



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:23 PM GMT

PDB ID : 4I2N  
Title : Crystal structure of 31kD Heat Shock Protein, VcHsp31 from *Vibrio cholerae*  
Authors : Das, S.; Sen, U.  
Deposited on : 2012-11-22  
Resolution : 1.90 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

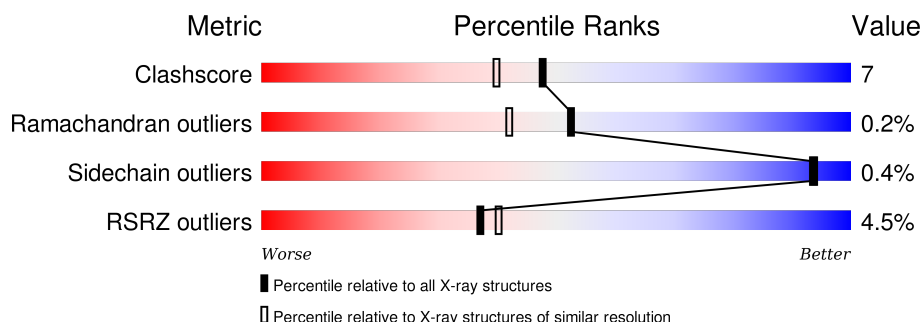
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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))
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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. 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	286	<div> <div>3%</div> <div>84%</div> <div>14%</div> <div>.</div> </div>
1	B	286	<div> <div>5%</div> <div>85%</div> <div>14%</div> <div>.</div> </div>
1	C	286	<div> <div>3%</div> <div>84%</div> <div>14%</div> <div>.</div> </div>
1	D	286	<div> <div>2%</div> <div>85%</div> <div>13%</div> <div>.</div> </div>
1	E	286	<div> <div>7%</div> <div>85%</div> <div>13%</div> <div>.</div> </div>
1	F	286	<div> <div>7%</div> <div>79%</div> <div>19%</div> <div>.</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MPD	A	301	-	-	X	X
2	MPD	B	301	-	-	-	X
2	MPD	D	301	-	-	X	X
2	MPD	E	301	-	-	-	X
2	MPD	F	301	-	-	X	X

## 2 Entry composition [i](#)

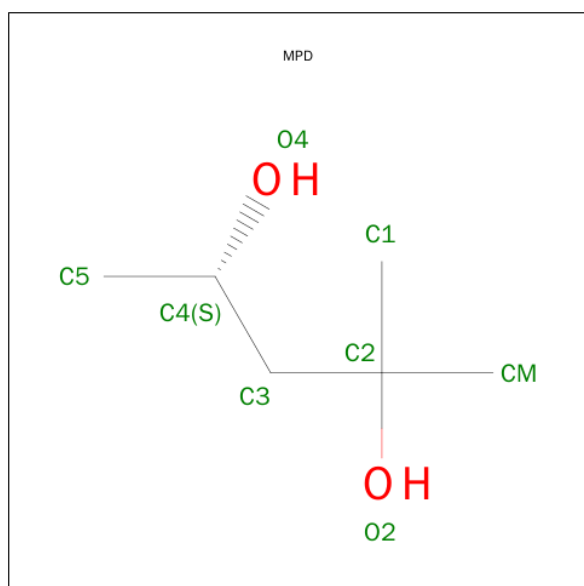
There are 4 unique types of molecules in this entry. The entry contains 14800 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Intracellular protease/amidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	281	Total	C	N	O	S	0	0	0
			2163	1390	352	411	10			
1	B	281	Total	C	N	O	S	0	0	0
			2163	1390	352	411	10			
1	C	281	Total	C	N	O	S	0	0	0
			2163	1390	352	411	10			
1	D	281	Total	C	N	O	S	0	0	0
			2163	1390	352	411	10			
1	E	281	Total	C	N	O	S	0	0	0
			2163	1390	352	411	10			
1	F	281	Total	C	N	O	S	0	0	0
			2163	1390	352	411	10			

