



Full wwPDB EM Validation Report ⓘ

Apr 19, 2026 – 12:21 AM JST

PDB ID : 9MB8 / pdb_00009mb8
EMDB ID : EMD-63769
Title : the complex of D14 and RGSV P3
Authors : Huang, Y.C.
Deposited on : 2025-03-15
Resolution : 3.67 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>

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:

EMDB validation analysis : **FAILED**
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

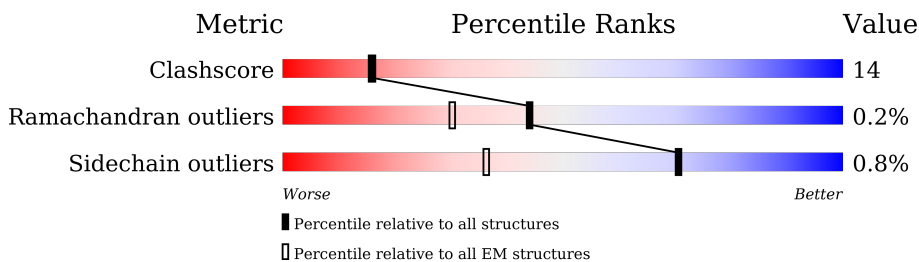
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.67 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)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	270	66% 33%
1	B	270	67% 33%
2	C	197	64% 26% 10%
2	D	197	57% 31% • 11%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7112 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Strigolactone esterase D14.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	270	Total	C	N	O	S	0	0
			2079	1326	372	373	8		
1	A	270	Total	C	N	O	S	0	0
			2079	1326	372	373	8		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	49	GLY	-	expression tag	UNP Q10QA5
B	50	PRO	-	expression tag	UNP Q10QA5
B	51	LEU	-	expression tag	UNP Q10QA5
B	52	GLY	-	expression tag	UNP Q10QA5
B	53	SER	-	expression tag	UNP Q10QA5
A	49	GLY	-	expression tag	UNP Q10QA5
A	50	PRO	-	expression tag	UNP Q10QA5
A	51	LEU	-	expression tag	UNP Q10QA5
A	52	GLY	-	expression tag	UNP Q10QA5
A	53	SER	-	expression tag	UNP Q10QA5

- Molecule 2 is a protein called p3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	178	Total	C	N	O	S	0	0
			1487	946	263	270	8		
2	D	176	Total	C	N	O	S	0	0
			1467	934	257	268	8		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	196	HIS	-	expression tag	UNP E5AXV2
C	197	HIS	-	expression tag	UNP E5AXV2
D	196	HIS	-	expression tag	UNP E5AXV2

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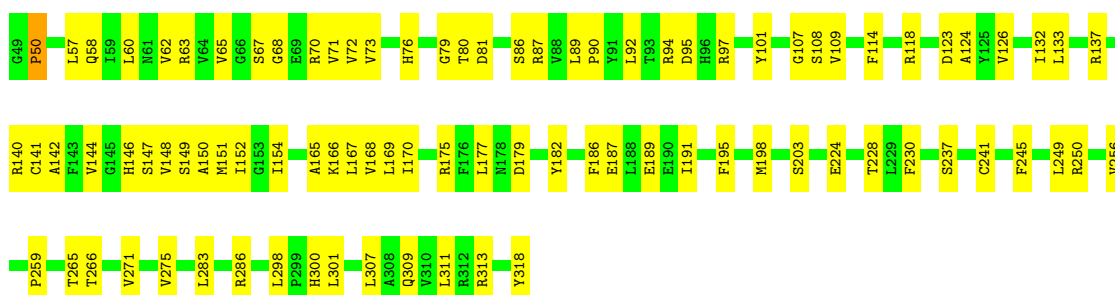
Chain	Residue	Modelled	Actual	Comment	Reference
D	197	HIS	-	expression tag	UNP E5AXV2

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

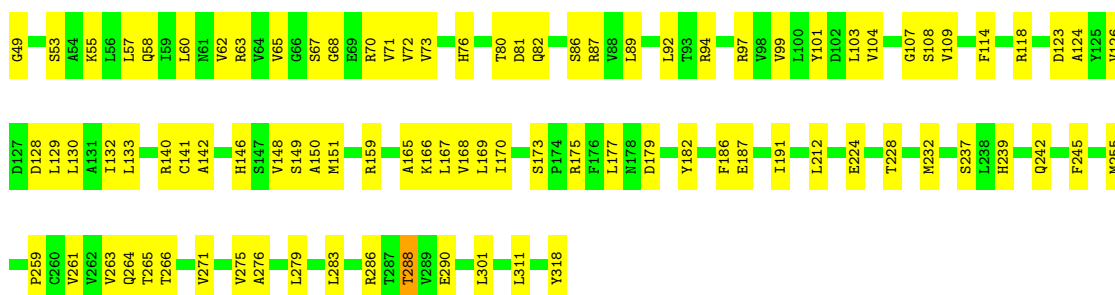
• Molecule 1: Strigolactone esterase D14

