Full wwPDB X-ray Structure Validation Report ⓘ

Oct 29, 2024 – 08:10 AM EDT

PDB ID	:	3QQ5
Title	:	Crystal structure of the [FeFe]-hydrogenase maturation protein HydF
Authors	:	Cendron, L.; Berto, P.; D'Adamo, S.; Vallese, F.; Govoni, C.; Posewitz, M.C.; Giacometti, G.M.; Costantini, P.; Zanotti, G.
Deposited on	:	2011-02-15
Resolution	:	2.99 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:

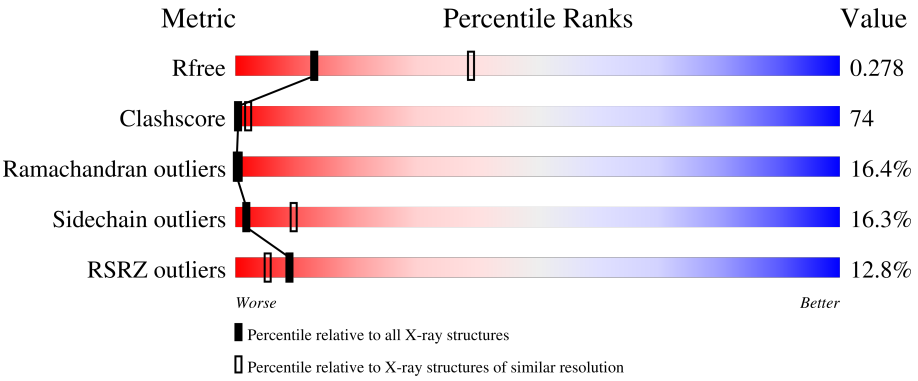
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.99 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}	164625	2511 (3.00-3.00)
Clashscore	180529	2866 (3.00-3.00)
Ramachandran outliers	177936	2778 (3.00-3.00)
Sidechain outliers	177891	2781 (3.00-3.00)
RSRZ outliers	164620	2523 (3.00-3.00)

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	423	12% 25% 46% 18% • 9%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2996 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 Small GTP-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	384	2996	1907	517	556	16	0	0	0

There are 27 discrepancies between the modelled and reference sequences:

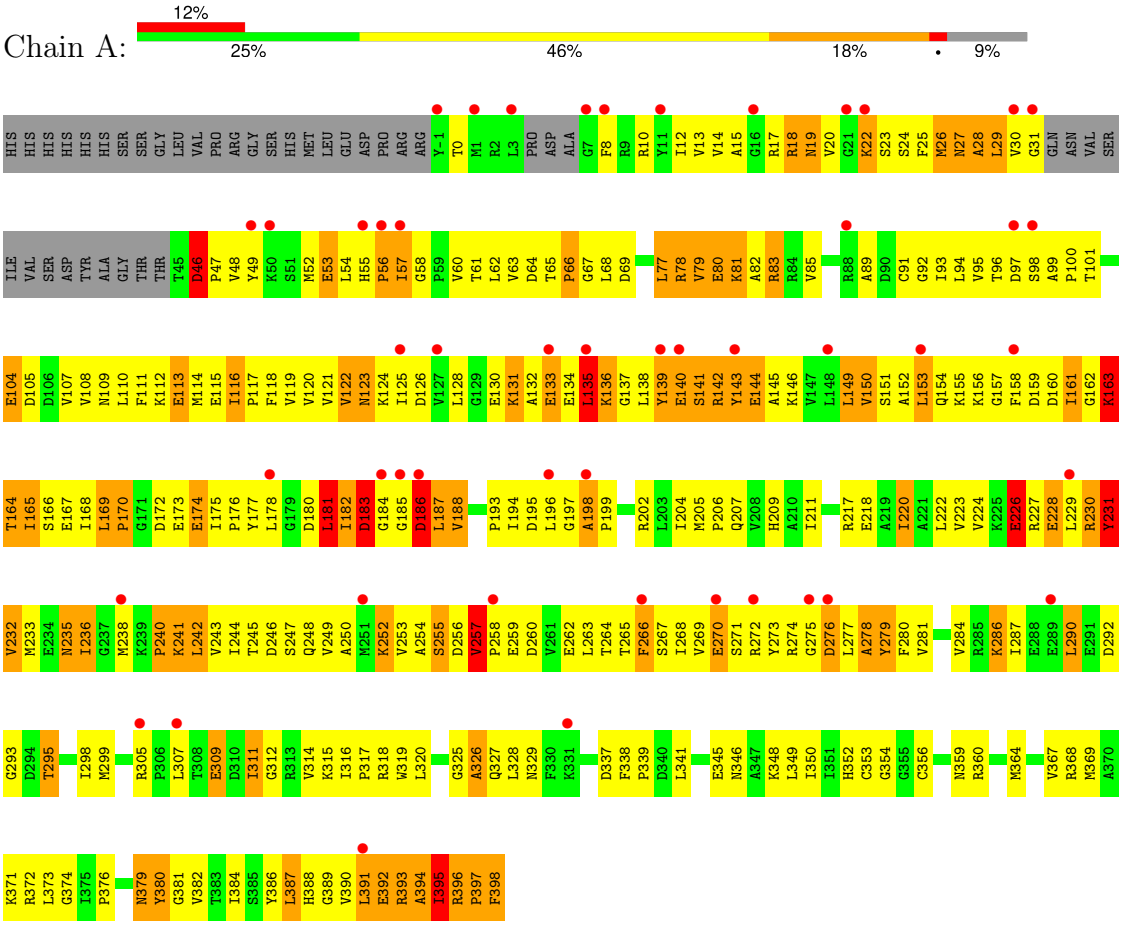
Chain	Residue	Modelled	Actual	Comment	Reference
A	-24	HIS	-	expression tag	UNP B9KBK7
A	-23	HIS	-	expression tag	UNP B9KBK7
A	-22	HIS	-	expression tag	UNP B9KBK7
A	-21	HIS	-	expression tag	UNP B9KBK7
A	-20	HIS	-	expression tag	UNP B9KBK7
A	-19	HIS	-	expression tag	UNP B9KBK7
A	-18	SER	-	expression tag	UNP B9KBK7
A	-17	SER	-	expression tag	UNP B9KBK7
A	-16	GLY	-	expression tag	UNP B9KBK7
A	-15	LEU	-	expression tag	UNP B9KBK7
A	-14	VAL	-	expression tag	UNP B9KBK7
A	-13	PRO	-	expression tag	UNP B9KBK7
A	-12	ARG	-	expression tag	UNP B9KBK7
A	-11	GLY	-	expression tag	UNP B9KBK7
A	-10	SER	-	expression tag	UNP B9KBK7
A	-9	HIS	-	expression tag	UNP B9KBK7
A	-8	MET	-	expression tag	UNP B9KBK7
A	-7	LEU	-	expression tag	UNP B9KBK7
A	-6	GLU	-	expression tag	UNP B9KBK7
A	-5	ASP	-	expression tag	UNP B9KBK7
A	-4	PRO	-	expression tag	UNP B9KBK7
A	-3	ARG	-	expression tag	UNP B9KBK7
A	-2	ARG	-	expression tag	UNP B9KBK7
A	-1	TYR	-	expression tag	UNP B9KBK7
A	0	THR	-	expression tag	UNP B9KBK7
A	1	MET	-	expression tag	UNP B9KBK7
A	250	ALA	VAL	conflict	UNP B9KBK7

