



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 09:51 pm BST

PDB ID : 6J8V  
Title : Structure of MOEN5-SSO7D fusion protein in complex with ligand 2  
Authors : Ko, T.P.; Zhang, L.L.; Chen, C.C.; Guo, R.T.  
Deposited on : 2019-01-21  
Resolution : 2.23 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](mailto: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.

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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

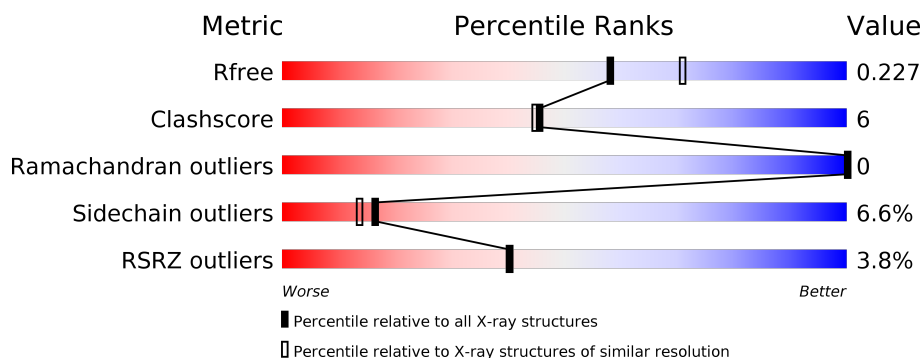
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.23 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	2391 (2.26-2.22)
Clashscore	141614	2539 (2.26-2.22)
Ramachandran outliers	138981	2489 (2.26-2.22)
Sidechain outliers	138945	2490 (2.26-2.22)
RSRZ outliers	127900	2353 (2.26-2.22)

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  $\geq 3$ , 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	343	<div> <div>3%</div> <div>66%</div> <div>7%</div> <div>25%</div> </div>
1	B	343	<div> <div>6%</div> <div>85%</div> <div>11%</div> <div>• •</div> </div>
1	C	343	<div> <div>64%</div> <div>9%</div> <div>24%</div> </div>
1	D	343	<div> <div>3%</div> <div>74%</div> <div>10%</div> <div>15%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9300 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 MoeN5,DNA-binding protein 7d.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	S	0	0	0
			1969	1220	364	374	11			
1	B	332	Total	C	N	O	S	0	0	0
			2533	1571	463	485	14			
1	C	261	Total	C	N	O	S	0	0	0
			1990	1230	371	378	11			
1	D	291	Total	C	N	O	S	0	0	0
			2234	1387	414	421	12			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	expression tag	UNP A0A010
A	-12	ALA	-	expression tag	UNP A0A010
A	-11	HIS	-	expression tag	UNP A0A010
A	-10	HIS	-	expression tag	UNP A0A010
A	-9	HIS	-	expression tag	UNP A0A010
A	-8	HIS	-	expression tag	UNP A0A010
A	-7	HIS	-	expression tag	UNP A0A010
A	-6	HIS	-	expression tag	UNP A0A010
A	-5	VAL	-	expression tag	UNP A0A010
A	-4	ASP	-	expression tag	UNP A0A010
A	-3	ASP	-	expression tag	UNP A0A010
A	-2	ASP	-	expression tag	UNP A0A010
A	-1	ASP	-	expression tag	UNP A0A010
A	0	LYS	-	expression tag	UNP A0A010
A	261	ALA	-	linker	UNP A0A010
A	262	GLY	-	linker	UNP A0A010
A	263	ALA	-	linker	UNP A0A010
A	264	GLY	-	linker	UNP A0A010
A	265	ALA	-	linker	UNP A0A010
B	-13	MET	-	expression tag	UNP A0A010
B	-12	ALA	-	expression tag	UNP A0A010

