



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 07:11 am BST

PDB ID : 1K5M
Title : Crystal Structure of a Human Rhinovirus Type 14:Human Immunodeficiency Virus Type 1 V3 Loop Chimeric Virus MN-III-2
Authors : Ding, J.; Smith, A.D.; Geisler, S.C.; Ma, X.; Arnold, G.F.; Arnold, E.
Deposited on : 2001-10-11
Resolution : 2.70 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 : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

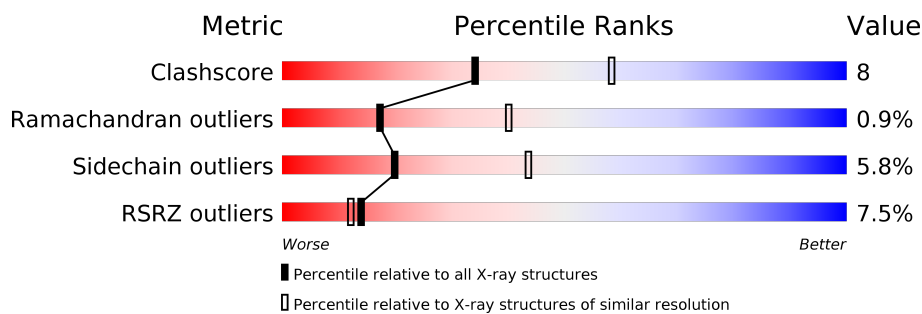
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 ≥ 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	289	<div> <div>8%</div> <div>82%</div> <div>15%</div> <div>.</div> </div>
2	B	277	<div> <div>10%</div> <div>77%</div> <div>17%</div> <div>.</div> <div>.</div> </div>
3	C	236	<div> <div>%</div> <div>81%</div> <div>16%</div> <div>.</div> </div>
4	D	68	<div> <div>12%</div> <div>56%</div> <div>41%</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
5	SPH	A	1971	X	-	-	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7117 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 COAT PROTEIN VP1 (P1D).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	283	Total	C	N	O	S	0	0	0
			2248	1422	388	430	8			

- Molecule 2 is a protein called CHIMERA OF HRV14 COAT PROTEIN VP2 (P1B) AND the V3 loop of HIV-1 gp120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	270	Total	C	N	O	S	0	0	0
			2065	1309	350	394	12			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1460	ALA	-	LINKER	UNP P05877
B	1461	ASP	-	LINKER	UNP P05877
B	1462	THR	-	LINKER	UNP P05877

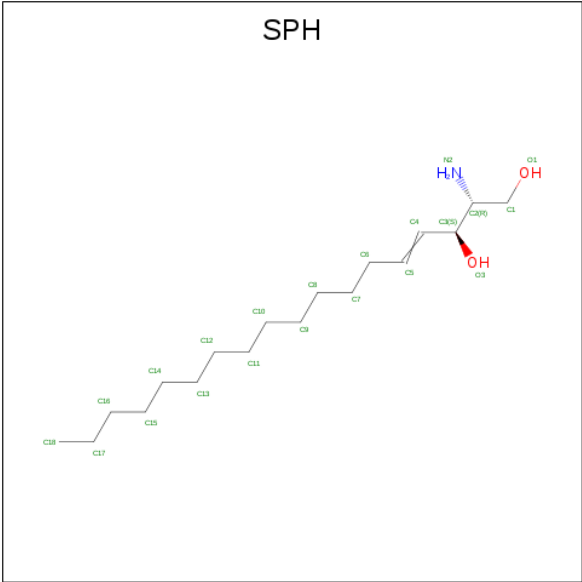
- Molecule 3 is a protein called COAT PROTEIN VP3 (P1C).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	236	Total	C	N	O	S	0	0	0
			1849	1184	305	353	7			

- Molecule 4 is a protein called COAT PROTEIN VP4 (P1A).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	40	Total	C	N	O	S	0	0	0
			297	186	47	62	2			

- Molecule 5 is SPHINGOSINE (three-letter code: SPH) (formula: C₁₈H₃₇NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			21	18	1	2		

