



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:10 PM GMT

PDB ID : 1EAH  
Title : PV2L COMPLEXED WITH ANTIVIRAL AGENT SCH48973  
Authors : Lentz, K.; Arnold, E.  
Deposited on : 1997-07-22  
Resolution : 2.90 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

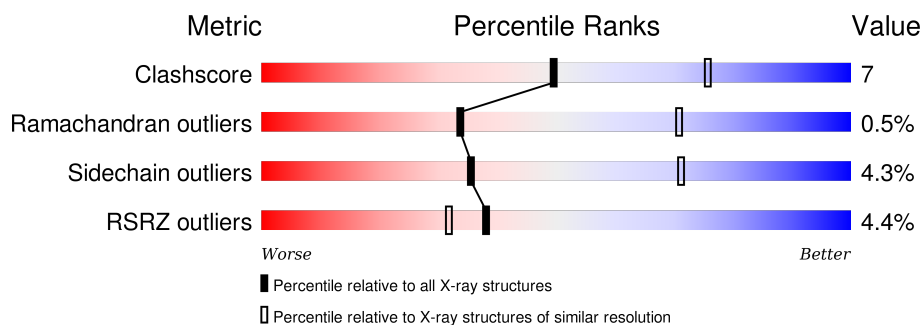
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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	1	301	 4% 67% 22% 10%
2	2	271	 3% 81% 14% 2% 2%
3	3	238	 2% 87% 9% 2% 2%
4	4	68	 18% 76% 19% 1%

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6823 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 POLIOVIRUS TYPE 2 COAT PROTEINS VP1 TO VP4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	272	Total	C	N	O	S	0	0	0
			2129	1361	363	400	5			

- Molecule 2 is a protein called POLIOVIRUS TYPE 2 COAT PROTEINS VP1 TO VP4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	262	Total	C	N	O	S	0	0	0
			2042	1298	346	384	14			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	11	VAL	ASP	CONFLICT	UNP P06210

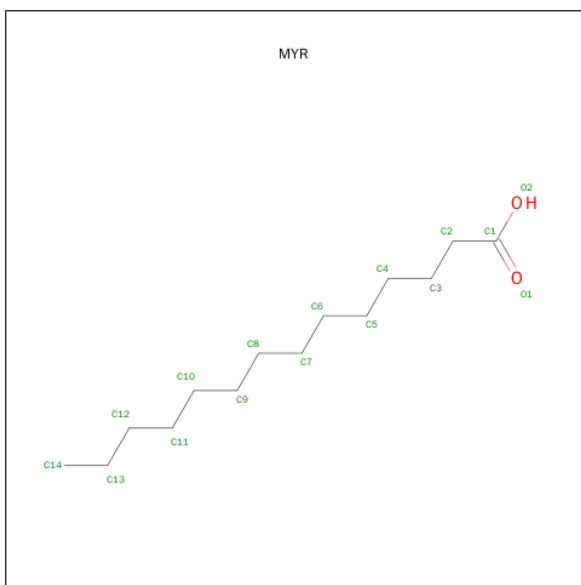
- Molecule 3 is a protein called POLIOVIRUS TYPE 2 COAT PROTEINS VP1 TO VP4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	235	Total	C	N	O	S	3	0	0
			1825	1156	303	349	17			

- Molecule 4 is a protein called POLIOVIRUS TYPE 2 COAT PROTEINS VP1 TO VP4.