Chain B: 



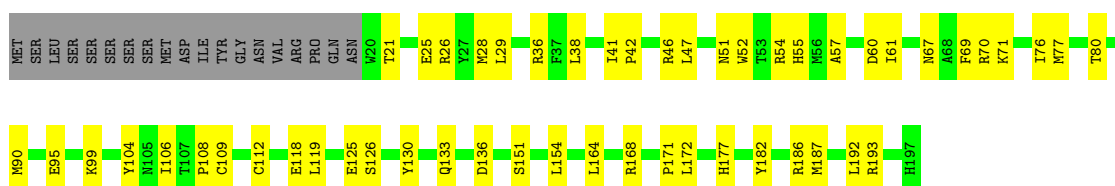
• Molecule 1: Strigolactone esterase D14

Chain A: 



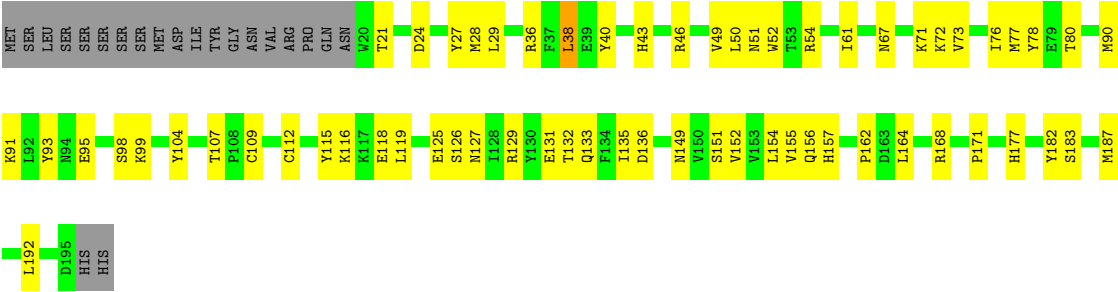
• Molecule 2: p3

Chain C: 



• Molecule 2: p3

Chain D: 57% 31% 11%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	103509	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

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	0.15	0/2125	0.44	2/2894 (0.1%)
1	B	0.17	0/2125	0.42	1/2894 (0.0%)
2	C	0.15	0/1524	0.44	0/2066
2	D	0.17	0/1502	0.42	0/2036
All	All	0.16	0/7276	0.43	3/9890 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	271	VAL	CA-C-N	7.30	127.06	119.76
1	A	271	VAL	C-N-CA	7.30	127.06	119.76
1	B	50	PRO	CA-N-CD	-6.51	102.88	112.00

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	2079	0	2089	64	0
1	B	2079	0	2089	64	0
2	C	1487	0	1467	42	0
2	D	1467	0	1453	43	0
All	All	7112	0	7098	205	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 14.

