Full wwPDB X-ray Structure Validation Report (i)

Oct 16, 2023 – 05:29 PM EDT

PDB ID	:	1V5W
Title	:	Crystal structure of the human Dmc1 protein
Authors	:	Kinebuchi, T.; Kagawa, W.; Enomoto, R.; Ikawa, S.; Shibata, T.; Kurumizaka, H.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2003-11-26
Resolution	:	3.20 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

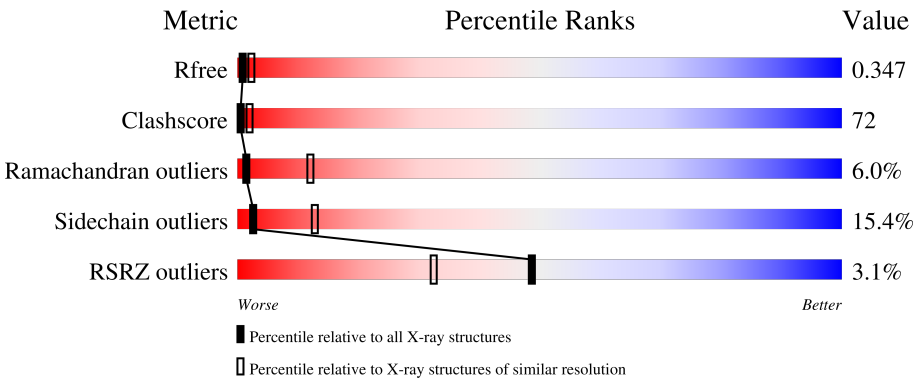
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 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}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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

Mol	Chain	Length	Quality of chain
1	A	343	2% 17% 43% 10% 30%
1	B	343	3% 18% 40% 11% 30%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 3767 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 Meiotic recombination protein DMC1/LIM15 homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	239	1875	1186	325	356	8	0	0	0
1	B	239	1875	1186	325	356	8	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	cloning artifact	UNP Q14565
A	-1	SER	-	cloning artifact	UNP Q14565
A	0	HIS	-	cloning artifact	UNP Q14565
B	-2	GLY	-	cloning artifact	UNP Q14565
B	-1	SER	-	cloning artifact	UNP Q14565
B	0	HIS	-	cloning artifact	UNP Q14565

- Molecule 2 is water.

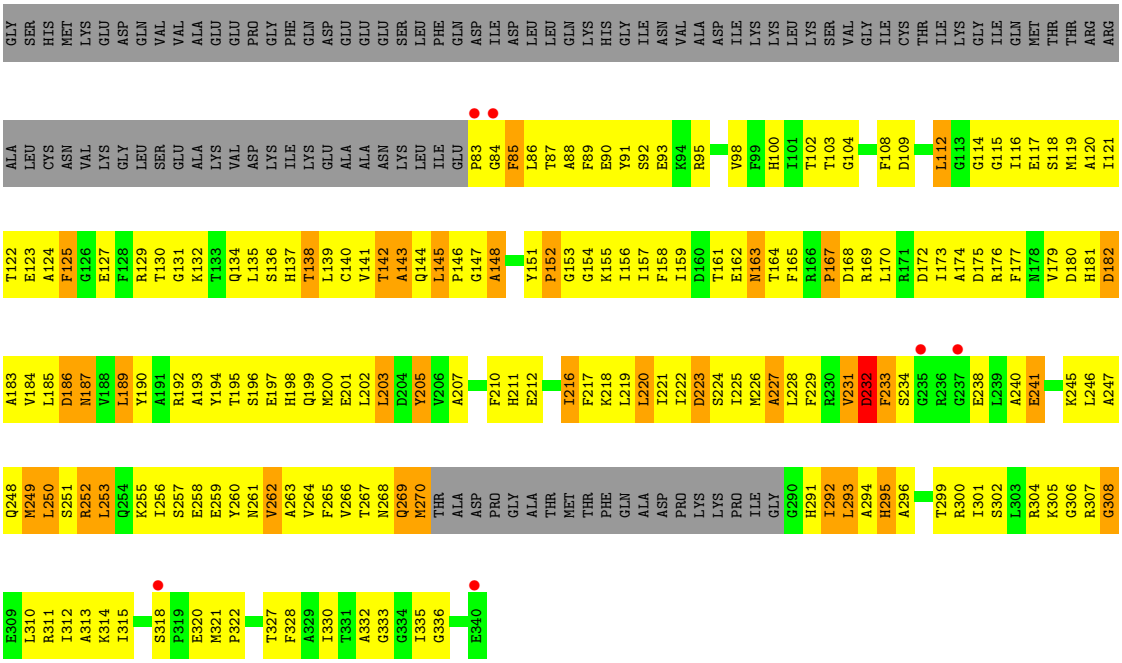
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	8	8	8	0	0
2	B	9	9	9	0	0

3 Residue-property plots (i)

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

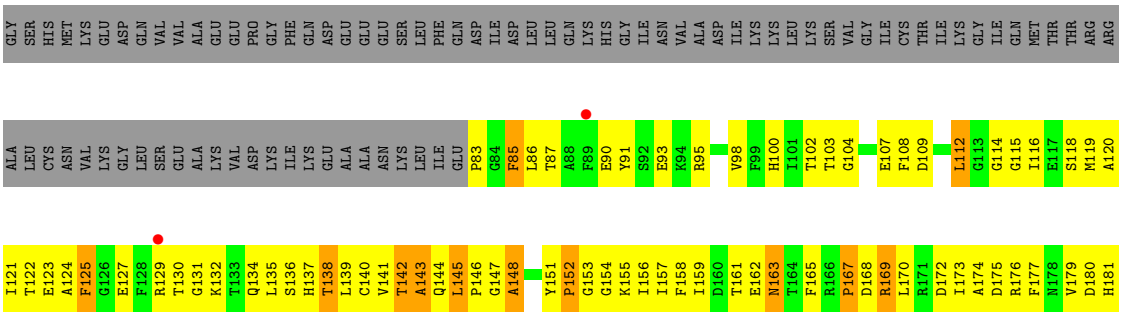
• Molecule 1: Meiotic recombination protein DMC1/LIM15 homolog