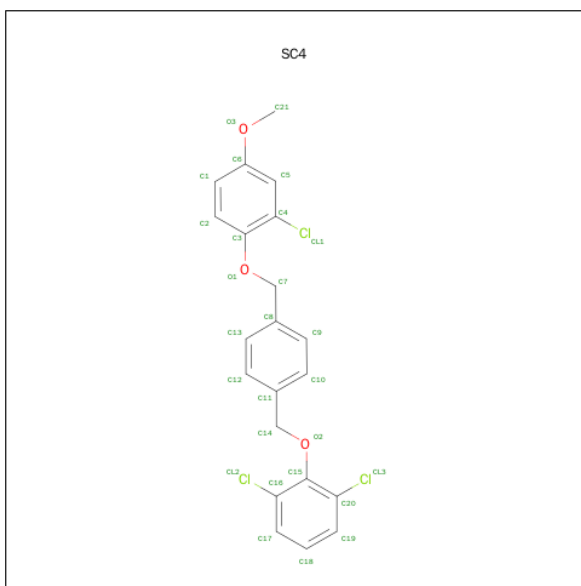
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	4	68	Total	C	N	O	0	0	0
			518	318	91	109			

- Molecule 5 is MYRISTIC ACID (three-letter code: MYR) (formula: C<sub>14</sub>H<sub>28</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	4	1	Total	C	O		0	0
			11	10	1			

- Molecule 6 is 1[2-CHLORO-4-METHOXY-PHENYL-OXYMETHYL]-4-[2,6-DICHLORO-PHENYL-OXYMETHYL]-BENZENE (three-letter code: SC4) (formula:  $C_{21}H_{17}Cl_3O_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	1	1	Total	C	Cl	O	0	0
			27	21	3	3		

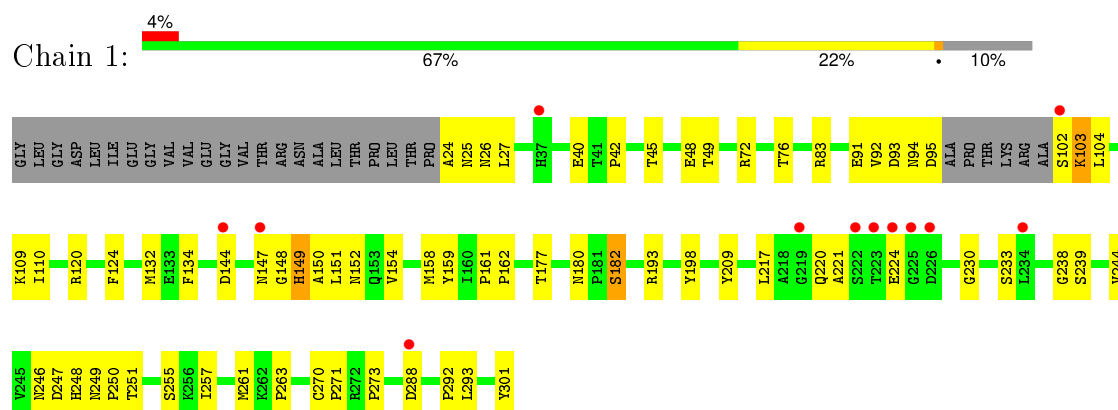
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	1	93	Total 93	O 93	0	0
7	2	83	Total 83	O 83	0	0
7	3	71	Total 71	O 71	0	0
7	4	24	Total 24	O 24	0	0

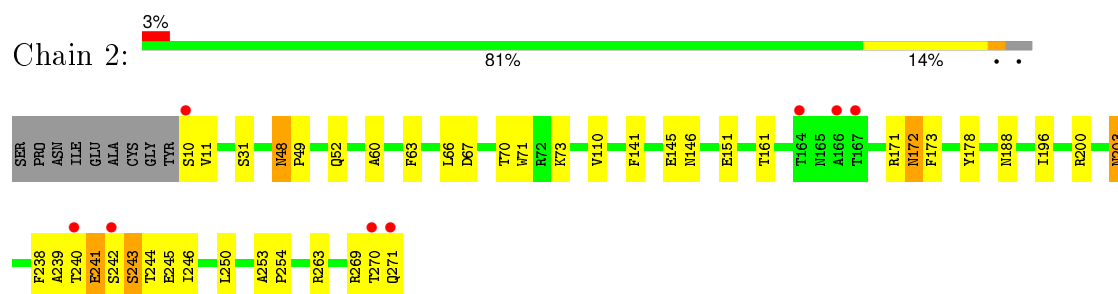
### 3 Residue-property plots [i](#)

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.

