



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 09:20 AM GMT

PDB ID : 4AED  
Title : Crystal structure of Human enterovirus 71  
Authors : Plevka, P.; Perera, R.; Kuhn, R.J.; Rossmann, M.G.  
Deposited on : 2012-01-09  
Resolution : 3.80 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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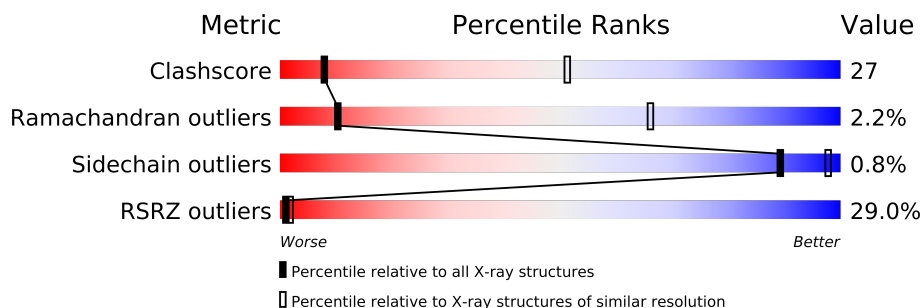
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.80 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	79885	1100 (4.10-3.50)
Ramachandran outliers	78287	1050 (4.10-3.50)
Sidechain outliers	78261	1042 (4.10-3.50)
RSRZ outliers	66119	1163 (4.20-3.40)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	297	
2	B	254	
3	C	242	
4	D	69	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
5	DAO	A	1289	-	X
6	CA	C	1243	-	X
6	CA	C	1244	-	X
6	CA	C	1245	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6471 atoms, of which 0 are hydrogen and 0 are deuterium.

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 VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	0	0	0
			2299	1447	394	445	13			

- Molecule 2 is a protein called VP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	236	Total	C	N	O	S	0	0	0
			1844	1184	305	346	9			

- Molecule 3 is a protein called VP3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	242	Total	C	N	O	S	0	0	0
			1866	1198	311	345	12			

- Molecule 4 is a protein called VP4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	57	Total	C	N	O	S	0	0	0
			443	276	72	94	1			

- Molecule 5 is LAURIC ACID (three-letter code: DAO) (formula: C<sub>12</sub>H<sub>24</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			14	12	2		

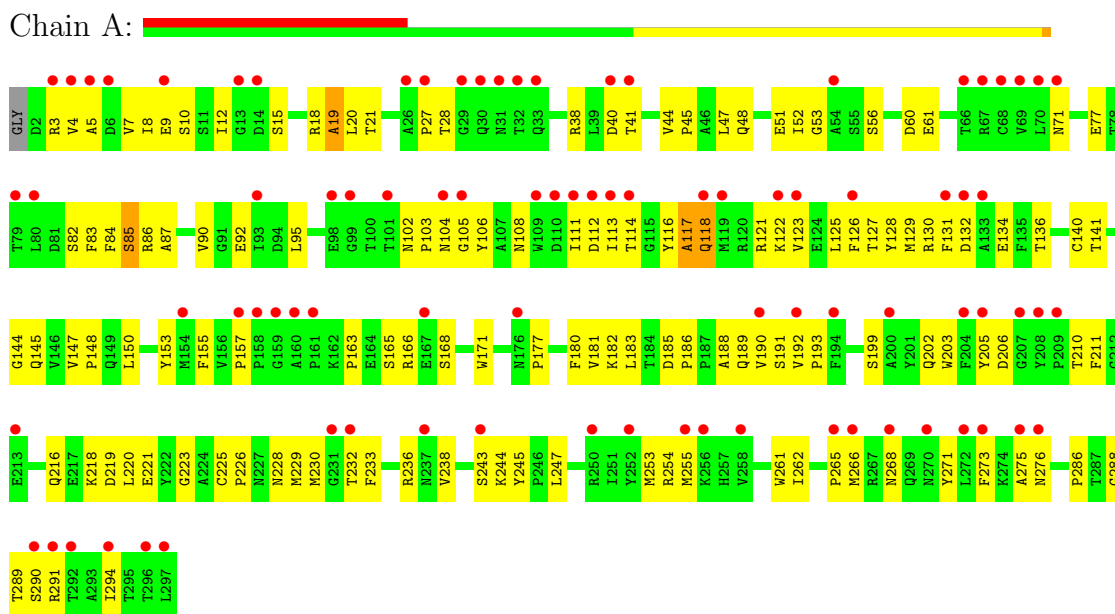
- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	2	Total	Ca	0	0
			2	2		
6	C	3	Total	Ca	0	0
			3	3		

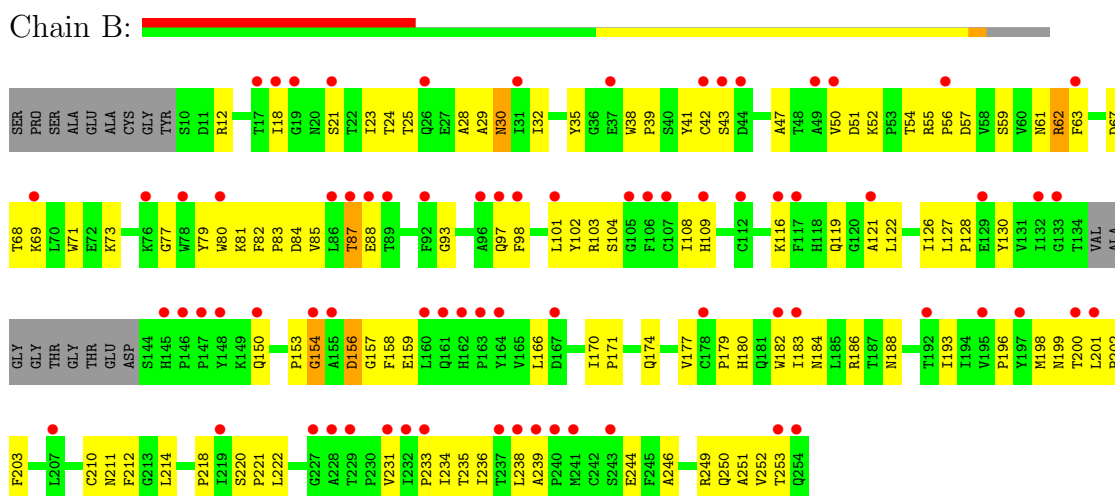
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: VP1