All (205) 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)
2:D:21:THR:OG1	2:D:46:ARG:NH1	2.15	0.79
2:C:51:ASN:OD1	2:C:54:ARG:NH2	2.16	0.74
1:B:76:HIS:ND1	1:B:80:THR:O	2.22	0.72
1:A:86:SER:OG	1:A:87:ARG:N	2.21	0.72
2:C:41:ILE:HD12	2:C:42:PRO:HD2	1.73	0.71
2:D:131:GLU:HG2	2:D:132:THR:HG23	1.73	0.70
2:D:132:THR:HG21	2:D:162:PRO:HG3	1.73	0.70
1:A:259:PRO:HB3	1:A:286:ARG:HB2	1.74	0.70
2:C:21:THR:HA	2:C:46:ARG:HE	1.56	0.69
2:C:164:LEU:HD12	2:C:168:ARG:HD3	1.75	0.68
1:A:76:HIS:ND1	1:A:80:THR:O	2.25	0.68
1:A:186:PHE:HB3	1:A:191:ILE:HD11	1.77	0.67
1:B:63:ARG:HD3	2:C:130:TYR:HE2	1.58	0.67
2:C:106:ILE:HG22	2:C:108:PRO:HD3	1.78	0.66
1:B:86:SER:OG	1:B:87:ARG:N	2.22	0.66
1:A:92:LEU:HD21	1:A:311:LEU:HD23	1.78	0.65
1:A:175:ARG:HH21	1:A:177:LEU:HD23	1.60	0.65
1:A:150:ALA:HB1	1:A:169:LEU:HB3	1.79	0.65
2:D:118:GLU:O	2:D:133:GLN:NE2	2.30	0.64
2:D:164:LEU:HD12	2:D:168:ARG:HD3	1.79	0.64
1:A:264:GLN:HG3	1:A:276:ALA:HB2	1.79	0.64
2:C:28:MET:HE3	2:C:28:MET:H	1.62	0.63
1:B:107:GLY:O	1:B:109:VAL:N	2.31	0.62
2:D:61:ILE:O	2:D:104:TYR:OH	2.16	0.62
1:A:107:GLY:O	1:A:109:VAL:N	2.33	0.62
1:A:148:VAL:O	1:A:151:MET:HB3	2.00	0.62
2:C:36:ARG:HA	2:C:36:ARG:NH1	2.15	0.61
1:B:148:VAL:O	1:B:151:MET:HB3	1.99	0.61
2:C:118:GLU:O	2:C:133:GLN:NE2	2.33	0.60
2:C:36:ARG:HA	2:C:36:ARG:HH11	1.66	0.60
1:A:146:HIS:O	1:A:149:SER:OG	2.19	0.60
1:A:94:ARG:HD3	1:A:94:ARG:H	1.66	0.60
1:B:72:VAL:HG12	1:B:142:ALA:HB3	1.83	0.60
1:B:150:ALA:HB1	1:B:169:LEU:HB3	1.83	0.60
1:B:259:PRO:HB3	1:B:286:ARG:HB2	1.84	0.60
1:B:63:ARG:HD3	2:C:130:TYR:CE2	2.37	0.59
1:B:141:CYS:SG	1:B:142:ALA:N	2.75	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:ARG:HD3	1:B:94:ARG:H	1.66	0.59
1:A:73:VAL:HG21	1:A:133:LEU:HD21	1.85	0.59
1:A:167:LEU:HD13	1:A:169:LEU:HD21	1.85	0.59
1:A:65:VAL:HG21	1:A:89:LEU:HD21	1.86	0.58
1:B:123:ASP:OD1	1:B:124:ALA:N	2.37	0.58
1:A:141:CYS:SG	1:A:142:ALA:N	2.77	0.57
1:A:72:VAL:HG12	1:A:142:ALA:HB3	1.86	0.57
1:A:62:VAL:HG13	1:A:101:TYR:HB3	1.87	0.56
1:B:177:LEU:HA	1:B:186:PHE:HB2	1.88	0.56
1:A:76:HIS:CD2	1:A:103:LEU:H	2.24	0.56
1:A:60:LEU:HD11	1:A:128:ASP:OD1	2.05	0.56
1:B:87:ARG:NH1	2:C:125:GLU:OE1	2.38	0.56
1:B:167:LEU:HD13	1:B:169:LEU:HD21	1.88	0.55
1:A:87:ARG:NH1	2:D:125:GLU:OE1	2.38	0.55
1:B:118:ARG:HH11	1:B:118:ARG:HG3	1.71	0.55
1:A:67:SER:OG	1:A:68:GLY:N	2.39	0.55
2:C:61:ILE:O	2:C:104:TYR:OH	2.21	0.55
2:D:36:ARG:O	2:D:36:ARG:NH1	2.39	0.54
1:A:263:VAL:HG22	1:A:290:GLU:HB2	1.89	0.54
1:A:286:ARG:HG3	1:A:286:ARG:HH11	1.72	0.54