- Molecule 2 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:  $C_6H_{14}O_2$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 8 6 2	0	0
2	B	1	Total C O 8 6 2	0	0
2	D	1	Total C O 8 6 2	0	0
2	E	1	Total C O 8 6 2	0	0
2	F	1	Total C O 8 6 2	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total Ca 1 1	0	0
3	E	1	Total Ca 1 1	0	0
3	B	1	Total Ca 1 1	0	0
3	C	1	Total Ca 1 1	0	0
3	A	1	Total Ca 1 1	0	0
3	F	1	Total Ca 1 1	0	0

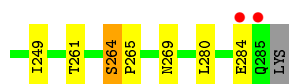
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	334	Total O 334 334	0	0
4	B	311	Total O 311 311	0	0
4	C	301	Total O 301 301	0	0
4	D	310	Total O 310 310	0	0
4	E	285	Total O 285 285	0	0
4	F	235	Total O 235 235	0	0

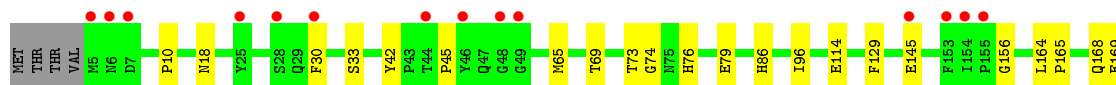
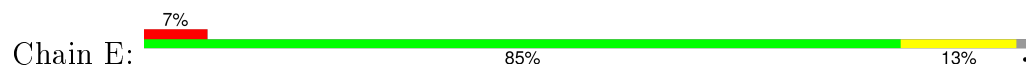


- Molecule 1: Intracellular protease/amidase

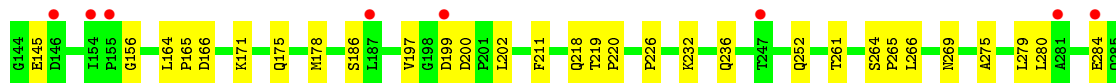
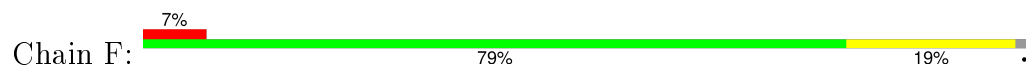




- Molecule 1: Intracellular protease/amidase



- Molecule 1: Intracellular protease/amidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.51Å 79.09Å 133.13Å 90.00° 95.22° 90.00°	Depositor
Resolution (Å)	29.54 – 1.90 29.54 – 1.90	Depositor EDS
% Data completeness (in resolution range)	94.7 (29.54-1.90) 94.8 (29.54-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.89 (at 1.91Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.187 , 0.223 0.193 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	22.6	Xtriage
Anisotropy	0.177	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 51.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 113579 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	14800	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.96% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: CA, MPD

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	0.33	0/2225	0.62	1/3023 (0.0%)
1	B	0.33	0/2225	0.62	1/3023 (0.0%)
1	C	0.33	0/2225	0.61	0/3023
1	D	0.33	0/2225	0.63	1/3023 (0.0%)
1	E	0.31	0/2225	0.59	0/3023
1	F	0.32	0/2225	0.58	0/3023
All	All	0.32	0/13350	0.61	3/18138 (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	D	6	ASN	N-CA-C	-6.83	92.55	111.00
1	A	157	GLY	N-CA-C	-5.12	100.30	113.10
1	B	157	GLY	N-CA-C	-5.04	100.51	113.10

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	2163	0	2072	36	0
1	B	2163	0	2072	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2163	0	2072	31	0
1	D	2163	0	2072	27	0
1	E	2163	0	2072	28	0
1	F	2163	0	2072	48	1
2	A	8	0	14	7	0
2	B	8	0	14	1	0
2	D	8	0	14	6	0
2	E	8	0	14	4	0
2	F	8	0	14	10	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	334	0	0	2	0
4	B	311	0	0	6	0
4	C	301	0	0	3	1
4	D	310	0	0	3	0
4	E	285	0	0	4	0
4	F	235	0	0	6	0
All	All	14800	0	12502	189	1

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 7.