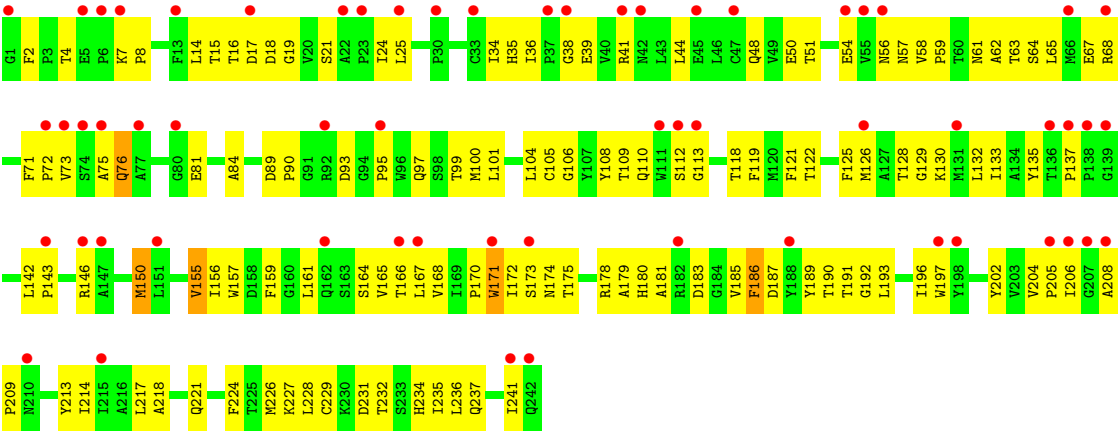


#### • Molecule 2: VP2



#### • Molecule 3: VP3





● Molecule 4: VP4

Chain D:



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	600.20Å 610.60Å 851.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.80 49.64 – 3.80	Depositor EDS
% Data completeness (in resolution range)	31.7 (50.00-3.80) 29.9 (49.64-3.80)	Depositor EDS
$R_{merge}$	0.24	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.33 (at 3.77Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, $R_{free}$	0.279 , (Not available) 0.323 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	58.5	Xtriage
Anisotropy	0.899	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 69.4	EDS
Estimated twinning fraction	0.023 for -1/2*h+1/2*k+1/2*l,1/2*h-1/2*k +1/2*l,h+k 0.025 for -1/2*h+1/2*k-1/2*l,1/2*h-1/2*k- 1/2*l,-h-k 0.064 for k,h,-l 0.000 for -1/2*h-1/2*k+1/2*l,-1/2*h-1/2*k- 1/2*l,h-k 0.014 for -1/2*h-1/2*k-1/2*l,-1/2*h-1/2*k+ 1/2*l,-h+k	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	0 of 459076 reflections	Xtriage
$F_o, F_c$ correlation	0.74	EDS
Total number of atoms	6471	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.93% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	0.27	0/2358	0.50	0/3213
2	B	0.26	0/1898	0.50	0/2600
3	C	0.27	0/1920	0.50	0/2626
4	D	0.29	0/452	0.52	0/611
All	All	0.27	0/6628	0.50	0/9050

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2299	0	2231	132	0
2	B	1844	0	1784	109	0
3	C	1866	0	1837	138	0
4	D	443	0	420	28	0
5	A	14	0	23	1	0
6	B	2	0	0	0	0
6	C	3	0	0	0	0
All	All	6471	0	6295	344	0



Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 27.