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: Small GTP-binding protein

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 3	Depositor
Cell constants a, b, c, α, β, γ	138.26Å 138.26Å 138.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	79.71 – 2.99 79.71 – 2.99	Depositor EDS
% Data completeness (in resolution range)	99.7 (79.71-2.99) 99.9 (79.71-2.99)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.94 (at 3.01Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.274 , 0.309 0.286 , 0.278	Depositor DCC
R_{free} test set	918 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	97.4	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 122.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.043 for l,-k,h	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	2996	wwPDB-VP
Average B, all atoms (Å^2)	107.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.51	0/3043	0.78	0/4111

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

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	2996	0	3068	447	0
All	All	2996	0	3068	447	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 74.

All (447) 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:22:LYS:HD3	1:A:95:VAL:CG1	1.55	1.35
1:A:22:LYS:CD	1:A:95:VAL:HG11	1.59	1.30
1:A:311:ILE:HD12	1:A:311:ILE:H	1.15	1.12
1:A:187:LEU:HD21	1:A:241:LYS:HG2	1.22	1.10
1:A:181:LEU:HG	1:A:217:ARG:HD2	1.35	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:ILE:HB	1:A:187:LEU:HD22	1.06	1.03
1:A:182:ILE:HB	1:A:187:LEU:CD2	1.88	1.02
1:A:263:LEU:HB3	1:A:395:ILE:HD12	1.40	1.02
1:A:181:LEU:HD22	1:A:182:ILE:H	1.26	0.99
1:A:139:TYR:HD1	1:A:140:GLU:HG3	1.27	0.99
1:A:79:VAL:HG23	1:A:80:GLU:H	1.27	0.98
1:A:245:THR:HG22	1:A:246:ASP:H	1.28	0.98
1:A:18:ARG:HD2	1:A:97:ASP:HB2	1.49	0.94
1:A:28:ALA:HB1	1:A:153:LEU:HD21	1.51	0.93
1:A:18:ARG:HA	1:A:18:ARG:NE	1.83	0.93
1:A:139:TYR:CD1	1:A:140:GLU:HG3	2.04	0.92
1:A:188:VAL:HG12	1:A:240:PRO:HA	1.48	0.92
1:A:186:ASP:O	1:A:187:LEU:HB2	1.65	0.92
1:A:181:LEU:CD2	1:A:182:ILE:H	1.83	0.92
1:A:396:ARG:N	1:A:397:PRO:HD2	1.84	0.91
1:A:18:ARG:HA	1:A:18:ARG:CZ	2.01	0.90
1:A:177:TYR:O	1:A:178:LEU:HG	1.70	0.90
1:A:161:ILE:O	1:A:165:ILE:HG22	1.71	0.90
1:A:182:ILE:CB	1:A:187:LEU:HD22	1.99	0.89
1:A:47:PRO:HB3	1:A:66:PRO:HB3	1.55	0.89
1:A:229:LEU:HD23	1:A:230:ARG:H	1.38	0.88
1:A:46:ASP:H	1:A:47:PRO:HD2	1.38	0.87
1:A:236:ILE:HD11	1:A:238:MET:SD	2.16	0.86
1:A:242:LEU:HD12	1:A:243:VAL:N	1.91	0.86
1:A:232:VAL:HG13	1:A:233:MET:H	1.40	0.85
1:A:99:ALA:HB1	1:A:100:PRO:HD2	1.56	0.85
1:A:31:GLY:H	1:A:52:MET:HE1	1.39	0.84
1:A:396:ARG:H	1:A:397:PRO:HD2	1.40	0.84
1:A:136:LYS:HD3	1:A:140:GLU:OE2	1.78	0.84
1:A:144:GLU:O	1:A:146:LYS:HG2	1.78	0.83
1:A:254:ALA:O	1:A:257:VAL:HG13	1.78	0.83
1:A:379:ASN:C	1:A:379:ASN:HD22	1.79	0.83
1:A:150:VAL:HG22	1:A:152:ALA:H	1.43	0.82
1:A:109:ASN:O	1:A:113:GLU:HB2	1.79	0.82
1:A:128:LEU:HD22	1:A:130:GLU:HG3	1.62	0.81
1:A:107:VAL:HG23	1:A:108:VAL:N	1.94	0.81
1:A:266:PHE:HB3	1:A:268:ILE:HG12	1.63	0.80
1:A:31:GLY:HA2	1:A:158:PHE:CE2	2.16	0.80
1:A:165:ILE:C	1:A:165:ILE:HD13	2.02	0.80
1:A:352:HIS:O	1:A:379:ASN:HB2	1.82	0.80
1:A:396:ARG:HG2	1:A:396:ARG:HH11	1.47	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:THR:H	1:A:104:GLU:CG	1.95	0.79
1:A:18:ARG:HG3	1:A:19:ASN:H	1.46	0.79
1:A:311:ILE:H	1:A:311:ILE:CD1	1.90	0.78
1:A:15:ALA:HA	1:A:65:THR:HG23	1.67	0.77
1:A:188:VAL:HG23	1:A:220:ILE:HD12	1.67	0.76
1:A:268:ILE:O	1:A:272:ARG:HD3	1.84	0.76
1:A:60:VAL:HG22	1:A:61:THR:N	2.01	0.75
1:A:160:ASP:HA	1:A:163:LYS:HD3	1.66	0.75
1:A:100:PRO:HA	1:A:104:GLU:HG3	1.69	0.74
1:A:31:GLY:N	1:A:52:MET:HE1	2.01	0.74
1:A:393:ARG:H	1:A:393:ARG:HD3	1.52	0.74
1:A:173:GLU:CB	1:A:360:ARG:HE	1.99	0.74
1:A:228:GLU:O	1:A:232:VAL:HG12	1.88	0.74
1:A:232:VAL:O	1:A:236:ILE:HG22	1.88	0.73
1:A:250:ALA:HB2	1:A:266:PHE:CE2	2.24	0.73
1:A:60:VAL:HG22	1:A:61:THR:H	1.53	0.73
1:A:24:SER:O	1:A:28:ALA:HB3	1.88	0.72
1:A:77:LEU:HD21	1:A:82:ALA:HB2	1.70	0.72
1:A:47:PRO:CB	1:A:66:PRO:HB3	2.19	0.72