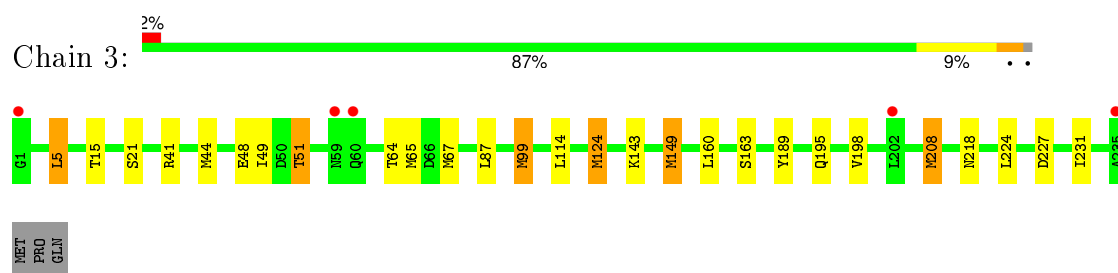
#### • Molecule 1: POLIOVIRUS TYPE 2 COAT PROTEINS VP1 TO VP4



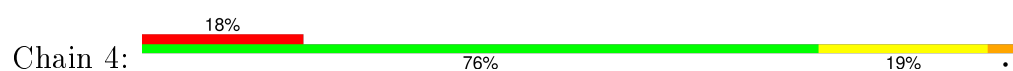
#### • Molecule 2: POLIOVIRUS TYPE 2 COAT PROTEINS VP1 TO VP4

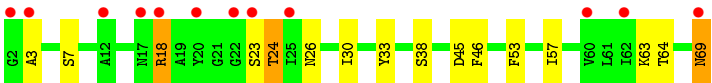


#### • Molecule 3: POLIOVIRUS TYPE 2 COAT PROTEINS VP1 TO VP4



#### • Molecule 4: POLIOVIRUS TYPE 2 COAT PROTEINS VP1 TO VP4





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	345.70 Å   497.20 Å   485.90 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	(Not available) – 2.90 29.93 – 2.90	Depositor EDS
% Data completeness (in resolution range)	45.4 ((Not available)-2.90) 48.9 (29.93-2.90)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.25 (at 2.90 Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.185 , (Not available) 0.175 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	18.4	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 135.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 444634 reflections	Xtriage
$F_o, F_c$ correlation	0.09	EDS
Total number of atoms	6823	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.25% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SC4, MYR

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	1	0.43	0/2193	0.68	1/2996 (0.0%)
2	2	0.44	0/2098	0.72	1/2863 (0.0%)
3	3	0.43	0/1869	0.67	1/2549 (0.0%)
4	4	0.52	0/527	0.68	0/713
All	All	0.44	0/6687	0.69	3/9121 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	288	ASP	N-CA-C	5.96	127.10	111.00
2	2	203	ASN	CB-CA-C	-5.75	98.89	110.40
3	3	5	LEU	CA-CB-CG	5.19	127.24	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	198	TYR	Sidechain

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	2129	0	2068	45	75
2	2	2042	0	1969	26	0
3	3	1825	0	1800	22	0
4	4	518	0	495	16	0
5	4	11	0	16	0	0
6	1	27	0	17	2	0
7	1	93	0	0	2	7
7	2	83	0	0	1	0
7	3	71	0	0	1	0
7	4	24	0	0	1	0
All	All	6823	0	6365	91	76

