



Full wwPDB X-ray Structure Validation Report ⓘ

May 27, 2020 – 11:20 pm BST

PDB ID : 3MH5
Title : HtrA proteases are activated by a conserved mechanism that can be triggered by distinct molecular cues
Authors : Krojer, T.; Sawa, J.; Huber, R.; Clausen, T.
Deposited on : 2010-04-07
Resolution : 3.00 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

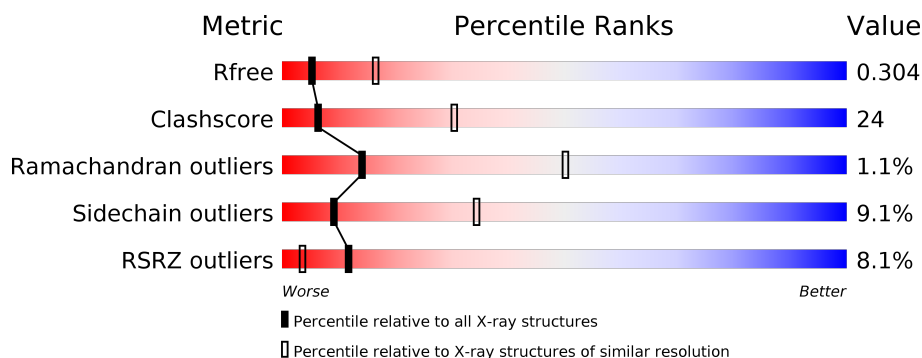
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (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 on 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	456	<div> <div>4%</div> <div>22% 17% • 58%</div> </div>
1	B	456	<div> <div>4%</div> <div>27% 15% • 56%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2922 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.

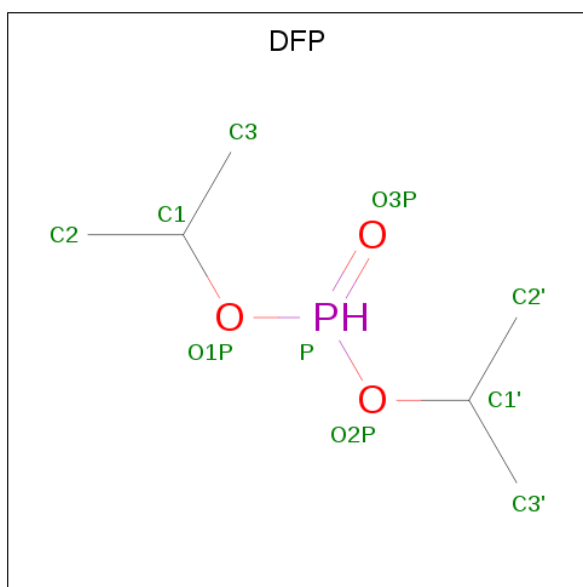
- Molecule 1 is a protein called Protease do.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	191	Total	C	N	O	S	0	0	0
			1409	883	241	277	8			
1	B	202	Total	C	N	O	S	0	0	0
			1484	926	259	290	9			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	449	ARG	-	EXPRESSION TAG	UNP P0C0V0
A	450	SER	-	EXPRESSION TAG	UNP P0C0V0
A	451	HIS	-	EXPRESSION TAG	UNP P0C0V0
A	452	HIS	-	EXPRESSION TAG	UNP P0C0V0
A	453	HIS	-	EXPRESSION TAG	UNP P0C0V0
A	454	HIS	-	EXPRESSION TAG	UNP P0C0V0
A	455	HIS	-	EXPRESSION TAG	UNP P0C0V0
A	456	HIS	-	EXPRESSION TAG	UNP P0C0V0
B	449	ARG	-	EXPRESSION TAG	UNP P0C0V0
B	450	SER	-	EXPRESSION TAG	UNP P0C0V0
B	451	HIS	-	EXPRESSION TAG	UNP P0C0V0
B	452	HIS	-	EXPRESSION TAG	UNP P0C0V0
B	453	HIS	-	EXPRESSION TAG	UNP P0C0V0
B	454	HIS	-	EXPRESSION TAG	UNP P0C0V0
B	455	HIS	-	EXPRESSION TAG	UNP P0C0V0
B	456	HIS	-	EXPRESSION TAG	UNP P0C0V0