1:A:161:ILE:HD13	1:A:162:GLY:H	1.55	0.72
1:A:395:ILE:HD13	1:A:395:ILE:H	1.55	0.71
1:A:149:LEU:HD21	1:A:157:GLY:HA2	1.72	0.71
1:A:169:LEU:HB3	1:A:170:PRO:HD2	1.72	0.71
1:A:152:ALA:O	1:A:154:GLN:HG3	1.91	0.71
1:A:181:LEU:HD13	1:A:181:LEU:H	1.56	0.71
1:A:187:LEU:HD21	1:A:241:LYS:CG	2.12	0.71
1:A:29:LEU:HD22	1:A:29:LEU:H	1.55	0.71
1:A:111:PHE:HA	1:A:116:ILE:HG23	1.73	0.70
1:A:379:ASN:C	1:A:379:ASN:ND2	2.45	0.70
1:A:101:THR:H	1:A:104:GLU:HG3	1.56	0.70
1:A:232:VAL:HG13	1:A:233:MET:N	2.06	0.70
1:A:386:TYR:HA	1:A:390:VAL:HG12	1.73	0.70
1:A:142:ARG:HD3	1:A:142:ARG:N	2.07	0.70
1:A:396:ARG:N	1:A:397:PRO:CD	2.55	0.70
1:A:141:SER:C	1:A:142:ARG:HD3	2.11	0.69
1:A:161:ILE:CD1	1:A:162:GLY:H	2.04	0.69
1:A:79:VAL:HG23	1:A:80:GLU:N	2.04	0.69
1:A:107:VAL:HG23	1:A:108:VAL:H	1.57	0.69
1:A:220:ILE:HD13	1:A:220:ILE:C	2.13	0.69
1:A:395:ILE:HD13	1:A:395:ILE:N	2.08	0.69
1:A:180:ASP:O	1:A:182:ILE:HG13	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:TYR:HD1	1:A:380:TYR:H	1.40	0.68
1:A:177:TYR:CD2	1:A:274:ARG:HD2	2.29	0.68
1:A:393:ARG:C	1:A:395:ILE:HG12	2.14	0.68
1:A:390:VAL:O	1:A:393:ARG:HD2	1.94	0.68
1:A:161:ILE:HG12	1:A:162:GLY:N	2.10	0.67
1:A:255:SER:O	1:A:257:VAL:N	2.26	0.67
1:A:396:ARG:HG2	1:A:396:ARG:NH1	2.09	0.67
1:A:390:VAL:O	1:A:390:VAL:HG22	1.94	0.67
1:A:19:ASN:N	1:A:22:LYS:HB3	2.08	0.67
1:A:143:TYR:O	1:A:145:ALA:N	2.27	0.67
1:A:48:VAL:HG22	1:A:64:ASP:OD1	1.93	0.67
1:A:393:ARG:HH21	1:A:394:ALA:HA	1.60	0.67
1:A:257:VAL:HG23	1:A:258:PRO:HA	1.77	0.66
1:A:396:ARG:H	1:A:397:PRO:CD	2.07	0.66
1:A:12:ILE:HB	1:A:62:LEU:HD23	1.78	0.66
1:A:101:THR:H	1:A:104:GLU:HG2	1.59	0.66
1:A:395:ILE:O	1:A:396:ARG:HD3	1.95	0.66
1:A:18:ARG:HD2	1:A:97:ASP:CB	2.23	0.66
1:A:165:ILE:O	1:A:168:ILE:HB	1.96	0.66
1:A:268:ILE:HG13	1:A:269:VAL:N	2.09	0.66
1:A:28:ALA:O	1:A:29:LEU:C	2.33	0.66
1:A:151:SER:C	1:A:153:LEU:H	1.99	0.65
1:A:120:VAL:HG13	1:A:145:ALA:HB1	1.79	0.65
1:A:187:LEU:CD2	1:A:241:LYS:HG2	2.13	0.65
1:A:284:VAL:O	1:A:287:ILE:HG13	1.96	0.65
1:A:193:PRO:HD2	1:A:224:VAL:O	1.96	0.65
1:A:222:LEU:HD23	1:A:222:LEU:C	2.16	0.65
1:A:205:MET:HB3	1:A:209:HIS:NE2	2.12	0.65
1:A:341:LEU:HD13	1:A:373:LEU:HD13	1.79	0.64
1:A:117:PRO:HB2	1:A:168:ILE:CG2	2.27	0.64
1:A:18:ARG:NH1	1:A:20:VAL:H	1.96	0.63
1:A:107:VAL:CG2	1:A:108:VAL:N	2.59	0.63
1:A:245:THR:HG22	1:A:246:ASP:N	2.06	0.63
1:A:29:LEU:HD22	1:A:29:LEU:N	2.14	0.63
1:A:55:HIS:HA	1:A:57:ILE:H	1.63	0.63
1:A:309:GLU:HB2	1:A:315:LYS:HZ3	1.62	0.63
1:A:259:GLU:O	1:A:262:GLU:HB3	1.99	0.62
1:A:31:GLY:H	1:A:52:MET:CE	2.12	0.62
1:A:169:LEU:HB3	1:A:170:PRO:CD	2.29	0.62
1:A:22:LYS:O	1:A:25:PHE:HB3	1.99	0.62
1:A:23:SER:O	1:A:26:MET:HB2	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:LEU:HD12	1:A:157:GLY:CA	2.30	0.62
1:A:393:ARG:O	1:A:395:ILE:HG12	1.98	0.62
1:A:95:VAL:HA	1:A:121:VAL:CG2	2.30	0.62
1:A:394:ALA:O	1:A:396:ARG:N	2.32	0.61
1:A:161:ILE:CG1	1:A:162:GLY:N	2.63	0.61
1:A:175:ILE:HD12	1:A:176:PRO:HD2	1.82	0.61
1:A:107:VAL:CG2	1:A:108:VAL:H	2.13	0.61
1:A:110:LEU:O	1:A:111:PHE:C	2.39	0.61
1:A:183:ASP:HB3	1:A:217:ARG:O	2.00	0.61
1:A:173:GLU:HB3	1:A:360:ARG:HE	1.66	0.61
1:A:222:LEU:HD23	1:A:223:VAL:N	2.16	0.60
1:A:349:LEU:HD12	1:A:376:PRO:O	2.01	0.60
1:A:173:GLU:HB2	1:A:360:ARG:HE	1.65	0.60
1:A:392:GLU:HG3	1:A:392:GLU:O	2.02	0.60
1:A:263:LEU:HD22	1:A:395:ILE:HD13	1.84	0.60
1:A:386:TYR:C	1:A:388:HIS:H	2.04	0.60
1:A:14:VAL:HG22	1:A:63:VAL:O	2.02	0.60
1:A:161:ILE:CG1	1:A:162:GLY:H	2.13	0.60
1:A:163:LYS:O	1:A:166:SER:HB3	2.02	0.60
1:A:195:ASP:CG	1:A:196:LEU:N	2.55	0.60
1:A:47:PRO:HB3	1:A:66:PRO:CB	2.31	0.60
1:A:247:SER:O	1:A:266:PHE:HZ	1.85	0.60
1:A:305:ARG:HB3	1:A:305:ARG:NH1	2.16	0.60
1:A:176:PRO:C	1:A:178:LEU:H	2.05	0.59
1:A:231:TYR:HD1	1:A:232:VAL:N	1.99	0.59
1:A:47:PRO:HG2	1:A:49:TYR:HE1	1.66	0.59
1:A:252:LYS:O	1:A:255:SER:HB2	2.01	0.59
1:A:30:VAL:HG23	1:A:52:MET:SD	2.43	0.59
1:A:164:THR:O	1:A:167:GLU:HB3	2.03	0.59
1:A:47:PRO:HD3	1:A:66:PRO:HB3	1.83	0.59
1:A:150:VAL:HG22	1:A:151:SER:N	2.17	0.59
1:A:292:ASP:HB3	1:A:327:GLN:HB2	1.85	0.59
1:A:176:PRO:C	1:A:178:LEU:N	2.56	0.58