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 (91) 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)
1:1:24:ALA:HB2	1:1:76:THR:HG21	1.58	0.85
2:2:11:VAL:HA	7:4:85:HOH:O	1.78	0.83
1:1:148:GLY:HA3	1:1:251:THR:HG23	1.63	0.80
1:1:233:SER:HB3	7:1:1044:HOH:O	1.82	0.78
2:2:48:ASN:HB3	2:2:49:PRO:HD3	1.66	0.77
2:2:178:TYR:HA	3:3:65:MET:HE3	1.66	0.77
1:1:177:THR:HG21	1:1:182:SER:OG	1.89	0.73
3:3:51:THR:HG21	3:3:99:MET:H	1.53	0.73
1:1:109:LYS:HA	1:1:239:SER:HB3	1.73	0.70
2:2:145:GLU:OE2	2:2:269:ARG:HD2	1.94	0.67
1:1:102:SER:O	1:1:104:LEU:N	2.29	0.65
1:1:158:MET:SD	1:1:177:THR:HG23	2.36	0.65
3:3:64:THR:O	3:3:67:MET:HG2	2.03	0.59
2:2:66:LEU:HD12	2:2:250:LEU:HD23	1.86	0.58
1:1:24:ALA:HB2	1:1:76:THR:CG2	2.33	0.58
2:2:110:VAL:HG22	2:2:250:LEU:HD12	1.86	0.58
1:1:27:LEU:HD21	1:1:72:ARG:HG3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:60:ALA:O	2:2:254:PRO:HG2	2.03	0.57
3:3:198:VAL:HG11	3:3:208:MET:CE	2.34	0.57
2:2:73:LYS:HE2	2:2:242:SER:HA	1.87	0.56
4:4:18:ARG:HG3	4:4:24:THR:HG21	1.87	0.56
1:1:301:TYR:CE1	3:3:189:TYR:HB3	2.41	0.55
1:1:132:MET:HG2	1:1:261:MET:CE	2.37	0.55
1:1:249:ASN:OD1	1:1:250:PRO:HD2	2.07	0.54
1:1:132:MET:HG2	1:1:261:MET:HE2	1.89	0.53
2:2:270:THR:O	2:2:271:GLN:HG2	2.07	0.53
2:2:172:ASN:ND2	2:2:173:PHE:H	2.07	0.52
1:1:40:GLU:HB3	4:4:64:THR:HB	1.91	0.52
1:1:217:LEU:O	1:1:220:GLN:HG2	2.09	0.52
1:1:132:MET:CG	1:1:261:MET:HE2	2.41	0.51
1:1:209:TYR:O	1:1:230:GLY:HA2	2.11	0.51
1:1:93:ASP:C	1:1:95:ASP:H	2.14	0.51
2:2:10:SER:HB2	4:4:69:ASN:O	2.10	0.50
3:3:198:VAL:HG11	3:3:208:MET:HE1	1.93	0.50
1:1:45:THR:HG23	3:3:163:SER:HB2	1.94	0.50
2:2:63:PHE:CD1	2:2:253:ALA:HB2	2.47	0.49
2:2:178:TYR:HA	3:3:65:MET:CE	2.41	0.49
1:1:273:PRO:HB3	2:2:188:ASN:HB3	1.93	0.49
2:2:241:GLU:CD	2:2:241:GLU:N	2.66	0.49
2:2:241:GLU:HB3	2:2:243:SER:O	2.11	0.49
1:1:221:ALA:O	1:1:224:GLU:HB2	2.13	0.48
1:1:49:THR:O	4:4:57:ILE:HD11	2.13	0.48
1:1:273:PRO:HB3	2:2:188:ASN:CB	2.43	0.48
3:3:41:ARG:NH1	4:4:46:PHE:CE1	2.82	0.48