All (344) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:41:ARG:HH22	4:D:24:THR:HG21	1.24	1.01
2:B:83:PRO:HG2	2:B:211:ASN:H	1.27	0.96
1:A:268:ASN:HB2	2:B:171:PRO:HD3	1.49	0.93
3:C:38:GLY:HA2	4:D:52:LYS:HD3	1.57	0.87
1:A:48:GLN:HA	4:D:67:PRO:HG2	1.57	0.86
3:C:75:ALA:HA	3:C:202:TYR:HB3	1.59	0.84
2:B:183:ILE:HA	2:B:188:ASN:HD21	1.43	0.83
3:C:206:ILE:HG13	3:C:206:ILE:O	1.77	0.82
2:B:83:PRO:HG2	2:B:211:ASN:N	1.94	0.81
2:B:57:ASP:HA	2:B:61:ASN:HD22	1.44	0.81
3:C:228:LEU:HG	3:C:229:CYS:H	1.45	0.80
2:B:186:ARG:HH11	3:C:121:PHE:HD2	1.29	0.79
3:C:232:THR:HG22	3:C:234:HIS:H	1.44	0.79
1:A:112:ASP:OD1	1:A:114:THR:HG22	1.82	0.79
3:C:108:TYR:HA	3:C:229:CYS:HA	1.65	0.79
4:D:13:HIS:O	4:D:14:GLU:HB2	1.81	0.77
3:C:48:GLN:HG3	4:D:50:PRO:HB3	1.65	0.76
1:A:230:MET:HG3	5:A:1289:DAO:H102	1.69	0.74
1:A:150:LEU:HD23	1:A:238:VAL:HG21	1.67	0.74
4:D:31:ASN:HB2	4:D:39:ALA:HB2	1.69	0.74
2:B:54:THR:HG22	2:B:56:PRO:HD3	1.69	0.74
2:B:82:PHE:HE1	2:B:214:LEU:HB2	1.54	0.72
1:A:189:GLN:HG3	3:C:21:SER:HB3	1.72	0.72
2:B:62:ARG:HB2	2:B:62:ARG:NH1	2.05	0.71
3:C:142:LEU:HD12	3:C:143:PRO:HD2	1.71	0.71
3:C:58:VAL:HB	3:C:59:PRO:HD3	1.74	0.70
2:B:62:ARG:HH11	2:B:62:ARG:HB2	1.56	0.69
4:D:16:SER:HB3	4:D:21:GLU:OE2	1.91	0.69
1:A:243:SER:O	1:A:244:LYS:HB3	1.91	0.69
3:C:109:THR:HB	3:C:228:LEU:HD23	1.73	0.69
1:A:273:PHE:HB2	1:A:276:ASN:HB3	1.74	0.69
1:A:87:ALA:HB3	3:C:15:THR:HG23	1.75	0.68
1:A:21:THR:HG22	4:D:49:ASP:OD1	1.93	0.68
1:A:254:ARG:HH22	3:C:19:GLY:H	1.41	0.68
1:A:121:ARG:HH11	1:A:121:ARG:HG2	1.57	0.67
3:C:174:ASN:OD1	3:C:175:THR:HG23	1.94	0.67
1:A:262:ILE:H	1:A:262:ILE:HD12	1.60	0.67
2:B:183:ILE:HA	2:B:188:ASN:ND2	2.10	0.67
1:A:86:ARG:HG2	3:C:16:THR:HG22	1.76	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:226:PRO:HA	1:A:229:MET:HG2	1.77	0.66
1:A:291:ARG:HD3	3:C:57:ASN:OD1	1.96	0.66
4:D:61:PHE:O	4:D:62:THR:HB	1.97	0.64
1:A:86:ARG:NH1	3:C:16:THR:HG21	2.13	0.64
3:C:105:CYS:HB3	3:C:180:HIS:CE1	2.33	0.64
2:B:67:ASP:OD2	2:B:69:LYS:HE2	1.98	0.64
1:A:294:ILE:HG22	3:C:56:ASN:HA	1.78	0.64
1:A:192:VAL:HG22	3:C:24:ILE:HD13	1.80	0.63
1:A:86:ARG:HH11	3:C:16:THR:HG21	1.62	0.63
1:A:262:ILE:N	1:A:262:ILE:HD12	2.14	0.63
3:C:56:ASN:O	3:C:68:ARG:HA	1.99	0.62
1:A:265:PRO:HG3	2:B:174:GLN:O	1.98	0.62
4:D:25:ILE:HG23	4:D:45:SER:HB3	1.81	0.62
1:A:268:ASN:HB2	2:B:171:PRO:CD	2.26	0.62
1:A:18:ARG:HB2	2:B:38:TRP:HB2	1.81	0.62
3:C:54:GLU:O	3:C:95:PRO:HB3	2.00	0.61
1:A:286:PRO:HB3	3:C:68:ARG:CZ	2.30	0.61
3:C:24:ILE:HG13	3:C:25:LEU:HG	1.82	0.61
1:A:288:GLY:CA	3:C:97:GLN:HG2	2.30	0.61
1:A:114:THR:HG21	1:A:275:ALA:N	2.15	0.61
1:A:193:PRO:HB3	4:D:37:TYR:CD2	2.36	0.61
1:A:226:PRO:HA	1:A:229:MET:CG	2.31	0.61
2:B:83:PRO:HG2	2:B:210:CYS:HA	1.81	0.61
3:C:61:ASN:O	3:C:62:ALA:HB3	2.01	0.61
2:B:82:PHE:CE1	2:B:214:LEU:HB2	2.34	0.60
1:A:288:GLY:HA3	3:C:97:GLN:HG2	1.84	0.60
2:B:73:LYS:HG2	2:B:222:LEU:O	2.02	0.60
1:A:261:TRP:CE3	3:C:36:ILE:HB	2.37	0.60
3:C:109:THR:CB	3:C:228:LEU:HD23	2.32	0.60
3:C:126:MET:HB3	3:C:205:PRO:HG2	1.84	0.59
3:C:112:SER:O	3:C:224:PHE:HA	2.02	0.59
1:A:44:VAL:HB	1:A:47:LEU:HB2	1.84	0.59
1:A:15:SER:HB2	2:B:43:SER:OG	2.03	0.59
3:C:181:ALA:HA	3:C:186:PHE:O	2.02	0.59
3:C:132:LEU:HD11	3:C:150:MET:HB3	1.83	0.59
4:D:17:ASN:O	4:D:37:TYR:HB3	2.02	0.59
2:B:231:VAL:O	2:B:233:PRO:HD3	2.02	0.59
1:A:132:ASP:OD1	1:A:193:PRO:HA	2.03	0.59
2:B:32:ILE:HD12	2:B:180:HIS:O	2.02	0.59
1:A:266:MET:O	2:B:171:PRO:HD2	2.02	0.59
1:A:125:LEU:HD23	1:A:266:MET:SD	2.43	0.58
2:B:67:ASP:OD2	2:B:156:ASP:HA	2.03	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:18:SER:O	4:D:20:THR:N	2.37	0.58
2:B:127:LEU:HD23	2:B:130:TYR:CD1	2.38	0.58
2:B:57:ASP:HA	2:B:61:ASN:ND2	2.17	0.58
2:B:184:ASN:HD21	3:C:122:THR:HA	1.67	0.58
1:A:147:VAL:O	1:A:183:LEU:HB2	2.03	0.58