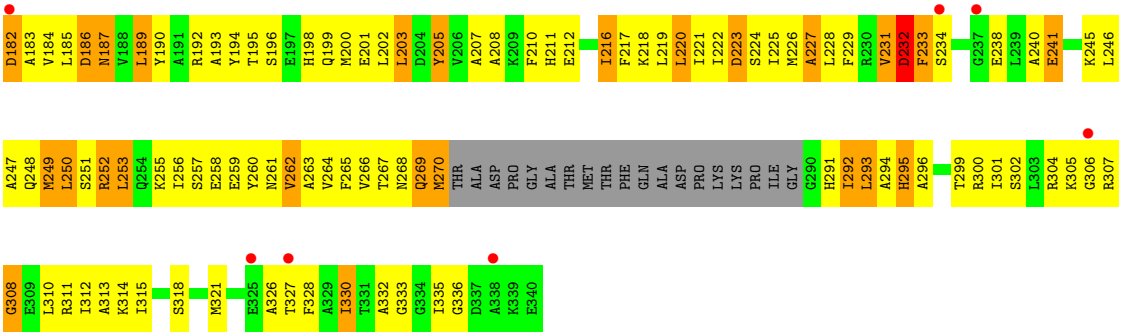
Chain A: 2% 17% 43% 10% 30%



• Molecule 1: Meiotic recombination protein DMC1/LIM15 homolog

Chain B: 3% 18% 40% 11% 30%




D182 A183 V184 L185 D186 N187 V188 L189 Y190 A191 R192 A193 Y194 T195 S196 E197 H198 Q199 M200 E201 L202 L203 D204 Y205 V206 A207 A208 K209 F210 H211 E212 I216 F217 K218 L219 L220 I221 I222 D223 S224 I225 M226 A227 L228 F229 R230 V231 D232 F233 S234 G237 E238 L239 A240 E241 K245 L246
A247 Q248 M249 L250 S251 R252 L253 Q254 K255 I256 S257 E258 E259 Y260 N261 V262 A263 V264 F265 V266 T267 N268 Q269 M270 THR ALA ASP PRO GLY ALA THR MET THR PHE GLN ALA ASP PRO LYS LYS PRO ILE GLY G290 H291 I292 L293 A294 H295 A296 T299 R300 I301 S302 L303 R304 K305 G306 R307
G308 E309 L310 R311 I312 A313 K314 I315 S318 M321 E325 A326 T327 F328 A329 I330 T331 A332 G333 G334 I335 G336 D337 A338 K339 E340

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α, β, γ	124.09Å 124.09Å 218.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.20 19.98 – 3.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-3.20) 97.9 (19.98-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.41 (at 3.22Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.294 , 0.346 0.293 , 0.347	Depositor DCC
R_{free} test set	1436 reflections (10.15%)	wwPDB-VP
Wilson B-factor (Å^2)	78.8	Xtriage
Anisotropy	0.608	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.20 , 74.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	3767	wwPDB-VP
Average B, all atoms (Å^2)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.45% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (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	0.49	0/1908	0.69	0/2564
1	B	0.49	0/1908	0.68	0/2564
All	All	0.49	0/3816	0.68	0/5128

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1875	0	1856	267	0
1	B	1875	0	1856	275	0
2	A	8	0	0	2	0
2	B	9	0	0	1	0
All	All	3767	0	3712	534	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 72.