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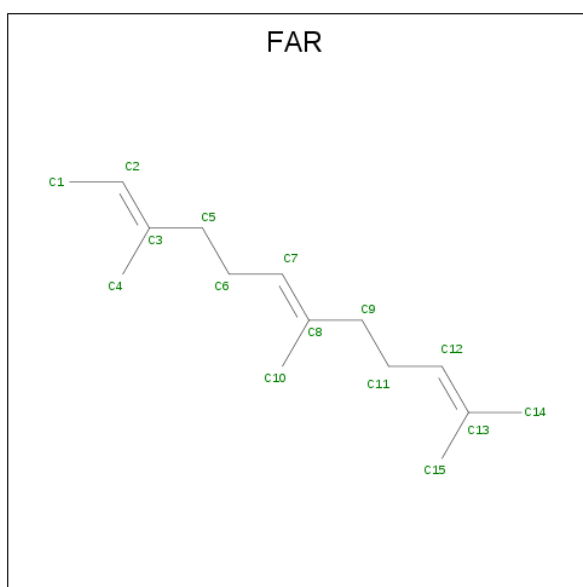
Chain	Residue	Modelled	Actual	Comment	Reference
B	-11	HIS	-	expression tag	UNP A0A010
B	-10	HIS	-	expression tag	UNP A0A010
B	-9	HIS	-	expression tag	UNP A0A010
B	-8	HIS	-	expression tag	UNP A0A010
B	-7	HIS	-	expression tag	UNP A0A010
B	-6	HIS	-	expression tag	UNP A0A010
B	-5	VAL	-	expression tag	UNP A0A010
B	-4	ASP	-	expression tag	UNP A0A010
B	-3	ASP	-	expression tag	UNP A0A010
B	-2	ASP	-	expression tag	UNP A0A010
B	-1	ASP	-	expression tag	UNP A0A010
B	0	LYS	-	expression tag	UNP A0A010
B	261	ALA	-	linker	UNP A0A010
B	262	GLY	-	linker	UNP A0A010
B	263	ALA	-	linker	UNP A0A010
B	264	GLY	-	linker	UNP A0A010
B	265	ALA	-	linker	UNP A0A010
C	-13	MET	-	expression tag	UNP A0A010
C	-12	ALA	-	expression tag	UNP A0A010
C	-11	HIS	-	expression tag	UNP A0A010
C	-10	HIS	-	expression tag	UNP A0A010
C	-9	HIS	-	expression tag	UNP A0A010
C	-8	HIS	-	expression tag	UNP A0A010
C	-7	HIS	-	expression tag	UNP A0A010
C	-6	HIS	-	expression tag	UNP A0A010
C	-5	VAL	-	expression tag	UNP A0A010
C	-4	ASP	-	expression tag	UNP A0A010
C	-3	ASP	-	expression tag	UNP A0A010
C	-2	ASP	-	expression tag	UNP A0A010
C	-1	ASP	-	expression tag	UNP A0A010
C	0	LYS	-	expression tag	UNP A0A010
C	261	ALA	-	linker	UNP A0A010
C	262	GLY	-	linker	UNP A0A010
C	263	ALA	-	linker	UNP A0A010
C	264	GLY	-	linker	UNP A0A010
C	265	ALA	-	linker	UNP A0A010
D	-13	MET	-	expression tag	UNP A0A010
D	-12	ALA	-	expression tag	UNP A0A010
D	-11	HIS	-	expression tag	UNP A0A010
D	-10	HIS	-	expression tag	UNP A0A010
D	-9	HIS	-	expression tag	UNP A0A010
D	-8	HIS	-	expression tag	UNP A0A010

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-7	HIS	-	expression tag	UNP A0A010
D	-6	HIS	-	expression tag	UNP A0A010
D	-5	VAL	-	expression tag	UNP A0A010
D	-4	ASP	-	expression tag	UNP A0A010
D	-3	ASP	-	expression tag	UNP A0A010
D	-2	ASP	-	expression tag	UNP A0A010
D	-1	ASP	-	expression tag	UNP A0A010
D	0	LYS	-	expression tag	UNP A0A010
D	261	ALA	-	linker	UNP A0A010
D	262	GLY	-	linker	UNP A0A010
D	263	ALA	-	linker	UNP A0A010
D	264	GLY	-	linker	UNP A0A010
D	265	ALA	-	linker	UNP A0A010

- Molecule 2 is FARNESYL (three-letter code: FAR) (formula: C<sub>15</sub>H<sub>26</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total C 15 15	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	147	Total O 147 147	0	0
3	B	144	Total O 144 144	0	0

