



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 20, 2021 – 04:08 PM JST

PDB ID : 7DF9
Title : Crystal of Arrestin2-V2Rpp-1-Fab30 complex
Authors : Sun, J.P.; Yu, X.; Xiao, P.; He, Q.T.; Lin, J.Y.; Zhu, Z.L.
Deposited on : 2020-11-06
Resolution : 3.17 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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 : 2.22
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) : 2.22

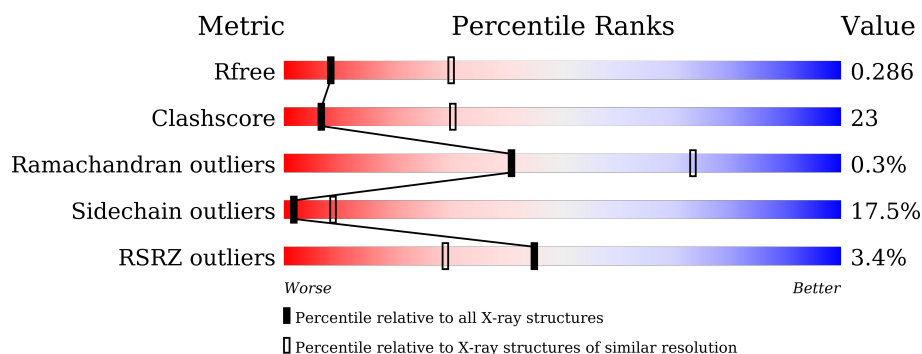
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.17 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	1467 (3.20-3.16)
Clashscore	141614	1599 (3.20-3.16)
Ramachandran outliers	138981	1574 (3.20-3.16)
Sidechain outliers	138945	1573 (3.20-3.16)
RSRZ outliers	127900	1423 (3.20-3.16)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	426	<div> <div>13%</div> <div>50% 31% 15%</div> </div>
2	V	23	<div> <div>13%</div> <div>43% 26% 17% 13%</div> </div>
3	L	227	<div> <div>6%</div> <div>53% 33% 7% 7%</div> </div>
4	H	249	<div> <div>2%</div> <div>45% 31% 8% 16%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5747 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 Beta-arrestin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	360	Total	C	N	O	S	0	0	0
			2624	1670	451	493	10			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	419	LEU	-	expression tag	UNP P17870
A	420	GLU	-	expression tag	UNP P17870
A	421	HIS	-	expression tag	UNP P17870
A	422	HIS	-	expression tag	UNP P17870
A	423	HIS	-	expression tag	UNP P17870
A	424	HIS	-	expression tag	UNP P17870
A	425	HIS	-	expression tag	UNP P17870
A	426	HIS	-	expression tag	UNP P17870

- Molecule 2 is a protein called VASOPRESSIN V2 RECEPTOR PHOSPHOPEPTIDE.

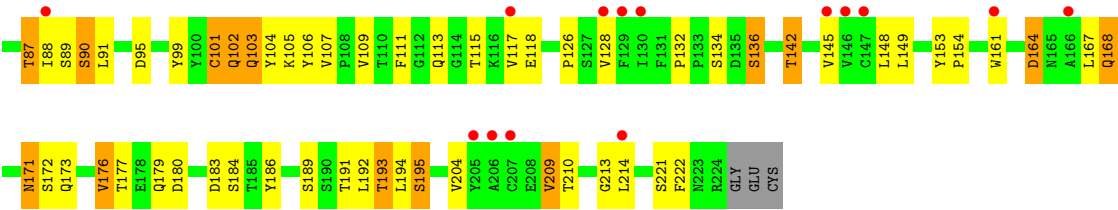
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	V	20	Total	C	N	O	P	S	0	0
			151	72	20	51	7	1		

- Molecule 3 is a protein called FAB30 LIGHT CHAIN.

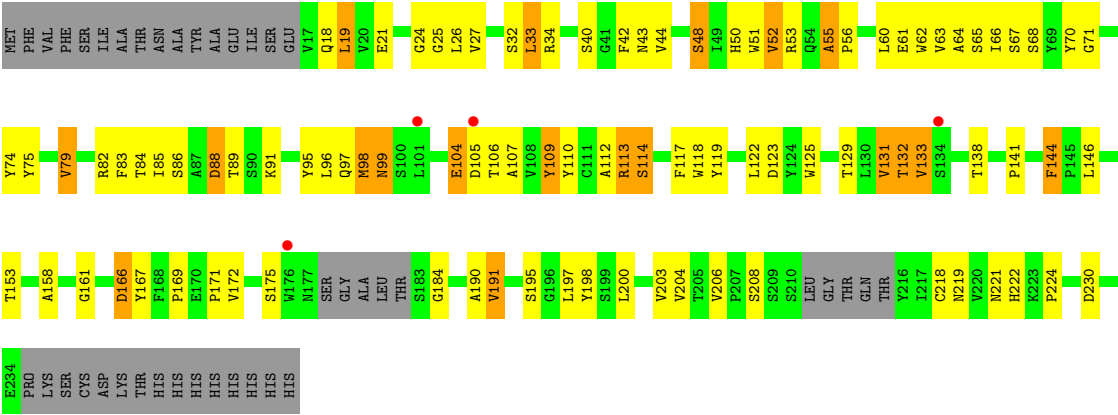
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	212	Total	C	N	O	S	0	0	0
			1517	948	245	319	5			