All (534) 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:220:LEU:HB3	1:B:264:VAL:HG12	1.24	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:ALA:HB2	1:A:292:ILE:HD11	1.18	1.16
1:A:220:LEU:HB3	1:A:264:VAL:HG12	1.22	1.16
1:B:247:ALA:HB2	1:B:292:ILE:HD11	1.17	1.13
1:A:141:VAL:HG12	1:A:145:LEU:HD21	1.25	1.13
1:B:141:VAL:HG12	1:B:145:LEU:HD21	1.28	1.05
1:A:216:ILE:HD13	1:A:216:ILE:H	1.27	1.00
1:B:216:ILE:HD13	1:B:216:ILE:H	1.30	0.96
1:B:247:ALA:HB2	1:B:292:ILE:CD1	1.97	0.93
1:B:228:LEU:HD23	1:B:228:LEU:O	1.69	0.93
1:A:247:ALA:HB2	1:A:292:ILE:CD1	1.97	0.93
1:A:228:LEU:O	1:A:228:LEU:HD23	1.70	0.92
1:A:194:TYR:H	1:A:198:HIS:HD2	1.17	0.91
1:B:194:TYR:H	1:B:198:HIS:HD2	1.18	0.91
1:A:121:ILE:HA	1:A:264:VAL:HG23	1.50	0.90
1:B:247:ALA:CB	1:B:292:ILE:HD11	2.02	0.89
1:B:145:LEU:N	1:B:145:LEU:HD22	1.86	0.89
1:A:145:LEU:HD22	1:A:145:LEU:N	1.88	0.88
1:B:121:ILE:HA	1:B:264:VAL:HG23	1.53	0.88
1:A:247:ALA:CB	1:A:292:ILE:HD11	2.02	0.87
1:A:121:ILE:HG12	1:A:264:VAL:HG21	1.56	0.86
1:A:219:LEU:HD23	1:A:220:LEU:N	1.91	0.85
1:B:167:PRO:HB3	1:B:185:LEU:HD11	1.59	0.84
1:B:219:LEU:HD23	1:B:220:LEU:N	1.92	0.84
1:B:121:ILE:HG12	1:B:264:VAL:HG21	1.57	0.84
1:A:174:ALA:HB2	1:A:184:VAL:HG21	1.61	0.83
1:B:142:THR:HA	1:B:145:LEU:HD23	1.58	0.83
1:A:130:THR:HG22	1:A:132:LYS:H	1.44	0.82
1:A:157:ILE:HD13	1:A:189:LEU:HB3	1.62	0.82
1:B:130:THR:HG22	1:B:132:LYS:H	1.45	0.82
1:B:174:ALA:HB2	1:B:184:VAL:HG21	1.61	0.82
1:A:238:GLU:HG3	1:A:241:GLU:HB2	1.62	0.81
1:B:238:GLU:HG3	1:B:241:GLU:HB2	1.62	0.81
1:A:262:VAL:HG23	1:A:263:ALA:N	1.96	0.81
1:B:262:VAL:HG23	1:B:263:ALA:N	1.96	0.80
1:A:157:ILE:HD13	1:A:189:LEU:CB	2.11	0.80
1:A:142:THR:HA	1:A:145:LEU:HD23	1.63	0.79
1:A:167:PRO:HB3	1:A:185:LEU:HD11	1.65	0.79
1:B:142:THR:CA	1:B:145:LEU:HD23	2.12	0.79
1:A:145:LEU:HD22	1:A:145:LEU:H	1.47	0.78
1:B:157:ILE:HD13	1:B:189:LEU:HB3	1.64	0.78
1:A:234:SER:HB2	1:A:238:GLU:CB	2.14	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:LEU:HD22	1:B:145:LEU:H	1.46	0.78
1:A:141:VAL:HG22	1:A:184:VAL:CG1	2.14	0.77
1:B:234:SER:HB2	1:B:238:GLU:CB	2.14	0.77
1:A:194:TYR:H	1:A:198:HIS:CD2	2.03	0.77
1:B:157:ILE:HD13	1:B:189:LEU:CB	2.15	0.77
1:A:304:ARG:HG3	1:A:312:ILE:HB	1.66	0.76
1:B:145:LEU:H	1:B:145:LEU:CD2	1.99	0.76
1:B:119:MET:HG2	1:B:258:GLU:HA	1.68	0.76
1:B:194:TYR:H	1:B:198:HIS:CD2	2.03	0.76
1:A:216:ILE:H	1:A:216:ILE:CD1	1.98	0.76
1:A:252:ARG:CA	1:A:252:ARG:HH11	1.98	0.75
1:B:304:ARG:HG3	1:B:312:ILE:HB	1.66	0.75
1:B:252:ARG:CA	1:B:252:ARG:HH11	2.00	0.75
1:A:234:SER:HB2	1:A:238:GLU:HB3	1.69	0.75
1:A:145:LEU:H	1:A:145:LEU:CD2	1.99	0.75
1:A:231:VAL:HG12	1:A:232:ASP:N	2.02	0.74
1:B:234:SER:HB2	1:B:238:GLU:HB3	1.70	0.73
1:A:129:ARG:HE	1:A:129:ARG:HA	1.54	0.73
1:A:142:THR:CA	1:A:145:LEU:HD23	2.18	0.73
1:A:140:CYS:O	1:A:144:GLN:NE2	2.22	0.73
1:B:138:THR:OG1	1:B:335:ILE:HD13	1.89	0.72
1:B:140:CYS:O	1:B:144:GLN:NE2	2.22	0.72
1:A:172:ASP:OD2	1:A:332:ALA:HB1	1.88	0.72
1:A:119:MET:HG2	1:A:258:GLU:HA	1.72	0.72
1:B:172:ASP:OD2	1:B:332:ALA:HB1	1.89	0.72
1:B:161:THR:HA	1:B:193:ALA:HB3	1.71	0.72
1:B:129:ARG:HE	1:B:129:ARG:HA	1.54	0.72
1:A:83:PRO:HB3	1:B:205:TYR:OH	1.90	0.72
1:B:252:ARG:NH1	1:B:252:ARG:HB3	2.05	0.71
1:B:121:ILE:HD13	1:B:253:LEU:HD13	1.71	0.71
1:B:124:ALA:HB3	1:B:267:THR:HA	1.72	0.71
1:A:130:THR:HB	1:A:132:LYS:HE2	1.72	0.71
1:A:138:THR:OG1	1:A:335:ILE:HD13	1.90	0.71
1:A:161:THR:HA	1:A:193:ALA:HB3	1.72	0.71
1:A:157:ILE:HB	1:A:220:LEU:HD23	1.70	0.71
1:B:132:LYS:NZ	1:B:269:GLN:HG3	2.06	0.71
1:B:216:ILE:H	1:B:216:ILE:CD1	2.02	0.70
1:B:141:VAL:HG22	1:B:184:VAL:CG1	2.21	0.70
1:A:132:LYS:NZ	1:A:269:GLN:HG3	2.06	0.70
1:B:145:LEU:N	1:B:145:LEU:CD2	2.54	0.70
1:A:203:LEU:HD21	1:A:222:ILE:HD11	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:THR:HB	1:B:132:LYS:HE2	1.72	0.69
1:B:157:ILE:HB	1:B:220:LEU:HD23	1.73	0.69
1:A:124:ALA:HB3	1:A:267:THR:HA	1.75	0.69
1:B:121:ILE:HG12	1:B:264:VAL:CG2	2.23	0.69
1:B:231:VAL:HG12	1:B:232:ASP:N	2.07	0.68
1:B:252:ARG:O	1:B:256:ILE:HG13	1.94	0.68
1:B:120:ALA:N	1:B:257:SER:OG	2.27	0.68
1:A:121:ILE:HG12	1:A:264:VAL:CG2	2.24	0.67
1:A:252:ARG:O	1:A:256:ILE:HG13	1.94	0.67
1:A:112:LEU:HB3	1:A:115:GLY:O	1.94	0.67
1:A:252:ARG:HB3	1:A:252:ARG:NH1	2.09	0.67
1:B:203:LEU:HD21	1:B:222:ILE:HD11	1.76	0.67
1:A:120:ALA:N	1:A:257:SER:OG	2.27	0.67
1:A:158:PHE:HA	1:A:221:ILE:HG23	1.77	0.67
1:B:112:LEU:HB3	1:B:115:GLY:O	1.94	0.67
1:A:233:PHE:HD2	1:A:233:PHE:O	1.77	0.67
1:A:137:HIS:O	1:A:140:CYS:HB2	1.95	0.67
1:A:141:VAL:HG22	1:A:184:VAL:HG11	1.77	0.67
1:A:221:ILE:HD13	1:A:265:PHE:HD2	1.60	0.67
1:A:132:LYS:HD2	1:A:267:THR:HB	1.76	0.66
1:A:135:LEU:HD22	1:A:265:PHE:CE2	2.30	0.66
1:A:121:ILE:HD13	1:A:253:LEU:HD13	1.75	0.66
1:A:252:ARG:HH11	1:A:252:ARG:HA	1.60	0.66
1:A:176:ARG:HH21	1:A:177:PHE:HZ	1.42	0.66
1:B:158:PHE:HA	1:B:221:ILE:HG23	1.77	0.66
1:A:221:ILE:HD13	1:A:265:PHE:HB3	1.78	0.66
1:A:104:GLY:O	1:A:336:GLY:HA2	1.96	0.65
1:A:221:ILE:HD13	1:A:265:PHE:CD2	2.31	0.65
1:B:141:VAL:O	1:B:144:GLN:N	2.30	0.65
1:B:132:LYS:HD2	1:B:267:THR:HB	1.78	0.65
1:B:196:SER:HB3	1:B:229:PHE:CE2	2.31	0.65
1:B:221:ILE:HD13	1:B:265:PHE:HD2	1.60	0.65
1:B:249:MET:O	1:B:252:ARG:N	2.29	0.65
1:B:176:ARG:HH21	1:B:177:PHE:HZ	1.43	0.65
1:A:249:MET:O	1:A:252:ARG:N	2.29	0.65
1:B:137:HIS:O	1:B:140:CYS:HB2	1.97	0.65
1:A:132:LYS:HZ2	1:A:269:GLN:HG3	1.61	0.64
1:B:233:PHE:HD2	1:B:233:PHE:O	1.80	0.64
1:B:221:ILE:HD13	1:B:265:PHE:HB3	1.79	0.64
1:B:141:VAL:HG22	1:B:184:VAL:HG11	1.79	0.64
1:B:305:LYS:HE3	1:B:311:ARG:HG3	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:LYS:HE3	1:A:311:ARG:HG3	1.80	0.64
1:A:141:VAL:O	1:A:144:GLN:N	2.31	0.64
1:B:154:GLY:HA3	1:B:218:LYS:HG2	1.79	0.63
1:B:221:ILE:HD13	1:B:265:PHE:CD2	2.32	0.63
1:A:224:SER:HB2	1:A:268:ASN:ND2	2.14	0.63
1:B:104:GLY:O	1:B:336:GLY:HA2	1.97	0.62
1:B:291:HIS:CD2	1:B:292:ILE:HG22	2.34	0.62