1:A:253:VAL:O	1:A:257:VAL:HA	2.02	0.58
1:A:391:LEU:N	1:A:391:LEU:HD22	2.17	0.58
1:A:266:PHE:CB	1:A:268:ILE:HG12	2.33	0.58
1:A:386:TYR:HA	1:A:390:VAL:CG1	2.33	0.58
1:A:122:VAL:HG23	1:A:123:ASN:N	2.18	0.58
1:A:250:ALA:HB2	1:A:266:PHE:HE2	1.66	0.58
1:A:268:ILE:CG1	1:A:269:VAL:N	2.66	0.58
1:A:55:HIS:HB2	1:A:56:PRO:HA	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:PHE:HA	1:A:116:ILE:CG2	2.33	0.58
1:A:29:LEU:HD12	1:A:157:GLY:HA3	1.84	0.58
1:A:124:LYS:NZ	1:A:126:ASP:OD1	2.35	0.58
1:A:266:PHE:HD1	1:A:268:ILE:CD1	2.17	0.57
1:A:181:LEU:HD13	1:A:181:LEU:N	2.18	0.57
1:A:345:GLU:O	1:A:346:ASN:HB2	2.05	0.57
1:A:95:VAL:HA	1:A:121:VAL:HG23	1.85	0.57
1:A:316:ILE:HB	1:A:317:PRO:HD3	1.86	0.57
1:A:80:GLU:OE1	1:A:80:GLU:HA	2.05	0.57
1:A:181:LEU:CG	1:A:217:ARG:HD2	2.24	0.57
1:A:94:LEU:O	1:A:121:VAL:HG22	2.05	0.57
1:A:292:ASP:HB3	1:A:327:GLN:CB	2.35	0.56
1:A:305:ARG:HB3	1:A:305:ARG:HH11	1.69	0.56
1:A:47:PRO:CG	1:A:66:PRO:HB3	2.35	0.56
1:A:188:VAL:HA	1:A:220:ILE:HG23	1.87	0.56
1:A:60:VAL:CG2	1:A:61:THR:H	2.19	0.56
1:A:184:GLY:C	1:A:186:ASP:H	2.07	0.56
1:A:255:SER:C	1:A:257:VAL:H	2.08	0.56
1:A:318:ARG:HG2	1:A:319:TRP:N	2.19	0.56
1:A:393:ARG:HD3	1:A:393:ARG:N	2.19	0.56
1:A:26:MET:O	1:A:28:ALA:N	2.38	0.56
1:A:47:PRO:CD	1:A:66:PRO:HB3	2.35	0.56
1:A:91:CYS:CB	1:A:117:PRO:HG2	2.35	0.56
1:A:18:ARG:NH1	1:A:19:ASN:N	2.54	0.56
1:A:25:PHE:HA	1:A:29:LEU:HD23	1.88	0.56
1:A:79:VAL:O	1:A:82:ALA:N	2.39	0.56
1:A:295:THR:HA	1:A:329:ASN:O	2.06	0.55
1:A:91:CYS:HB3	1:A:117:PRO:HG2	1.88	0.55
1:A:176:PRO:HB3	1:A:217:ARG:NH2	2.22	0.55
1:A:255:SER:C	1:A:257:VAL:N	2.60	0.55
1:A:311:ILE:HD12	1:A:311:ILE:N	2.01	0.55
1:A:18:ARG:HG3	1:A:19:ASN:N	2.20	0.55
1:A:165:ILE:HD13	1:A:165:ILE:O	2.07	0.55
1:A:28:ALA:O	1:A:30:VAL:N	2.40	0.55
1:A:229:LEU:HD23	1:A:230:ARG:N	2.17	0.55
1:A:263:LEU:HD22	1:A:395:ILE:CD1	2.37	0.55
1:A:53:GLU:C	1:A:54:LEU:HD12	2.28	0.55
1:A:13:VAL:HG23	1:A:13:VAL:O	2.06	0.55
1:A:110:LEU:O	1:A:113:GLU:N	2.40	0.55
1:A:117:PRO:HB2	1:A:168:ILE:HG22	1.89	0.54
1:A:143:TYR:C	1:A:145:ALA:N	2.58	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:VAL:HG11	1:A:260:ASP:OD2	2.07	0.54
1:A:77:LEU:O	1:A:78:ARG:CB	2.55	0.54
1:A:232:VAL:CG1	1:A:233:MET:H	2.18	0.54
1:A:390:VAL:O	1:A:393:ARG:CD	2.55	0.54
1:A:46:ASP:H	1:A:47:PRO:CD	2.17	0.54
1:A:154:GLN:O	1:A:156:LYS:N	2.40	0.54
1:A:142:ARG:C	1:A:144:GLU:N	2.55	0.54
1:A:18:ARG:O	1:A:19:ASN:HB2	2.07	0.54
1:A:48:VAL:HG23	1:A:48:VAL:O	2.08	0.54
1:A:60:VAL:CG2	1:A:61:THR:N	2.70	0.54
1:A:18:ARG:CZ	1:A:18:ARG:CA	2.83	0.53
1:A:116:ILE:HD13	1:A:116:ILE:C	2.29	0.53
1:A:393:ARG:C	1:A:393:ARG:NE	2.62	0.53
1:A:110:LEU:O	1:A:114:MET:N	2.30	0.53
1:A:82:ALA:O	1:A:83:ARG:C	2.47	0.53
1:A:235:ASN:O	1:A:236:ILE:C	2.46	0.53
1:A:279:TYR:HD1	1:A:367:VAL:HG13	1.72	0.53
1:A:57:ILE:HG23	1:A:58:GLY:N	2.24	0.53
1:A:281:VAL:O	1:A:284:VAL:HG12	2.09	0.53
1:A:247:SER:O	1:A:266:PHE:CZ	2.62	0.53
1:A:353:CYS:HA	1:A:380:TYR:CD1	2.43	0.53
1:A:22:LYS:HD3	1:A:95:VAL:HG11	0.68	0.53
1:A:242:LEU:HD12	1:A:243:VAL:H	1.72	0.53
1:A:309:GLU:CB	1:A:315:LYS:HZ3	2.22	0.53
1:A:63:VAL:HG22	1:A:64:ASP:N	2.25	0.52
1:A:119:VAL:HG12	1:A:120:VAL:N	2.24	0.52
1:A:18:ARG:HD2	1:A:97:ASP:OD2	2.10	0.52
1:A:77:LEU:O	1:A:78:ARG:HB2	2.08	0.52
1:A:181:LEU:CD2	1:A:182:ILE:N	2.64	0.52
1:A:164:THR:O	1:A:167:GLU:N	2.43	0.52
1:A:82:ALA:O	1:A:85:VAL:N	2.23	0.52
1:A:130:GLU:O	1:A:131:LYS:HB2	2.10	0.52
1:A:120:VAL:HG13	1:A:145:ALA:CB	2.40	0.52
1:A:188:VAL:HG12	1:A:240:PRO:CA	2.31	0.52
1:A:229:LEU:CD2	1:A:230:ARG:H	2.16	0.51
1:A:380:TYR:HD1	1:A:380:TYR:N	2.08	0.51
1:A:380:TYR:CD1	1:A:380:TYR:N	2.76	0.51
1:A:182:ILE:CG2	1:A:187:LEU:HD13	2.39	0.51
1:A:183:ASP:O	1:A:186:ASP:O	2.28	0.51
1:A:270:GLU:O	1:A:270:GLU:OE1	2.29	0.51
1:A:116:ILE:HD13	1:A:117:PRO:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:GLY:HA2	1:A:165:ILE:CG2	2.40	0.51
1:A:91:CYS:HA	1:A:117:PRO:O	2.10	0.51
1:A:231:TYR:CD1	1:A:232:VAL:N	2.78	0.51
1:A:242:LEU:HD12	1:A:242:LEU:C	2.30	0.51
1:A:131:LYS:HG2	1:A:134:GLU:OE2	2.11	0.51
1:A:157:GLY:O	1:A:161:ILE:HG23	2.10	0.51