- Molecule 4 is a protein called FAB30 HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	208	Total	C	N	O	S	0	0	0
			1455	927	239	284	5			



● Molecule 4: FAB30 HEAVY CHAIN



4 Data and refinement statistics

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	116.17Å 121.54Å 144.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.25 – 3.17 39.01 – 3.17	Depositor EDS
% Data completeness (in resolution range)	99.0 (38.25-3.17) 98.8 (39.01-3.17)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 3.18Å)	Xtriage
Refinement program	PHENIX 1.14 _3260	Depositor
R, R_{free}	0.255 , 0.281 0.254 , 0.286	Depositor DCC
R_{free} test set	908 reflections (5.18%)	wwPDB-VP
Wilson B-factor (Å ²)	102.2	Xtriage
Anisotropy	0.493	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 48.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.004 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	5747	wwPDB-VP
Average B, all atoms (Å ²)	107.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.07% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: TPO, SEP

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	0.54	0/2681	0.71	0/3672
2	V	0.56	0/77	0.64	0/101
3	L	0.47	0/1551	0.68	0/2128
4	H	0.52	0/1494	0.71	1/2052 (0.0%)
All	All	0.52	0/5803	0.70	1/7953 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	109	TYR	CB-CA-C	5.56	121.52	110.40

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	2624	0	2486	100	0
2	V	151	0	91	4	0
3	L	1517	0	1364	66	0
4	H	1455	0	1266	98	0
All	All	5747	0	5207	257	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 23.