2:B:18:ILE:HG22	2:B:61:ASN:O	2.04	0.57
1:A:125:LEU:HD13	1:A:125:LEU:O	2.05	0.57
2:B:24:THR:HG22	2:B:25:THR:N	2.19	0.57
3:C:112:SER:HA	3:C:171:TRP:CZ3	2.40	0.57
1:A:294:ILE:CG2	3:C:56:ASN:HA	2.35	0.57
1:A:51:GLU:HA	2:B:182:TRP:HB2	1.87	0.57
1:A:95:LEU:HD23	1:A:102:ASN:HB3	1.87	0.56
1:A:191:SER:HB3	3:C:21:SER:OG	2.06	0.56
2:B:81:LYS:HE2	2:B:130:TYR:HD2	1.68	0.56
1:A:117:ALA:HB2	3:C:237:GLN:HG3	1.87	0.56
4:D:61:PHE:O	4:D:62:THR:CB	2.53	0.56
1:A:48:GLN:CA	4:D:67:PRO:HG2	2.34	0.56
3:C:64:SER:HB3	3:C:67:GLU:OE2	2.06	0.56
3:C:156:ILE:N	3:C:156:ILE:HD12	2.21	0.55
1:A:147:VAL:HG11	1:A:245:TYR:CG	2.41	0.55
2:B:249:ARG:HG3	2:B:249:ARG:HH11	1.72	0.55
1:A:206:ASP:OD2	2:B:210:CYS:HB2	2.07	0.55
2:B:87:THR:HG22	2:B:88:GLU:HG3	1.89	0.55
3:C:232:THR:HG22	3:C:234:HIS:N	2.20	0.55
2:B:62:ARG:HH11	2:B:62:ARG:CB	2.20	0.55
1:A:225:CYS:HB3	1:A:228:ASN:ND2	2.22	0.55
1:A:3:ARG:CB	1:A:8:ILE:HD11	2.37	0.54
3:C:185:VAL:C	3:C:187:ASP:H	2.09	0.54
1:A:216:GLN:HA	1:A:219:ASP:OD2	2.07	0.54
4:D:49:ASP:OD2	4:D:52:LYS:HB2	2.07	0.54
2:B:153:PRO:HG3	2:B:158:PHE:HB2	1.90	0.54
1:A:127:THR:HB	1:A:262:ILE:HB	1.88	0.54
3:C:18:ASP:OD2	4:D:40:THR:HB	2.08	0.54
2:B:122:LEU:HD21	2:B:218:PRO:HG3	1.88	0.54
1:A:126:PHE:HD2	1:A:129:MET:HE1	1.73	0.54
2:B:42:CYS:SG	2:B:47:ALA:HB2	2.48	0.54
3:C:34:ILE:HG22	3:C:35:HIS:N	2.23	0.54
2:B:98:PHE:CE1	2:B:251:ALA:HB2	2.41	0.54
1:A:56:SER:OG	3:C:166:THR:HG21	2.08	0.53
3:C:41:ARG:NH2	4:D:24:THR:HG21	2.08	0.53
2:B:81:LYS:HE2	2:B:130:TYR:CD2	2.43	0.53
1:A:134:GLU:HA	1:A:190:VAL:O	2.09	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:51:GLU:OE2	2:B:184:ASN:HB3	2.07	0.53
2:B:52:LYS:HG3	2:B:52:LYS:O	2.09	0.53
3:C:128:THR:HG22	3:C:129:GLY:N	2.23	0.53
2:B:32:ILE:HB	2:B:193:ILE:HD13	1.91	0.53
3:C:73:VAL:HG13	3:C:73:VAL:O	2.09	0.53
3:C:51:THR:HG21	3:C:100:MET:HB2	1.90	0.53
1:A:12:ILE:HG13	1:A:12:ILE:O	2.09	0.53
2:B:81:LYS:O	2:B:85:VAL:HG23	2.08	0.53
1:A:77:GLU:HA	1:A:82:SER:OG	2.09	0.53
2:B:77:GLY:O	2:B:159:GLU:HG3	2.09	0.52
3:C:75:ALA:HB2	3:C:202:TYR:HD2	1.75	0.52
1:A:123:VAL:HB	1:A:203:TRP:CZ2	2.44	0.52
3:C:232:THR:CG2	3:C:234:HIS:H	2.19	0.52
3:C:173:SER:HB2	3:C:178:ARG:CZ	2.39	0.52
1:A:5:ALA:O	1:A:9:GLU:HG2	2.09	0.52
1:A:262:ILE:H	1:A:262:ILE:CD1	2.23	0.52
1:A:118:GLN:HE22	3:C:231:ASP:HB3	1.74	0.52
1:A:114:THR:HG21	1:A:275:ALA:H	1.74	0.52
2:B:71:TRP:CE2	2:B:222:LEU:HB2	2.45	0.51
3:C:41:ARG:HH22	4:D:24:THR:CG2	2.11	0.51
1:A:155:PHE:CE2	1:A:157:PRO:HG3	2.46	0.51
2:B:67:ASP:CG	2:B:156:ASP:HA	2.30	0.51
2:B:41:TYR:HE2	2:B:55:ARG:HG2	1.76	0.51
1:A:238:VAL:HG23	1:A:238:VAL:O	2.11	0.51
1:A:153:TYR:HB3	1:A:233:PHE:HE1	1.76	0.51
2:B:71:TRP:HB2	2:B:234:ILE:HD11	1.92	0.51
3:C:110:GLN:HB2	3:C:227:LYS:HG2	1.93	0.51
1:A:236:ARG:HH11	1:A:236:ARG:HG3	1.76	0.51
1:A:121:ARG:NH1	1:A:121:ARG:HG2	2.25	0.50
3:C:157:TRP:CD2	3:C:165:VAL:HG11	2.47	0.50
3:C:161:LEU:N	3:C:161:LEU:HD12	2.26	0.50
1:A:48:GLN:HG3	1:A:56:SER:OG	2.10	0.50
2:B:101:LEU:HB3	2:B:203:PHE:HB3	1.93	0.50
1:A:136:THR:HA	1:A:188:ALA:O	2.10	0.50
3:C:161:LEU:H	3:C:161:LEU:HD12	1.75	0.50
2:B:83:PRO:CG	2:B:210:CYS:HA	2.42	0.50
1:A:53:GLY:HA3	2:B:32:ILE:HD11	1.92	0.50
1:A:199:SER:OG	3:C:34:ILE:HG13	2.12	0.50
1:A:140:CYS:SG	1:A:144:GLY:HA2	2.52	0.50
2:B:56:PRO:HB2	2:B:59:SER:OG	2.12	0.50
1:A:193:PRO:HD3	4:D:37:TYR:CE1	2.47	0.50
2:B:63:PHE:CD1	2:B:239:ALA:HB2	2.47	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:71:PHE:CE1	3:C:84:ALA:HB2	2.46	0.50
3:C:187:ASP:OD1	3:C:190:THR:HB	2.11	0.50
3:C:128:THR:HG22	3:C:129:GLY:H	1.77	0.50
1:A:141:THR:OG1	1:A:145:GLN:HB3	2.11	0.50
3:C:59:PRO:O	3:C:68:ARG:HD3	2.11	0.49
3:C:71:PHE:HB3	3:C:214:ILE:O	2.12	0.49
3:C:192:GLY:O	3:C:193:LEU:HD23	2.12	0.49
2:B:166:LEU:HD12	2:B:170:ILE:HG13	1.93	0.49
3:C:135:TYR:O	3:C:137:PRO:HD3	2.13	0.49