2:2:11:VAL:HG23	4:4:69:ASN:HB3	1.94	0.48
1:1:48:GLU:HA	2:2:196:ILE:HB	1.96	0.48
1:1:159:TYR:CE2	1:1:161:PRO:HG3	2.49	0.48
3:3:149:MET:O	3:3:149:MET:HG2	2.13	0.48
1:1:158:MET:SD	1:1:177:THR:CG2	3.02	0.47
1:1:120:ARG:HD2	3:3:231:ILE:HB	1.96	0.47
1:1:257:ILE:HD12	1:1:257:ILE:N	2.29	0.47
2:2:146:ASN:HB3	2:2:172:ASN:ND2	2.29	0.47
2:2:71:TRP:CE3	2:2:246:ILE:HD11	2.50	0.46
1:1:132:MET:HE1	6:1:999:SC4:H71	1.98	0.46
1:1:261:MET:HE1	1:1:263:PRO:HG3	1.98	0.45
1:1:94:ASN:OD1	1:1:248:HIS:HB3	2.16	0.45
3:3:87:LEU:HD11	3:3:114:LEU:HD12	1.98	0.45
1:1:110:ILE:HG13	1:1:239:SER:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:238:PHE:O	2:2:240:THR:N	2.51	0.44
3:3:49:ILE:HD11	4:4:53:PHE:HB3	2.00	0.43
1:1:42:PRO:HA	4:4:63:LYS:O	2.18	0.43
3:3:51:THR:HB	7:3:256:HOH:O	2.17	0.43
3:3:231:ILE:HD12	3:3:231:ILE:HA	1.96	0.43
4:4:7:SER:HA	4:4:26:ASN:HA	2.01	0.42
3:3:44:MET:O	3:3:48:GLU:HG3	2.20	0.42
4:4:33:TYR:HB2	4:4:38:SER:HB2	2.00	0.42
2:2:110:VAL:HG22	2:2:250:LEU:CD1	2.47	0.42
2:2:67:ASP:N	7:2:331:HOH:O	2.51	0.42
1:1:134:PHE:O	1:1:193:ARG:HA	2.19	0.42
3:3:195:GLN:OE1	3:3:195:GLN:HA	2.20	0.42
4:4:3:ALA:HA	4:4:30:ILE:HG12	2.01	0.42
3:3:41:ARG:NH1	4:4:46:PHE:HE1	2.18	0.42
1:1:162:PRO:HD3	1:1:238:GLY:CA	2.50	0.42
1:1:25:ASN:HB3	1:1:26:ASN:H	1.52	0.41
1:1:24:ALA:HB3	4:4:45:ASP:O	2.21	0.41
3:3:65:MET:HE2	3:3:65:MET:HA	2.02	0.41
4:4:57:ILE:HD13	4:4:57:ILE:HA	1.78	0.41
1:1:292:PRO:HG2	1:1:293:LEU:HD12	2.02	0.41
1:1:92:VAL:HG23	1:1:255:SER:HB2	2.02	0.41
1:1:132:MET:HE3	6:1:999:SC4:C13	2.51	0.41
1:1:94:ASN:O	1:1:95:ASP:HB2	2.21	0.41
1:1:91:GLU:O	1:1:103:LYS:HE3	2.21	0.41
2:2:141:PHE:CE2	2:2:171:ARG:HG2	2.56	0.41
1:1:177:THR:HG22	1:1:180:ASN:HB2	2.04	0.40
3:3:124:MET:HG3	3:3:124:MET:O	2.18	0.40
3:3:143:LYS:HD3	3:3:143:LYS:HA	1.75	0.40
4:4:23:SER:HA	4:4:26:ASN:HD22	1.86	0.40
1:1:24:ALA:N	7:1:1036:HOH:O	2.54	0.40
2:2:241:GLU:C	2:2:243:SER:N	2.74	0.40
3:3:21:SER:O	4:4:38:SER:HB3	2.22	0.40
1:1:124:PHE:O	1:1:271:PRO:HA	2.22	0.40

