1:B:154:ALA:HB3	2.00	0.42
1:C:41:TYR:CD1	1:C:258:ALA:HB1	2.55	0.42
1:C:124:PRO:CG	1:C:125:ARG:H	2.29	0.42
1:C:187:SER:O	1:C:191:SER:OG	2.37	0.42
1:A:82:ILE:O	1:A:86:LEU:HD13	2.19	0.42
1:A:120:ILE:HG21	1:A:250:GLN:HE22	1.84	0.42
1:B:189:PHE:O	1:B:190:VAL:C	2.63	0.42
1:D:66:PHE:HD1	1:D:189:PHE:CD2	2.37	0.42
1:D:117:LEU:CB	1:D:210:THR:HG23	2.50	0.42
1:D:247:HIS:CD2	1:D:248:LEU:CD1	3.02	0.42
1:A:32:GLN:HG2	1:A:52:ASP:CG	2.45	0.42
1:A:151:ASN:OD1	1:A:154:ALA:HB2	2.20	0.42
1:A:168:VAL:HG12	1:A:171:ALA:H	1.85	0.42
1:C:79:LEU:HD11	1:C:93:TYR:CE1	2.55	0.42
1:C:116:LYS:HE2	1:C:264:ALA:HB1	2.02	0.42
1:C:225:VAL:C	1:C:227:GLU:N	2.77	0.42
1:C:230:ARG:HB2	1:C:239:VAL:HG21	2.01	0.42
1:A:109:ARG:C	1:A:110:ARG:HG2	2.44	0.42
1:A:152:TYR:O	1:A:156:VAL:HG23	2.19	0.42
1:B:121:GLY:H	1:B:213:ILE:CG2	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:227:GLU:OE1	1:D:230:ARG:HB3	2.19	0.42
1:A:17:THR:HG22	1:A:47:ARG:NH2	2.35	0.42
1:A:112:GLU:CG	1:A:113:LEU:HD13	2.50	0.42
1:A:117:LEU:CB	1:A:210:THR:HG23	2.49	0.42
1:B:28:PHE:CG	1:B:29:GLY:N	2.88	0.42
1:B:169:PRO:HA	1:B:172:VAL:CG1	2.50	0.42
1:B:189:PHE:O	1:B:191:SER:N	2.53	0.42
1:D:38:ILE:HD11	1:D:258:ALA:HA	2.02	0.42
1:A:26:HIS:N	1:A:35:TRP:HE1	2.18	0.41
1:A:189:PHE:O	1:A:191:SER:N	2.53	0.41
1:A:223:ALA:O	1:A:224:SER:C	2.63	0.41
1:B:43:THR:HG23	1:B:44:GLN:CD	2.45	0.41
1:C:36:HIS:C	1:C:38:ILE:N	2.78	0.41
1:C:254:PRO:O	1:C:255:ALA:C	2.63	0.41
1:D:230:ARG:HB2	1:D:239:VAL:HG21	2.02	0.41
1:D:240:GLU:HG3	1:D:241:THR:H	1.84	0.41
1:B:172:VAL:O	1:B:172:VAL:HG22	2.20	0.41
1:C:28:PHE:CG	1:C:29:GLY:N	2.87	0.41
1:D:57:GLY:C	1:D:59:VAL:H	2.27	0.41
1:D:101:MET:O	1:D:102:ILE:C	2.64	0.41
1:A:169:PRO:HA	1:A:172:VAL:CG1	2.50	0.41
1:B:32:GLN:HG2	1:B:52:ASP:OD1	2.20	0.41
1:B:68:ARG:O	1:B:70:THR:HG23	2.20	0.41
1:B:73:ASP:N	1:B:74:PRO:HD2	2.35	0.41
1:B:109:ARG:CZ	1:D:207:ARG:HH22	2.33	0.41
1:B:145:PHE:HZ	1:B:192:ARG:HA	1.85	0.41
1:C:39:LEU:CD1	1:C:48:VAL:HG11	2.51	0.41
1:C:74:PRO:O	1:C:77:ASP:HB2	2.20	0.41
1:D:152:TYR:O	1:D:156:VAL:HG23	2.20	0.41
1:D:200:ARG:O	1:D:201:GLY:C	2.63	0.41
1:A:110:ARG:HD3	1:A:112:GLU:OE1	2.20	0.41
1:D:28:PHE:O	1:D:30:THR:N	2.54	0.41
1:D:39:LEU:O	1:D:40:PRO:C	2.62	0.41
1:D:76:VAL:HG13	1:D:106:ALA:HB2	2.02	0.41
1:D:144:VAL:O	1:D:148:MET:HB2	2.20	0.41
1:B:39:LEU:O	1:B:40:PRO:C	2.63	0.41