2:B:82:PHE:HB2	2:B:83:PRO:HD3	1.93	0.49
2:B:87:THR:HG22	2:B:88:GLU:N	2.27	0.49
1:A:92:GLU:HB3	1:A:116:TYR:OH	2.12	0.49
3:C:101:LEU:HD23	3:C:101:LEU:C	2.31	0.49
3:C:204:VAL:CG1	3:C:208:ALA:HB3	2.43	0.49
1:A:38:ARG:HG3	1:A:38:ARG:HH11	1.77	0.49
3:C:44:LEU:O	3:C:48:GLN:HG2	2.13	0.49
2:B:128:PRO:HA	2:B:212:PHE:HB3	1.94	0.49
1:A:19:ALA:O	1:A:20:LEU:HB2	2.13	0.49
2:B:29:ALA:O	2:B:30:ASN:CB	2.61	0.49
2:B:196:PRO:O	2:B:198:MET:HG3	2.13	0.49
1:A:85:SER:OG	1:A:254:ARG:HD3	2.13	0.48
1:A:155:PHE:HB3	1:A:177:PRO:HG2	1.94	0.48
2:B:79:TYR:HA	2:B:214:LEU:O	2.13	0.48
2:B:63:PHE:HA	2:B:239:ALA:HB2	1.95	0.48
1:A:18:ARG:CG	2:B:38:TRP:HB2	2.44	0.48
3:C:132:LEU:C	3:C:132:LEU:HD23	2.34	0.48
1:A:147:VAL:HG13	1:A:148:PRO:HD2	1.95	0.48
1:A:10:SER:HB3	1:A:12:ILE:HG12	1.94	0.48
2:B:108:ILE:HD13	2:B:126:ILE:HD11	1.96	0.48
3:C:93:ASP:HA	3:C:97:GLN:OE1	2.14	0.48
4:D:19:ALA:C	4:D:21:GLU:H	2.17	0.48
3:C:14:LEU:HB3	3:C:17:ASP:HB2	1.95	0.48
1:A:4:VAL:O	1:A:5:ALA:HB3	2.14	0.48
1:A:218:LYS:C	1:A:220:LEU:H	2.17	0.48
2:B:200:THR:HA	3:C:36:ILE:HD11	1.95	0.47
3:C:178:ARG:HD3	3:C:189:TYR:O	2.14	0.47
1:A:27:PRO:HG2	1:A:28:THR:H	1.79	0.47
3:C:228:LEU:HG	3:C:229:CYS:N	2.24	0.47
1:A:166:ARG:HH12	1:A:243:SER:N	2.11	0.47
1:A:105:GLY:HA3	1:A:166:ARG:HD2	1.96	0.47
1:A:60:ASP:OD1	3:C:168:VAL:HG11	2.14	0.47
1:A:171:TRP:CZ3	1:A:236:ARG:HG2	2.49	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:105:CYS:HB3	3:C:180:HIS:HE1	1.79	0.47
4:D:46:LEU:N	4:D:46:LEU:HD12	2.29	0.47
2:B:82:PHE:O	2:B:83:PRO:C	2.53	0.47
3:C:50:GLU:HB3	3:C:217:LEU:HB3	1.96	0.47
1:A:48:GLN:HA	4:D:67:PRO:CG	2.38	0.47
3:C:130:LYS:HA	3:C:157:TRP:O	2.14	0.47
3:C:159:PHE:CD1	3:C:159:PHE:N	2.83	0.47
1:A:52:ILE:O	2:B:32:ILE:HD11	2.15	0.47
3:C:161:LEU:CD1	3:C:161:LEU:H	2.28	0.47
3:C:100:MET:O	3:C:104:LEU:HG	2.15	0.46
3:C:119:PHE:HE2	3:C:133:ILE:HG21	1.79	0.46
3:C:228:LEU:CG	3:C:229:CYS:H	2.18	0.46
2:B:21:SER:OG	2:B:63:PHE:HB2	2.15	0.46
3:C:71:PHE:O	3:C:213:TYR:HA	2.15	0.46
2:B:116:LYS:HB3	3:C:125:PHE:HD2	1.81	0.46
2:B:202:PRO:HD3	3:C:34:ILE:CD1	2.45	0.46
2:B:202:PRO:HG2	2:B:203:PHE:H	1.80	0.46
2:B:12:ARG:O	2:B:28:ALA:HB3	2.15	0.46
2:B:174:GLN:O	2:B:177:VAL:HG22	2.15	0.46
2:B:252:VAL:HG12	2:B:253:THR:N	2.30	0.46
1:A:130:ARG:O	1:A:131:PHE:HB3	2.15	0.46
3:C:170:PRO:O	3:C:172:ILE:HG13	2.16	0.45
3:C:155:VAL:CG1	3:C:167:LEU:HD13	2.46	0.45
2:B:101:LEU:HB2	2:B:246:ALA:HB3	1.97	0.45
3:C:99:THR:HG21	3:C:218:ALA:HB3	1.97	0.45
2:B:93:GLY:O	2:B:97:GLN:HG3	2.15	0.45
3:C:173:SER:HB2	3:C:178:ARG:NH2	2.32	0.45
2:B:97:GLN:HB3	2:B:252:VAL:O	2.16	0.45
4:D:25:ILE:HB	4:D:27:TYR:CE1	2.52	0.45
3:C:76:GLN:HB3	3:C:81:GLU:OE2	2.16	0.45
1:A:189:GLN:HG3	3:C:21:SER:CB	2.44	0.45
3:C:235:ILE:O	3:C:236:LEU:HD23	2.16	0.45
1:A:18:ARG:CB	2:B:38:TRP:HB2	2.47	0.45
2:B:85:VAL:HA	2:B:154:GLY:HA2	1.99	0.45
2:B:23:ILE:HG21	2:B:109:HIS:CD2	2.52	0.45
3:C:61:ASN:O	3:C:62:ALA:CB	2.65	0.44
2:B:199:ASN:C	2:B:201:LEU:H	2.20	0.44
1:A:271:TYR:HB2	3:C:241:ILE:CD1	2.47	0.44
1:A:127:THR:N	1:A:262:ILE:O	2.47	0.44
1:A:165:SER:H	1:A:168:SER:HB2	1.81	0.44
3:C:146:ARG:HG3	3:C:197:TRP:HB2	1.99	0.44
3:C:97:GLN:NE2	3:C:234:HIS:ND1	2.65	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:103:ARG:HD3	2:B:244:GLU:OE1	2.17	0.44
2:B:153:PRO:O	2:B:154:GLY:C	2.55	0.44
1:A:262:ILE:HG23	2:B:35:TYR:OH	2.17	0.44
3:C:71:PHE:CD1	3:C:72:PRO:HD2	2.52	0.44
1:A:253:MET:HG2	1:A:254:ARG:N	2.33	0.44
1:A:18:ARG:O	1:A:19:ALA:HB3	2.17	0.44
3:C:113:GLY:HA3	3:C:224:PHE:HA	1.99	0.44
3:C:71:PHE:HD2	3:C:214:ILE:HB	1.82	0.44
3:C:118:THR:HA	3:C:166:THR:HA	2.00	0.44
1:A:288:GLY:HA2	3:C:97:GLN:HG2	1.99	0.43
2:B:41:TYR:CE2	2:B:55:ARG:HG2	2.53	0.43
1:A:111:ILE:HG13	1:A:232:THR:HA	2.00	0.43
2:B:50:VAL:HG23	2:B:50:VAL:O	2.18	0.43
1:A:40:ASP:OD1	1:A:41:THR:N	2.49	0.43