All (76) 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)
1:1:149:HIS:CG	1:1:246:ASN:OD1[3_555]	0.35	1.85
1:1:247:ASP:C	1:1:249:ASN:OD1[3_555]	0.64	1.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:247:ASP:O	1:1:249:ASN:CG[3_555]	0.65	1.55
1:1:150:ALA:O	1:1:151:LEU:C[3_555]	0.76	1.44
1:1:247:ASP:CB	1:1:251:THR:N[3_555]	0.79	1.41
1:1:149:HIS:CA	1:1:246:ASN:ND2[3_555]	0.93	1.27
1:1:149:HIS:CD2	1:1:246:ASN:OD1[3_555]	1.02	1.18
1:1:149:HIS:C	1:1:246:ASN:ND2[3_555]	1.04	1.16
7:1:1070:HOH:O	7:1:1089:HOH:O[3_555]	1.09	1.11
1:1:247:ASP:O	1:1:249:ASN:CB[3_555]	1.17	1.03
1:1:247:ASP:CG	1:1:250:PRO:C[3_555]	1.24	0.96
1:1:150:ALA:C	1:1:151:LEU:O[3_555]	1.24	0.96
1:1:247:ASP:O	1:1:249:ASN:OD1[3_555]	1.26	0.94
1:1:149:HIS:CD2	1:1:246:ASN:CG[3_555]	1.28	0.92
1:1:149:HIS:CG	1:1:246:ASN:CG[3_555]	1.31	0.89
1:1:150:ALA:C	1:1:151:LEU:C[3_555]	1.32	0.88
1:1:247:ASP:CB	1:1:250:PRO:C[3_555]	1.36	0.84
1:1:247:ASP:CG	1:1:251:THR:N[3_555]	1.39	0.81
1:1:151:LEU:N	1:1:151:LEU:O[3_555]	1.42	0.78
1:1:251:THR:CG2	7:1:1063:HOH:O[3_555]	1.44	0.76
1:1:149:HIS:ND1	1:1:246:ASN:OD1[3_555]	1.46	0.74
1:1:151:LEU:N	1:1:151:LEU:N[3_555]	1.48	0.72
1:1:247:ASP:C	1:1:249:ASN:CG[3_555]	1.48	0.72
1:1:247:ASP:OD2	1:1:250:PRO:O[3_555]	1.49	0.71
1:1:149:HIS:CB	1:1:246:ASN:ND2[3_555]	1.50	0.70
1:1:150:ALA:O	1:1:152:ASN:N[3_555]	1.50	0.70
1:1:150:ALA:O	1:1:151:LEU:CA[3_555]	1.51	0.69
1:1:248:HIS:N	1:1:249:ASN:OD1[3_555]	1.51	0.69
1:1:248:HIS:N	1:1:250:PRO:CD[3_555]	1.55	0.65
1:1:147:ASN:CA	7:1:1062:HOH:O[3_555]	1.57	0.63
1:1:247:ASP:OD2	1:1:251:THR:CA[3_555]	1.58	0.62
1:1:247:ASP:CG	1:1:250:PRO:O[3_555]	1.61	0.59
1:1:149:HIS:ND1	1:1:154:VAL:N[3_555]	1.61	0.59
1:1:149:HIS:O	1:1:246:ASN:CB[3_555]	1.64	0.56
1:1:150:ALA:O	1:1:151:LEU:O[3_555]	1.64	0.56
1:1:251:THR:CB	7:1:1063:HOH:O[3_555]	1.65	0.55
1:1:150:ALA:C	1:1:151:LEU:CA[3_555]	1.66	0.54