All (257) 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)
4:H:55:ALA:HB1	4:H:56:PRO:HD3	1.23	1.17
4:H:55:ALA:HB1	4:H:56:PRO:CD	1.93	0.97
4:H:84:THR:HB	4:H:97:GLN:HB3	1.52	0.88
4:H:109:TYR:HE2	4:H:131:VAL:HG11	1.44	0.82
4:H:53:ARG:CB	4:H:109:TYR:HE1	1.95	0.79
4:H:109:TYR:CE2	4:H:131:VAL:HG11	2.16	0.79
1:A:34:VAL:HB	1:A:119:ILE:HB	1.66	0.78
4:H:64:ALA:HB1	4:H:85:ILE:HD12	1.64	0.78
4:H:52:VAL:HG21	4:H:125:TRP:CZ3	2.20	0.77
4:H:32:SER:HA	4:H:98:MET:O	1.86	0.76
1:A:8:VAL:O	2:V:362:SEP:HB3	1.85	0.76
3:L:171:ASN:HD22	3:L:194:LEU:HD21	1.50	0.76
1:A:101:GLN:HE21	1:A:114:PRO:HB2	1.49	0.75
3:L:161:TRP:HB2	3:L:168:GLN:HG2	1.67	0.75
4:H:24:GLY:HA2	4:H:33:LEU:HD21	1.69	0.75
4:H:53:ARG:CB	4:H:109:TYR:CE1	2.70	0.75
4:H:106:THR:HG23	4:H:132:THR:HA	1.71	0.71
4:H:222:HIS:CD2	4:H:224:PRO:HD2	2.26	0.71
4:H:55:ALA:CB	4:H:56:PRO:CD	2.66	0.70
1:A:101:GLN:NE2	1:A:114:PRO:HB2	2.06	0.70
3:L:104:TYR:HB2	4:H:119:TYR:HE2	1.57	0.70
1:A:37:VAL:HB	1:A:117:PHE:HB2	1.74	0.69
1:A:182:PRO:HG2	1:A:203:LEU:HB2	1.75	0.69
1:A:14:PRO:HG2	1:A:161:ARG:HA	1.74	0.68
4:H:107:ALA:H	4:H:131:VAL:HG12	1.60	0.67
1:A:58:THR:HA	1:A:81:VAL:HG22	1.77	0.67
4:H:172:VAL:HG22	4:H:222:HIS:HA	1.78	0.65
4:H:169:PRO:HD2	4:H:222:HIS:CE1	2.32	0.65
4:H:166:ASP:HA	4:H:197:LEU:HB3	1.79	0.64
4:H:113:ARG:NE	4:H:114:SER:O	2.22	0.64
1:A:31:ILE:HG21	1:A:307:ARG:HA	1.78	0.64
1:A:331:ARG:HE	1:A:340:SER:HA	1.62	0.64
4:H:82:ARG:HB2	4:H:99:ASN:O	1.97	0.64
4:H:65:SER:OG	4:H:74:TYR:HB2	1.97	0.63
1:A:190:PHE:HE2	1:A:224:THR:HG21	1.63	0.63
2:V:347:THR:OG1	2:V:348:PRO:HD2	1.98	0.63
3:L:47:ALA:HA	3:L:61:ILE:O	1.99	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:173:GLN:HG3	4:H:191:VAL:HG11	1.81	0.63
1:A:9:PHE:O	1:A:21:TYR:HA	1.98	0.62
2:V:358:CYS:SG	2:V:359:TPO:N	2.72	0.62
4:H:79:VAL:HB	4:H:83:PHE:HB2	1.80	0.62
1:A:61:PHE:CE1	1:A:243:LEU:HB2	2.35	0.61
1:A:12:ALA:HB2	1:A:19:THR:HG23	1.81	0.61
4:H:33:LEU:HD22	4:H:131:VAL:HG23	1.83	0.61
4:H:107:ALA:H	4:H:131:VAL:CG1	2.14	0.61
4:H:117:PHE:HA	4:H:118:TRP:CD1	2.36	0.61
3:L:75:PHE:HE1	3:L:99:TYR:HE1	1.49	0.60
3:L:31:ARG:HG2	3:L:89:SER:HA	1.83	0.60
4:H:86:SER:OG	4:H:95:TYR:HB2	2.01	0.60
1:A:238:TYR:CE2	1:A:322:LYS:HB2	2.37	0.60
3:L:42:VAL:HG11	3:L:103:GLN:NE2	2.16	0.60
4:H:153:THR:HA	4:H:158:ALA:HA	1.83	0.59
3:L:192:LEU:HD21	3:L:194:LEU:HD12	1.84	0.59
4:H:112:ALA:HB1	4:H:122:LEU:HD23	1.83	0.59
4:H:75:TYR:CZ	4:H:85:ILE:HG22	2.37	0.59
3:L:148:LEU:HD22	4:H:203:VAL:HG11	1.84	0.59
4:H:88:ASP:OD1	4:H:91:LYS:HD2	2.03	0.59
1:A:98:THR:H	1:A:101:GLN:HB2	1.68	0.58
1:A:61:PHE:O	1:A:76:ARG:HA	2.03	0.58
3:L:78:SER:OG	3:L:79:ARG:N	2.36	0.58
3:L:42:VAL:HG23	3:L:42:VAL:O	2.03	0.58
1:A:52:ARG:HB3	1:A:151:ALA:O	2.04	0.58
4:H:171:PRO:HG3	4:H:198:TYR:CE1	2.38	0.58
1:A:238:TYR:HE2	1:A:322:LYS:HB2	1.67	0.58
4:H:62:TRP:HZ2	4:H:65:SER:HB3	1.68	0.58
4:H:53:ARG:N	4:H:61:GLU:O	2.35	0.58
3:L:179:GLN:HE21	3:L:186:TYR:HE1	1.53	0.57
4:H:107:ALA:HB3	4:H:109:TYR:CE2	2.38	0.57
1:A:366:PRO:HB2	3:L:107:VAL:HG23	1.85	0.57
3:L:128:VAL:HG21	3:L:209:VAL:HG11	1.87	0.57
1:A:79:LEU:HD22	1:A:315:LEU:HD22	1.87	0.56
4:H:75:TYR:OH	4:H:85:ILE:HG22	2.05	0.56
4:H:169:PRO:HD2	4:H:222:HIS:HE1	1.68	0.56
3:L:180:ASP:HB3	3:L:183:ASP:HB3	1.88	0.55
4:H:32:SER:OG	4:H:99:ASN:HA	2.06	0.55
1:A:33:LEU:HG	1:A:33:LEU:O	2.07	0.55
1:A:197:LEU:HD23	1:A:343:VAL:HG21	1.88	0.55
1:A:165:ARG:NH2	2:V:350:SEP:O1P	2.39	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:LEU:HD22	1:A:327:LEU:HG	1.89	0.55
1:A:283:GLU:HG2	1:A:284:LYS:N	2.22	0.55
4:H:97:GLN:HG3	4:H:99:ASN:ND2	2.22	0.55
1:A:224:THR:O	1:A:264:PRO:HB3	2.06	0.55
1:A:79:LEU:HB3	1:A:315:LEU:HD13	1.88	0.54
1:A:201:ALA:HB1	1:A:347:LEU:HD11	1.89	0.54
3:L:45:ALA:HA	3:L:104:TYR:CZ	2.42	0.54
1:A:238:TYR:CE2	1:A:322:LYS:HD2	2.43	0.54
4:H:34:ARG:HA	4:H:96:LEU:O	2.08	0.54
4:H:83:PHE:CZ	4:H:98:MET:SD	3.01	0.54
4:H:141:PRO:HB3	4:H:167:TYR:HD1	1.71	0.54
4:H:171:PRO:HG3	4:H:198:TYR:CD1	2.43	0.54
1:A:61:PHE:CD1	1:A:243:LEU:HB2	2.43	0.53
1:A:278:LEU:HG	1:A:278:LEU:O	2.08	0.53
1:A:40:VAL:HG22	1:A:104:LEU:HD13	1.90	0.53
4:H:190:ALA:HB2	4:H:200:LEU:HD23	1.91	0.53
3:L:171:ASN:ND2	3:L:194:LEU:HD21	2.22	0.53
1:A:277:PHE:CE1	1:A:279:ALA:HB3	2.42	0.53
3:L:48:TRP:CZ3	3:L:101:CYS:HB2	2.43	0.53
1:A:187:THR:OG1	1:A:198:HIS:ND1	2.42	0.53
1:A:335:LEU:O	1:A:338:LEU:HB2	2.09	0.53
3:L:103:GLN:O	3:L:103:GLN:HG3	2.09	0.53
3:L:118:GLU:OE1	3:L:186:TYR:OH	2.26	0.52
1:A:65:ARG:HB2	1:A:68:LEU:CB	2.39	0.52
1:A:298:THR:O	4:H:70:TYR:OH	2.22	0.52
4:H:117:PHE:HA	4:H:118:TRP:CG	2.44	0.52
3:L:128:VAL:HG11	3:L:209:VAL:HG11	1.92	0.52
3:L:136:SER:HB2	4:H:144:PHE:HD2	1.75	0.52
4:H:50:HIS:HA	4:H:64:ALA:O	2.10	0.52
1:A:209:TYR:CE1	1:A:354:PRO:HG3	2.45	0.51
3:L:104:TYR:HA	3:L:109:VAL:HG12	1.92	0.51
4:H:167:TYR:O	4:H:198:TYR:N	2.43	0.51
1:A:233:ILE:HG12	1:A:325:VAL:HG13	1.92	0.51
3:L:20:SER:OG	3:L:21:PRO:HD3	2.11	0.51
3:L:72:PRO:HB2	3:L:75:PHE:CD2	2.46	0.51
4:H:172:VAL:HG13	4:H:221:ASN:C	2.31	0.51
4:H:18:GLN:OE1	4:H:19:LEU:N	2.43	0.50
4:H:51:TRP:HD1	4:H:64:ALA:HB3	1.76	0.50
4:H:141:PRO:HB3	4:H:167:TYR:CD1	2.46	0.50
1:A:275:THR:HG22	1:A:276:PRO:O	2.12	0.50
4:H:219:ASN:HA	4:H:230:ASP:HA	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:ILE:O	1:A:109:GLY:N	2.34	0.49
4:H:33:LEU:O	4:H:98:MET:CG	2.60	0.49
4:H:48:SER:O	4:H:114:SER:HB2	2.12	0.49
4:H:51:TRP:CD1	4:H:64:ALA:HB3	2.47	0.49
3:L:126:PRO:O	3:L:128:VAL:HG23	2.12	0.49
1:A:205:LYS:HD2	1:A:207:ILE:O	2.12	0.49
1:A:325:VAL:O	1:A:344:ALA:HA	2.13	0.49
4:H:33:LEU:O	4:H:98:MET:HG3	2.13	0.49
1:A:277:PHE:HD1	1:A:279:ALA:H	1.60	0.49
4:H:107:ALA:N	4:H:131:VAL:HG12	2.25	0.49
1:A:312:ARG:H	1:A:314:ILE:HD11	1.78	0.49
4:H:62:TRP:CZ2	4:H:65:SER:HB3	2.46	0.49
4:H:167:TYR:O	4:H:198:TYR:HB2	2.13	0.49
4:H:195:SER:OG	4:H:197:LEU:HD13	2.13	0.49
3:L:164:ASP:HA	3:L:204:VAL:HB	1.95	0.49
1:A:53:VAL:HG22	1:A:150:CYS:HB3	1.94	0.48