1:A:316:ILE:O	1:A:320:LEU:HB2	2.11	0.51
1:A:143:TYR:C	1:A:145:ALA:H	2.14	0.51
1:A:395:ILE:C	1:A:396:ARG:HD3	2.30	0.51
1:A:47:PRO:HD3	1:A:66:PRO:CB	2.41	0.51
1:A:46:ASP:N	1:A:47:PRO:HD2	2.16	0.50
1:A:92:GLY:O	1:A:118:PHE:HA	2.11	0.50
1:A:101:THR:N	1:A:104:GLU:HG3	2.25	0.50
1:A:292:ASP:HB3	1:A:327:GLN:HG3	1.92	0.50
1:A:393:ARG:NH2	1:A:394:ALA:HA	2.24	0.50
1:A:79:VAL:CG2	1:A:80:GLU:H	2.11	0.50
1:A:65:THR:HB	1:A:68:LEU:HB2	1.93	0.50
1:A:182:ILE:HG22	1:A:187:LEU:HD13	1.93	0.50
1:A:391:LEU:HD22	1:A:391:LEU:H	1.77	0.49
1:A:279:TYR:CE1	1:A:371:LYS:HG3	2.46	0.49
1:A:18:ARG:HH12	1:A:20:VAL:H	1.60	0.49
1:A:183:ASP:OD2	1:A:183:ASP:N	2.33	0.49
1:A:386:TYR:O	1:A:388:HIS:N	2.46	0.49
1:A:117:PRO:HA	1:A:143:TYR:HE1	1.77	0.49
1:A:256:ASP:O	1:A:257:VAL:C	2.51	0.49
1:A:108:VAL:O	1:A:112:LYS:HB2	2.12	0.49
1:A:161:ILE:HG12	1:A:162:GLY:H	1.74	0.49
1:A:229:LEU:HD11	1:A:230:ARG:NH2	2.28	0.49
1:A:132:ALA:O	1:A:134:GLU:N	2.46	0.49
1:A:236:ILE:HG23	1:A:236:ILE:O	2.13	0.49
1:A:116:ILE:HB	1:A:372:ARG:NH2	2.28	0.48
1:A:157:GLY:C	1:A:159:ASP:H	2.16	0.48
1:A:26:MET:O	1:A:27:ASN:C	2.51	0.48
1:A:83:ARG:HG3	1:A:83:ARG:HH21	1.79	0.48
1:A:162:GLY:O	1:A:165:ILE:HG23	2.13	0.48
1:A:305:ARG:NH1	1:A:305:ARG:CB	2.75	0.48
1:A:338:PHE:CG	1:A:339:PRO:HD2	2.48	0.48
1:A:14:VAL:HA	1:A:93:ILE:O	2.14	0.48
1:A:320:LEU:HD12	1:A:320:LEU:HA	1.55	0.48
1:A:25:PHE:O	1:A:26:MET:O	2.31	0.48
1:A:379:ASN:HD21	1:A:382:VAL:H	1.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:ASN:O	1:A:23:SER:N	2.35	0.48
1:A:205:MET:HB3	1:A:209:HIS:CD2	2.48	0.48
1:A:309:GLU:HB2	1:A:315:LYS:NZ	2.29	0.48
1:A:387:LEU:O	1:A:388:HIS:HD2	1.96	0.48
1:A:177:TYR:HD2	1:A:274:ARG:HD2	1.77	0.47
1:A:151:SER:C	1:A:153:LEU:N	2.67	0.47
1:A:280:PHE:HB3	1:A:382:VAL:HG21	1.96	0.47
1:A:252:LYS:HE2	1:A:252:LYS:HA	1.96	0.47
1:A:309:GLU:CB	1:A:315:LYS:NZ	2.77	0.47
1:A:19:ASN:CA	1:A:22:LYS:HB3	2.44	0.47
1:A:281:VAL:HA	1:A:284:VAL:HG12	1.97	0.47
1:A:393:ARG:O	1:A:394:ALA:C	2.52	0.47
1:A:125:ILE:HG13	1:A:125:ILE:O	2.13	0.47
1:A:245:THR:O	1:A:267:SER:N	2.47	0.47
1:A:128:LEU:HD13	1:A:130:GLU:CG	2.45	0.47
1:A:182:ILE:HD12	1:A:241:LYS:HG2	1.97	0.47
1:A:241:LYS:O	1:A:241:LYS:HG3	2.14	0.47
1:A:256:ASP:OD1	1:A:258:PRO:HB3	2.14	0.47
1:A:287:ILE:O	1:A:290:LEU:HB2	2.13	0.47
1:A:14:VAL:HG23	1:A:14:VAL:O	2.14	0.47
1:A:247:SER:OG	1:A:248:GLN:N	2.48	0.46
1:A:207:GLN:O	1:A:211:ILE:HG13	2.16	0.46
1:A:77:LEU:C	1:A:77:LEU:HD23	2.36	0.46
1:A:393:ARG:NH1	1:A:393:ARG:HG2	2.30	0.46
1:A:93:ILE:CD1	1:A:119:VAL:HB	2.45	0.46
1:A:152:ALA:O	1:A:153:LEU:C	2.54	0.46
1:A:181:LEU:H	1:A:181:LEU:CD1	2.26	0.46
1:A:348:LYS:O	1:A:376:PRO:CG	2.64	0.46
1:A:12:ILE:HB	1:A:62:LEU:CD2	2.44	0.46
1:A:104:GLU:O	1:A:108:VAL:HG23	2.16	0.46
1:A:162:GLY:CA	1:A:165:ILE:CG2	2.94	0.46
1:A:257:VAL:HG23	1:A:258:PRO:CA	2.45	0.46
1:A:386:TYR:C	1:A:388:HIS:N	2.69	0.46
1:A:22:LYS:HA	1:A:95:VAL:HG21	1.97	0.46
1:A:165:ILE:C	1:A:165:ILE:CD1	2.76	0.46
1:A:67:GLY:C	1:A:69:ASP:H	2.19	0.45
1:A:325:GLY:O	1:A:326:ALA:O	2.33	0.45
1:A:142:ARG:C	1:A:144:GLU:H	2.19	0.45
1:A:352:HIS:O	1:A:379:ASN:CB	2.61	0.45
1:A:122:VAL:CG2	1:A:149:LEU:H	2.30	0.45
1:A:149:LEU:CD2	1:A:150:VAL:H	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:TYR:CD1	1:A:231:TYR:C	2.90	0.45
1:A:181:LEU:HD22	1:A:182:ILE:N	2.11	0.45
1:A:230:ARG:NH2	1:A:256:ASP:HB2	2.32	0.45
1:A:15:ALA:HA	1:A:65:THR:CG2	2.41	0.45
1:A:128:LEU:HB3	1:A:130:GLU:OE1	2.17	0.45
1:A:293:GLY:N	1:A:327:GLN:O	2.49	0.45
1:A:169:LEU:O	1:A:170:PRO:O	2.35	0.45
1:A:159:ASP:N	1:A:161:ILE:HD12	2.32	0.45
1:A:292:ASP:CB	1:A:327:GLN:HB2	2.47	0.45
1:A:314:VAL:C	1:A:317:PRO:HD2	2.37	0.45
1:A:57:ILE:CG2	1:A:58:GLY:N	2.80	0.44
1:A:136:LYS:H	1:A:136:LYS:HG2	1.57	0.44
1:A:276:ASP:HB2	1:A:364:MET:CE	2.48	0.44
1:A:99:ALA:HB1	1:A:100:PRO:CD	2.37	0.44
1:A:114:MET:O	1:A:115:GLU:C	2.55	0.44
1:A:18:ARG:NH1	1:A:19:ASN:H	2.14	0.44
1:A:195:ASP:OD1	1:A:196:LEU:N	2.46	0.44
1:A:205:MET:O	1:A:206:PRO:C	2.56	0.44
1:A:229:LEU:CG	1:A:230:ARG:N	2.81	0.44
1:A:79:VAL:O	1:A:80:GLU:C	2.54	0.44