All (189) 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:178:MET:HG3	1:A:202:LEU:HD21	1.29	1.08
1:F:265:PRO:HD2	2:F:301:MPD:H12	1.38	1.00
1:F:265:PRO:HD2	2:F:301:MPD:C1	1.99	0.91
1:F:266:LEU:HD21	2:F:301:MPD:H51	1.53	0.90
1:F:265:PRO:CD	2:F:301:MPD:H12	2.10	0.81
1:F:211:PHE:HE1	2:F:301:MPD:H11	1.51	0.76
1:D:197:VAL:HG11	1:D:202:LEU:HD21	1.70	0.74
1:C:140:GLU:HB3	1:F:143:LEU:HB2	1.70	0.71
1:D:30:PHE:CD1	2:D:301:MPD:H11	2.27	0.69
1:D:264:SER:HB2	1:D:265:PRO:CD	2.21	0.69
1:E:30:PHE:CD1	2:E:301:MPD:H11	2.29	0.68
1:C:264:SER:HB2	1:C:265:PRO:CD	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:116:GLN:OE1	4:F:570:HOH:O	2.12	0.67
1:E:30:PHE:CE1	2:E:301:MPD:H11	2.30	0.67
1:F:265:PRO:CD	2:F:301:MPD:C1	2.72	0.66
1:C:135:LEU:O	1:C:139:ILE:HG12	1.94	0.66
1:E:30:PHE:HB3	2:E:301:MPD:H31	1.79	0.65
1:F:79:GLU:OE2	1:F:265:PRO:HG3	1.97	0.65
1:B:197:VAL:HG11	1:B:202:LEU:HD21	1.79	0.64
2:B:301:MPD:HM3	4:B:465:HOH:O	1.98	0.64
1:E:264:SER:HB2	1:E:265:PRO:CD	2.29	0.62
1:A:264:SER:HB2	1:A:265:PRO:CD	2.30	0.62
1:C:59:ASP:HB3	1:C:98:THR:HB	1.83	0.59
1:A:211:PHE:HE1	2:A:301:MPD:C1	2.16	0.59
1:D:249:ILE:CD1	2:D:301:MPD:HM1	2.32	0.58
1:F:280:LEU:O	1:F:284:GLU:HG3	2.04	0.58
1:A:136:SER:O	1:A:140:GLU:HG3	2.04	0.58
1:F:211:PHE:CE1	2:F:301:MPD:H11	2.36	0.58
1:C:214:GLU:HG2	4:C:682:HOH:O	2.04	0.58
1:F:264:SER:HB2	1:F:265:PRO:CD	2.33	0.58
1:C:79:GLU:OE2	1:C:265:PRO:HG3	2.03	0.57
1:D:264:SER:HB2	1:D:265:PRO:HD2	1.85	0.57
1:A:186:SER:O	1:A:261:THR:HA	2.04	0.57
1:D:42:TYR:OH	1:D:86:HIS:HD2	1.88	0.57
1:C:186:SER:O	1:C:261:THR:HA	2.04	0.56
1:A:178:MET:HG3	1:A:202:LEU:CD2	2.20	0.56
1:E:164:LEU:HB2	1:E:165:PRO:HD3	1.86	0.56
1:E:18:ASN:ND2	1:E:69:THR:HA	2.20	0.56
1:F:65:MET:HG3	1:F:226:PRO:HG2	1.88	0.56
1:B:264:SER:HB2	1:B:265:PRO:CD	2.35	0.56
1:E:145:GLU:HG3	4:E:619:HOH:O	2.05	0.55
1:F:197:VAL:HG11	1:F:202:LEU:HD21	1.89	0.55
1:B:140:GLU:HB3	4:B:519:HOH:O	2.06	0.55
1:B:86:HIS:HE1	1:B:269:ASN:OD1	1.89	0.54
1:E:79:GLU:OE1	1:E:156:GLY:HA3	2.08	0.54
1:B:52:LYS:HG2	1:B:93:SER:HB3	1.88	0.54