4:H:25:GLY:O	4:H:132:THR:HG23	2.12	0.48
1:A:323:VAL:HG23	1:A:349:PHE:CE2	2.49	0.48
4:H:169:PRO:HG2	4:H:224:PRO:HB2	1.94	0.48
4:H:106:THR:HG23	4:H:133:VAL:H	1.77	0.48
1:A:199:LEU:HD23	1:A:345:VAL:HG23	1.95	0.48
1:A:323:VAL:HG23	1:A:349:PHE:HE2	1.79	0.48
4:H:63:VAL:HG13	4:H:79:VAL:HG21	1.95	0.47
4:H:107:ALA:O	4:H:131:VAL:O	2.31	0.47
4:H:125:TRP:CD1	4:H:125:TRP:N	2.82	0.47
1:A:323:VAL:N	1:A:347:LEU:O	2.47	0.47
1:A:366:PRO:CB	3:L:107:VAL:HG23	2.44	0.47
1:A:201:ALA:CB	1:A:347:LEU:HD11	2.45	0.47
3:L:42:VAL:HG11	3:L:103:GLN:HE21	1.79	0.47
1:A:31:ILE:HD11	1:A:305:LEU:HB3	1.96	0.47
4:H:105:ASP:O	4:H:109:TYR:OH	2.28	0.47
1:A:290:ASP:C	1:A:298:THR:HG21	2.35	0.46
3:L:46:VAL:HG21	3:L:84:PHE:CD1	2.50	0.46
4:H:44:VAL:HG11	4:H:89:THR:HB	1.96	0.46
3:L:176:VAL:HG23	3:L:177:THR:O	2.15	0.46
1:A:235:VAL:HG22	1:A:323:VAL:HG22	1.96	0.46
1:A:196:PRO:O	1:A:223:ASN:HB2	2.15	0.46
1:A:292:LYS:HG3	1:A:298:THR:OG1	2.16	0.46
3:L:105:LYS:HG2	3:L:106:TYR:CE2	2.49	0.46
3:L:142:THR:HG22	3:L:195:SER:HA	1.97	0.46
4:H:166:ASP:OD1	4:H:166:ASP:N	2.48	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:113:ARG:HD3	4:H:123:ASP:HB2	1.97	0.46
3:L:148:LEU:HD21	4:H:203:VAL:HG21	1.98	0.46
4:H:97:GLN:HG3	4:H:99:ASN:HD21	1.80	0.46
1:A:10:LYS:HA	1:A:20:VAL:O	2.15	0.46
1:A:292:LYS:NZ	1:A:298:THR:OG1	2.48	0.46
3:L:41:SER:O	3:L:41:SER:OG	2.33	0.46
4:H:112:ALA:CB	4:H:122:LEU:HD23	2.45	0.46
1:A:182:PRO:CG	1:A:203:LEU:HB2	2.45	0.45
1:A:210:HIS:HD2	1:A:353:HIS:CE1	2.34	0.45
1:A:334:LEU:HG	1:A:335:LEU:HD23	1.96	0.45
1:A:28:VAL:HG23	1:A:30:HIS:CE1	2.51	0.45
3:L:74:ARG:O	3:L:88:ILE:HA	2.16	0.45
3:L:191:THR:HG22	3:L:193:THR:HG23	1.98	0.45
3:L:32:VAL:O	3:L:87:THR:HA	2.16	0.45
1:A:285:ARG:HG3	1:A:286:GLY:N	2.32	0.45
3:L:153:TYR:CE2	3:L:154:PRO:HB3	2.51	0.45
1:A:129:LEU:HD23	1:A:288:ALA:HA	1.98	0.45
3:L:90:SER:O	3:L:90:SER:OG	2.29	0.45
4:H:184:GLY:O	4:H:204:VAL:HA	2.17	0.45
1:A:240:ASP:HB2	1:A:318:ILE:HB	2.00	0.44
4:H:67:SER:O	4:H:71:GLY:N	2.47	0.44
1:A:32:ASP:OD2	1:A:33:LEU:HD23	2.17	0.44
1:A:302:SER:HB3	1:A:352:MET:HB3	1.99	0.44
1:A:322:LYS:HA	1:A:348:PRO:HA	2.00	0.44
4:H:83:PHE:CE2	4:H:98:MET:SD	3.11	0.44
1:A:52:ARG:HB2	1:A:52:ARG:CZ	2.48	0.44
3:L:29:GLY:O	3:L:90:SER:HA	2.18	0.44
1:A:236:ARG:HA	1:A:252:PRO:HA	1.99	0.44
1:A:260:ASP:OD1	1:A:260:ASP:N	2.50	0.44
4:H:169:PRO:HB2	4:H:224:PRO:HG2	2.00	0.44
4:H:51:TRP:HA	4:H:110:TYR:O	2.17	0.44
1:A:128:THR:HG21	1:A:292:LYS:HD2	1.99	0.44
4:H:107:ALA:HB3	4:H:109:TYR:CZ	2.53	0.44
3:L:61:ILE:HG23	3:L:66:SER:O	2.18	0.43
4:H:24:GLY:HA3	4:H:129:THR:HG21	2.00	0.43
1:A:123:LEU:HD13	1:A:123:LEU:HA	1.65	0.43
1:A:209:TYR:CD1	1:A:354:PRO:HG3	2.53	0.43
3:L:161:TRP:O	3:L:167:LEU:HA	2.17	0.43
1:A:52:ARG:O	1:A:151:ALA:N	2.51	0.43
1:A:277:PHE:HE1	1:A:279:ALA:HB3	1.80	0.43
3:L:75:PHE:CE1	3:L:99:TYR:HE1	2.34	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:27:VAL:HG13	4:H:133:VAL:HG13	1.99	0.43
4:H:33:LEU:O	4:H:98:MET:N	2.49	0.43
1:A:322:LYS:HA	1:A:347:LEU:O	2.18	0.43
4:H:146:LEU:N	4:H:161:GLY:O	2.49	0.43
1:A:337:ASP:OD1	1:A:337:ASP:N	2.51	0.43
4:H:119:TYR:OH	4:H:122:LEU:HD11	2.19	0.43
1:A:167:VAL:HG12	1:A:293:LEU:HD23	2.00	0.43
4:H:175:SER:N	4:H:219:ASN:O	2.35	0.43
3:L:34:ILE:HD13	3:L:115:THR:HG21	2.00	0.43
1:A:14:PRO:HD2	1:A:161:ARG:O	2.18	0.42
1:A:27:PHE:CE1	1:A:37:VAL:HA	2.54	0.42
3:L:31:ARG:HE	3:L:31:ARG:HB3	1.59	0.42
3:L:145:VAL:HG23	3:L:192:LEU:HB3	2.01	0.42
1:A:97:LEU:HD23	1:A:97:LEU:H	1.85	0.42
1:A:181:GLN:HG3	1:A:182:PRO:N	2.35	0.42
1:A:270:LYS:HD3	1:A:272:TYR:CZ	2.54	0.42
1:A:29:ASP:OD1	1:A:34:VAL:HG22	2.19	0.42
3:L:50:GLN:HB3	3:L:60:LEU:HD11	2.00	0.42
4:H:117:PHE:HA	4:H:118:TRP:HA	1.78	0.42
4:H:138:THR:HG23	4:H:169:PRO:HG2	2.01	0.42
3:L:25:SER:OG	3:L:118:GLU:OE2	2.38	0.42
3:L:75:PHE:CE1	3:L:88:ILE:HG12	2.55	0.42
1:A:45:PRO:HA	1:A:48:LEU:CB	2.49	0.42
1:A:75:PHE:N	1:A:75:PHE:CD2	2.88	0.42
3:L:132:PRO:HG3	3:L:222:PHE:CD1	2.55	0.42
1:A:62:ARG:NH1	1:A:74:THR:OG1	2.53	0.41
3:L:128:VAL:HG22	3:L:149:LEU:HG	2.02	0.41
3:L:50:GLN:HG2	3:L:60:LEU:HD21	2.01	0.41
4:H:106:THR:HA	4:H:133:VAL:HG23	2.01	0.41
3:L:22:SER:O	3:L:115:THR:HA	2.21	0.41
3:L:59:LEU:HG	3:L:60:LEU:N	2.36	0.41
3:L:72:PRO:HG2	3:L:75:PHE:HE2	1.86	0.41
3:L:184:SER:O	3:L:184:SER:OG	2.35	0.41
3:L:213:GLY:O	3:L:214:LEU:HD12	2.21	0.41
4:H:51:TRP:HB2	4:H:64:ALA:HB3	2.03	0.41
3:L:17:MET:HB2	3:L:111:PHE:O	2.21	0.41
3:L:17:MET:SD	3:L:103:GLN:HB3	2.61	0.41
3:L:47:ALA:N	3:L:102:GLN:O	2.47	0.41
1:A:41:VAL:O	1:A:112:ALA:HA	2.21	0.41
1:A:98:THR:HG23	1:A:101:GLN:OE1	2.21	0.41
1:A:128:THR:O	1:A:289:LEU:N	2.49	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:179:GLN:NE2	3:L:186:TYR:HE1	2.16	0.41
1:A:34:VAL:CB	1:A:119:ILE:HB	2.43	0.41
1:A:129:LEU:HD22	1:A:286:GLY:O	2.20	0.41
1:A:222:ASN:O	1:A:265:SER:HA	2.21	0.41
1:A:298:THR:HG22	1:A:299:ASN:H	1.86	0.41
4:H:32:SER:OG	4:H:99:ASN:HB3	2.21	0.41
1:A:7:ARG:HA	1:A:7:ARG:HD2	1.91	0.40
1:A:219:HIS:ND1	1:A:269:CYS:SG	2.88	0.40
3:L:111:PHE:CD2	4:H:60:LEU:HD13	2.56	0.40
3:L:149:LEU:N	3:L:149:LEU:HD12	2.37	0.40
4:H:104:GLU:H	4:H:104:GLU:HG2	1.34	0.40
4:H:66:ILE:HD13	4:H:66:ILE:HG21	1.88	0.40
3:L:46:VAL:HA	3:L:102:GLN:O	2.20	0.40
1:A:172:GLN:HB3	1:A:352:MET:HE1	2.04	0.40
4:H:96:LEU:HD12	4:H:96:LEU:HA	1.95	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	356/426 (84%)	307 (86%)	49 (14%)	0	100	100
2	V	10/23 (44%)	8 (80%)	1 (10%)	1 (10%)	0	3
3	L	210/227 (92%)	180 (86%)	30 (14%)	0	100	100
4	H	202/249 (81%)	177 (88%)	24 (12%)	1 (0%)	29	66
All	All	778/925 (84%)	672 (86%)	104 (13%)	2 (0%)	41	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	H	55	ALA
2	V	349	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	265/380 (70%)	226 (85%)	39 (15%)	3	14
2	V	7/14 (50%)	5 (71%)	2 (29%)	0	1
3	L	162/199 (81%)	129 (80%)	33 (20%)	1	5
4	H	137/209 (66%)	111 (81%)	26 (19%)	1	7
All	All	571/802 (71%)	471 (82%)	100 (18%)	2	9