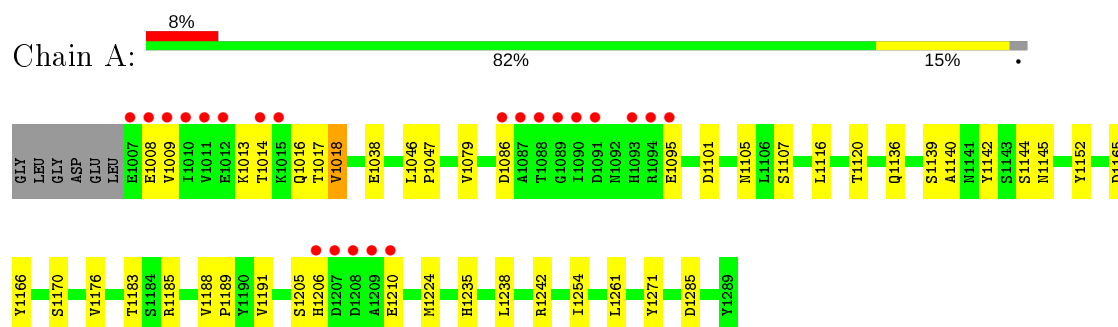
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	246	Total	O	0	0
			246	246		
6	B	194	Total	O	0	0
			194	194		
6	C	166	Total	O	0	0
			166	166		
6	D	31	Total	O	0	0
			31	31		

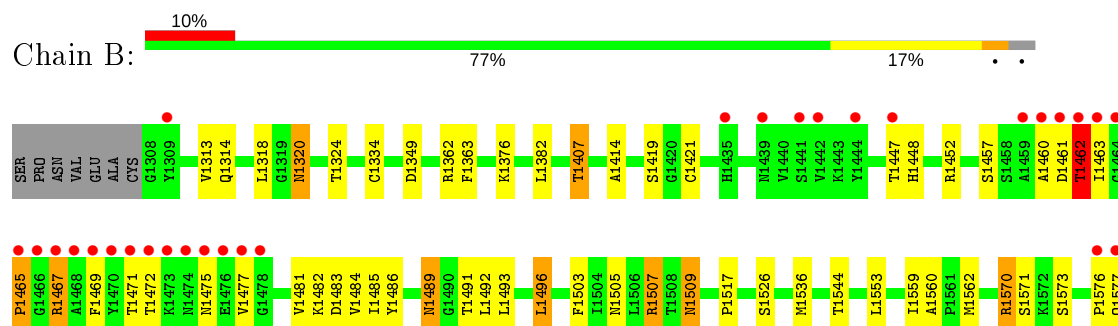
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

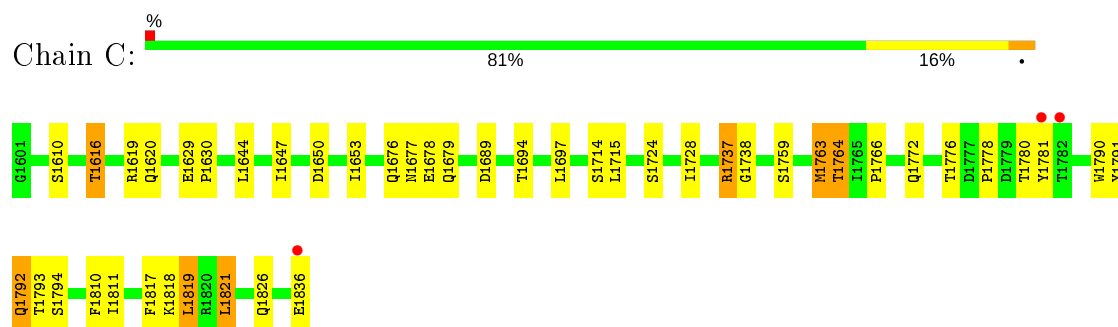
- Molecule 1: COAT PROTEIN VP1 (P1D)



- Molecule 2: CHIMERA OF HRV14 COAT PROTEIN VP2 (P1B) AND the V3 loop of HIV-1 gp120

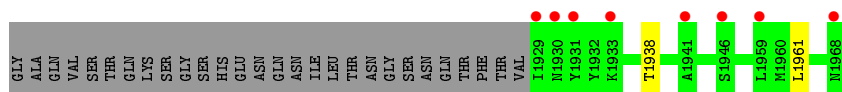


- Molecule 3: COAT PROTEIN VP3 (P1C)



- Molecule 4: COAT PROTEIN VP4 (P1A)