2:C:25:GLU:O	2:C:26:ARG:HG2	2.08	0.54
2:C:28:MET:HE3	2:C:28:MET:N	2.23	0.54
1:B:187:GLU:O	1:B:191:ILE:HG12	2.08	0.53
2:C:76:ILE:O	2:C:80:THR:HG23	2.08	0.53
1:A:57:LEU:HD23	1:A:132:ILE:HD12	1.90	0.53
2:C:171:PRO:HA	2:C:192:LEU:HD23	1.89	0.53
2:D:155:VAL:O	2:D:177:HIS:NE2	2.42	0.53
1:A:123:ASP:OD1	1:A:124:ALA:N	2.42	0.53
1:A:168:VAL:HG11	1:A:311:LEU:HD12	1.90	0.53
2:D:67:ASN:O	2:D:71:LYS:HG2	2.09	0.53
1:B:189:GLU:N	1:B:189:GLU:OE2	2.42	0.53
2:D:171:PRO:HA	2:D:192:LEU:HD23	1.90	0.52
1:B:57:LEU:HD23	1:B:132:ILE:HD12	1.92	0.51
2:C:119:LEU:HG	2:C:154:LEU:HD21	1.92	0.51
2:D:119:LEU:HG	2:D:154:LEU:HD21	1.90	0.51
1:B:203:SER:HA	1:B:230:PHE:HE1	1.75	0.51
2:C:21:THR:HA	2:C:46:ARG:NE	2.25	0.51
1:A:53:SER:O	1:A:55:LYS:N	2.42	0.51
2:C:47:LEU:O	2:C:51:ASN:N	2.34	0.51
2:D:38:LEU:HD22	2:D:46:ARG:NH1	2.26	0.51
2:D:36:ARG:HH11	2:D:36:ARG:HA	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:152:VAL:HG12	2:D:154:LEU:H	1.77	0.50
1:B:170:ILE:HD11	1:B:307:LEU:HD11	1.94	0.50
1:B:224:GLU:HG2	1:B:301:LEU:HD11	1.94	0.50
1:B:60:LEU:HD12	1:B:132:ILE:HD11	1.94	0.50
1:A:71:VAL:HA	1:A:97:ARG:O	2.12	0.49
1:B:90:PRO:HG3	2:C:126:SER:OG	2.11	0.49
2:C:55:HIS:HB3	2:C:61:ILE:HD13	1.94	0.49
2:C:186:ARG:NH1	2:C:187:MET:O	2.44	0.49
2:D:27:TYR:O	2:D:28:MET:HG2	2.12	0.49
1:A:168:VAL:O	1:A:168:VAL:HG12	2.12	0.49
2:D:24:ASP:HB3	2:D:50:LEU:HD23	1.93	0.49
1:B:265:THR:OG1	1:B:266:THR:N	2.46	0.49
1:B:92:LEU:HD21	1:B:311:LEU:HD23	1.94	0.49
1:A:191:ILE:HD12	1:A:245:PHE:HE2	1.77	0.49
1:B:168:VAL:HG11	1:B:311:LEU:HD12	1.94	0.48
2:D:107:THR:O	2:D:107:THR:HG23	2.13	0.48
2:D:76:ILE:O	2:D:80:THR:OG1	2.31	0.48
1:B:140:ARG:HD2	1:B:165:ALA:HB2	1.95	0.48
1:A:80:THR:HG22	1:A:228:THR:HG21	1.96	0.48
2:C:70:ARG:NH2	2:C:108:PRO:HG3	2.28	0.48
2:C:71:LYS:HA	2:C:71:LYS:HE2	1.95	0.48
1:A:92:LEU:HD12	1:A:92:LEU:O	2.14	0.48
1:B:70:ARG:HH12	1:B:318:TYR:HB3	1.79	0.48
1:A:179:ASP:H	1:A:182:TYR:HB3	1.78	0.47
2:D:129:ARG:NH2	2:D:156:GLN:OE1	2.47	0.47
2:C:112:CYS:HB3	2:C:177:HIS:CE1	2.50	0.47
1:B:118:ARG:HG3	1:B:118:ARG:NH1	2.29	0.47
1:A:104:VAL:HA	1:A:109:VAL:HG11	1.95	0.47
1:A:232:MET:HE3	1:A:237:SER:HB2	1.96	0.47
2:C:29:LEU:HD22	2:C:57:ALA:HA	1.96	0.47
2:D:27:TYR:CD2	2:D:54:ARG:HG3	2.50	0.47
1:B:147:SER:OG	1:B:148:VAL:N	2.47	0.47
1:A:49:GLY:O	1:A:118:ARG:NH2	2.47	0.47
1:A:63:ARG:NE	1:A:82:GLN:OE1	2.48	0.47
1:B:62:VAL:HG13	1:B:101:TYR:HB3	1.96	0.46
1:B:50:PRO:O	1:B:118:ARG:NH1	2.47	0.46
1:A:224:GLU:HG2	1:A:301:LEU:HD11	1.98	0.46
2:C:151:SER:HB2	2:C:182:TYR:CZ	2.51	0.46