1:F:266:LEU:CD2	2:F:301:MPD:H51	2.31	0.54
1:C:277:LYS:HB3	1:C:277:LYS:NZ	2.23	0.54
1:B:186:SER:O	1:B:261:THR:HA	2.08	0.54
1:C:171:LYS:O	1:C:175:GLN:HG3	2.08	0.53
1:C:139:ILE:HD11	1:C:173:VAL:HG23	1.90	0.53
1:D:30:PHE:HD1	2:D:301:MPD:H11	1.73	0.53
1:C:52:LYS:HG2	1:C:93:SER:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:ASP:HB3	1:A:98:THR:HB	1.90	0.53
1:D:166:ASP:HB3	4:D:648:HOH:O	2.08	0.53
1:B:59:ASP:HB3	1:B:98:THR:HB	1.90	0.53
1:E:264:SER:HB2	1:E:265:PRO:HD2	1.90	0.52
1:F:218:GLN:HG2	4:F:585:HOH:O	2.08	0.52
1:F:76:HIS:HD2	1:F:79:GLU:H	1.58	0.52
1:D:59:ASP:HB3	1:D:98:THR:HB	1.91	0.52
1:A:42:TYR:OH	1:A:86:HIS:HD2	1.93	0.51
1:A:211:PHE:CE1	2:A:301:MPD:H13	2.45	0.51
1:C:264:SER:HB2	1:C:265:PRO:HD2	1.92	0.51
1:E:280:LEU:O	1:E:284:GLU:HG2	2.11	0.51
1:D:249:ILE:HD12	2:D:301:MPD:HM1	1.92	0.51
1:C:42:TYR:OH	1:C:86:HIS:HD2	1.93	0.51
1:D:235:GLU:HA	1:D:238:GLN:HE21	1.76	0.51
1:D:186:SER:O	1:D:261:THR:HA	2.10	0.51
1:A:266:LEU:HD21	2:A:301:MPD:H51	1.93	0.51
1:B:65:MET:HG3	1:B:226:PRO:HG2	1.93	0.51
1:A:86:HIS:HE1	1:A:269:ASN:OD1	1.94	0.50
1:E:42:TYR:O	1:E:45:PRO:HD3	2.10	0.50
1:F:264:SER:HB2	1:F:265:PRO:HD2	1.92	0.50
1:A:65:MET:HG3	1:A:226:PRO:HG2	1.92	0.50
1:A:171:LYS:HG3	1:A:197:VAL:HA	1.93	0.50
1:E:65:MET:HG3	1:E:226:PRO:HG2	1.94	0.50
1:F:265:PRO:CG	2:F:301:MPD:H12	2.41	0.50
1:D:280:LEU:O	1:D:284:GLU:HG3	2.12	0.49
1:F:186:SER:O	1:F:261:THR:HA	2.13	0.49
1:C:137:ASP:OD1	1:F:145:GLU:HG3	2.12	0.49
1:A:199:ASP:OD1	1:C:50:ARG:HD2	2.12	0.49
1:C:143:LEU:HB2	1:F:140:GLU:HB3	1.93	0.49
1:D:197:VAL:HB	1:D:200:ASP:HB3	1.95	0.49
1:D:249:ILE:HD11	2:D:301:MPD:HM1	1.95	0.48
1:D:37:LEU:HD21	1:D:85:TYR:CE2	2.48	0.48
1:F:236:GLN:HG3	4:F:457:HOH:O	2.13	0.48
1:F:219:THR:N	1:F:220:PRO:CD	2.75	0.48
1:E:186:SER:O	1:E:261:THR:HA	2.13	0.48
1:D:86:HIS:HE1	1:D:269:ASN:OD1	1.97	0.48
1:A:136:SER:HB3	1:A:169:GLU:OE2	2.13	0.48
1:F:252:GLN:HG2	4:F:439:HOH:O	2.14	0.48
1:F:18:ASN:ND2	1:F:69:THR:HA	2.29	0.48
1:A:202:LEU:HD23	1:A:202:LEU:C	2.35	0.48
1:A:253:VAL:HG12	1:A:262:GLY:HA2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:86:HIS:HE1	1:F:269:ASN:OD1	1.96	0.47