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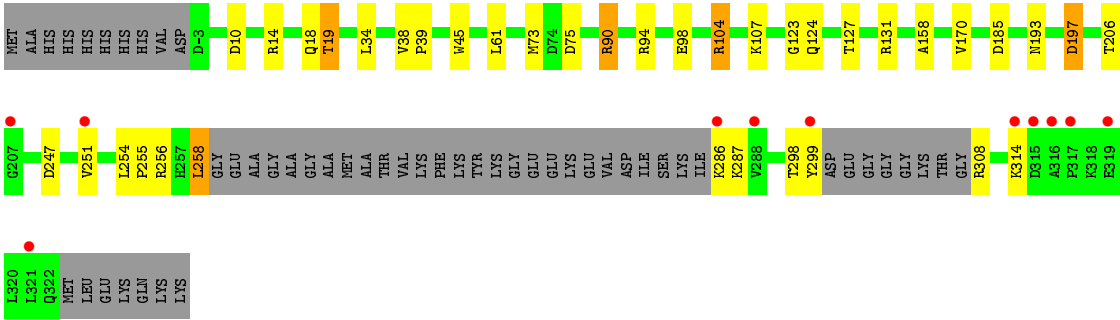
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	123	Total 123	O 123	0	0
3	D	145	Total 145	O 145	0	0

**i**

- Molecule 1: MoeN5,DNA-binding protein 7d







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	137.86Å 217.34Å 104.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.23 24.98 – 2.23	Depositor EDS
% Data completeness (in resolution range)	99.5 (25.00-2.23) 99.6 (24.98-2.23)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.82 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, $R_{free}$	0.172 , 0.225 0.179 , 0.227	Depositor DCC
$R_{free}$ test set	3628 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.5	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 34.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	9300	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.72	0/2000	0.88	0/2719
1	B	0.75	0/2572	0.84	0/3478
1	C	0.75	0/2022	0.87	0/2748
1	D	0.77	0/2269	0.85	0/3075
All	All	0.75	0/8863	0.86	0/12020

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	1969	0	1960	29	0
1	B	2533	0	2532	28	0
1	C	1990	0	1979	32	0
1	D	2234	0	2233	27	0
2	D	15	0	26	4	0
3	A	147	0	0	4	0
3	B	144	0	0	1	0
3	C	123	0	0	6	0
3	D	145	0	0	1	0
All	All	9300	0	8730	112	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 6.