1:B:241:CYS:O	1:B:245:PHE:HB2	2.16	0.46
2:C:52:TRP:HE3	2:C:69:PHE:CE1	2.33	0.46
2:C:95:GLU:OE2	2:C:95:GLU:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:VAL:HG21	1:B:133:LEU:HD21	1.97	0.46
1:A:70:ARG:HH12	1:A:318:TYR:HB3	1.81	0.46
1:B:179:ASP:H	1:B:182:TYR:HB3	1.80	0.46
2:D:72:LYS:HB2	2:D:72:LYS:HE3	1.74	0.46
1:A:212:LEU:HD12	1:A:212:LEU:HA	1.83	0.45
1:B:65:VAL:HG21	1:B:89:LEU:HD21	1.99	0.45
2:C:67:ASN:O	2:C:71:LYS:HG2	2.16	0.45
2:D:71:LYS:HE3	2:D:116:LYS:HE3	1.99	0.45
2:D:112:CYS:HB3	2:D:177:HIS:CE1	2.51	0.45
2:D:51:ASN:OD1	2:D:54:ARG:NE	2.42	0.45
1:B:154:ILE:HG13	1:B:256:VAL:HG11	1.99	0.45
2:D:115:TYR:CD1	2:D:135:ILE:HD11	2.52	0.44
1:B:137:ARG:HH11	1:B:137:ARG:HG2	1.82	0.44
1:B:167:LEU:HD23	1:B:167:LEU:HA	1.86	0.44
1:A:301:LEU:HD23	1:A:301:LEU:HA	1.76	0.44
1:B:67:SER:OG	1:B:68:GLY:N	2.50	0.44
1:A:170:ILE:HD13	1:A:170:ILE:HA	1.89	0.44
2:C:77:MET:HE1	2:C:90:MET:SD	2.58	0.44
2:C:95:GLU:O	2:C:99:LYS:HG3	2.18	0.44
1:A:187:GLU:O	1:A:191:ILE:HG12	2.17	0.44
2:C:41:ILE:HD12	2:C:42:PRO:CD	2.45	0.44
1:A:123:ASP:O	1:A:126:VAL:HG12	2.18	0.44
1:A:133:LEU:HD23	1:A:133:LEU:HA	1.84	0.44
1:A:101:TYR:CZ	1:A:129:LEU:HD13	2.53	0.44
2:D:151:SER:HB2	2:D:182:TYR:CZ	2.53	0.44
2:D:77:MET:HE1	2:D:90:MET:SD	2.58	0.43
1:B:271:VAL:HB	1:B:275:VAL:HG11	2.00	0.43
1:A:255:MET:N	1:A:255:MET:HE2	2.33	0.43
1:A:261:VAL:HG22	1:A:288:THR:HB	2.00	0.43
2:D:51:ASN:O	2:D:54:ARG:HB3	2.17	0.43
2:D:95:GLU:O	2:D:99:LYS:HG3	2.18	0.43
1:A:173:SER:HA	1:A:275:VAL:HG21	2.00	0.43
1:A:81:ASP:OD1	1:A:81:ASP:C	2.62	0.43
2:C:193:ARG:NH2	2:D:98:SER:OG	2.51	0.43
1:A:265:THR:OG1	1:A:266:THR:N	2.51	0.43
1:A:279:LEU:HD12	1:A:279:LEU:HA	1.84	0.43
2:D:91:LYS:O	2:D:95:GLU:HG2	2.19	0.43
1:B:114:PHE:C	1:B:114:PHE:CD1	2.97	0.43
1:A:58:GLN:HE21	2:D:136:ASP:HB2	1.84	0.43
2:D:27:TYR:O	2:D:29:LEU:N	2.52	0.43
1:A:165:ALA:O	1:A:166:LYS:HE2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:GLN:HA	1:A:242:GLN:OE1	2.18	0.42
2:C:28:MET:O	2:C:28:MET:HG2	2.19	0.42
1:A:130:LEU:HD12	1:A:159:ARG:HD2	2.00	0.42
2:D:40:TYR:HD2	2:D:76:ILE:HG23	1.84	0.42
2:D:126:SER:OG	2:D:127:ASN:N	2.53	0.42
2:D:187:MET:HE1	2:D:192:LEU:HB2	2.00	0.42
1:B:195:PHE:O	1:B:198:MET:HG3	2.19	0.42
1:A:114:PHE:C	1:A:114:PHE:CD1	2.97	0.42
1:B:92:LEU:HD12	1:B:92:LEU:O	2.20	0.42
1:A:123:ASP:OD1	1:A:123:ASP:C	2.61	0.42
2:D:43:HIS:O	2:D:46:ARG:HB2	2.19	0.42
2:D:149:ASN:O	2:D:183:SER:OG	2.29	0.42
1:B:144:VAL:HG22	1:B:168:VAL:HB	2.01	0.42
1:B:146:HIS:H	1:B:149:SER:HB3	1.85	0.42