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	SER
1	A	18	LEU
1	A	28	VAL
1	A	30	HIS
1	A	32	ASP
1	A	33	LEU
1	A	55	VAL
1	A	61	PHE
1	A	75	PHE
1	A	86	SER
1	A	92	GLU
1	A	97	LEU
1	A	111	HIS
1	A	123	LEU
1	A	126	SER
1	A	146	VAL
1	A	150	CYS
1	A	181	GLN
1	A	194	ASP
1	A	202	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	215	SER
1	A	225	ASN
1	A	251	CYS
1	A	259	ASP
1	A	261	THR
1	A	262	VAL
1	A	285	ARG
1	A	290	ASP
1	A	294	LYS
1	A	297	ASP
1	A	299	ASN
1	A	303	SER
1	A	304	THR
1	A	306	LEU
1	A	320	SER
1	A	325	VAL
1	A	337	ASP
1	A	338	LEU
1	A	352	MET
2	V	347	THR
2	V	368	ASP
3	L	13	SER
3	L	25	SER
3	L	27	SER
3	L	32	VAL
3	L	34	ILE
3	L	39	SER
3	L	49	TYR
3	L	71	VAL
3	L	73	SER
3	L	76	SER
3	L	87	THR
3	L	90	SER
3	L	91	LEU
3	L	95	ASP
3	L	101	CYS
3	L	102	GLN
3	L	103	GLN
3	L	113	GLN
3	L	117	VAL
3	L	134	SER
3	L	136	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	L	142	THR
3	L	164	ASP
3	L	168	GLN
3	L	171	ASN
3	L	172	SER
3	L	176	VAL
3	L	189	SER
3	L	193	THR
3	L	195	SER
3	L	209	VAL
3	L	210	THR
3	L	221	SER
4	H	19	LEU
4	H	21	GLU
4	H	26	LEU
4	H	33	LEU
4	H	40	SER
4	H	42	PHE
4	H	43	ASN
4	H	48	SER
4	H	52	VAL
4	H	68	SER
4	H	79	VAL
4	H	88	ASP
4	H	98	MET
4	H	99	ASN
4	H	104	GLU
4	H	113	ARG
4	H	114	SER
4	H	131	VAL
4	H	132	THR
4	H	133	VAL
4	H	144	PHE
4	H	166	ASP
4	H	191	VAL
4	H	206	VAL
4	H	208	SER
4	H	218	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
3	L	103	GLN
4	H	99	ASN
4	H	222	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