2:B:83:PRO:HB2	2:B:210:CYS:HA	2.00	0.43
1:A:106:TYR:CE2	1:A:165:SER:HA	2.52	0.43
3:C:62:ALA:HA	3:C:65:LEU:CD1	2.49	0.43
2:B:102:TYR:CE1	2:B:104:SER:HB3	2.53	0.43
2:B:150:GLN:HG3	2:B:158:PHE:CE2	2.53	0.43
3:C:51:THR:HG21	3:C:100:MET:CB	2.49	0.43
1:A:87:ALA:HA	1:A:253:MET:O	2.18	0.43
2:B:119:GLN:HG2	3:C:209:PRO:HG2	2.00	0.43
3:C:61:ASN:C	3:C:63:THR:H	2.21	0.43
1:A:103:PRO:O	1:A:104:ASN:HB2	2.18	0.43
1:A:205:TYR:O	1:A:223:GLY:HA2	2.19	0.43
1:A:171:TRP:CH2	1:A:236:ARG:HG2	2.54	0.43
1:A:28:THR:HB	1:A:71:ASN:O	2.19	0.43
2:B:121:ALA:HB3	2:B:220:SER:HB3	2.00	0.43
2:B:102:TYR:CD1	2:B:103:ARG:N	2.87	0.43
2:B:55:ARG:HG3	2:B:244:GLU:HG2	2.00	0.43
3:C:89:ASP:HA	3:C:90:PRO:HD3	1.85	0.43
1:A:181:VAL:HG12	1:A:182:LYS:N	2.33	0.43
2:B:83:PRO:CB	2:B:210:CYS:HA	2.49	0.42
1:A:261:TRP:HA	3:C:39:GLU:HA	1.99	0.42
1:A:289:THR:HG22	1:A:290:SER:N	2.34	0.42
3:C:7:LYS:HB3	3:C:8:PRO:HD2	2.00	0.42
1:A:254:ARG:NH2	3:C:19:GLY:H	2.13	0.42
3:C:171:TRP:CH2	3:C:178:ARG:HG3	2.54	0.42
3:C:191:THR:HG22	3:C:191:THR:O	2.19	0.42
1:A:180:PHE:N	1:A:180:PHE:CD1	2.88	0.42
1:A:61:GLU:OE1	1:A:61:GLU:N	2.51	0.42
3:C:224:PHE:CE1	3:C:226:MET:HG3	2.54	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:150:LEU:HD12	1:A:181:VAL:O	2.19	0.42
4:D:31:ASN:HB2	4:D:39:ALA:CB	2.45	0.42
1:A:210:THR:HG21	1:A:221:GLU:OE2	2.19	0.42
2:B:12:ARG:NH2	3:C:161:LEU:HB3	2.34	0.42
3:C:221:GLN:HA	3:C:221:GLN:OE1	2.20	0.42
3:C:183:ASP:O	3:C:187:ASP:HB2	2.20	0.42
3:C:206:ILE:CG1	3:C:206:ILE:O	2.57	0.42
3:C:106:GLY:HA3	3:C:234:HIS:CD2	2.54	0.42
1:A:128:TYR:CE1	1:A:202:GLN:HG3	2.54	0.42
1:A:286:PRO:HG3	3:C:65:LEU:HD21	2.02	0.42
2:B:80:TRP:HB3	2:B:85:VAL:HG21	2.01	0.42
1:A:117:ALA:O	1:A:118:GLN:C	2.57	0.42
3:C:119:PHE:O	3:C:164:SER:HA	2.20	0.42
1:A:45:PRO:HG3	4:D:64:MET:SD	2.60	0.42
2:B:24:THR:CG2	2:B:25:THR:N	2.83	0.42
2:B:87:THR:O	2:B:88:GLU:HB2	2.19	0.42
2:B:32:ILE:HB	2:B:193:ILE:CD1	2.49	0.42
3:C:185:VAL:O	3:C:187:ASP:N	2.48	0.42
2:B:122:LEU:CD2	2:B:218:PRO:HG3	2.48	0.42
1:A:185:ASP:HB3	1:A:186:PRO:HD2	2.02	0.42
1:A:210:THR:O	1:A:211:PHE:CB	2.68	0.41
3:C:95:PRO:C	3:C:97:GLN:H	2.22	0.41
2:B:103:ARG:HH11	2:B:103:ARG:HG3	1.85	0.41
2:B:108:ILE:CD1	2:B:126:ILE:HD11	2.51	0.41
4:D:25:ILE:HA	4:D:47:LYS:NZ	2.36	0.41
1:A:261:TRP:CZ3	3:C:36:ILE:HB	2.55	0.41
3:C:133:ILE:CD1	3:C:196:ILE:HG23	2.50	0.41
1:A:90:VAL:HB	1:A:113:ILE:HG22	2.02	0.41
2:B:235:THR:HG22	2:B:236:ILE:N	2.36	0.41
1:A:87:ALA:HB3	3:C:15:THR:HA	2.02	0.41
2:B:81:LYS:C	2:B:85:VAL:HG23	2.40	0.41
3:C:155:VAL:O	3:C:155:VAL:HG13	2.20	0.41
1:A:4:VAL:CG2	1:A:7:VAL:HG23	2.50	0.41
4:D:62:THR:HG22	4:D:63:GLU:N	2.36	0.41
3:C:204:VAL:HA	3:C:205:PRO:HD3	1.91	0.41
2:B:38:TRP:HA	2:B:39:PRO:HD3	1.95	0.41
2:B:250:GLN:HG2	2:B:251:ALA:N	2.34	0.41
3:C:155:VAL:HG12	3:C:167:LEU:HD13	2.02	0.41
3:C:228:LEU:O	3:C:229:CYS:HB3	2.21	0.41
2:B:67:ASP:OD1	2:B:68:THR:N	2.47	0.41
1:A:108:ASN:OD1	1:A:163:PRO:HG2	2.20	0.41
3:C:2:PHE:O	3:C:4:THR:HG23	2.20	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:38:ARG:HG3	1:A:38:ARG:NH1	2.35	0.41
3:C:71:PHE:CZ	3:C:84:ALA:HB2	2.56	0.40
1:A:84:PHE:HB3	1:A:255:MET:HE3	2.03	0.40
1:A:183:LEU:HD21	1:A:247:LEU:HD22	2.02	0.40
1:A:87:ALA:O	3:C:15:THR:HG23	2.21	0.40
1:A:83:PHE:CZ	1:A:122:LYS:HD2	2.57	0.40
3:C:179:ALA:HB3	3:C:189:TYR:CD2	2.56	0.40
2:B:126:ILE:HG23	2:B:212:PHE:CD2	2.57	0.40
2:B:220:SER:HA	2:B:221:PRO:HD2	1.92	0.40
3:C:7:LYS:HB3	3:C:8:PRO:CD	2.52	0.40
2:B:238:LEU:O	2:B:238:LEU:HD12	2.22	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	294/297 (99%)	243 (83%)	47 (16%)	4 (1%)	16	74
2	B	232/254 (91%)	193 (83%)	33 (14%)	6 (3%)	8	62
3	C	240/242 (99%)	203 (85%)	33 (14%)	4 (2%)	14	71
4	D	55/69 (80%)	46 (84%)	5 (9%)	4 (7%)	2	33
All	All	821/862 (95%)	685 (83%)	118 (14%)	18 (2%)	10	66