1:A:225:ILE:HG23	1:A:226:MET:H	1.64	0.62
1:A:216:ILE:HD13	1:A:216:ILE:N	2.07	0.62
1:B:226:MET:HB2	1:B:268:ASN:ND2	2.14	0.62
1:A:196:SER:HB3	1:A:229:PHE:CE2	2.35	0.62
1:A:291:HIS:CD2	1:A:292:ILE:HG22	2.34	0.62
1:B:177:PHE:O	1:B:179:VAL:HG23	1.99	0.62
1:A:220:LEU:CB	1:A:264:VAL:HG12	2.15	0.62
1:B:216:ILE:HD13	1:B:216:ILE:N	2.10	0.62
1:A:103:THR:HG23	1:A:109:ASP:OD1	2.00	0.61
1:B:135:LEU:HD22	1:B:265:PHE:CE2	2.35	0.61
1:B:252:ARG:HH11	1:B:252:ARG:HA	1.64	0.61
1:A:92:SER:HB2	1:B:167:PRO:HB2	1.83	0.61
1:A:226:MET:HB2	1:A:268:ASN:ND2	2.15	0.61
1:A:174:ALA:CB	1:A:184:VAL:HG21	2.30	0.60
1:A:225:ILE:HD11	1:A:249:MET:SD	2.40	0.60
1:B:129:ARG:HA	1:B:129:ARG:NE	2.17	0.60
1:B:165:PHE:CD1	1:B:190:TYR:CD1	2.89	0.60
1:B:225:ILE:HD11	1:B:249:MET:SD	2.40	0.60
1:B:103:THR:HG23	1:B:109:ASP:OD1	2.02	0.60
1:B:116:ILE:HG22	1:B:263:ALA:HB1	1.84	0.60
1:A:141:VAL:HG12	1:A:145:LEU:CD2	2.17	0.60
1:A:255:LYS:O	1:A:259:GLU:HB3	2.02	0.60
1:B:224:SER:HB2	1:B:268:ASN:ND2	2.15	0.60
1:B:255:LYS:O	1:B:259:GLU:HB3	2.01	0.60
1:A:246:LEU:HD23	1:A:292:ILE:HD13	1.83	0.60
1:A:116:ILE:HG22	1:A:263:ALA:HB1	1.84	0.60
1:A:129:ARG:HA	1:A:129:ARG:NE	2.16	0.60
1:B:174:ALA:CB	1:B:184:VAL:HG21	2.30	0.60
1:B:182:ASP:O	1:B:186:ASP:HB2	2.01	0.60
1:B:252:ARG:HH11	1:B:252:ARG:CB	2.14	0.59
1:B:223:ASP:HB2	1:B:267:THR:HG23	1.84	0.59
1:B:145:LEU:HG	1:B:177:PHE:CD2	2.38	0.59
1:B:121:ILE:HD11	1:B:253:LEU:HB3	1.85	0.59
1:A:137:HIS:O	1:A:140:CYS:N	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:ILE:N	1:B:335:ILE:HD12	2.18	0.59
1:A:182:ASP:O	1:A:186:ASP:HB2	2.03	0.59
1:A:177:PHE:O	1:A:179:VAL:HG23	2.03	0.59
1:A:225:ILE:HG23	1:A:226:MET:N	2.17	0.59
1:A:223:ASP:HB2	1:A:267:THR:HG23	1.84	0.58
1:A:233:PHE:C	1:A:233:PHE:CD2	2.77	0.58
1:B:162:GLU:O	1:B:163:ASN:HB3	2.02	0.58
1:B:250:LEU:HD13	1:B:296:ALA:CB	2.34	0.58
1:A:227:ALA:H	1:A:268:ASN:ND2	2.02	0.58
1:B:225:ILE:HG23	1:B:226:MET:H	1.69	0.58
1:A:162:GLU:O	1:A:163:ASN:HB3	2.03	0.58
1:B:167:PRO:HB3	1:B:185:LEU:CD1	2.32	0.58
1:A:121:ILE:HD11	1:A:253:LEU:HB3	1.85	0.58
1:A:163:ASN:HA	1:A:192:ARG:HH12	1.69	0.58
1:A:195:THR:C	1:A:228:LEU:HD21	2.24	0.58
1:A:335:ILE:N	1:A:335:ILE:HD12	2.19	0.58
1:B:139:LEU:HA	1:B:142:THR:OG1	2.04	0.58
1:A:161:THR:HG21	1:A:224:SER:O	2.03	0.58
1:B:137:HIS:O	1:B:140:CYS:N	2.36	0.57
1:A:145:LEU:HG	1:A:177:PHE:CD2	2.39	0.57
1:B:151:TYR:CZ	1:B:153:GLY:HA2	2.39	0.57
1:A:252:ARG:HH11	1:A:252:ARG:CB	2.17	0.57
1:A:92:SER:HB2	1:B:167:PRO:CB	2.35	0.57
1:A:141:VAL:O	1:A:143:ALA:N	2.37	0.57
1:A:156:ILE:HG22	1:A:157:ILE:N	2.20	0.57
1:B:245:LYS:HD3	1:B:248:GLN:OE1	2.05	0.57
1:A:165:PHE:CD1	1:A:190:TYR:CD1	2.92	0.57
1:A:249:MET:O	1:A:251:SER:N	2.37	0.57
1:A:318:SER:O	1:A:321:MET:HB3	2.05	0.57
1:B:313:ALA:HB2	1:B:328:PHE:HE2	1.70	0.57
1:A:151:TYR:CZ	1:A:153:GLY:HA2	2.39	0.57
1:A:314:LYS:HG2	1:A:315:ILE:N	2.20	0.57
1:B:249:MET:O	1:B:251:SER:N	2.37	0.57
1:B:314:LYS:HG2	1:B:315:ILE:N	2.20	0.57
1:B:135:LEU:HD23	1:B:135:LEU:C	2.25	0.56
1:B:161:THR:HG21	1:B:224:SER:O	2.05	0.56
1:B:227:ALA:H	1:B:268:ASN:ND2	2.02	0.56
1:B:233:PHE:C	1:B:233:PHE:CD2	2.78	0.56
1:A:154:GLY:HA3	1:A:218:LYS:HG2	1.88	0.56
1:A:313:ALA:HB2	1:A:328:PHE:HE2	1.70	0.56
1:B:162:GLU:O	1:B:163:ASN:CB	2.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:ASN:CA	1:A:192:ARG:HH12	2.17	0.56
1:A:226:MET:HG3	1:A:270:MET:SD	2.45	0.56
1:B:194:TYR:N	1:B:198:HIS:HD2	1.97	0.56
1:B:141:VAL:HG12	1:B:145:LEU:CD2	2.19	0.56
1:B:195:THR:C	1:B:228:LEU:HD21	2.26	0.56
1:B:225:ILE:HG23	1:B:226:MET:N	2.20	0.56
1:B:299:THR:HA	1:B:318:SER:OG	2.05	0.56
1:A:250:LEU:HD11	1:A:293:LEU:HG	1.87	0.56
1:A:122:THR:O	1:A:266:VAL:HG22	2.05	0.56
1:A:139:LEU:HA	1:A:142:THR:OG1	2.06	0.55
1:A:156:ILE:O	1:A:189:LEU:HB2	2.06	0.55
1:A:162:GLU:O	1:A:163:ASN:CB	2.54	0.55
1:B:125:PHE:CB	1:B:302:SER:HA	2.36	0.55
1:B:203:LEU:HD21	1:B:222:ILE:CD1	2.37	0.55
1:A:159:ILE:HD12	1:A:222:ILE:HD11	1.88	0.55
1:B:252:ARG:NH1	1:B:252:ARG:CB	2.69	0.55
1:A:224:SER:HB2	1:A:268:ASN:CG	2.27	0.55
1:B:163:ASN:CA	1:B:192:ARG:HH12	2.19	0.55
1:A:135:LEU:C	1:A:135:LEU:HD23	2.26	0.55
1:A:85:PHE:HB2	1:B:190:TYR:O	2.05	0.55
1:A:203:LEU:HD21	1:A:222:ILE:CD1	2.36	0.55
1:A:250:LEU:HD13	1:A:296:ALA:CB	2.37	0.55
1:A:141:VAL:O	1:A:142:THR:C	2.44	0.55
1:A:299:THR:HA	1:A:318:SER:OG	2.06	0.55
1:B:156:ILE:HG22	1:B:157:ILE:N	2.20	0.55
1:B:318:SER:O	1:B:321:MET:HB3	2.07	0.55
1:A:216:ILE:HG12	1:A:217:PHE:N	2.22	0.55
1:A:220:LEU:O	1:A:264:VAL:HA	2.07	0.55
1:B:156:ILE:O	1:B:189:LEU:HB2	2.07	0.55
1:A:125:PHE:CB	1:A:302:SER:HA	2.37	0.55
1:B:163:ASN:HA	1:B:192:ARG:HH12	1.72	0.55
1:A:207:ALA:O	1:A:210:PHE:N	2.39	0.54
1:B:132:LYS:HZ1	1:B:269:GLN:HG3	1.71	0.54
1:A:245:LYS:HD3	1:A:248:GLN:OE1	2.08	0.54
1:B:165:PHE:CD1	1:B:190:TYR:CE1	2.95	0.54
1:A:119:MET:HB3	1:A:258:GLU:HG2	1.90	0.54
1:A:181:HIS:O	1:A:183:ALA:N	2.40	0.54
1:B:291:HIS:HD2	1:B:292:ILE:HG22	1.71	0.54
1:A:100:HIS:ND1	1:A:114:GLY:HA3	2.23	0.54
1:B:100:HIS:ND1	1:B:114:GLY:HA3	2.23	0.53
1:B:180:ASP:O	1:B:184:VAL:HG23	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:LEU:O	1:B:264:VAL:HA	2.09	0.53
1:B:226:MET:HG3	1:B:270:MET:SD	2.47	0.53
1:A:291:HIS:HD2	1:A:292:ILE:HG22	1.72	0.53
1:B:216:ILE:HG12	1:B:217:PHE:N	2.23	0.53
1:A:135:LEU:HD23	1:A:135:LEU:O	2.09	0.53
1:A:310:LEU:HD23	1:A:327:THR:CG2	2.39	0.53
1:B:306:GLY:O	1:B:307:ARG:HB2	2.09	0.53
1:A:167:PRO:HB3	1:A:185:LEU:CD1	2.37	0.53
1:A:200:MET:SD	1:A:249:MET:HG3	2.49	0.53
1:A:144:GLN:OE1	1:A:184:VAL:HG13	2.08	0.53
1:A:252:ARG:NH1	1:A:252:ARG:CB	2.71	0.53
1:A:267:THR:O	1:A:268:ASN:OD1	2.27	0.53
1:A:238:GLU:CG	1:A:241:GLU:HB2	2.38	0.53
1:A:310:LEU:N	1:A:310:LEU:HD12	2.24	0.53
1:B:122:THR:O	1:B:266:VAL:HG22	2.09	0.53
1:B:207:ALA:O	1:B:210:PHE:N	2.41	0.52
1:B:223:ASP:HB2	1:B:267:THR:CG2	2.39	0.52
1:A:314:LYS:HG2	1:A:315:ILE:H	1.74	0.52