7 non-standard protein/DNA/RNA residues 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
2	SEP	V	350	2	8,9,10	1.69	2 (25%)	8,12,14	1.86	1 (12%)
2	SEP	V	364	2	8,9,10	0.77	0	8,12,14	0.76	0
2	TPO	V	359	2	8,10,11	1.77	1 (12%)	10,14,16	1.04	1 (10%)
2	SEP	V	362	2	8,9,10	1.11	0	8,12,14	1.51	1 (12%)
2	TPO	V	360	2	8,10,11	0.82	0	10,14,16	1.07	1 (10%)
2	SEP	V	357	2	8,9,10	1.59	1 (12%)	8,12,14	1.48	1 (12%)
2	SEP	V	363	2	8,9,10	0.99	0	8,12,14	0.80	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	SEP	V	350	2	-	5/5/8/10	-
2	SEP	V	364	2	-	2/5/8/10	-
2	TPO	V	359	2	-	6/9/11/13	-
2	SEP	V	362	2	-	2/5/8/10	-
2	TPO	V	360	2	-	2/9/11/13	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SEP	V	357	2	-	4/5/8/10	-
2	SEP	V	363	2	-	1/5/8/10	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	V	359	TPO	P-O1P	3.49	1.61	1.50
2	V	350	SEP	P-O1P	3.47	1.61	1.50
2	V	357	SEP	P-O1P	3.39	1.61	1.50
2	V	350	SEP	P-O3P	2.18	1.63	1.54