All (112) 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:260:GLU:HG2	1:C:137:GLU:OE2	1.67	0.93
1:C:33:ARG:HD3	3:C:495:HOH:O	1.69	0.91
1:A:115:GLN:HG3	3:A:538:HOH:O	1.71	0.88
1:D:10:ASP:HB2	3:D:596:HOH:O	1.75	0.86
1:C:10:ASP:HB3	1:C:14:ARG:NH2	1.97	0.79
1:D:254:LEU:HG	1:D:258:LEU:HD22	1.66	0.78
1:B:179:MET:CE	1:B:217:LEU:HD11	2.14	0.77
1:A:18:GLN:HG2	3:A:450:HOH:O	1.87	0.75
1:B:229:VAL:HG13	1:B:235:ALA:O	1.87	0.74
1:C:187:LEU:HD21	1:C:204:MET:CE	2.19	0.72
1:D:247:ASP:O	1:D:251:VAL:HG13	1.90	0.72
1:C:219:GLU:OE2	1:C:222:ARG:NH2	2.20	0.71
1:C:1:MET:SD	1:C:37:ARG:HD3	2.31	0.71
1:A:104:ARG:HD3	1:A:163:GLU:HG3	1.73	0.69
1:A:11:HIS:CE1	1:A:57:ARG:NH1	2.62	0.68
1:B:172:GLU:OE2	1:B:224:ARG:HD2	1.96	0.66
1:C:187:LEU:CD2	1:C:204:MET:HE3	2.27	0.65
3:C:512:HOH:O	1:D:107:LYS:HG2	1.97	0.64
1:C:187:LEU:HD21	1:C:204:MET:HE3	1.80	0.63
1:A:11:HIS:CE1	1:A:57:ARG:HH11	2.16	0.63
1:C:15:CYS:O	1:C:19:THR:HG22	1.97	0.63
1:C:140:ALA:O	1:C:144:THR:HG23	1.99	0.62
1:B:187:LEU:HD21	1:B:204:MET:CE	2.30	0.62
1:B:179:MET:HE3	1:B:217:LEU:HD11	1.82	0.60
1:D:34:LEU:HD23	2:D:401:FAR:H13	1.83	0.59
1:D:104:ARG:NH1	1:D:158:ALA:O	2.37	0.58
1:B:229:VAL:CG1	1:B:235:ALA:O	2.52	0.58
1:C:5:GLU:OE2	1:C:33:ARG:HG3	2.02	0.58
1:D:61:LEU:HD13	1:D:94:ARG:HG3	1.86	0.58
1:A:187:LEU:HD21	1:A:204:MET:HE1	1.86	0.56
1:C:254:LEU:N	1:C:255:PRO:CD	2.68	0.56
1:D:34:LEU:CD2	2:D:401:FAR:H13	2.37	0.55
1:A:139:ARG:HD3	1:A:179:MET:CE	2.37	0.55
1:D:10:ASP:O	1:D:14:ARG:CG	2.55	0.55
1:C:70:ASP:OD1	1:C:128:LYS:HE3	2.07	0.55
1:B:187:LEU:HD21	1:B:204:MET:HE3	1.88	0.55
1:C:166:PRO:HD3	1:C:233:PRO:HD2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:ARG:NE	1:A:163:GLU:HG2	2.23	0.54
1:B:254:LEU:N	1:B:255:PRO:CD	2.71	0.54
1:A:33:ARG:HG2	1:A:33:ARG:HH11	1.73	0.54
1:D:38:VAL:HG12	1:D:39:PRO:HD3	1.89	0.53
1:A:12:VAL:HG12	1:A:29:THR:HG23	1.89	0.53
1:A:232:PRO:HA	1:A:233:PRO:C	2.29	0.53
1:D:298:THR:HA	1:D:308:ARG:HG3	1.91	0.53
1:A:179:MET:HE2	1:A:221:LEU:HD21	1.91	0.52
1:A:139:ARG:HD3	1:A:179:MET:HE3	1.91	0.52
1:C:38:VAL:HG12	1:C:39:PRO:HD3	1.92	0.52
1:C:57:ARG:NE	3:C:403:HOH:O	2.42	0.52
1:D:10:ASP:O	1:D:14:ARG:HG2	2.09	0.52
1:D:94:ARG:HD2	1:D:98:GLU:OE2	2.10	0.52
1:B:200:LEU:HG	1:B:204:MET:CE	2.41	0.51
1:B:214:VAL:HG11	1:B:254:LEU:HD21	1.93	0.51
1:A:104:ARG:CZ	1:A:163:GLU:HG2	2.41	0.51
1:D:123:GLY:O	1:D:127:THR:HG23	2.10	0.50
1:C:57:ARG:CZ	3:C:403:HOH:O	2.59	0.50
1:D:94:ARG:HD3	1:D:98:GLU:HG3	1.94	0.50
1:A:254:LEU:HB2	1:A:255:PRO:HD3	1.93	0.49
1:A:187:LEU:CD2	1:A:204:MET:CE	2.91	0.49
1:A:38:VAL:HG12	1:A:39:PRO:HD3	1.94	0.49
1:D:19:THR:CG2	1:D:90:ARG:HG3	2.43	0.48
1:D:131:ARG:HD2	1:D:197:ASP:OD1	2.12	0.48
1:A:187:LEU:CD2	1:A:204:MET:HE1	2.43	0.48