4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	318.90Å 349.30Å 368.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.70 49.77 – 2.70	Depositor EDS
% Data completeness (in resolution range)	89.0 (50.00-2.70) 92.7 (49.77-2.70)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.85 (at 2.69Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.216 , (Not available) 0.222 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	11.6	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 24.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	7117	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.60% 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: SPH

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	0.53	0/2306	0.50	0/3135
2	B	0.51	1/2117 (0.0%)	0.52	0/2893
3	C	0.48	0/1898	0.50	0/2597
4	D	0.45	0/302	0.44	0/406
All	All	0.51	1/6623 (0.0%)	0.50	0/9031

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	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1421	CYS	CB-SG	-5.60	1.72	1.81

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1166	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	A	2248	0	2190	26	0
2	B	2065	0	2036	58	0
3	C	1849	0	1830	29	0
4	D	297	0	294	1	0
5	A	21	0	36	3	0
6	A	246	0	0	6	0
6	B	194	0	0	8	0
6	C	166	0	0	4	0
6	D	31	0	0	0	0
All	All	7117	0	6386	108	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 8.

All (108) 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)
2:B:1461:ASP:CG	2:B:1485:ILE:HG22	1.37	1.41
2:B:1461:ASP:OD2	2:B:1485:ILE:HG22	1.34	1.28
2:B:1461:ASP:CG	2:B:1485:ILE:CG2	2.08	1.20
2:B:1461:ASP:OD2	2:B:1485:ILE:CG2	1.91	1.19
2:B:1376:LYS:HD2	2:B:1462:THR:CG2	2.00	0.90
1:A:1008:GLU:O	1:A:1018:VAL:HG22	1.75	0.85
2:B:1376:LYS:HD2	2:B:1462:THR:HG23	1.59	0.83
2:B:1461:ASP:CB	2:B:1485:ILE:HG22	2.13	0.78
1:A:1047:PRO:HA	3:C:1764:THR:HG21	1.67	0.75
2:B:1376:LYS:HG3	2:B:1460:ALA:CB	2.18	0.73
2:B:1376:LYS:CD	2:B:1462:THR:HG23	2.20	0.72
2:B:1461:ASP:CG	2:B:1485:ILE:HG21	2.09	0.72
2:B:1320:ASN:HD21	2:B:1362:ARG:HH21	1.38	0.71
2:B:1461:ASP:OD1	2:B:1485:ILE:HG21	1.92	0.69
1:A:1210:GLU:HB3	6:A:2201:HOH:O	1.96	0.65
2:B:1376:LYS:CE	2:B:1462:THR:HG23	2.27	0.64
2:B:1376:LYS:HB3	2:B:1484:VAL:HG21	1.80	0.63
2:B:1447:THR:HG21	6:B:2375:HOH:O	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1152:TYR:HB2	5:A:1971:SPH:H171	1.81	0.63
2:B:1376:LYS:CD	2:B:1462:THR:CG2	2.74	0.63
1:A:1016:GLN:HG2	6:A:2022:HOH:O	1.99	0.62
2:B:1376:LYS:HE3	2:B:1462:THR:HG23	1.79	0.62
1:A:1105:ASN:ND2	1:A:1107:SER:H	1.96	0.62
2:B:1447:THR:HG23	2:B:1448:HIS:ND1	2.14	0.62
3:C:1793:THR:HG22	3:C:1794:SER:N	2.15	0.61
1:A:1008:GLU:HA	6:A:2688:HOH:O	2.00	0.61
3:C:1826:GLN:HG2	6:C:2507:HOH:O	2.01	0.60
2:B:1461:ASP:OD1	2:B:1485:ILE:CG2	2.44	0.60
2:B:1457:SER:HB2	6:B:2389:HOH:O	2.02	0.60
3:C:1792:GLN:HA	3:C:1792:GLN:HE21	1.67	0.60
2:B:1507:ARG:HD3	6:B:2398:HOH:O	2.02	0.59
1:A:1189:PRO:O	1:A:1191:VAL:HG13	2.03	0.59
1:A:1014:THR:O	1:A:1014:THR:HG22	2.03	0.58
2:B:1471:THR:HG22	2:B:1472:THR:H	1.68	0.58
2:B:1509:ASN:N	2:B:1509:ASN:HD22	2.01	0.56
2:B:1509:ASN:HD22	2:B:1509:ASN:H	1.54	0.56
1:A:1009:VAL:O	1:A:1017:THR:HG23	2.05	0.56
2:B:1489:ASN:HD22	2:B:1489:ASN:C	2.10	0.56