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	154	GLY
1	A	117	ALA
2	B	157	GLY
4	D	19	ALA
4	D	62	THR
1	A	118	GLN
3	C	186	PHE

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Mol	Chain	Res	Type
4	D	14	GLU
1	A	19	ALA
2	B	30	ASN
2	B	87	THR
3	C	76	GLN
1	A	85	SER
2	B	51	ASP
3	C	171	TRP
4	D	20	THR
3	C	155	VAL
2	B	179	PRO

### 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	253/253 (100%)	253 (100%)	0	100	100
2	B	204/215 (95%)	201 (98%)	3 (2%)	76	95
3	C	203/203 (100%)	202 (100%)	1 (0%)	94	98
4	D	48/58 (83%)	46 (96%)	2 (4%)	40	84
All	All	708/729 (97%)	702 (99%)	6 (1%)	89	98

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

Mol	Chain	Res	Type
2	B	62	ARG
2	B	84	ASP
2	B	156	ASP
3	C	150	MET
4	D	17	ASN
4	D	61	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA chains 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 6 ligands modelled in this entry, 5 are monoatomic - leaving 1 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	$\# Z  > 2$
5	DAO	A	1289	-	13,13,13	0.47	0	13,13,13	1.02	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
5	DAO	A	1289	-	-	0/11/11/11	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.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	296/297 (99%)	1.54	86 (29%) 1 2	50, 81, 124, 154	0
2	B	236/254 (92%)	1.72	75 (31%) 1 2	45, 74, 105, 125	0
3	C	242/242 (100%)	1.40	60 (24%) 1 2	51, 75, 104, 142	0
4	D	57/69 (82%)	1.62	18 (31%) 1 2	56, 87, 134, 147	0
All	All	831/862 (96%)	1.56	239 (28%) 1 2	45, 77, 119, 154	0