- Molecule 2 is DIISOPROPYL PHOSPHONATE (three-letter code: DFP) (formula: C₆H₁₅O₃P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			10	6	3	1		
2	B	1	Total	C	O	P	0	0
			10	6	3	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	O	0	0
			2	2		
3	B	7	Total	O	0	0
			7	7		

These plots are drawn for all protein, RNA and DNA 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.

Chain A:

Chain B:

Amino Acid	Frequency Category
ALA	Grey
GLU	Grey
THR	Grey
SER	Grey
SER	Grey
ALA	Grey
THR	Grey
THR	Grey
ALA	Grey
GLN	Grey
Q11	Green
M12	Yellow
A16	Yellow
P17	Yellow
M18	Yellow
L19	Yellow
E20	Yellow
M23	Yellow
ARG	Grey
V31	Yellow
V37	Green
M38	Yellow
T39	Green
P40	Yellow
R41	Green
M42	Green
P40	Grey
ARG	Grey
ASN	Grey
PHE	Grey
GLN	Grey
PHE	Grey
PHE	Grey
ASP	Grey
ASP	Grey
SER	Grey
P40	Grey
PHE	Grey
CYS	Grey
GLU	Grey
GLY	Grey
SER	Grey
P40	Grey
PHE	Grey
GLN	Grey
GLN	Grey
SER	Grey
SER	Grey
P40	Grey
PHE	Grey
CYS	Grey
GLY	Grey
GLY	Grey
GLN	Grey

Amino Acid	Frequency Category
GLY	Green
ASN	Grey
GLY	Green
GLY	Green
G79	Green
Q80	Yellow
Q81	Yellow
Q82	Green
M85	Yellow
A86	Yellow
L87	Yellow
G88	Yellow
S89	Yellow
G90	Yellow
V91	Yellow
I92	Yellow
I93	Yellow
D94	Yellow
GLY	Yellow
V100	Yellow
V101	Green
I102	Yellow
M103	Yellow
M104	Yellow
H105	Yellow
V106	Yellow
G120	Yellow
F123	Yellow
K126	Yellow
M127	Yellow
V128	Yellow
G129	Yellow
K130	Yellow
R133	Yellow
S134	Yellow
D135	Yellow
L138	Yellow
I139	Yellow
O140	Yellow
I141	Yellow
Q142	Yellow
M143	Yellow
P144	Yellow
K145	Yellow
M146	Yellow
L147	Yellow
I150	Yellow
K151	Yellow
M152	Yellow
K153	Yellow
D154	Yellow

[illegible]

4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α , β , γ	121.45Å 121.45Å 226.65Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.00 24.94 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.1 (20.00-3.00) 99.2 (24.94-3.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.46 (at 2.99Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.281 , 0.309 0.276 , 0.304	Depositor DCC
R_{free} test set	942 reflections (4.60%)	wwPDB-VP
Wilson B-factor (Å ²)	85.1	Xtriage
Anisotropy	0.718	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 99.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	2922	wwPDB-VP
Average B, all atoms (Å ²)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% 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

5.1 Standard geometry

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

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	0.37	0/1422	0.65	0/1920
1	B	0.38	0/1497	0.63	0/2021
All	All	0.38	0/2919	0.64	0/3941

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	1409	0	1436	79	0
1	B	1484	0	1515	65	0
2	A	10	0	14	1	0
2	B	10	0	14	1	0
3	A	2	0	0	0	0
3	B	7	0	0	0	0
All	All	2922	0	2979	142	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 24.