3:C:1653:ILE:HD11	3:C:1811:ILE:HB	1.87	0.56
3:C:1689:ASP:HB2	3:C:1778:PRO:HB3	1.87	0.56
1:A:1105:ASN:HD22	1:A:1107:SER:H	1.55	0.55
2:B:1570:ARG:HG2	2:B:1571:SER:N	2.22	0.54
2:B:1376:LYS:HG3	2:B:1460:ALA:HB3	1.89	0.54
2:B:1486:TYR:HA	2:B:1491:THR:O	2.07	0.54
2:B:1414:ALA:HB2	2:B:1553:LEU:HD21	1.89	0.54
1:A:1038:GLU:HA	2:B:1503:PHE:HB2	1.89	0.54
3:C:1776:THR:HG22	6:C:2508:HOH:O	2.06	0.54
1:A:1188:VAL:HG21	5:A:1971:SPH:H141	1.91	0.53
2:B:1461:ASP:OD2	2:B:1485:ILE:HG23	1.99	0.53
3:C:1793:THR:O	3:C:1794:SER:HB3	2.09	0.52
3:C:1780:THR:HG22	3:C:1781:TYR:N	2.24	0.51
1:A:1145:ASN:HB3	6:A:2157:HOH:O	2.10	0.51
1:A:1116:LEU:HD13	5:A:1971:SPH:H2	1.93	0.50
2:B:1419:SER:HB2	2:B:1544:THR:HB	1.93	0.50
2:B:1505:ASN:H	2:B:1509:ASN:HD21	1.60	0.49
2:B:1320:ASN:HD21	2:B:1362:ARG:NH2	2.08	0.49
3:C:1650:ASP:HB2	3:C:1810:PHE:HB3	1.96	0.48
2:B:1407:THR:HG23	2:B:1560:ALA:HB3	1.95	0.48
1:A:1285:ASP:HB2	6:A:2258:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1009:VAL:O	1:A:1009:VAL:HG12	2.13	0.47
3:C:1616:THR:HG23	3:C:1616:THR:O	2.14	0.47
2:B:1382:LEU:HD21	2:B:1559:ILE:HD13	1.96	0.47
3:C:1714:SER:HB2	3:C:1810:PHE:HB2	1.97	0.46
1:A:1013:LYS:O	1:A:1016:GLN:HB2	2.15	0.46
3:C:1763:MET:HG3	3:C:1764:THR:N	2.31	0.46
2:B:1576:PRO:O	2:B:1577:GLN:HB3	2.15	0.46
2:B:1509:ASN:N	2:B:1509:ASN:ND2	2.65	0.45
6:B:2398:HOH:O	3:C:1759:SER:HB3	2.15	0.45
1:A:1142:TYR:CE2	1:A:1235:HIS:HE1	2.35	0.45
2:B:1334:CYS:HB2	2:B:1517:PRO:HD2	1.98	0.45
1:A:1120:THR:HB	1:A:1254:ILE:HB	1.99	0.45
2:B:1363:PHE:CD1	2:B:1560:ALA:HB2	2.51	0.45
3:C:1676:GLN:O	3:C:1791:TYR:HB2	2.16	0.45
2:B:1376:LYS:HG3	2:B:1460:ALA:HB2	1.96	0.45
2:B:1463:ILE:HD11	6:B:2387:HOH:O	2.17	0.45
3:C:1780:THR:CG2	3:C:1781:TYR:N	2.80	0.44
3:C:1728:ILE:HG23	3:C:1790:TRP:HB2	1.99	0.44
2:B:1320:ASN:HD22	2:B:1320:ASN:C	2.20	0.44
2:B:1448:HIS:HD2	6:B:2412:HOH:O	2.00	0.44
3:C:1737:ARG:HD2	3:C:1738:GLY:O	2.18	0.44
2:B:1492:LEU:HD12	3:C:1694:THR:HB	1.99	0.44
2:B:1460:ALA:HB3	2:B:1465:PRO:HD2	1.98	0.44
2:B:1467:ARG:HD3	6:B:2671:HOH:O	2.17	0.43
1:A:1101:ASP:HA	1:A:1224:MET:O	2.18	0.43
2:B:1320:ASN:HD21	2:B:1362:ARG:HE	1.67	0.43
2:B:1460:ALA:HA	2:B:1482:LYS:O	2.19	0.43
1:A:1271:TYR:OH	2:B:1483:ASP:HB2	2.19	0.43
1:A:1095:GLU:HG3	6:A:2702:HOH:O	2.19	0.42
3:C:1764:THR:O	3:C:1766:PRO:HD3	2.19	0.42
2:B:1469:PHE:HB3	2:B:1471:THR:O	2.20	0.42
3:C:1724:SER:HB2	6:C:2525:HOH:O	2.19	0.42
3:C:1780:THR:HB	6:C:2536:HOH:O	2.18	0.42
2:B:1407:THR:HG22	2:B:1562:MET:SD	2.59	0.42
2:B:1481:VAL:O	2:B:1481:VAL:HG13	2.19	0.42
1:A:1136:GLN:HE21	1:A:1140:ALA:CB	2.33	0.41
3:C:1715:LEU:HA	3:C:1715:LEU:HD12	1.94	0.41
2:B:1461:ASP:HB3	2:B:1485:ILE:H	1.84	0.41
3:C:1620:GLN:HE21	4:D:1938:THR:HA	1.85	0.41
1:A:1079:VAL:HG22	1:A:1242:ARG:HG2	2.03	0.41
3:C:1817:PHE:HE2	3:C:1819:LEU:HD11	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1261:LEU:HD11	2:B:1486:TYR:CD2	2.56	0.41
2:B:1313:VAL:C	2:B:1314:GLN:HG2	2.40	0.41
3:C:1818:LYS:O	3:C:1819:LEU:HD13	2.21	0.41
3:C:1679:GLN:HB2	3:C:1790:TRP:CZ3	2.56	0.41
3:C:1644:LEU:HD23	3:C:1647:ILE:HD11	2.02	0.41
2:B:1493:LEU:O	2:B:1496:LEU:HB2	2.22	0.40
2:B:1576:PRO:HA	6:B:2444:HOH:O	2.21	0.40
3:C:1629:GLU:HA	3:C:1630:PRO:HD2	1.98	0.40