1:C:164:LEU:HB2	1:C:165:PRO:HD3	1.96	0.47
1:A:264:SER:HB2	1:A:265:PRO:HD2	1.96	0.47
4:C:597:HOH:O	1:E:168:GLN:HG2	2.15	0.47
1:A:79:GLU:OE2	1:A:265:PRO:HG3	2.15	0.47
1:D:143:LEU:O	1:D:147:SER:HB2	2.15	0.47
1:B:164:LEU:HB2	1:B:165:PRO:HD3	1.96	0.47
1:E:30:PHE:CE2	1:E:222:ILE:HD11	2.50	0.47
1:C:52:LYS:HD2	4:C:522:HOH:O	2.13	0.47
1:F:164:LEU:HB2	1:F:165:PRO:HD3	1.97	0.47
1:C:73:THR:OG1	1:C:74:GLY:N	2.48	0.47
1:D:30:PHE:CD1	2:D:301:MPD:C1	2.97	0.46
4:B:710:HOH:O	1:F:284:GLU:HG3	2.15	0.46
1:A:17:ASP:HA	4:A:604:HOH:O	2.16	0.46
1:A:211:PHE:CE1	2:A:301:MPD:C1	2.97	0.46
1:F:199:ASP:HB2	4:F:604:HOH:O	2.14	0.46
1:F:79:GLU:OE1	1:F:156:GLY:HA3	2.15	0.46
1:B:73:THR:OG1	1:B:74:GLY:N	2.48	0.46
1:B:141:THR:HG22	4:B:656:HOH:O	2.16	0.46
1:B:5:MET:CB	1:B:9:HIS:CE1	2.99	0.46
1:C:65:MET:HG3	1:C:226:PRO:HG2	1.96	0.46
1:E:73:THR:OG1	1:E:74:GLY:N	2.48	0.46
1:A:140:GLU:HG3	4:A:569:HOH:O	2.16	0.45
1:B:234:GLY:O	1:B:238:GLN:HG3	2.15	0.45
1:B:76:HIS:HE1	4:B:418:HOH:O	2.00	0.45
1:A:73:THR:OG1	1:A:74:GLY:N	2.47	0.45
1:E:171:LYS:O	1:E:175:GLN:HG3	2.16	0.45
1:C:5:MET:O	1:C:6:ASN:ND2	2.49	0.45
1:F:171:LYS:O	1:F:175:GLN:HG3	2.16	0.45
1:E:86:HIS:HE1	1:E:269:ASN:OD1	2.00	0.45
1:B:6:ASN:HB3	1:B:8:LYS:H	1.82	0.44
1:B:136:SER:HB3	1:B:169:GLU:OE2	2.17	0.44
1:A:211:PHE:HE1	2:A:301:MPD:H13	1.81	0.44
1:F:73:THR:OG1	1:F:74:GLY:N	2.51	0.44
1:C:79:GLU:OE1	1:C:156:GLY:HA3	2.17	0.44
1:A:178:MET:CG	1:A:202:LEU:HD21	2.22	0.44
1:F:219:THR:OG1	1:F:220:PRO:HD3	2.18	0.44
1:A:266:LEU:HD11	2:A:301:MPD:H51	1.99	0.44
1:C:274:LEU:HD12	1:C:277:LYS:NZ	2.32	0.44
1:A:259:MET:C	1:A:260:LEU:HD12	2.39	0.44
1:D:65:MET:HG3	1:D:226:PRO:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:SER:CB	1:A:265:PRO:CD	2.95	0.43
4:E:533:HOH:O	1:F:14:PRO:HG2	2.18	0.43
1:A:200:ASP:C	1:A:202:LEU:H	2.21	0.43
1:E:264:SER:CB	1:E:265:PRO:CD	2.97	0.43
1:B:30:PHE:CE2	1:B:222:ILE:HD11	2.53	0.43
1:C:139:ILE:HD11	1:C:173:VAL:CG2	2.48	0.43
1:A:265:PRO:HD2	2:A:301:MPD:H12	2.00	0.43