1:1:149:HIS:CD2	1:1:246:ASN:CB[3_555]	1.67	0.53
1:1:248:HIS:C	1:1:249:ASN:CA[3_555]	1.68	0.52
1:1:247:ASP:N	1:1:251:THR:OG1[3_555]	1.68	0.52
1:1:247:ASP:CA	1:1:249:ASN:OD1[3_555]	1.72	0.48
1:1:149:HIS:CB	1:1:246:ASN:CG[3_555]	1.76	0.44
1:1:149:HIS:CB	1:1:246:ASN:OD1[3_555]	1.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:149:HIS:NE2	1:1:244:VAL:CG1[3_555]	1.79	0.41
1:1:247:ASP:OD2	1:1:250:PRO:C[3_555]	1.81	0.39
1:1:248:HIS:O	1:1:248:HIS:O[3_555]	1.83	0.37
1:1:247:ASP:OD2	1:1:251:THR:N[3_555]	1.83	0.37
1:1:251:THR:OG1	7:1:1063:HOH:O[3_555]	1.84	0.36
1:1:149:HIS:CA	1:1:246:ASN:CG[3_555]	1.86	0.34
1:1:151:LEU:N	1:1:151:LEU:C[3_555]	1.87	0.33
1:1:149:HIS:O	1:1:246:ASN:ND2[3_555]	1.89	0.31
1:1:149:HIS:NE2	1:1:246:ASN:OD1[3_555]	1.90	0.30
1:1:247:ASP:O	1:1:249:ASN:ND2[3_555]	1.90	0.30
1:1:149:HIS:C	1:1:246:ASN:CG[3_555]	1.96	0.24
1:1:247:ASP:CB	1:1:250:PRO:CA[3_555]	1.96	0.24
1:1:150:ALA:N	1:1:246:ASN:ND2[3_555]	1.99	0.21
1:1:149:HIS:O	1:1:246:ASN:CG[3_555]	2.00	0.20
1:1:247:ASP:CG	1:1:251:THR:CA[3_555]	2.02	0.18
1:1:151:LEU:CD2	7:1:1071:HOH:O[3_555]	2.05	0.15
1:1:151:LEU:N	1:1:151:LEU:CA[3_555]	2.05	0.15
1:1:149:HIS:CE1	1:1:246:ASN:OD1[3_555]	2.07	0.13
1:1:149:HIS:N	1:1:246:ASN:ND2[3_555]	2.08	0.12
1:1:247:ASP:O	1:1:249:ASN:CA[3_555]	2.10	0.10
1:1:247:ASP:CB	1:1:250:PRO:N[3_555]	2.10	0.10
1:1:247:ASP:OD2	1:1:251:THR:C[3_555]	2.10	0.10
1:1:247:ASP:OD1	1:1:250:PRO:C[3_555]	2.11	0.09
1:1:151:LEU:CA	1:1:151:LEU:O[3_555]	2.11	0.09
1:1:149:HIS:CG	1:1:246:ASN:ND2[3_555]	2.12	0.08
1:1:151:LEU:CA	1:1:151:LEU:C[3_555]	2.12	0.08
1:1:149:HIS:CE1	1:1:244:VAL:CG1[3_555]	2.13	0.07
1:1:149:HIS:CD2	1:1:246:ASN:N[3_555]	2.13	0.07
1:1:247:ASP:C	1:1:250:PRO:N[3_555]	2.16	0.04
1:1:247:ASP:CA	1:1:251:THR:N[3_555]	2.17	0.03
1:1:247:ASP:N	1:1:249:ASN:OD1[3_555]	2.19	0.01
1:1:147:ASN:C	7:1:1062:HOH:O[3_555]	2.19	0.01
1:1:247:ASP:CB	1:1:251:THR:CA[3_555]	2.19	0.01