1:B:86:LEU:O	1:B:87:GLY:O	2.39	0.41
1:C:28:PHE:O	1:C:30:THR:N	2.53	0.41
1:C:32:GLN:HG2	1:C:52:ASP:OD1	2.21	0.41
1:C:100:ALA:HB1	1:C:122:PHE:HB2	2.03	0.41
1:C:119:LEU:HB3	1:C:122:PHE:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:169:PRO:HA	1:D:172:VAL:CG1	2.51	0.41
1:A:97:SER:O	1:A:100:ALA:HB3	2.21	0.41
1:A:145:PHE:HZ	1:A:192:ARG:HA	1.85	0.41
1:C:53:LEU:HA	1:C:53:LEU:HD13	1.81	0.41
1:C:256:GLN:H	1:C:256:GLN:HG2	1.65	0.41
1:A:35:TRP:O	1:A:38:ILE:N	2.48	0.41
1:A:60:ASN:HD22	1:A:61:PRO:N	2.19	0.41
1:A:147:ALA:HA	1:A:150:ALA:HB3	2.02	0.41
1:C:104:ILE:HG13	1:C:122:PHE:CZ	2.55	0.41
1:D:9:ALA:HA	1:D:63:TYR:CE1	2.56	0.41
1:D:151:ASN:OD1	1:D:154:ALA:HB2	2.21	0.41
1:A:37:LEU:HA	1:A:37:LEU:HD13	1.89	0.41
1:A:102:ILE:H	1:A:102:ILE:HG13	1.71	0.41
1:C:55:CYS:HB2	1:C:190:VAL:HG21	2.01	0.41
1:C:73:ASP:O	1:C:74:PRO:C	2.62	0.41
1:C:162:LEU:O	1:C:163:ALA:C	2.64	0.41
1:C:225:VAL:C	1:C:227:GLU:H	2.27	0.41
1:D:189:PHE:O	1:D:191:SER:N	2.53	0.41
1:A:54:VAL:HG11	1:A:69:TYR:CE1	2.55	0.41
1:A:86:LEU:O	1:A:87:GLY:O	2.38	0.41
1:A:137:GLU:O	1:A:138:GLU:C	2.64	0.41
1:A:200:ARG:O	1:A:201:GLY:C	2.64	0.41
1:A:257:LEU:HG	1:A:261:LEU:HD12	2.02	0.41
1:B:36:HIS:C	1:B:38:ILE:N	2.77	0.41
1:B:117:LEU:CB	1:B:210:THR:HG23	2.50	0.41
1:B:265:LEU:HA	1:B:266:PRO:HA	1.92	0.41
1:C:42:PHE:HE2	1:C:265:LEU:HD11	1.85	0.41
1:C:57:GLY:C	1:C:59:VAL:H	2.29	0.41
1:C:120:ILE:O	1:C:121:GLY:C	2.64	0.41
1:C:215:THR:HG21	1:C:246:GLY:O	2.19	0.41
1:D:39:LEU:CD1	1:D:48:VAL:HG11	2.50	0.41
1:D:66:PHE:HD1	1:D:189:PHE:HD2	1.67	0.41
1:A:66:PHE:HD1	1:A:189:PHE:CD2	2.39	0.41
1:A:156:VAL:HG22	1:A:179:LEU:HD12	2.03	0.41
1:A:175:PHE:CZ	1:A:179:LEU:HD23	2.56	0.41
1:B:108:ILE:HG23	1:B:207:ARG:HH11	1.86	0.41
1:B:249:PRO:C	1:B:251:LEU:H	2.29	0.41
1:D:26:HIS:CD2	1:D:31:ASP:HA	2.56	0.41
1:D:137:GLU:H	1:D:140:GLU:HB2	1.85	0.41
1:D:244:THR:HB	1:D:256:GLN:NE2	2.36	0.41
1:B:21:ILE:HA	1:B:47:ARG:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:CYS:CB	1:B:190:VAL:HG21	2.51	0.40
1:D:114:PHE:HB3	1:D:117:LEU:HD21	2.03	0.40
1:D:172:VAL:O	1:D:172:VAL:HG22	2.20	0.40
1:D:229:LEU:C	1:D:231:SER:N	2.76	0.40
1:D:245:GLU:CD	1:D:246:GLY:H	2.29	0.40
1:A:43:THR:HG23	1:A:44:GLN:CD	2.46	0.40
1:D:116:LYS:HE2	1:D:264:ALA:HB1	2.04	0.40
1:C:121:GLY:H	1:C:213:ILE:CG2	2.25	0.40
1:C:245:GLU:CD	1:C:246:GLY:N	2.79	0.40
1:D:36:HIS:C	1:D:38:ILE:N	2.77	0.40