1:F:76:HIS:CD2	1:F:78:VAL:HB	2.53	0.43
1:B:6:ASN:C	1:B:8:LYS:H	2.20	0.43
1:D:164:LEU:HB2	1:D:165:PRO:HD3	2.01	0.43
1:F:78:VAL:HG13	1:F:82:LEU:HD13	2.00	0.43
1:C:204:ALA:HA	1:C:241:GLY:HA3	2.01	0.43
1:E:96:ILE:HD13	1:E:129:PHE:CD1	2.54	0.43
1:E:10:PRO:HB3	4:E:421:HOH:O	2.18	0.42
1:D:73:THR:OG1	1:D:74:GLY:N	2.52	0.42
1:F:178:MET:HG3	1:F:202:LEU:HD12	2.02	0.42
1:D:44:THR:HG23	4:D:615:HOH:O	2.19	0.42
1:B:236:GLN:HG3	4:B:510:HOH:O	2.19	0.42
1:A:76:HIS:CE1	1:A:78:VAL:HB	2.55	0.42
1:F:53:ILE:HB	1:F:94:PHE:CD1	2.54	0.42
1:C:168:GLN:HE22	1:C:171:LYS:HD3	1.85	0.42
1:F:211:PHE:CE1	2:F:301:MPD:C1	3.02	0.42
1:D:66:ASP:OD2	1:D:228:HIS:HB2	2.20	0.42
1:A:79:GLU:OE1	1:A:156:GLY:HA3	2.20	0.42
1:C:76:HIS:CD2	1:C:78:VAL:H	2.38	0.42
1:F:59:ASP:HB3	1:F:98:THR:HB	2.02	0.42
1:E:76:HIS:HE1	4:E:509:HOH:O	2.03	0.42
1:F:232:LYS:O	1:F:236:GLN:HG2	2.20	0.41
1:D:121:LEU:C	1:D:121:LEU:HD13	2.41	0.41
1:E:33:SER:HB2	1:E:114:GLU:HG3	2.02	0.41
1:B:200:ASP:OD2	1:B:202:LEU:HD22	2.20	0.41
1:F:171:LYS:HG3	1:F:197:VAL:HA	2.02	0.41
1:A:42:TYR:HA	1:A:43:PRO:HD2	1.85	0.41
1:E:42:TYR:OH	1:E:86:HIS:HD2	2.03	0.41
1:F:275:ALA:O	1:F:279:LEU:HD13	2.20	0.41
1:D:219:THR:N	1:D:220:PRO:CD	2.83	0.41
1:A:103:PRO:HB3	1:A:130:ARG:O	2.20	0.41
1:F:115:ASP:HA	4:F:568:HOH:O	2.20	0.41
1:A:53:ILE:HD13	1:A:87:LEU:HD13	2.02	0.41
1:E:30:PHE:CE1	2:E:301:MPD:C1	3.02	0.41
1:E:190:GLY:N	1:E:191:PRO:CD	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:197:VAL:HB	1:F:200:ASP:HB3	2.02	0.41
1:C:76:HIS:HD2	1:C:78:VAL:H	1.67	0.41
1:D:205:GLY:HA2	4:D:540:HOH:O	2.21	0.41
1:C:171:LYS:HG3	1:C:197:VAL:HA	2.02	0.40
1:C:13:ASP:HA	1:C:21:PHE:CE2	2.56	0.40
1:B:219:THR:N	1:B:220:PRO:CD	2.84	0.40
1:E:169:GLU:O	1:E:173:VAL:HG23	2.22	0.40
1:B:13:ASP:HA	1:B:21:PHE:CE2	2.57	0.40
1:A:164:LEU:HB2	1:A:165:PRO:HD3	2.03	0.40
1:F:46:TYR:O	1:F:91:GLY:HA3	2.20	0.40
1:C:42:TYR:O	1:C:45:PRO:HD3	2.21	0.40
1:F:75:ASN:HD22	1:F:75:ASN:HA	1.78	0.40
1:E:219:THR:N	1:E:220:PRO:CD	2.85	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:116:GLN:NE2	4:C:526:HOH:O[1_565]	2.17	0.03