All (142) 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:104:ASN:HD21	1:B:130:LYS:HE3	1.23	1.04
1:A:104:ASN:HD21	1:A:130:LYS:HE3	1.27	0.99
1:B:253:GLN:HG2	1:B:260:VAL:HA	1.52	0.91
1:B:171:PHE:HB2	1:B:173:LEU:HD12	1.52	0.91
1:A:198:PHE:HB3	1:A:243:PRO:HD3	1.51	0.90
1:A:171:PHE:HB2	1:A:173:LEU:HD12	1.55	0.88
1:A:94:ASP:HB3	1:A:99:TYR:HB2	1.57	0.85
1:B:94:ASP:HB3	1:B:99:TYR:HB2	1.58	0.83
1:B:167:ILE:O	1:B:212:GLY:HA3	1.84	0.76
1:A:198:PHE:HB3	1:A:243:PRO:CD	2.16	0.76
1:B:104:ASN:HD22	1:B:130:LYS:HB2	1.49	0.75
1:A:104:ASN:HD22	1:A:130:LYS:HB2	1.51	0.75
1:B:104:ASN:ND2	1:B:130:LYS:HE3	1.99	0.75
1:A:104:ASN:ND2	1:A:130:LYS:HB2	2.02	0.74
1:B:197:ASN:HD22	1:B:243:PRO:HG3	1.51	0.74
1:B:104:ASN:ND2	1:B:130:LYS:HB2	2.02	0.73
1:A:104:ASN:ND2	1:A:130:LYS:HE3	2.03	0.71
1:B:205:ILE:HD11	2:B:500:DFP:H3'3	1.75	0.69
1:B:145:LYS:HE2	1:B:146:ASN:HD21	1.57	0.68
1:A:134:SER:HB2	1:A:242:ILE:HD12	1.74	0.68
1:A:253:GLN:HG2	1:A:260:VAL:HA	1.74	0.67
1:A:183:SER:OG	1:A:238:ILE:HD11	1.97	0.65
1:B:225:ASN:HD22	1:B:241:ALA:HB2	1.61	0.64
1:B:260:VAL:HG23	1:B:262:ARG:HD2	1.80	0.64
1:A:16:ALA:HB3	1:A:17:PRO:HD3	1.80	0.64
1:A:207:ARG:HB3	1:A:209:ASN:OD1	1.98	0.64
1:A:206:ASN:HB2	1:A:238:ILE:O	1.97	0.63
1:B:87:LEU:HD23	1:B:87:LEU:O	1.97	0.63
1:B:16:ALA:O	1:B:20:GLU:HG3	1.97	0.63
1:A:87:LEU:HD23	1:A:87:LEU:O	1.97	0.63
1:A:183:SER:CB	1:A:238:ILE:HD11	2.31	0.61
1:B:170:PRO:HA	1:B:209:ASN:HB2	1.80	0.61
1:B:16:ALA:HB3	1:B:17:PRO:HD3	1.82	0.61
1:B:253:GLN:OE1	1:B:261:LYS:N	2.33	0.61
1:A:243:PRO:HG2	1:A:246:MET:HB2	1.84	0.60
1:B:198:PHE:CE2	1:B:240:PHE:HB3	2.37	0.59
1:B:206:ASN:HB2	1:B:236:ILE:HG22	1.85	0.59
1:A:145:LYS:HE2	1:A:146:ASN:HD21	1.69	0.57
1:A:103:ASN:HA	1:A:135:ASP:O	2.05	0.56
1:A:207:ARG:HB2	1:A:210:SER:HB2	1.86	0.56
1:A:23:MET:CE	1:A:175:GLU:HG2	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:THR:O	1:A:36:THR:HG22	2.04	0.56
1:B:160:VAL:O	1:B:182:VAL:HB	2.05	0.56
1:A:16:ALA:O	1:A:20:GLU:HG3	2.03	0.56
1:B:173:LEU:H	1:B:173:LEU:CD1	2.17	0.56
1:B:145:LYS:HG2	1:B:146:ASN:ND2	2.21	0.56
1:A:200:GLN:HA	1:A:239:GLY:O	2.06	0.56
1:A:34:SER:O	1:A:109:ASN:HB3	2.05	0.55