1:A:33:ARG:NH1	1:A:33:ARG:HG2	2.29	0.48
1:B:200:LEU:HG	1:B:204:MET:HE2	1.94	0.47
1:B:179:MET:HE2	1:B:221:LEU:HD11	1.94	0.47
1:B:187:LEU:HD21	1:B:204:MET:HE1	1.95	0.47
1:C:219:GLU:OE2	1:C:222:ARG:HD2	2.15	0.47
1:D:124:GLN:HG2	2:D:401:FAR:H142	1.95	0.47
1:C:141:HIS:HD2	3:C:439:HOH:O	1.98	0.47
1:A:183:MET:O	1:A:187:LEU:HG	2.15	0.46
1:C:187:LEU:HD21	1:C:204:MET:HE1	1.97	0.46
1:B:205:ARG:NH1	1:C:131:ARG:HG2	2.31	0.46
1:C:44:GLU:HG2	1:C:238:LEU:HG	1.98	0.46
1:B:224:ARG:NH1	3:B:405:HOH:O	2.49	0.45
1:A:187:LEU:HD22	1:A:204:MET:CE	2.46	0.45
1:D:10:ASP:O	1:D:14:ARG:HG3	2.16	0.45
1:D:254:LEU:N	1:D:255:PRO:CD	2.79	0.45
1:B:131:ARG:HG2	1:B:197:ASP:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:14:ARG:HD3	3:C:438:HOH:O	2.17	0.45
1:C:90:ARG:C	1:C:90:ARG:HD3	2.37	0.45
1:B:172:GLU:CD	1:B:224:ARG:HH21	2.19	0.44
1:B:172:GLU:HA	1:B:172:GLU:OE1	2.17	0.44
1:A:18:GLN:CG	3:A:450:HOH:O	2.52	0.43
1:C:127:THR:HG21	1:C:145:TYR:CD2	2.53	0.43
1:A:14:ARG:HD3	3:A:424:HOH:O	2.18	0.43
1:B:195:GLU:O	1:B:196:ARG:NH1	2.49	0.43
1:A:187:LEU:HD22	1:A:204:MET:HE3	2.01	0.43
1:A:187:LEU:HD21	1:A:204:MET:CE	2.49	0.43
1:C:165:GLN:HB2	1:C:165:GLN:HE21	1.64	0.43
1:D:258:LEU:HA	1:D:258:LEU:HD12	1.73	0.43
1:D:38:VAL:N	1:D:39:PRO:CD	2.82	0.43
1:A:171:ARG:O	1:A:175:GLU:HG3	2.18	0.42
2:D:401:FAR:H112	2:D:401:FAR:H101	1.84	0.42
1:B:266:MET:HE3	1:B:266:MET:HA	2.00	0.42
1:A:254:LEU:N	1:A:255:PRO:CD	2.82	0.42
1:A:106:PRO:HB2	1:B:106:PRO:HB2	2.00	0.42
1:C:107:LYS:HD3	1:C:107:LYS:O	2.19	0.42
1:C:16:VAL:HG21	1:C:29:THR:HG21	2.02	0.42
1:D:251:VAL:O	1:D:255:PRO:HG2	2.20	0.42
1:B:172:GLU:OE1	1:B:224:ARG:NH2	2.52	0.42
1:B:272:LYS:HE2	1:B:275:GLY:O	2.20	0.41
1:D:45:TRP:CE3	1:D:170:VAL:HG22	2.54	0.41
1:B:179:MET:HE2	1:B:221:LEU:HD21	2.02	0.41
1:C:178:ALA:O	1:C:181:ILE:HG12	2.19	0.41
1:C:187:LEU:CD2	1:C:204:MET:CE	2.90	0.41
1:D:19:THR:HG21	1:D:90:ARG:HG3	2.03	0.41
1:A:38:VAL:N	1:A:39:PRO:CD	2.84	0.41
1:D:75:ASP:O	1:D:75:ASP:CG	2.59	0.41
1:B:256:ARG:HB3	1:C:129:ARG:O	2.21	0.41
1:B:201:ALA:HB1	1:B:257:HIS:CE1	2.56	0.40
1:C:38:VAL:N	1:C:39:PRO:CD	2.84	0.40
1:B:26:VAL:HG11	1:D:193:ASN:HA	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	254/343 (74%)	244 (96%)	10 (4%)	0	100	100
1	B	330/343 (96%)	320 (97%)	10 (3%)	0	100	100
1	C	259/343 (76%)	251 (97%)	8 (3%)	0	100	100
1	D	285/343 (83%)	277 (97%)	8 (3%)	0	100	100
All	All	1128/1372 (82%)	1092 (97%)	36 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	204/270 (76%)	194 (95%)	10 (5%)	25	25
1	B	260/270 (96%)	241 (93%)	19 (7%)	14	10
1	C	205/270 (76%)	189 (92%)	16 (8%)	12	9
1	D	231/270 (86%)	217 (94%)	14 (6%)	18	16
All	All	900/1080 (83%)	841 (93%)	59 (7%)	16	14