1:D:41:TYR:CD1	1:D:258:ALA:HB1	2.56	0.40
1:D:120:ILE:O	1:D:121:GLY:C	2.64	0.40
1:D:203:LEU:O	1:D:204:GLY:C	2.64	0.40
1:D:254:PRO:O	1:D:255:ALA:C	2.64	0.40
1:A:249:PRO:O	1:A:251:LEU:N	2.55	0.40
1:B:35:TRP:O	1:B:38:ILE:N	2.52	0.40
1:C:47:ARG:HH11	1:D:168:VAL:HG13	1.85	0.40
1:D:257:LEU:HG	1:D:261:LEU:HD12	2.03	0.40
1:B:10:LEU:CD2	1:B:54:VAL:HA	2.52	0.40
1:B:126:PHE:HD2	1:B:126:PHE:HA	1.78	0.40
1:C:249:PRO:C	1:C:251:LEU:H	2.30	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	259/267 (97%)	187 (72%)	52 (20%)	20 (8%)	1	8
1	B	259/267 (97%)	187 (72%)	53 (20%)	19 (7%)	1	9
1	C	259/267 (97%)	189 (73%)	52 (20%)	18 (7%)	1	10
1	D	259/267 (97%)	189 (73%)	49 (19%)	21 (8%)	1	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1036/1068 (97%)	752 (73%)	206 (20%)	78 (8%)	1 9

All (78) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	30	THR
1	A	37	LEU
1	A	150	ALA
1	B	11	ASN
1	B	30	THR
1	B	150	ALA
1	C	11	ASN
1	C	30	THR
1	C	150	ALA
1	C	236	ASP
1	D	11	ASN
1	D	30	THR
1	D	150	ALA
1	A	56	ALA
1	A	87	GLY
1	A	124	PRO
1	A	146	SER
1	A	236	ASP
1	B	37	LEU
1	B	87	GLY
1	B	124	PRO
1	B	236	ASP
1	C	29	GLY
1	C	37	LEU
1	C	87	GLY
1	C	124	PRO
1	D	37	LEU
1	D	56	ALA
1	D	87	GLY
1	D	124	PRO
1	D	236	ASP
1	A	200	ARG
1	B	29	GLY
1	B	107	SER
1	B	146	SER
1	B	166	ALA

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Mol	Chain	Res	Type
1	B	200	ARG
1	C	56	ALA
1	D	107	SER
1	D	146	SER
1	D	166	ALA
1	A	29	GLY
1	A	107	SER
1	A	113	LEU
1	A	166	ALA
1	A	211	CYS
1	A	258	ALA
1	B	113	LEU
1	B	255	ALA
1	B	258	ALA
1	C	107	SER
1	C	113	LEU
1	C	146	SER
1	C	200	ARG
1	C	255	ALA
1	D	29	GLY
1	D	113	LEU
1	D	200	ARG
1	A	69	TYR
1	A	190	VAL
1	B	56	ALA
1	B	211	CYS
1	C	166	ALA
1	C	211	CYS
1	D	211	CYS
1	D	250	GLN
1	D	255	ALA
1	D	258	ALA
1	D	69	TYR
1	D	190	VAL
1	B	190	VAL
1	C	165	GLY
1	A	38	ILE
1	B	38	ILE
1	C	190	VAL
1	A	165	GLY
1	D	165	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	220/226 (97%)	202 (92%)	18 (8%)	10	34
1	B	220/226 (97%)	202 (92%)	18 (8%)	10	34
1	C	220/226 (97%)	200 (91%)	20 (9%)	9	32
1	D	220/226 (97%)	203 (92%)	17 (8%)	12	37
All	All	880/904 (97%)	807 (92%)	73 (8%)	10	34

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	VAL
1	A	88	ILE
1	A	99	SER
1	A	126	PHE
1	A	128	ASN
1	A	140	GLU
1	A	179	LEU
1	A	196	ASN
1	A	199	LEU
1	A	200	ARG
1	A	202	VAL
1	A	210	THR