1:A:31:VAL:HG21	1:A:106:VAL:O	2.06	0.55
1:B:23:MET:HE3	1:B:175:GLU:HG2	1.87	0.55
1:A:180:GLY:CA	1:A:203:ALA:HB2	2.36	0.55
1:A:173:LEU:CD1	1:A:173:LEU:H	2.19	0.54
1:A:92:ILE:HD13	1:A:147:LEU:HG	1.90	0.54
1:A:169:ASN:HD21	1:A:172:GLY:HA2	1.72	0.54
1:B:91:VAL:CG2	1:B:213:ALA:HB2	2.38	0.54
1:A:169:ASN:HD21	1:A:172:GLY:CA	2.20	0.54
1:A:160:VAL:HG13	1:A:182:VAL:O	2.08	0.53
1:B:257:TYR:CE1	1:B:261:LYS:HE3	2.43	0.53
1:A:160:VAL:O	1:A:182:VAL:O	2.26	0.53
1:B:243:PRO:HG2	1:B:246:MET:HB2	1.89	0.53
1:A:23:MET:HE3	1:A:175:GLU:HG2	1.90	0.53
1:B:103:ASN:HA	1:B:135:ASP:O	2.09	0.52
1:A:141:ILE:HD12	1:A:147:LEU:HD21	1.90	0.52
1:A:180:GLY:HA3	1:A:203:ALA:HB2	1.91	0.52
1:A:160:VAL:O	1:A:182:VAL:HB	2.10	0.51
1:A:150:ILE:HG12	1:A:221:LEU:HB2	1.93	0.51
1:A:198:PHE:CG	1:A:243:PRO:HG3	2.45	0.51
1:B:169:ASN:HD21	1:B:172:GLY:CA	2.23	0.51
1:A:205:ILE:HB	1:A:207:ARG:HD3	1.92	0.51
1:A:214:LEU:HD13	1:A:222:ILE:HD11	1.91	0.51
1:B:169:ASN:HD21	1:B:172:GLY:HA2	1.75	0.50
1:B:225:ASN:ND2	1:B:241:ALA:HB2	2.27	0.49
1:B:145:LYS:HE2	1:B:146:ASN:ND2	2.26	0.49
1:A:199:ILE:O	1:A:240:PHE:HA	2.12	0.49
1:A:33:GLY:HA3	1:A:109:ASN:O	2.13	0.49
1:A:214:LEU:HD23	1:A:225:ASN:OD1	2.13	0.49
1:A:242:ILE:HG22	1:A:246:MET:HB3	1.93	0.49
1:B:184:ALA:HB3	1:B:200:GLN:HB2	1.94	0.49
1:B:173:LEU:HD13	1:B:173:LEU:H	1.78	0.49
1:B:23:MET:CE	1:B:175:GLU:HG2	2.43	0.48
1:A:173:LEU:HD22	1:A:173:LEU:C	2.33	0.48
1:A:134:SER:HB2	1:A:242:ILE:CD1	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:PRO:HB2	1:B:147:LEU:HD22	1.96	0.48
1:B:173:LEU:C	1:B:173:LEU:HD22	2.34	0.47
1:A:207:ARG:HG3	1:A:207:ARG:NH1	2.29	0.47
1:A:173:LEU:HD13	1:A:173:LEU:H	1.80	0.47
1:A:169:ASN:ND2	1:A:172:GLY:H	2.13	0.47
1:A:250:LEU:O	1:A:253:GLN:HB3	2.15	0.47
1:B:37:VAL:HG22	1:B:38:ASN:N	2.31	0.46
1:A:225:ASN:HD22	1:A:241:ALA:HB2	1.81	0.46
1:B:133:ARG:HH11	1:B:133:ARG:HG2	1.80	0.46
1:B:126:LYS:HE3	1:B:142:GLN:NE2	2.31	0.45
1:B:91:VAL:HG21	1:B:213:ALA:HB2	1.99	0.45
1:A:207:ARG:HH11	1:A:207:ARG:HG3	1.82	0.45
1:B:150:ILE:HG12	1:B:221:LEU:HB2	1.97	0.45
1:B:92:ILE:HD13	1:B:147:LEU:HG	1.98	0.45
1:B:257:TYR:HB2	1:B:259:GLN:O	2.17	0.45