1:A:233:MET:HG3	1:A:258:PRO:HG3	1.99	0.44
1:A:204:ILE:HG12	1:A:207:GLN:NE2	2.32	0.44
1:A:101:THR:N	1:A:104:GLU:CG	2.74	0.43
1:A:135:LEU:C	1:A:137:GLY:H	2.22	0.43
1:A:220:ILE:HD13	1:A:220:ILE:O	2.18	0.43
1:A:270:GLU:OE2	1:A:273:TYR:CD2	2.72	0.43
1:A:10:ARG:O	1:A:60:VAL:HG23	2.18	0.43
1:A:10:ARG:HB2	1:A:60:VAL:HG23	2.01	0.43
1:A:286:LYS:HB2	1:A:286:LYS:HE3	1.66	0.43
1:A:22:LYS:HZ1	1:A:64:ASP:HB2	1.83	0.43
1:A:292:ASP:HB3	1:A:327:GLN:CG	2.48	0.43
1:A:398:PHE:HD1	1:A:398:PHE:O	2.01	0.43
1:A:81:LYS:NZ	1:A:81:LYS:HB2	2.34	0.43
1:A:112:LYS:HE3	1:A:141:SER:OG	2.18	0.43
1:A:142:ARG:O	1:A:144:GLU:N	2.51	0.43
1:A:222:LEU:C	1:A:222:LEU:CD2	2.85	0.43
1:A:162:GLY:HA2	1:A:165:ILE:HG21	2.00	0.43
1:A:247:SER:C	1:A:249:VAL:H	2.22	0.43
1:A:277:LEU:O	1:A:278:ALA:C	2.57	0.43
1:A:298:ILE:HG21	1:A:312:GLY:O	2.19	0.43
1:A:368:ARG:O	1:A:369:MET:C	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:ARG:N	1:A:393:ARG:CD	2.81	0.43
1:A:53:GLU:N	1:A:53:GLU:CD	2.72	0.43
1:A:95:VAL:HA	1:A:121:VAL:HG22	2.01	0.43
1:A:161:ILE:HD13	1:A:161:ILE:N	2.34	0.43
1:A:305:ARG:CB	1:A:305:ARG:CZ	2.96	0.43
1:A:305:ARG:CZ	1:A:305:ARG:HB2	2.48	0.43
1:A:390:VAL:N	1:A:391:LEU:HD22	2.34	0.43
1:A:255:SER:O	1:A:257:VAL:HG22	2.19	0.43
1:A:390:VAL:O	1:A:390:VAL:CG2	2.64	0.43
1:A:105:ASP:O	1:A:109:ASN:OD1	2.37	0.42
1:A:176:PRO:O	1:A:178:LEU:N	2.52	0.42
1:A:114:MET:HE2	1:A:372:ARG:HB3	2.00	0.42
1:A:139:TYR:HD1	1:A:140:GLU:N	2.17	0.42
1:A:149:LEU:O	1:A:150:VAL:HB	2.19	0.42
1:A:265:THR:OG1	1:A:266:PHE:N	2.53	0.42
1:A:18:ARG:NE	1:A:18:ARG:CA	2.62	0.42
1:A:135:LEU:O	1:A:137:GLY:N	2.52	0.42
1:A:371:LYS:O	1:A:374:GLY:N	2.42	0.42
1:A:161:ILE:HD13	1:A:162:GLY:N	2.30	0.42
1:A:380:TYR:O	1:A:384:ILE:HG13	2.20	0.42
1:A:150:VAL:CG2	1:A:151:SER:N	2.83	0.42
1:A:160:ASP:CA	1:A:163:LYS:HD3	2.42	0.42
1:A:226:GLU:OE1	1:A:229:LEU:HD22	2.20	0.42
1:A:242:LEU:HD12	1:A:243:VAL:O	2.20	0.42
1:A:19:ASN:HA	1:A:22:LYS:HB3	2.02	0.42
1:A:396:ARG:NH1	1:A:396:ARG:CG	2.78	0.42
1:A:177:TYR:CD2	1:A:274:ARG:CD	3.01	0.41
1:A:229:LEU:HD11	1:A:230:ARG:HH21	1.83	0.41
1:A:26:MET:CE	1:A:48:VAL:HG23	2.49	0.41
1:A:138:LEU:O	1:A:139:TYR:O	2.37	0.41
1:A:204:ILE:HG13	1:A:206:PRO:HD2	2.01	0.41
1:A:29:LEU:N	1:A:29:LEU:CD2	2.82	0.41
1:A:65:THR:HB	1:A:68:LEU:CB	2.49	0.41
1:A:116:ILE:CD1	1:A:117:PRO:O	2.68	0.41
1:A:161:ILE:CD1	1:A:161:ILE:H	2.34	0.41
1:A:158:PHE:O	1:A:158:PHE:CG	2.74	0.41
1:A:185:GLY:O	1:A:186:ASP:HB2	2.20	0.41
1:A:220:ILE:C	1:A:220:ILE:CD1	2.83	0.41
1:A:230:ARG:HH21	1:A:256:ASP:HB2	1.85	0.41
1:A:245:THR:CG2	1:A:246:ASP:N	2.75	0.41
1:A:349:LEU:HG	1:A:350:ILE:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:ASP:C	1:A:276:ASP:OD1	2.59	0.41
1:A:328:LEU:HD12	1:A:328:LEU:HA	1.91	0.41
1:A:187:LEU:HG	1:A:241:LYS:CB	2.50	0.41
1:A:199:PRO:HG2	1:A:202:ARG:HG3	2.02	0.41
1:A:197:GLY:O	1:A:198:ALA:O	2.39	0.41
1:A:63:VAL:CG2	1:A:64:ASP:N	2.84	0.41
1:A:135:LEU:C	1:A:137:GLY:N	2.73	0.41
1:A:141:SER:HB3	1:A:142:ARG:H	1.67	0.41
1:A:252:LYS:HE2	1:A:252:LYS:CA	2.50	0.41
1:A:252:LYS:HA	1:A:252:LYS:CE	2.51	0.41
1:A:393:ARG:HG2	1:A:393:ARG:HH11	1.86	0.41
1:A:14:VAL:HG12	1:A:93:ILE:HB	2.03	0.41
1:A:143:TYR:HD2	1:A:143:TYR:HA	1.70	0.41
1:A:174:GLU:O	1:A:174:GLU:HG2	2.21	0.41
1:A:243:VAL:C	1:A:244:ILE:HG13	2.41	0.41
1:A:257:VAL:N	1:A:258:PRO:HA	2.36	0.41
1:A:287:ILE:HD12	1:A:386:TYR:CE2	2.56	0.41
1:A:31:GLY:HA2	1:A:158:PHE:CD2	2.53	0.40
1:A:272:ARG:NH2	1:A:354:GLY:HA3	2.36	0.40
1:A:93:ILE:HD13	1:A:93:ILE:HA	1.72	0.40
1:A:100:PRO:HB2	1:A:139:TYR:CZ	2.56	0.40
1:A:186:ASP:O	1:A:187:LEU:CB	2.51	0.40
1:A:266:PHE:CD1	1:A:268:ILE:CD1	3.01	0.40
1:A:292:ASP:CA	1:A:327:GLN:HB2	2.51	0.40
1:A:96:THR:HG21	1:A:136:LYS:NZ	2.35	0.40
1:A:299:MET:SD	1:A:339:PRO:HD3	2.62	0.40
1:A:62:LEU:HD23	1:A:62:LEU:HA	1.88	0.40
1:A:77:LEU:HD21	1:A:82:ALA:CB	2.44	0.40
1:A:98:SER:HB3	1:A:99:ALA:H	1.74	0.40
1:A:226:GLU:O	1:A:229:LEU:HD22	2.21	0.40
1:A:229:LEU:HG	1:A:230:ARG:N	2.36	0.40
1:A:231:TYR:O	1:A:232:VAL:C	2.59	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	378/423 (89%)	235 (62%)	81 (21%)	62 (16%)	0 0