There are no symmetry-related clashes.

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	281/289 (97%)	270 (96%)	11 (4%)	0	100	100
2	B	268/277 (97%)	241 (90%)	22 (8%)	5 (2%)	8	20
3	C	234/236 (99%)	220 (94%)	12 (5%)	2 (1%)	17	40
4	D	38/68 (56%)	34 (90%)	4 (10%)	0	100	100
All	All	821/870 (94%)	765 (93%)	49 (6%)	7 (1%)	17	40

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1467	ARG
2	B	1462	THR
2	B	1475	ASN
2	B	1465	PRO
2	B	1477	VAL
3	C	1678	GLU
3	C	1821	LEU

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	248/253 (98%)	235 (95%)	13 (5%)	23	49
2	B	234/240 (98%)	219 (94%)	15 (6%)	17	39
3	C	209/209 (100%)	196 (94%)	13 (6%)	18	40
4	D	33/57 (58%)	32 (97%)	1 (3%)	41	70
All	All	724/759 (95%)	682 (94%)	42 (6%)	20	43

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1018	VAL
1	A	1046	LEU
1	A	1086	ASP
1	A	1139	SER
1	A	1144	SER
1	A	1165	ASP
1	A	1170	SER
1	A	1176	VAL
1	A	1183	THR
1	A	1185	ARG
1	A	1205	SER
1	A	1206	HIS
1	A	1238	LEU
2	B	1318	LEU
2	B	1320	ASN
2	B	1324	THR
2	B	1349	ASP
2	B	1407	THR
2	B	1452	ARG
2	B	1462	THR
2	B	1489	ASN
2	B	1496	LEU
2	B	1507	ARG
2	B	1509	ASN

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Mol	Chain	Res	Type
2	B	1526	SER
2	B	1536	MET
2	B	1570	ARG
2	B	1573	SER
3	C	1610	SER
3	C	1616	THR
3	C	1619	ARG
3	C	1677	ASN
3	C	1697	LEU
3	C	1737	ARG
3	C	1763	MET
3	C	1764	THR
3	C	1772	GLN
3	C	1792	GLN
3	C	1819	LEU
3	C	1821	LEU
3	C	1836	GLU
4	D	1961	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1105	ASN
1	A	1136	GLN
1	A	1232	HIS
1	A	1235	HIS
2	B	1320	ASN
2	B	1435	HIS
2	B	1489	ASN
2	B	1509	ASN
3	C	1620	GLN
3	C	1792	GLN
4	D	1943	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	SPH	A	1971	-	19,20,20	1.29	1 (5%)	18,21,21	1.64	2 (11%)