1:B:93:ILE:HD11	1:B:152:MET:SD	2.57	0.45
1:A:225:ASN:ND2	1:A:241:ALA:HB2	2.31	0.44
1:A:166:ALA:HB1	2:A:500:DFP:H22	2.00	0.44
1:B:93:ILE:HD12	1:B:93:ILE:HA	1.88	0.44
1:A:211:GLY:O	1:A:225:ASN:HB2	2.18	0.44
1:B:184:ALA:HB3	1:B:200:GLN:CB	2.48	0.44
1:A:136:ILE:HD11	1:A:242:ILE:HG13	1.99	0.44
1:A:133:ARG:HH11	1:A:133:ARG:HG2	1.83	0.44
1:A:196:GLU:O	1:A:197:ASN:HB2	2.18	0.43
1:B:160:VAL:O	1:B:182:VAL:O	2.36	0.43
1:A:144:PRO:HB2	1:A:147:LEU:HD22	1.98	0.43
1:A:240:PHE:CD1	1:A:240:PHE:N	2.86	0.43
1:B:129:GLY:HA3	1:B:254:MET:HB3	2.01	0.43
1:A:119:ASP:C	1:A:119:ASP:OD1	2.57	0.43
1:A:254:MET:O	1:A:258:GLY:N	2.50	0.43
1:B:128:VAL:HG22	1:B:138:LEU:HB3	1.99	0.43
1:B:169:ASN:ND2	1:B:172:GLY:H	2.16	0.43
1:A:126:LYS:HE3	1:A:142:GLN:HE22	1.83	0.43
1:A:145:LYS:HG2	1:A:146:ASN:ND2	2.34	0.43
1:B:126:LYS:HE3	1:B:142:GLN:HE22	1.84	0.42
1:B:154:ASP:HA	1:B:245:ASN:HD21	1.84	0.42
1:B:19:LEU:O	1:B:23:MET:HG2	2.19	0.42
1:A:129:GLY:HA3	1:A:254:MET:HB3	2.01	0.42
1:A:145:LYS:HE2	1:A:146:ASN:ND2	2.32	0.42
1:A:103:ASN:HB2	1:A:106:VAL:HG23	2.01	0.42
1:A:32:GLU:O	1:A:111:THR:HB	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:ILE:HD11	1:A:152:MET:SD	2.59	0.42
1:B:250:LEU:O	1:B:253:GLN:HB3	2.20	0.42
1:A:23:MET:HE1	1:A:175:GLU:CB	2.50	0.42
1:B:253:GLN:HE21	1:B:253:GLN:HB2	1.59	0.42
1:A:19:LEU:HD11	1:A:177:VAL:HG11	2.01	0.41
1:A:198:PHE:HB3	1:A:243:PRO:CG	2.50	0.41
1:B:217:LEU:HD12	1:B:217:LEU:HA	1.94	0.41
1:B:206:ASN:CB	1:B:236:ILE:HG22	2.50	0.41
1:A:100:VAL:HB	1:A:139:ILE:HG13	2.02	0.41
1:B:31:VAL:HG21	1:B:106:VAL:O	2.20	0.41
1:A:255:VAL:O	1:B:143:ASN:HB3	2.20	0.41
1:A:19:LEU:O	1:A:23:MET:HG2	2.20	0.41
1:B:216:ASN:HD21	1:B:220:GLU:HB2	1.85	0.41
1:A:143:ASN:OD1	1:B:120:GLY:CA	2.68	0.41
1:B:141:ILE:HD12	1:B:147:LEU:HD21	2.02	0.41
1:A:263:GLY:O	1:A:264:GLU:HG2	2.21	0.41
1:B:100:VAL:HB	1:B:139:ILE:HG13	2.03	0.41
1:B:123:PHE:HB3	1:B:141:ILE:HG23	2.03	0.41
1:A:214:LEU:HA	1:A:214:LEU:HD22	1.71	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	183/456 (40%)	169 (92%)	11 (6%)	3 (2%)	9	40
1	B	194/456 (42%)	179 (92%)	14 (7%)	1 (0%)	29	68
All	All	377/912 (41%)	348 (92%)	25 (7%)	4 (1%)	14	50