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	V	350	SEP	OG-CB-CA	4.53	112.55	108.14
2	V	362	SEP	O3P-P-OG	-3.07	98.57	106.73
2	V	357	SEP	P-OG-CB	-3.07	109.85	118.30
2	V	360	TPO	O-C-CA	-2.81	117.43	124.78
2	V	359	TPO	P-OG1-CB	-2.03	117.08	123.21

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	V	350	SEP	CB-OG-P-O2P
2	V	350	SEP	CB-OG-P-O3P
2	V	357	SEP	CB-OG-P-O1P
2	V	357	SEP	CB-OG-P-O2P
2	V	357	SEP	CB-OG-P-O3P
2	V	359	TPO	N-CA-CB-CG2
2	V	359	TPO	N-CA-CB-OG1
2	V	359	TPO	C-CA-CB-CG2
2	V	359	TPO	CG2-CB-OG1-P
2	V	360	TPO	O-C-CA-CB
2	V	360	TPO	CB-OG1-P-O2P
2	V	362	SEP	N-CA-CB-OG
2	V	362	SEP	CA-CB-OG-P
2	V	363	SEP	N-CA-CB-OG
2	V	350	SEP	CB-OG-P-O1P
2	V	359	TPO	CB-OG1-P-O2P
2	V	350	SEP	N-CA-CB-OG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	V	357	SEP	N-CA-CB-OG
2	V	364	SEP	N-CA-CB-OG
2	V	364	SEP	CB-OG-P-O1P
2	V	359	TPO	CA-CB-OG1-P
2	V	350	SEP	CA-CB-OG-P