2:D:78:TYR:C	2:D:78:TYR:CD1	2.98	0.42
1:B:81:ASP:OD1	1:B:81:ASP:C	2.62	0.42
1:A:170:ILE:HD13	1:A:263:VAL:HB	2.02	0.42
2:C:28:MET:H	2:C:28:MET:CE	2.32	0.41
1:A:73:VAL:HG22	1:A:99:VAL:HB	2.02	0.41
2:D:73:VAL:HG11	2:D:93:TYR:HB2	2.01	0.41
1:B:123:ASP:O	1:B:126:VAL:HG12	2.20	0.41
2:C:76:ILE:HD13	2:C:76:ILE:HA	1.89	0.41
1:B:71:VAL:HA	1:B:97:ARG:O	2.20	0.41
1:B:94:ARG:HG2	1:B:95:ASP:N	2.35	0.41
2:C:38:LEU:HD12	2:C:38:LEU:HA	1.79	0.41
1:B:76:HIS:O	1:B:149:SER:HB2	2.20	0.41
1:B:87:ARG:O	1:B:90:PRO:HD2	2.20	0.41
2:C:172:LEU:HD12	2:C:172:LEU:HA	1.87	0.41
1:A:283:LEU:HD12	1:A:283:LEU:HA	1.84	0.41
1:B:168:VAL:HG12	1:B:168:VAL:O	2.20	0.41
1:B:175:ARG:HD3	1:B:250:ARG:HH12	1.84	0.41
1:B:309:GLN:O	1:B:313:ARG:HG3	2.21	0.41
2:D:49:VAL:O	2:D:52:TRP:HB2	2.21	0.41
1:B:79:GLY:O	1:B:228:THR:HG23	2.21	0.41
1:B:298:LEU:HD12	1:B:300:HIS:HE1	1.86	0.41
2:C:55:HIS:ND1	2:C:60:ASP:O	2.54	0.41
1:B:149:SER:HA	1:B:152:ILE:HG12	2.02	0.41
1:B:165:ALA:O	1:B:166:LYS:HE2	2.21	0.41
1:B:198:MET:HE1	1:B:237:SER:HB3	2.03	0.41
1:A:167:LEU:HD23	1:A:167:LEU:HA	1.87	0.40
1:B:58:GLN:HE21	2:C:136:ASP:HB2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:ARG:HD2	1:A:165:ALA:HB2	2.03	0.40
2:D:38:LEU:HD21	2:D:46:ARG:HG2	2.04	0.40
1:B:249:LEU:HA	1:B:249:LEU:HD12	1.85	0.40
1:B:283:LEU:HD12	1:B:283:LEU:HA	1.86	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 PDB entries followed by that with respect to all EM entries.

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	268/270 (99%)	242 (90%)	25 (9%)	1 (0%)	30	60
1	B	268/270 (99%)	245 (91%)	22 (8%)	1 (0%)	30	60
2	C	176/197 (89%)	152 (86%)	24 (14%)	0	100	100
2	D	174/197 (88%)	154 (88%)	20 (12%)	0	100	100
All	All	886/934 (95%)	793 (90%)	91 (10%)	2 (0%)	44	71

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	108	SER
1	A	108	SER

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 PDB entries followed by that with respect to all EM entries.

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	221/221 (100%)	219 (99%)	2 (1%)	70	75
1	B	221/221 (100%)	221 (100%)	0	100	100
2	C	167/185 (90%)	166 (99%)	1 (1%)	78	79
2	D	165/185 (89%)	162 (98%)	3 (2%)	51	66
All	All	774/812 (95%)	768 (99%)	6 (1%)	70	76

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	109	CYS
1	A	239	HIS
1	A	288	THR
2	D	38	LEU
2	D	109	CYS
2	D	157	HIS

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

Mol	Chain	Res	Type
1	B	82	GLN
2	C	157	HIS
2	C	190	GLN
2	D	157	HIS
2	D	190	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.