All (239) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	19	GLY	7.3
2	B	129	GLU	7.1
3	C	113	GLY	7.0
2	B	145	HIS	6.9
2	B	160	LEU	6.8
4	D	37	TYR	6.6
1	A	275	ALA	6.6
2	B	146	PRO	6.1
2	B	183	ILE	6.0
1	A	133	ALA	6.0
2	B	107	CYS	5.9
1	A	98	GLU	5.7
3	C	38	GLY	5.6
1	A	176	ASN	5.6
1	A	255	MET	5.3
2	B	254	GLN	5.2
1	A	111	ILE	5.1
1	A	4	VAL	5.1
2	B	228	ALA	5.1
4	D	68	LEU	5.0
2	B	37	GLU	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	119	MET	4.8
3	C	206	ILE	4.8
2	B	201	LEU	4.7
1	A	110	ASP	4.6
1	A	27	PRO	4.6
2	B	161	GLN	4.6
3	C	137	PRO	4.4
3	C	173	SER	4.4
3	C	5	GLU	4.3
3	C	54	GLU	4.3
2	B	87	THR	4.2
2	B	253	THR	4.2
1	A	123	VAL	4.2
1	A	104	ASN	4.2
1	A	71	ASN	4.1
2	B	121	ALA	4.1
2	B	132	ILE	4.0
3	C	56	ASN	4.0
3	C	7	LYS	4.0
3	C	146	ARG	4.0
3	C	45	GLU	4.0
1	A	67	ARG	4.0
1	A	272	LEU	3.9
3	C	242	GLN	3.9
4	D	34	LYS	3.9
3	C	55	VAL	3.9
4	D	61	PHE	3.9
2	B	238	LEU	3.9
3	C	136	THR	3.8
2	B	241	MET	3.8
2	B	239	ALA	3.8
3	C	1	GLY	3.8
1	A	122	LYS	3.8
4	D	54	ALA	3.8
3	C	138	PRO	3.8
3	C	6	PRO	3.7
2	B	18	ILE	3.7
1	A	276	ASN	3.7
1	A	232	THR	3.7
2	B	89	THR	3.7
1	A	99	GLY	3.6
2	B	86	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
2	B	76	LYS	3.5
4	D	28	THR	3.5
1	A	114	THR	3.5
2	B	197	TYR	3.5
1	A	79	THR	3.5
3	C	147	ALA	3.5
1	A	266	MET	3.5
3	C	171	TRP	3.4
1	A	157	PRO	3.4
1	A	109	TRP	3.4
2	B	147	PRO	3.4
3	C	210	ASN	3.3
2	B	195	VAL	3.3
1	A	290	SER	3.3
1	A	273	PHE	3.3
2	B	56	PRO	3.3
2	B	162	HIS	3.3
1	A	101	THR	3.3
1	A	105	GLY	3.3
1	A	208	TYR	3.3
1	A	5	ALA	3.2
1	A	190	VAL	3.2
4	D	25	ILE	3.2
2	B	240	PRO	3.2
2	B	154	GLY	3.2
2	B	49	ALA	3.2
1	A	294	ILE	3.2
2	B	44	ASP	3.2
2	B	150	GLN	3.2
3	C	80	GLY	3.2
4	D	32	TYR	3.2
1	A	66	THR	3.1
1	A	159	GLY	3.1
1	A	160	ALA	3.1
2	B	227	GLY	3.1
3	C	75	ALA	3.1
2	B	200	THR	3.1
4	D	69	LYS	3.0
3	C	207	GLY	3.0
2	B	69	LYS	3.0
1	A	112	ASP	3.0
3	C	205	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	231	GLY	3.0
1	A	192	VAL	3.0
1	A	131	PHE	3.0
2	B	21	SER	3.0
1	A	26	ALA	2.9
2	B	42	CYS	2.9
3	C	41	ARG	2.9
2	B	232	ILE	2.9
2	B	96	ALA	2.9
3	C	92	ARG	2.9
2	B	116	LYS	2.9
2	B	237	THR	2.9
3	C	74	SER	2.8
1	A	194	PHE	2.8
1	A	40	ASP	2.8
1	A	158	PRO	2.8
3	C	131	MET	2.8
3	C	17	ASP	2.8
3	C	167	LEU	2.8
4	D	62	THR	2.8
2	B	17	THR	2.8
2	B	207	LEU	2.8
2	B	167	ASP	2.8
1	A	265	PRO	2.8
1	A	237	ASN	2.7
1	A	33	GLN	2.7
1	A	93	ILE	2.7
1	A	80	LEU	2.7
1	A	126	PHE	2.7
1	A	204	PHE	2.7
2	B	229	THR	2.7
1	A	68	CYS	2.7
1	A	250	ARG	2.7
3	C	73	VAL	2.7
2	B	101	LEU	2.7
2	B	98	PHE	2.6
3	C	25	LEU	2.6
2	B	43	SER	2.6
3	C	66	MET	2.6
4	D	38	ALA	2.6
3	C	95	PRO	2.6
3	C	241	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	231	VAL	2.6
2	B	233	PRO	2.6
1	A	9	GLU	2.6
2	B	105	GLY	2.6
3	C	166	THR	2.5
1	A	207	GLY	2.5
3	C	112	SER	2.5
1	A	297	LEU	2.5
2	B	50	VAL	2.5
1	A	30	GLN	2.5
1	A	213	GLU	2.5
2	B	163	PRO	2.5
3	C	47	CYS	2.5
1	A	132	ASP	2.5
3	C	42	ASN	2.5
2	B	117	PHE	2.5
1	A	29	GLY	2.5
1	A	118	GLN	2.5
3	C	22	ALA	2.5
1	A	291	ARG	2.4
3	C	151	LEU	2.4
1	A	209	PRO	2.4
1	A	167	GLU	2.4
1	A	32	THR	2.4
2	B	63	PHE	2.4
4	D	47	LYS	2.4
1	A	205	TYR	2.4
1	A	41	THR	2.4
3	C	198	TYR	2.4
3	C	23	PRO	2.4
2	B	80	TRP	2.4
2	B	88	GLU	2.4
1	A	258	VAL	2.3
2	B	182	TRP	2.3
3	C	77	ALA	2.3
2	B	92	PHE	2.3
1	A	54	ALA	2.3
4	D	35	ASP	2.3
3	C	72	PRO	2.3
1	A	70	LEU	2.3
1	A	268	ASN	2.3
2	B	26	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	155	ALA	2.3
3	C	197	TRP	2.3
2	B	178	CYS	2.3
1	A	154	MET	2.3
1	A	31	ASN	2.3
1	A	113	ILE	2.3
2	B	219	ILE	2.3
2	B	164	TYR	2.2
2	B	109	HIS	2.2
2	B	133	GLY	2.2
3	C	162	GLN	2.2
2	B	192	THR	2.2
1	A	161	PRO	2.2
1	A	252	TYR	2.2
2	B	148	TYR	2.2
4	D	57	VAL	2.2
4	D	44	GLN	2.2
1	A	13	GLY	2.2
1	A	69	VAL	2.2
1	A	256	LYS	2.2
2	B	31	ILE	2.1
2	B	97	GLN	2.1
2	B	243	SER	2.1
2	B	106	PHE	2.1
1	A	6	ASP	2.1
1	A	200	ALA	2.1
3	C	37	PRO	2.1
1	A	270	ASN	2.1
1	A	243	SER	2.1
4	D	55	ASN	2.1
3	C	208	ALA	2.1
1	A	3	ARG	2.1
3	C	33	CYS	2.1
1	A	14	ASP	2.1
2	B	112	CYS	2.1
3	C	111	TRP	2.1
1	A	296	THR	2.1
3	C	215	ILE	2.1
3	C	143	PRO	2.1
3	C	188	TYR	2.1
4	D	27	TYR	2.1
4	D	46	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	78	TRP	2.0
1	A	292	THR	2.0
3	C	126	MET	2.0
3	C	13	PHE	2.0
3	C	182	ARG	2.0
3	C	30	PRO	2.0
3	C	139	GLY	2.0
3	C	68	ARG	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
6	CA	C	1244	1/1	2.19	7.06	83,83,83,83	1
6	CA	C	1245	1/1	1.49	3.03	77,77,77,77	1
5	DAO	A	1289	14/14	0.84	0.85	69,69,69,69	0
6	CA	C	1243	1/1	0.52	-1.22	97,97,97,97	0
6	CA	B	1255	1/1	0.20	-1.74	72,72,72,72	0
6	CA	B	1256	1/1	0.12	-3.36	85,85,85,85	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.