All (62) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	26	MET
1	A	27	ASN
1	A	28	ALA
1	A	66	PRO
1	A	78	ARG
1	A	79	VAL
1	A	131	LYS
1	A	139	TYR
1	A	144	GLU
1	A	153	LEU
1	A	155	LYS
1	A	163	LYS
1	A	170	PRO
1	A	187	LEU
1	A	194	ILE
1	A	231	TYR
1	A	236	ILE
1	A	255	SER
1	A	309	GLU
1	A	326	ALA
1	A	387	LEU
1	A	395	ILE
1	A	0	THR
1	A	19	ASN
1	A	29	LEU
1	A	46	ASP
1	A	89	ALA
1	A	122	VAL
1	A	123	ASN
1	A	133	GLU
1	A	141	SER
1	A	169	LEU
1	A	186	ASP
1	A	218	GLU

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Mol	Chain	Res	Type
1	A	232	VAL
1	A	235	ASN
1	A	275	GLY
1	A	276	ASP
1	A	356	CYS
1	A	394	ALA
1	A	135	LEU
1	A	278	ALA
1	A	286	LYS
1	A	56	PRO
1	A	57	ILE
1	A	77	LEU
1	A	136	LYS
1	A	174	GLU
1	A	183	ASP
1	A	226	GLU
1	A	227	ARG
1	A	83	ARG
1	A	150	VAL
1	A	181	LEU
1	A	240	PRO
1	A	397	PRO
1	A	182	ILE
1	A	389	GLY
1	A	396	ARG
1	A	198	ALA
1	A	381	GLY
1	A	257	VAL