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	V	350	SEP	1	0
2	V	359	TPO	1	0
2	V	362	SEP	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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, 95th 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 ²)	Q<0.9
1	A	360/426 (84%)	-0.04	6 (1%) 70 57	58, 94, 135, 150	0
2	V	13/23 (56%)	0.55	3 (23%) 0 0	107, 126, 146, 151	0
3	L	212/227 (93%)	0.32	14 (6%) 18 10	93, 123, 144, 153	0
4	H	208/249 (83%)	-0.07	4 (1%) 66 53	70, 120, 151, 165	0
All	All	793/925 (85%)	0.06	27 (3%) 45 29	58, 110, 144, 165	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	L	147	CYS	5.8
3	L	130	ILE	5.6
3	L	146	VAL	4.7
3	L	206	ALA	4.4
4	H	101	LEU	4.4
3	L	205	TYR	3.6
1	A	148	ALA	3.5
3	L	161	TRP	3.5
1	A	361	PRO	3.4
1	A	164	VAL	3.0
1	A	43	VAL	3.0
3	L	128	VAL	2.9
2	V	365	LEU	2.8
2	V	346	ARG	2.8
3	L	88	ILE	2.6
4	H	176	TRP	2.6
2	V	347	THR	2.6
1	A	111	HIS	2.4
3	L	207	CYS	2.3
4	H	105	ASP	2.2
3	L	117	VAL	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	L	145	VAL	2.1
3	L	214	LEU	2.1
3	L	129	PHE	2.0
4	H	134	SER	2.0
3	L	166	ALA	2.0
1	A	18	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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, 95th 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(Å ²)	Q<0.9
2	SEP	V	364	10/11	0.77	0.17	121,128,137,139	0
2	SEP	V	362	10/11	0.80	0.20	108,113,122,123	0
2	SEP	V	350	10/11	0.83	0.14	112,128,142,144	0
2	SEP	V	357	10/11	0.87	0.17	123,142,150,151	0
2	TPO	V	360	11/12	0.89	0.19	101,112,123,130	0
2	TPO	V	359	11/12	0.91	0.10	126,136,153,154	0
2	SEP	V	363	10/11	0.92	0.13	110,118,123,139	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.