1:B:250:LEU:HD11	1:B:293:LEU:HG	1.90	0.52
1:B:159:ILE:HD12	1:B:222:ILE:HD11	1.90	0.52
1:B:310:LEU:HD23	1:B:327:THR:CG2	2.39	0.52
1:A:200:MET:CG	1:A:249:MET:HB2	2.39	0.52
1:A:249:MET:C	1:A:251:SER:N	2.63	0.52
1:B:135:LEU:HD23	1:B:135:LEU:O	2.09	0.52
1:B:201:GLU:OE1	1:B:201:GLU:HA	2.09	0.52
1:B:310:LEU:HD12	1:B:310:LEU:N	2.24	0.52
1:A:121:ILE:HA	1:A:264:VAL:CG2	2.32	0.52
1:A:223:ASP:HB2	1:A:267:THR:CG2	2.40	0.52
1:B:314:LYS:HG2	1:B:315:ILE:H	1.74	0.52
1:A:201:GLU:HA	1:A:201:GLU:OE1	2.10	0.52
1:B:119:MET:CG	1:B:258:GLU:HA	2.39	0.52
1:B:173:ILE:HG12	1:B:333:GLY:C	2.29	0.52
1:B:200:MET:CG	1:B:249:MET:HB2	2.39	0.52
1:B:250:LEU:HD13	1:B:296:ALA:HB1	1.92	0.52
1:A:95:ARG:HH11	1:A:98:VAL:HG21	1.74	0.52
1:A:185:LEU:C	1:A:187:ASN:H	2.12	0.52
1:A:225:ILE:HG22	1:A:268:ASN:OD1	2.10	0.52
1:B:121:ILE:CD1	1:B:253:LEU:HD13	2.38	0.52
1:B:291:HIS:O	1:B:293:LEU:N	2.43	0.52
1:B:224:SER:HB2	1:B:268:ASN:CG	2.30	0.51
1:A:194:TYR:N	1:A:198:HIS:HD2	1.97	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:GLY:O	1:A:307:ARG:HB2	2.10	0.51
1:B:141:VAL:O	1:B:142:THR:C	2.46	0.51
1:A:198:HIS:O	1:A:201:GLU:HB2	2.10	0.51
1:B:132:LYS:HZ2	1:B:269:GLN:HG3	1.76	0.51
1:B:225:ILE:HG22	1:B:268:ASN:OD1	2.11	0.51
1:B:249:MET:C	1:B:251:SER:N	2.64	0.51
1:A:84:GLY:H	1:B:205:TYR:HE1	1.59	0.51
1:A:165:PHE:CD1	1:A:190:TYR:CE1	2.99	0.51
1:A:233:PHE:O	1:A:233:PHE:CD2	2.62	0.51
1:A:250:LEU:HD13	1:A:296:ALA:HB1	1.93	0.51
1:B:119:MET:HB3	1:B:258:GLU:HG2	1.93	0.51
1:B:141:VAL:O	1:B:143:ALA:N	2.44	0.51
1:B:144:GLN:OE1	1:B:184:VAL:HG13	2.11	0.51
1:B:181:HIS:O	1:B:183:ALA:N	2.44	0.50
1:B:246:LEU:HD23	1:B:292:ILE:HD13	1.91	0.50
1:A:121:ILE:CD1	1:A:253:LEU:HD13	2.41	0.50
1:A:130:THR:HG22	1:A:131:GLY:N	2.26	0.50
1:B:267:THR:O	1:B:268:ASN:OD1	2.30	0.50
1:B:86:LEU:HD11	1:B:91:TYR:HA	1.94	0.50
1:A:173:ILE:HG12	1:A:333:GLY:C	2.32	0.50
1:B:90:GLU:O	1:B:93:GLU:HB2	2.10	0.50
1:B:219:LEU:HD23	1:B:220:LEU:H	1.76	0.50
1:B:123:GLU:HA	1:B:266:VAL:HG23	1.94	0.50
1:B:250:LEU:HD11	1:B:293:LEU:HD23	1.93	0.50
1:A:185:LEU:C	1:A:187:ASN:N	2.65	0.49
1:B:95:ARG:HH11	1:B:98:VAL:HG21	1.77	0.49
1:B:227:ALA:H	1:B:268:ASN:HD21	1.59	0.49
1:B:125:PHE:HB3	1:B:302:SER:HA	1.95	0.49
1:A:123:GLU:OE2	1:A:125:PHE:HE1	1.95	0.49
1:B:127:GLU:N	1:B:130:THR:OG1	2.42	0.49
1:B:192:ARG:HG2	1:B:192:ARG:HH11	1.77	0.49
1:B:198:HIS:O	1:B:201:GLU:HB2	2.11	0.49
1:A:86:LEU:HD11	1:A:91:TYR:HA	1.94	0.49
1:A:163:ASN:HA	1:A:192:ARG:NH1	2.27	0.49
1:B:238:GLU:HG3	1:B:238:GLU:O	2.13	0.49
1:A:157:ILE:HD13	1:A:189:LEU:HB2	1.94	0.49
1:A:180:ASP:O	1:A:184:VAL:HG23	2.13	0.49
1:A:90:GLU:O	1:A:93:GLU:HB2	2.13	0.49
1:A:100:HIS:N	1:A:100:HIS:CD2	2.81	0.49
1:A:123:GLU:HA	1:A:266:VAL:HG23	1.94	0.49
1:B:123:GLU:OE2	1:B:125:PHE:HE1	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:HIS:O	1:A:293:LEU:N	2.46	0.48
1:A:295:HIS:ND1	1:A:295:HIS:C	2.66	0.48
1:B:102:THR:HG22	1:B:142:THR:HB	1.95	0.48
1:B:185:LEU:C	1:B:187:ASN:H	2.16	0.48
1:B:155:LYS:C	1:B:156:ILE:HG13	2.34	0.48
1:A:252:ARG:O	1:A:252:ARG:NH1	2.47	0.48
1:A:183:ALA:O	1:A:187:ASN:HB2	2.13	0.48
1:B:163:ASN:HA	1:B:192:ARG:NH1	2.29	0.48
1:B:200:MET:HG2	1:B:249:MET:HG3	1.96	0.48
1:B:130:THR:HG22	1:B:131:GLY:N	2.28	0.48
1:A:227:ALA:H	1:A:268:ASN:HD21	1.60	0.48
1:B:137:HIS:O	1:B:138:THR:C	2.53	0.48
1:A:147:GLY:O	1:A:148:ALA:O	2.32	0.47
1:A:238:GLU:HG3	1:A:238:GLU:O	2.13	0.47
1:A:246:LEU:HD23	1:A:292:ILE:HG21	1.95	0.47
1:B:159:ILE:HD12	1:B:222:ILE:CD1	2.44	0.47
1:B:118:SER:HA	1:B:262:VAL:O	2.14	0.47
1:B:125:PHE:HB2	1:B:301:ILE:O	2.13	0.47
1:A:119:MET:CG	1:A:258:GLU:HA	2.43	0.47
1:B:231:VAL:O	1:B:233:PHE:N	2.47	0.47
1:A:183:ALA:O	1:A:184:VAL:C	2.50	0.47
1:A:184:VAL:O	1:A:187:ASN:CB	2.63	0.47
1:A:127:GLU:N	1:A:130:THR:OG1	2.42	0.47
1:A:83:PRO:C	1:A:85:PHE:H	2.18	0.47
1:A:155:LYS:C	1:A:156:ILE:HG13	2.35	0.47
1:A:226:MET:SD	1:A:246:LEU:HD11	2.55	0.47
1:B:250:LEU:HD11	1:B:293:LEU:CD2	2.43	0.47
1:B:295:HIS:ND1	1:B:295:HIS:C	2.68	0.47
1:A:118:SER:HA	1:A:262:VAL:O	2.14	0.47
1:A:192:ARG:HG2	1:A:192:ARG:HH11	1.80	0.47
1:B:142:THR:C	1:B:144:GLN:H	2.17	0.47
1:B:183:ALA:O	1:B:184:VAL:C	2.51	0.47
1:B:233:PHE:O	1:B:233:PHE:CD2	2.65	0.47
1:A:102:THR:HG22	1:A:142:THR:HB	1.97	0.47
1:B:184:VAL:O	1:B:187:ASN:CB	2.63	0.47
1:A:125:PHE:HB2	1:A:302:SER:HA	1.97	0.46
1:A:159:ILE:HD12	1:A:222:ILE:CD1	2.44	0.46
1:B:335:ILE:N	1:B:335:ILE:CD1	2.78	0.46
1:A:136:SER:HB3	1:A:158:PHE:CE1	2.51	0.46
1:A:137:HIS:O	1:A:138:THR:C	2.53	0.46
1:A:200:MET:HG3	1:A:249:MET:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:LEU:C	1:A:141:VAL:N	2.67	0.46
1:A:241:GLU:HA	1:A:241:GLU:OE1	2.14	0.46
1:A:250:LEU:HD11	1:A:293:LEU:CG	2.46	0.46
1:B:100:HIS:HA	1:B:116:ILE:O	2.15	0.46
1:B:185:LEU:C	1:B:187:ASN:N	2.69	0.46
1:B:200:MET:SD	1:B:249:MET:HG3	2.55	0.46
1:B:200:MET:HG3	1:B:249:MET:HB2	1.95	0.46
1:A:335:ILE:N	1:A:335:ILE:CD1	2.78	0.46
1:A:123:GLU:OE2	1:A:125:PHE:CE1	2.69	0.46
1:B:139:LEU:C	1:B:141:VAL:N	2.68	0.46
1:A:258:GLU:OE2	1:B:192:ARG:NE	2.49	0.46
1:A:250:LEU:HD11	1:A:293:LEU:CD2	2.46	0.46
1:A:250:LEU:HD11	1:A:293:LEU:HD23	1.97	0.46
1:B:145:LEU:HG	1:B:177:PHE:HD2	1.80	0.46
1:B:226:MET:SD	1:B:246:LEU:HD11	2.56	0.46
1:A:170:LEU:O	1:A:173:ILE:N	2.40	0.46
1:A:233:PHE:HD2	1:A:233:PHE:C	2.17	0.46
1:A:249:MET:C	1:A:251:SER:H	2.18	0.46
1:A:138:THR:HG21	1:A:335:ILE:H	1.80	0.45
1:B:234:SER:HB2	1:B:238:GLU:HB2	1.96	0.45
1:A:267:THR:O	1:A:268:ASN:CG	2.54	0.45
1:B:123:GLU:OE2	1:B:125:PHE:CE1	2.70	0.45
1:B:250:LEU:HD11	1:B:293:LEU:CG	2.46	0.45
1:A:125:PHE:HB2	1:A:301:ILE:O	2.16	0.45
1:B:121:ILE:HA	1:B:264:VAL:CG2	2.36	0.45
1:A:100:HIS:HA	1:A:116:ILE:O	2.16	0.45
1:B:125:PHE:HB2	1:B:302:SER:HA	1.98	0.45
1:B:136:SER:HB3	1:B:158:PHE:CE1	2.52	0.45
1:B:305:LYS:CE	1:B:311:ARG:HG3	2.45	0.45
1:A:182:ASP:O	1:A:182:ASP:OD1	2.35	0.45
1:A:223:ASP:HA	1:A:224:SER:HA	1.58	0.45