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	35	THR
1	A	84	PHE
1	A	161	GLY
1	B	161	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	155/365 (42%)	140 (90%)	15 (10%)	8	31
1	B	163/365 (45%)	149 (91%)	14 (9%)	10	37
All	All	318/730 (44%)	289 (91%)	29 (9%)	9	34

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	MET
1	A	36	THR
1	A	84	PHE
1	A	85	MET
1	A	87	LEU
1	A	128	VAL
1	A	138	LEU
1	A	147	LEU
1	A	173	LEU
1	A	175	GLU
1	A	206	ASN
1	A	207	ARG
1	A	214	LEU
1	A	217	LEU
1	A	246	MET
1	B	12	MET
1	B	18	MET
1	B	80	GLN
1	B	85	MET
1	B	87	LEU

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Mol	Chain	Res	Type
1	B	128	VAL
1	B	138	LEU
1	B	147	LEU
1	B	173	LEU
1	B	175	GLU
1	B	198	PHE
1	B	206	ASN
1	B	217	LEU
1	B	246	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	ASN
1	A	146	ASN
1	A	169	ASN
1	A	206	ASN
1	A	245	ASN
1	A	249	ASN
1	A	259	GLN
1	B	38	ASN
1	B	80	GLN
1	B	104	ASN
1	B	142	GLN
1	B	146	ASN
1	B	169	ASN
1	B	197	ASN
1	B	206	ASN
1	B	225	ASN
1	B	245	ASN
1	B	249	ASN
1	B	259	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	DFP	A	500	1	6,9,9	1.28	0	6,11,11	0.42	0
2	DFP	B	500	1	6,9,9	1.18	0	6,11,11	0.41	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DFP	A	500	1	-	0/4/8/8	-
2	DFP	B	500	1	-	0/4/8/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	DFP	1	0
2	B	500	DFP	1	0

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	191/456 (41%)	0.25	16 (8%)	11 3	63, 91, 156, 197	0
1	B	202/456 (44%)	0.12	16 (7%)	12 4	59, 85, 151, 181	0
All	All	393/912 (43%)	0.18	32 (8%)	12 3	59, 88, 156, 197	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	11	GLN	4.8
1	A	263	GLY	4.0
1	A	197	ASN	3.9
1	A	206	ASN	3.9
1	A	228	ILE	3.8
1	A	33	GLY	3.6
1	B	42	MET	3.5
1	B	82	GLN	3.5
1	B	206	ASN	3.3
1	B	38	ASN	3.2
1	A	240	PHE	3.1
1	A	264	GLU	2.8
1	A	89	SER	2.8
1	A	90	GLY	2.7
1	B	40	PRO	2.7
1	A	212	GLY	2.6
1	B	259	GLN	2.6
1	B	263	GLY	2.6
1	B	213	ALA	2.5
1	B	90	GLY	2.4
1	B	101	VAL	2.4
1	A	213	ALA	2.4
1	A	34	SER	2.3
1	B	212	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	259	GLN	2.3
1	A	101	VAL	2.3
1	A	109	ASN	2.2
1	B	258	GLY	2.2
1	B	89	SER	2.2
1	B	39	THR	2.1
1	A	35	THR	2.1
1	B	37	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 carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	DFP	A	500	10/10	0.90	0.26	172,173,175,175	0
2	DFP	B	500	10/10	0.93	0.21	113,118,120,121	0

6.5 Other polymers [i](#)

There are no such residues in this entry.