## 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	279/286 (98%)	270 (97%)	8 (3%)	1 (0%)	39	27
1	B	279/286 (98%)	270 (97%)	9 (3%)	0	100	100
1	C	279/286 (98%)	268 (96%)	10 (4%)	1 (0%)	39	27
1	D	279/286 (98%)	269 (96%)	9 (3%)	1 (0%)	39	27
1	E	279/286 (98%)	269 (96%)	10 (4%)	0	100	100
1	F	279/286 (98%)	268 (96%)	11 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1674/1716 (98%)	1614 (96%)	57 (3%)	3 (0%)	52	42

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	6	ASN
1	A	264	SER
1	D	264	SER

### 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	226/233 (97%)	226 (100%)	0	100	100
1	B	226/233 (97%)	225 (100%)	1 (0%)	93	94
1	C	226/233 (97%)	225 (100%)	1 (0%)	93	94
1	D	226/233 (97%)	226 (100%)	0	100	100
1	E	226/233 (97%)	226 (100%)	0	100	100
1	F	226/233 (97%)	223 (99%)	3 (1%)	76	73
All	All	1356/1398 (97%)	1351 (100%)	5 (0%)	93	94

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	252	GLN
1	C	117	GLU
1	F	7	ASP
1	F	113	ARG
1	F	166	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:



Mol	Chain	Res	Type
1	A	86	HIS
1	A	102	ASN
1	B	9	HIS
1	B	76	HIS
1	B	86	HIS
1	B	102	ASN
1	B	252	GLN
1	C	6	ASN
1	C	76	HIS
1	C	86	HIS
1	C	102	ASN
1	C	168	GLN
1	C	252	GLN
1	D	18	ASN
1	D	76	HIS
1	D	86	HIS
1	D	102	ASN
1	D	238	GLN
1	E	18	ASN
1	E	47	GLN
1	E	76	HIS
1	E	86	HIS
1	E	168	GLN
1	E	180	GLN
1	F	18	ASN
1	F	76	HIS
1	F	86	HIS

### 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

Of 11 ligands modelled in this entry, 6 are monoatomic - leaving 5 for Mogul analysis.

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	MPD	A	301	-	6,7,7	0.36	0	7,10,10	0.93	0
2	MPD	B	301	-	6,7,7	0.39	0	7,10,10	0.64	0
2	MPD	D	301	-	6,7,7	0.47	0	7,10,10	0.38	0
2	MPD	E	301	-	6,7,7	0.70	0	7,10,10	0.51	0
2	MPD	F	301	-	6,7,7	0.49	0	7,10,10	0.74	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	MPD	A	301	-	-	0/5/5/5	0/0/0/0
2	MPD	B	301	-	-	0/5/5/5	0/0/0/0
2	MPD	D	301	-	-	0/5/5/5	0/0/0/0
2	MPD	E	301	-	-	0/5/5/5	0/0/0/0
2	MPD	F	301	-	-	0/5/5/5	0/0/0/0

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.