1	A	213	ILE
1	A	227	GLU
1	A	243	LYS
1	A	245	GLU
1	A	250	GLN
1	A	265	LEU
1	B	53	LEU
1	B	88	ILE
1	B	99	SER
1	B	126	PHE
1	B	128	ASN
1	B	129	ASP

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Mol	Chain	Res	Type
1	B	140	GLU
1	B	179	LEU
1	B	196	ASN
1	B	199	LEU
1	B	200	ARG
1	B	210	THR
1	B	213	ILE
1	B	227	GLU
1	B	243	LYS
1	B	245	GLU
1	B	250	GLN
1	B	265	LEU
1	C	11	ASN
1	C	53	LEU
1	C	88	ILE
1	C	99	SER
1	C	126	PHE
1	C	128	ASN
1	C	129	ASP
1	C	140	GLU
1	C	179	LEU
1	C	196	ASN
1	C	199	LEU
1	C	200	ARG
1	C	202	VAL
1	C	210	THR
1	C	213	ILE
1	C	227	GLU
1	C	243	LYS
1	C	245	GLU
1	C	250	GLN
1	C	265	LEU
1	D	88	ILE
1	D	99	SER
1	D	126	PHE
1	D	128	ASN
1	D	140	GLU
1	D	179	LEU
1	D	196	ASN
1	D	199	LEU
1	D	200	ARG
1	D	202	VAL

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Mol	Chain	Res	Type
1	D	210	THR
1	D	213	ILE
1	D	227	GLU
1	D	243	LYS
1	D	245	GLU
1	D	250	GLN
1	D	265	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	44	GLN
1	A	60	ASN
1	A	128	ASN
1	A	214	GLN
1	A	250	GLN
1	A	256	GLN
1	A	259	GLN
1	B	32	GLN
1	B	44	GLN
1	B	60	ASN
1	B	128	ASN
1	B	214	GLN
1	B	250	GLN
1	B	256	GLN
1	B	259	GLN
1	C	32	GLN
1	C	44	GLN
1	C	60	ASN
1	C	128	ASN
1	C	157	HIS
1	C	214	GLN
1	C	250	GLN
1	C	256	GLN
1	C	259	GLN
1	D	32	GLN
1	D	44	GLN
1	D	60	ASN
1	D	151	ASN
1	D	214	GLN
1	D	250	GLN

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Mol	Chain	Res	Type
1	D	256	GLN
1	D	259	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	261/267 (97%)	0.42	5 (1%) 66 41	2, 27, 56, 68	0
1	B	261/267 (97%)	0.48	4 (1%) 72 47	3, 34, 60, 67	0
1	C	261/267 (97%)	0.51	6 (2%) 61 37	5, 44, 71, 80	0
1	D	261/267 (97%)	0.63	14 (5%) 31 18	2, 41, 67, 83	0
All	All	1044/1068 (97%)	0.51	29 (2%) 55 32	2, 36, 63, 83	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	166	ALA	4.5
1	B	157	HIS	3.7
1	C	202	VAL	3.4
1	D	157	HIS	3.3
1	A	234	GLY	3.2
1	B	166	ALA	2.9
1	D	155	TRP	2.8
1	A	133	HIS	2.7
1	C	133	HIS	2.7
1	D	124	PRO	2.6
1	C	127	LEU	2.6
1	A	218	ASP	2.5
1	C	174	GLU	2.5
1	D	219	VAL	2.5
1	D	37	LEU	2.4
1	D	15	VAL	2.4
1	D	255	ALA	2.4
1	D	75	TYR	2.4
1	D	28	PHE	2.3
1	A	41	TYR	2.3
1	B	243	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	158	GLY	2.2
1	D	173	ARG	2.1
1	B	136	PHE	2.1
1	D	171	ALA	2.1
1	A	134	GLY	2.0
1	C	200	ARG	2.0
1	D	163	ALA	2.0
1	D	12	VAL	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.