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	29	THR

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Mol	Chain	Res	Type
1	A	90	ARG
1	A	107	LYS
1	A	128	LYS
1	A	131	ARG
1	A	139	ARG
1	A	163	GLU
1	A	189	ASP
1	A	254	LEU
1	B	-4	ASP
1	B	18	GLN
1	B	19	THR
1	B	38	VAL
1	B	90	ARG
1	B	107	LYS
1	B	130	SER
1	B	131	ARG
1	B	163	GLU
1	B	186	ASP
1	B	197	ASP
1	B	206	THR
1	B	266	MET
1	B	272	LYS
1	B	274	LYS
1	B	283	SER
1	B	288	VAL
1	B	308	ARG
1	B	324	LEU
1	C	-2	ASP
1	C	-1	ASP
1	C	18	GLN
1	C	19	THR
1	C	29	THR
1	C	52	ARG
1	C	90	ARG
1	C	107	LYS
1	C	131	ARG
1	C	139	ARG
1	C	141	HIS
1	C	144	THR
1	C	165	GLN
1	C	181	ILE
1	C	222	ARG

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Mol	Chain	Res	Type
1	C	254	LEU
1	D	18	GLN
1	D	19	THR
1	D	73	MET
1	D	90	ARG
1	D	104	ARG
1	D	185	ASP
1	D	197	ASP
1	D	206	THR
1	D	256	ARG
1	D	258	LEU
1	D	286	LYS
1	D	287	LYS
1	D	299	TYR
1	D	314	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	165	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is 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	FAR	D	401	-	14,14,14	2.05	5 (35%)	16,16,16	1.89	5 (31%)

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	FAR	D	401	-	-	3/14/14/14	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	FAR	C5-C3	3.73	1.59	1.51
2	D	401	FAR	C9-C8	3.70	1.59	1.51
2	D	401	FAR	C7-C8	2.56	1.39	1.33
2	D	401	FAR	C6-C7	2.50	1.58	1.50
2	D	401	FAR	C11-C12	2.38	1.58	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	FAR	C10-C8-C7	-3.91	113.65	123.68
2	D	401	FAR	C4-C3-C5	3.10	120.48	115.27
2	D	401	FAR	C9-C8-C7	2.86	126.91	121.12
2	D	401	FAR	C6-C5-C3	2.63	121.63	112.98
2	D	401	FAR	C10-C8-C9	2.43	119.36	115.27

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	401	FAR	C10-C8-C9-C11
2	D	401	FAR	C7-C8-C9-C11
2	D	401	FAR	C3-C5-C6-C7

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	401	FAR	4	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	258/343 (75%)	-0.28	10 (3%)	39 39	31, 41, 75, 120	0
1	B	332/343 (96%)	-0.04	21 (6%)	20 19	30, 45, 89, 122	0
1	C	261/343 (76%)	-0.39	1 (0%)	92 93	29, 44, 70, 108	0
1	D	291/343 (84%)	-0.22	11 (3%)	40 40	29, 42, 94, 132	0
All	All	1142/1372 (83%)	-0.22	43 (3%)	40 40	29, 43, 85, 132	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	299	TYR	5.4
1	A	190	TYR	5.3
1	B	304	GLY	5.1
1	D	316	ALA	4.6
1	B	261	ALA	4.5
1	B	277	GLU	4.3
1	D	314	LYS	4.1
1	B	-4	ASP	4.0
1	B	326	LYS	3.8
1	B	276	GLU	3.8
1	A	-5	VAL	3.8
1	A	164	GLY	3.5
1	B	274	LYS	3.5
1	A	189	ASP	3.4
1	D	317	PRO	3.4
1	D	315	ASP	3.3
1	B	194	GLY	3.2
1	B	302	GLY	3.2
1	B	163	GLU	3.1
1	A	163	GLU	3.0
1	B	322	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	265	ALA	2.9
1	B	273	TYR	2.8
1	B	197	ASP	2.8
1	B	303	GLY	2.7
1	A	131	ARG	2.7
1	D	321	LEU	2.7
1	C	-2	ASP	2.6
1	B	325	GLU	2.6
1	A	130	SER	2.5
1	D	319	GLU	2.5
1	B	305	LYS	2.4
1	B	190	TYR	2.3
1	A	162	GLY	2.3
1	D	207	GLY	2.3
1	A	191	ASP	2.3
1	A	95	ALA	2.3
1	D	251	VAL	2.2
1	B	314	LYS	2.2
1	D	288	VAL	2.2
1	D	286	LYS	2.2
1	B	300	ASP	2.2
1	B	131	ARG	2.1

## 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	FAR	D	401	15/15	0.84	0.33	56,76,93,98	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.