## 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	1	268/301 (89%)	250 (93%)	16 (6%)	2 (1%)	26	63
2	2	260/271 (96%)	245 (94%)	13 (5%)	2 (1%)	24	60
3	3	233/238 (98%)	226 (97%)	7 (3%)	0	100	100
4	4	66/68 (97%)	62 (94%)	4 (6%)	0	100	100
All	All	827/878 (94%)	783 (95%)	40 (5%)	4 (0%)	34	71

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	103	LYS
2	2	239	ALA
2	2	48	ASN
1	1	270	CYS

### 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	1	231/253 (91%)	227 (98%)	4 (2%)	68	91
2	2	221/228 (97%)	208 (94%)	13 (6%)	24	58
3	3	207/210 (99%)	196 (95%)	11 (5%)	28	63
4	4	56/56 (100%)	53 (95%)	3 (5%)	27	62
All	All	715/747 (96%)	684 (96%)	31 (4%)	35	71

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	83	ARG
1	1	144	ASP
1	1	149	HIS
1	1	182	SER

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Mol	Chain	Res	Type
2	2	31	SER
2	2	52	GLN
2	2	70	THR
2	2	151	GLU
2	2	161	THR
2	2	172	ASN
2	2	200	ARG
2	2	203	ASN
2	2	241	GLU
2	2	243	SER
2	2	244	THR
2	2	245	GLU
2	2	263	ARG
3	3	5	LEU
3	3	15	THR
3	3	51	THR
3	3	99	MET
3	3	124	MET
3	3	149	MET
3	3	160	LEU
3	3	208	MET
3	3	218	ASN
3	3	224	LEU
3	3	227	ASP
4	4	18	ARG
4	4	24	THR
4	4	69	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	62	GLN
1	1	65	HIS
1	1	149	HIS
1	1	220	GLN
2	2	172	ASN
2	2	203	ASN
3	3	218	ASN
3	3	233	GLN
4	4	69	ASN



### 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](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
6	SC4	1	999	-	29,29,29	1.30	4 (13%)	39,39,39	1.34	5 (12%)
5	MYR	4	1	4	10,10,15	0.66	0	8,9,15	0.64	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
6	SC4	1	999	-	-	0/12/12/12	0/3/3/3
5	MYR	4	1	4	-	0/7/8/13	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	1	999	SC4	C3-C4	2.07	1.43	1.39
6	1	999	SC4	C18-C19	2.14	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	1	999	SC4	C15-C16	2.38	1.45	1.40
6	1	999	SC4	C5-C6	3.23	1.44	1.38

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	1	999	SC4	O1-C3-C2	-2.85	118.05	124.01
6	1	999	SC4	C15-C20-CL3	2.40	121.38	118.43
6	1	999	SC4	C15-C16-CL2	2.53	121.53	118.43
6	1	999	SC4	C21-O3-C6	2.57	123.53	117.51
6	1	999	SC4	O1-C3-C4	4.21	121.88	116.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	1	999	SC4	2	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	1	272/301 (90%)	-0.16	12 (4%) 38 32	5, 11, 39, 60	0
2	2	262/271 (96%)	-0.23	8 (3%) 52 45	5, 9, 34, 61	0
3	3	235/238 (98%)	-0.21	5 (2%) 67 62	5, 9, 26, 58	2 (0%)
4	4	68/68 (100%)	0.94	12 (17%) 2 1	7, 23, 45, 53	0
All	All	837/878 (95%)	-0.11	37 (4%) 38 32	5, 10, 39, 61	2 (0%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1	223	THR	4.8
1	1	102	SER	4.5
3	3	235	ALA	4.2
2	2	167	THR	4.0
4	4	62	ILE	4.0
2	2	164	THR	4.0
3	3	1	GLY	4.0
4	4	17	ASN	3.9
2	2	271	GLN	3.5
1	1	222	SER	3.1
4	4	69	ASN	2.9
4	4	2	GLY	2.8
2	2	166	ALA	2.7
4	4	22	GLY	2.6
4	4	60	VAL	2.6
4	4	20	TYR	2.5
2	2	270	THR	2.4
3	3	60	GLN	2.4
4	4	25	ILE	2.4
4	4	18	ARG	2.4
3	3	59	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
2	2	242	SER	2.3
1	1	144	ASP	2.2
1	1	224	GLU	2.2
4	4	12	ALA	2.2
1	1	288	ASP	2.2
1	1	234	LEU	2.2
4	4	3	ALA	2.1
1	1	226	ASP	2.1
3	3	202	LEU	2.1
1	1	37	HIS	2.1
1	1	219	GLY	2.1
1	1	147	ASN	2.1
1	1	225	GLY	2.1
4	4	23	SER	2.1
2	2	240	THR	2.0
2	2	10	SER	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( $\text{\AA}^2$ )	Q<0.9
6	SC4	1	999	27/27	0.98	0.13	-0.90	5,5,9,9	0
5	MYR	4	1	11/16	0.87	0.49	-	30,36,40,40	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.