1:A:305:LYS:CE	1:A:311:ARG:HG3	2.45	0.45
1:B:249:MET:C	1:B:251:SER:H	2.20	0.45
1:B:252:ARG:NH1	1:B:252:ARG:O	2.50	0.45
1:A:125:PHE:HB3	1:A:302:SER:HA	1.98	0.45
1:A:131:GLY:O	1:A:134:GLN:N	2.49	0.45
1:B:119:MET:HA	1:B:258:GLU:HA	1.99	0.45
1:A:119:MET:HA	1:A:258:GLU:HA	1.99	0.45
1:B:159:ILE:HB	1:B:222:ILE:HG12	1.99	0.45
1:A:145:LEU:HG	1:A:177:PHE:HD2	1.82	0.45
1:B:131:GLY:O	1:B:134:GLN:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:THR:HB	2:A:347:HOH:O	2.17	0.44
1:B:100:HIS:N	1:B:100:HIS:CD2	2.84	0.44
1:B:199:GLN:O	1:B:202:LEU:HB2	2.17	0.44
1:B:267:THR:O	1:B:268:ASN:CG	2.55	0.44
1:A:305:LYS:HE2	1:A:308:GLY:O	2.18	0.44
1:B:291:HIS:O	1:B:294:ALA:N	2.50	0.44
1:A:89:PHE:HB2	1:B:185:LEU:HB3	1.99	0.44
1:B:241:GLU:OE1	1:B:241:GLU:HA	2.16	0.44
1:B:295:HIS:ND1	1:B:296:ALA:N	2.66	0.44
1:A:112:LEU:HD23	1:A:115:GLY:HA2	1.99	0.44
1:A:159:ILE:HB	1:A:222:ILE:HG12	1.99	0.44
1:B:170:LEU:O	1:B:173:ILE:N	2.40	0.44
1:B:184:VAL:O	1:B:187:ASN:HB3	2.17	0.44
1:B:231:VAL:C	1:B:233:PHE:H	2.21	0.44
1:A:142:THR:C	1:A:144:GLN:H	2.21	0.44
1:A:181:HIS:C	1:A:183:ALA:N	2.70	0.44
1:B:238:GLU:CG	1:B:241:GLU:HB2	2.38	0.44
1:B:250:LEU:HD23	1:B:250:LEU:HA	1.74	0.44
1:B:183:ALA:O	1:B:187:ASN:HB2	2.16	0.44
1:B:246:LEU:HD23	1:B:292:ILE:HG21	1.99	0.44
1:A:173:ILE:C	1:A:175:ASP:N	2.68	0.44
1:A:130:THR:CG2	1:A:131:GLY:N	2.79	0.43
1:A:295:HIS:ND1	1:A:296:ALA:N	2.66	0.43
1:B:130:THR:CG2	1:B:131:GLY:N	2.81	0.43
1:A:88:ALA:HB1	1:B:185:LEU:HD13	2.00	0.43
1:A:173:ILE:O	1:A:175:ASP:N	2.51	0.43
1:B:253:LEU:HD23	1:B:256:ILE:HD12	2.00	0.43
1:A:252:ARG:HA	1:A:252:ARG:HD2	1.83	0.43
1:B:86:LEU:HD12	1:B:90:GLU:CB	2.48	0.43
1:A:135:LEU:HD23	1:A:139:LEU:HG	1.99	0.43
1:A:146:PRO:HG3	1:A:152:PRO:O	2.18	0.43
1:A:223:ASP:OD1	1:A:223:ASP:O	2.37	0.43
1:B:155:LYS:HB3	1:B:217:PHE:CE2	2.53	0.43
1:B:173:ILE:C	1:B:175:ASP:N	2.70	0.43
1:B:223:ASP:O	1:B:223:ASP:OD1	2.36	0.43
1:A:184:VAL:O	1:A:187:ASN:HB3	2.17	0.43
1:A:226:MET:O	1:A:228:LEU:N	2.51	0.43
1:A:231:VAL:O	1:A:233:PHE:N	2.51	0.43
1:B:124:ALA:N	1:B:266:VAL:O	2.51	0.43
1:B:147:GLY:O	1:B:148:ALA:O	2.35	0.43
1:B:330:ILE:HD12	1:B:330:ILE:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:ASN:HB2	1:B:192:ARG:NH2	2.34	0.43
1:B:182:ASP:O	1:B:182:ASP:OD1	2.37	0.43
1:B:196:SER:HA	1:B:228:LEU:HD22	2.01	0.43
1:A:144:GLN:HA	2:A:341:HOH:O	2.19	0.43
1:B:233:PHE:HA	2:B:347:HOH:O	2.17	0.43
1:A:116:ILE:CG2	1:A:263:ALA:HB1	2.48	0.43
1:A:200:MET:HG2	1:A:249:MET:HG3	2.01	0.43
1:A:250:LEU:HA	1:A:250:LEU:HD23	1.75	0.43
1:B:252:ARG:HA	1:B:252:ARG:HD2	1.87	0.43
1:A:196:SER:HA	1:A:228:LEU:HD22	2.01	0.43
1:B:83:PRO:C	1:B:85:PHE:H	2.22	0.43
1:B:116:ILE:CG2	1:B:263:ALA:HB1	2.48	0.43
1:B:123:GLU:HA	1:B:266:VAL:O	2.19	0.43
1:B:135:LEU:HA	1:B:138:THR:OG1	2.19	0.42
1:B:293:LEU:O	1:B:300:ARG:NH1	2.52	0.42
1:A:200:MET:O	1:A:201:GLU:C	2.57	0.42
1:B:226:MET:HG3	1:B:293:LEU:HD12	2.01	0.42
1:A:112:LEU:N	1:A:112:LEU:CD1	2.82	0.42
1:A:253:LEU:HD23	1:A:256:ILE:HD12	2.00	0.42
1:A:292:ILE:O	1:A:296:ALA:HB2	2.19	0.42
1:A:293:LEU:O	1:A:300:ARG:NH1	2.52	0.42
1:B:176:ARG:NH2	1:B:177:PHE:CE1	2.84	0.42
1:B:221:ILE:HG23	1:B:221:ILE:O	2.19	0.42
1:A:163:ASN:HB2	1:A:192:ARG:NH2	2.34	0.42
1:B:138:THR:HG21	1:B:335:ILE:H	1.83	0.42
1:B:205:TYR:O	1:B:205:TYR:CD2	2.72	0.42
1:B:305:LYS:HE2	1:B:308:GLY:O	2.19	0.42
1:A:221:ILE:HG23	1:A:221:ILE:O	2.20	0.42
1:B:119:MET:CB	1:B:258:GLU:HA	2.49	0.42
1:A:86:LEU:HD12	1:A:90:GLU:CB	2.50	0.42
1:A:291:HIS:O	1:A:294:ALA:N	2.52	0.42
1:B:112:LEU:CD1	1:B:112:LEU:N	2.83	0.42
1:B:181:HIS:C	1:B:183:ALA:N	2.73	0.42
1:B:200:MET:O	1:B:201:GLU:C	2.56	0.42
1:B:305:LYS:HE3	1:B:311:ARG:CG	2.48	0.42
1:B:112:LEU:HD23	1:B:115:GLY:HA2	2.01	0.42
1:B:233:PHE:HD2	1:B:233:PHE:C	2.18	0.42
1:B:138:THR:CG2	1:B:335:ILE:H	2.32	0.42
1:A:231:VAL:C	1:A:233:PHE:H	2.23	0.41
1:B:199:GLN:OE1	1:B:225:ILE:HG13	2.20	0.41
1:B:183:ALA:O	1:B:186:ASP:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:GLU:OE1	1:A:238:GLU:HA	2.20	0.41
1:B:107:GLU:OE2	1:B:326:ALA:HA	2.20	0.41
1:B:123:GLU:OE1	1:B:293:LEU:HD13	2.20	0.41
1:B:223:ASP:HA	1:B:224:SER:HA	1.56	0.41
1:A:238:GLU:C	1:A:240:ALA:N	2.73	0.41
1:B:146:PRO:HG3	1:B:152:PRO:O	2.20	0.41
1:B:229:PHE:C	1:B:231:VAL:N	2.73	0.41
1:B:238:GLU:C	1:B:240:ALA:N	2.74	0.41
1:A:199:GLN:O	1:A:202:LEU:HB2	2.20	0.41
1:A:231:VAL:HG12	1:A:232:ASP:OD1	2.20	0.41
1:B:205:TYR:CD2	1:B:205:TYR:C	2.93	0.41
1:B:304:ARG:CG	1:B:312:ILE:HB	2.45	0.41
1:A:117:GLU:CG	1:A:118:SER:N	2.83	0.41
1:B:167:PRO:O	1:B:170:LEU:HB2	2.21	0.41
1:B:183:ALA:O	1:B:187:ASN:N	2.54	0.41
1:B:211:HIS:HA	1:B:260:TYR:HE2	1.86	0.41
1:A:135:LEU:HA	1:A:138:THR:OG1	2.21	0.41
1:A:247:ALA:CA	1:A:292:ILE:HD11	2.50	0.41
1:B:192:ARG:HG2	1:B:192:ARG:NH1	2.36	0.41
1:B:207:ALA:O	1:B:208:ALA:C	2.59	0.41
1:A:127:GLU:N	1:A:130:THR:HG1	2.18	0.41
1:A:138:THR:CG2	1:A:335:ILE:H	2.33	0.41
1:A:181:HIS:O	1:A:182:ASP:C	2.59	0.41
1:A:234:SER:HB2	1:A:238:GLU:HB2	1.98	0.41
1:B:165:PHE:HD1	1:B:190:TYR:CE1	2.37	0.41
1:A:183:ALA:O	1:A:187:ASN:N	2.54	0.40
1:A:123:GLU:OE1	1:A:293:LEU:HD13	2.20	0.40
1:A:197:GLU:O	1:A:201:GLU:HG2	2.22	0.40
1:B:169:ARG:HA	1:B:169:ARG:HD3	1.71	0.40
1:B:199:GLN:HE21	1:B:199:GLN:HB2	1.68	0.40
1:B:292:ILE:O	1:B:296:ALA:HB2	2.21	0.40
1:A:112:LEU:HD23	1:A:115:GLY:C	2.41	0.40
1:A:211:HIS:HA	1:A:260:TYR:HE2	1.86	0.40
1:A:219:LEU:HD23	1:A:219:LEU:C	2.41	0.40
1:A:205:TYR:C	1:A:205:TYR:CD2	2.95	0.40
1:A:216:ILE:CG1	1:A:217:PHE:N	2.84	0.40
1:A:320:GLU:O	1:A:322:PRO:HD3	2.21	0.40
1:B:173:ILE:O	1:B:175:ASP:N	2.54	0.40
1:A:132:LYS:HB2	1:A:267:THR:CG2	2.51	0.40
1:B:132:LYS:HB2	1:B:267:THR:CG2	2.52	0.40
1:B:313:ALA:HB2	1:B:328:PHE:CE2	2.54	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	235/343 (68%)	184 (78%)	37 (16%)	14 (6%)	1 12
1	B	235/343 (68%)	185 (79%)	36 (15%)	14 (6%)	1 12
All	All	470/686 (68%)	369 (78%)	73 (16%)	28 (6%)	1 12