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	326/365 (89%)	273 (84%)	53 (16%)	2 9

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	PHE
1	A	17	ARG
1	A	18	ARG
1	A	22	LYS
1	A	46	ASP
1	A	53	GLU
1	A	80	GLU
1	A	81	LYS
1	A	104	GLU
1	A	113	GLU
1	A	116	ILE
1	A	133	GLU
1	A	135	LEU
1	A	140	GLU
1	A	142	ARG
1	A	143	TYR
1	A	149	LEU
1	A	161	ILE
1	A	163	LYS
1	A	164	THR
1	A	165	ILE
1	A	172	ASP
1	A	181	LEU
1	A	183	ASP
1	A	186	ASP
1	A	188	VAL
1	A	220	ILE
1	A	226	GLU
1	A	228	GLU
1	A	230	ARG
1	A	231	TYR
1	A	241	LYS
1	A	242	LEU
1	A	252	LYS
1	A	257	VAL
1	A	264	THR
1	A	266	PHE
1	A	270	GLU
1	A	271	SER
1	A	279	TYR
1	A	290	LEU
1	A	295	THR
1	A	307	LEU

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Mol	Chain	Res	Type
1	A	311	ILE
1	A	337	ASP
1	A	359	ASN
1	A	379	ASN
1	A	380	TYR
1	A	391	LEU
1	A	392	GLU
1	A	393	ARG
1	A	395	ILE
1	A	398	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	ASN
1	A	154	GLN
1	A	207	GLN
1	A	359	ASN
1	A	379	ASN
1	A	388	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 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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	384/423 (90%)	0.79	49 (12%) 9 5	52, 101, 164, 215	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	140	GLU	8.8
1	A	49	TYR	7.2
1	A	22	LYS	5.5
1	A	139	TYR	5.0
1	A	307	LEU	4.8
1	A	185	GLY	4.7
1	A	56	PRO	4.6
1	A	31	GLY	4.5
1	A	275	GLY	4.5
1	A	50	LYS	4.1
1	A	57	ILE	3.8
1	A	186	ASP	3.7
1	A	143	TYR	3.5
1	A	125	ILE	3.5
1	A	158	PHE	3.3
1	A	127	VAL	3.2
1	A	391	LEU	3.2
1	A	21	GLY	3.1
1	A	251	MET	3.1
1	A	8	PHE	3.0
1	A	135	LEU	3.0
1	A	196	LEU	2.9
1	A	7	GLY	2.9
1	A	98	SER	2.8
1	A	305	ARG	2.7
1	A	148	LEU	2.7
1	A	238	MET	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	11	TYR	2.6
1	A	272	ARG	2.6
1	A	97	ASP	2.5
1	A	270	GLU	2.5
1	A	3	LEU	2.4
1	A	88	ARG	2.4
1	A	184	GLY	2.4
1	A	289	GLU	2.4
1	A	198	ALA	2.4
1	A	178	LEU	2.3
1	A	-1	TYR	2.3
1	A	55	HIS	2.3
1	A	133	GLU	2.2
1	A	30	VAL	2.1
1	A	276	ASP	2.1
1	A	266	PHE	2.1
1	A	331	LYS	2.1
1	A	153	LEU	2.1
1	A	229	LEU	2.0
1	A	258	PRO	2.0
1	A	1	MET	2.0
1	A	16	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.