5 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	MPD	7	0
2	B	301	MPD	1	0
2	D	301	MPD	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	301	MPD	4	0
2	F	301	MPD	10	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	281/286 (98%)	0.15	9 (3%)	51 54	13, 19, 30, 48	0
1	B	281/286 (98%)	0.17	13 (4%)	36 39	13, 18, 31, 63	0
1	C	281/286 (98%)	0.18	8 (2%)	56 60	14, 20, 33, 59	0
1	D	281/286 (98%)	0.05	5 (1%)	71 74	13, 19, 32, 61	0
1	E	281/286 (98%)	0.42	20 (7%)	19 21	16, 24, 39, 67	0
1	F	281/286 (98%)	0.56	21 (7%)	17 19	16, 25, 47, 63	0
All	All	1686/1716 (98%)	0.25	76 (4%)	37 40	13, 21, 38, 67	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	5	MET	11.5
1	D	285	GLN	7.3
1	D	5	MET	6.0
1	B	285	GLN	5.8
1	E	5	MET	5.7
1	B	5	MET	5.7
1	D	6	ASN	5.3
1	C	6	ASN	5.3
1	E	283	VAL	4.0
1	F	9	HIS	4.0
1	E	6	ASN	4.0
1	F	43	PRO	3.8
1	E	285	GLN	3.6
1	F	247	THR	3.6
1	E	44	THR	3.5
1	E	284	GLU	3.5
1	D	284	GLU	3.4
1	A	153	PHE	3.4
1	F	44	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	E	48	GLY	3.3
1	F	116	GLN	3.2
1	F	5	MET	3.2
1	F	6	ASN	3.1
1	A	141	THR	3.0
1	B	154	ILE	2.9
1	C	55	VAL	2.9
1	A	6	ASN	2.8
1	E	145	GLU	2.8
1	E	153	PHE	2.8
1	F	114	GLU	2.7
1	F	199	ASP	2.7
1	E	199	ASP	2.7
1	F	146	ASP	2.7
1	A	185	ILE	2.6
1	A	154	ILE	2.6
1	E	154	ILE	2.6
1	B	141	THR	2.6
1	F	33	SER	2.6
1	E	46	TYR	2.6
1	B	6	ASN	2.6
1	B	155	PRO	2.5
1	A	187	LEU	2.5
1	F	113	ARG	2.5
1	E	187	LEU	2.5
1	B	153	PHE	2.5
1	C	154	ILE	2.5
1	C	284	GLU	2.5
1	F	7	ASP	2.4
1	B	185	ILE	2.4
1	C	155	PRO	2.4
1	F	284	GLU	2.4
1	B	284	GLU	2.3
1	B	184	ILE	2.3
1	E	155	PRO	2.3
1	E	28	SER	2.3
1	E	30	PHE	2.3
1	F	154	ILE	2.3
1	B	55	VAL	2.3
1	C	153	PHE	2.3
1	F	155	PRO	2.3
1	F	281	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	29	GLN	2.3
1	A	25	TYR	2.3
1	E	7	ASP	2.2
1	A	55	VAL	2.2
1	F	32	ALA	2.2
1	B	199	ASP	2.2
1	F	41	HIS	2.2
1	F	187	LEU	2.1
1	C	199	ASP	2.1
1	E	25	TYR	2.1
1	E	49	GLY	2.1
1	D	24	ALA	2.0
1	E	185	ILE	2.0
1	A	5	MET	2.0
1	B	146	ASP	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	MPD	F	301	8/8	0.73	0.47	14.47	47,48,49,49	0
2	MPD	D	301	8/8	0.79	0.34	10.43	43,43,44,46	0
2	MPD	A	301	8/8	0.74	0.21	6.02	42,44,45,46	0
2	MPD	E	301	8/8	0.68	0.32	4.34	40,42,44,45	0
2	MPD	B	301	8/8	0.83	0.21	3.05	38,39,42,43	0
3	CA	C	301	1/1	0.96	0.08	-1.62	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CA	B	302	1/1	0.99	0.06	-2.37	23,23,23,23	0
3	CA	E	302	1/1	1.00	0.07	-2.59	31,31,31,31	0
3	CA	A	302	1/1	0.99	0.05	-3.68	26,26,26,26	0
3	CA	F	302	1/1	0.98	0.04	-4.18	35,35,35,35	0
3	CA	D	302	1/1	0.99	0.04	-4.71	28,28,28,28	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.