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	148	ALA
1	A	163	ASN
1	A	227	ALA
1	A	292	ILE
1	A	308	GLY
1	B	148	ALA
1	B	227	ALA
1	B	292	ILE
1	B	308	GLY
1	A	142	THR
1	A	182	ASP
1	A	212	GLU
1	A	232	ASP
1	A	250	LEU
1	B	163	ASN
1	B	182	ASP
1	B	232	ASP
1	B	250	LEU
1	B	142	THR
1	B	212	GLU
1	A	231	VAL
1	B	143	ALA

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Mol	Chain	Res	Type
1	B	231	VAL
1	A	261	ASN
1	B	261	ASN
1	A	143	ALA
1	A	152	PRO
1	B	152	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	195/282 (69%)	165 (85%)	30 (15%)	2 13
1	B	195/282 (69%)	165 (85%)	30 (15%)	2 13
All	All	390/564 (69%)	330 (85%)	60 (15%)	2 13

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	85	PHE
1	A	87	THR
1	A	108	PHE
1	A	112	LEU
1	A	125	PHE
1	A	138	THR
1	A	145	LEU
1	A	167	PRO
1	A	168	ASP
1	A	169	ARG
1	A	186	ASP
1	A	187	ASN
1	A	189	LEU
1	A	203	LEU
1	A	205	TYR
1	A	216	ILE
1	A	220	LEU

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Mol	Chain	Res	Type
1	A	223	ASP
1	A	232	ASP
1	A	233	PHE
1	A	241	GLU
1	A	249	MET
1	A	252	ARG
1	A	253	LEU
1	A	262	VAL
1	A	269	GLN
1	A	270	MET
1	A	293	LEU
1	A	295	HIS
1	A	330	ILE
1	B	85	PHE
1	B	87	THR
1	B	108	PHE
1	B	112	LEU
1	B	125	PHE
1	B	138	THR
1	B	145	LEU
1	B	167	PRO
1	B	168	ASP
1	B	169	ARG
1	B	186	ASP
1	B	187	ASN
1	B	189	LEU
1	B	203	LEU
1	B	205	TYR
1	B	216	ILE
1	B	220	LEU
1	B	223	ASP
1	B	232	ASP
1	B	233	PHE
1	B	241	GLU
1	B	249	MET
1	B	252	ARG
1	B	253	LEU
1	B	262	VAL
1	B	269	GLN
1	B	270	MET
1	B	293	LEU
1	B	295	HIS

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Mol	Chain	Res	Type
1	B	330	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	198	HIS
1	A	291	HIS
1	B	198	HIS
1	B	254	GLN
1	B	291	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	239/343 (69%)	-0.23	6 (2%)	57	43	15, 69, 145, 200	0
1	B	239/343 (69%)	-0.09	9 (3%)	40	26	25, 76, 165, 200	0
All	All	478/686 (69%)	-0.16	15 (3%)	49	32	15, 73, 160, 200	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	327	THR	5.4
1	A	83	PRO	4.0
1	B	325	GLU	3.6
1	A	84	GLY	3.1
1	B	338	ALA	3.0
1	A	318	SER	2.8
1	A	340	GLU	2.5
1	B	182	ASP	2.5
1	B	234	SER	2.4
1	B	306	GLY	2.4
1	B	129	ARG	2.3
1	A	237	GLY	2.2
1	A	235	GLY	2.1
1	B	89	PHE	2.0
1	B	237	GLY	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 monosaccharides 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.