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	SPH	A	1971	-	2/2/2/4	10/21/21/21	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1971	SPH	C4-C5	4.45	1.50	1.31

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1971	SPH	C3-C4-C5	-5.49	112.56	124.79
5	A	1971	SPH	C6-C5-C4	-2.72	113.21	125.39

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	1971	SPH	C2
5	A	1971	SPH	C3

All (10) torsion outliers are listed below:

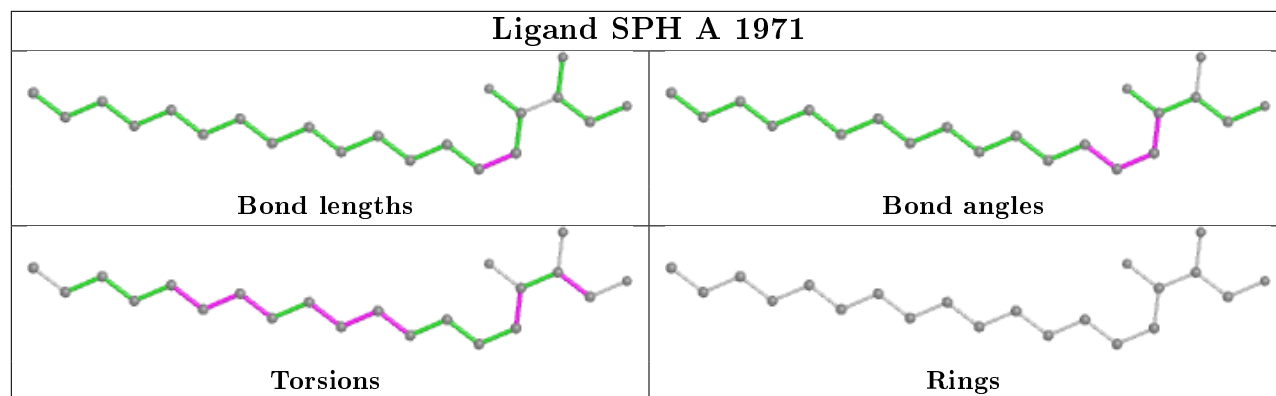
Mol	Chain	Res	Type	Atoms
5	A	1971	SPH	O1-C1-C2-N2
5	A	1971	SPH	C2-C3-C4-C5
5	A	1971	SPH	O3-C3-C4-C5
5	A	1971	SPH	C11-C12-C13-C14
5	A	1971	SPH	C11-C10-C9-C8
5	A	1971	SPH	C6-C7-C8-C9
5	A	1971	SPH	C12-C13-C14-C15
5	A	1971	SPH	O1-C1-C2-C3
5	A	1971	SPH	C7-C8-C9-C10
5	A	1971	SPH	C10-C11-C12-C13

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1971	SPH	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	283/289 (97%)	-0.01	22 (7%) 13 11	5, 8, 62, 78	0
2	B	270/277 (97%)	0.35	29 (10%) 6 4	5, 7, 74, 82	0
3	C	236/236 (100%)	-0.18	3 (1%) 77 78	5, 7, 31, 55	0
4	D	40/68 (58%)	0.88	8 (20%) 1 0	7, 32, 68, 74	0
All	All	829/870 (95%)	0.10	62 (7%) 14 12	5, 7, 61, 82	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1461	ASP	12.3
2	B	1465	PRO	11.0
2	B	1460	ALA	9.3
2	B	1459	ALA	8.6
2	B	1464	GLY	8.3
1	A	1008	GLU	8.1
2	B	1471	THR	7.9
1	A	1014	THR	7.8
1	A	1009	VAL	7.2
2	B	1474	ASN	7.0
2	B	1473	LYS	7.0
1	A	1010	ILE	6.8
2	B	1468	ALA	6.7
2	B	1469	PHE	6.6
2	B	1470	TYR	6.6
2	B	1475	ASN	6.4
2	B	1472	THR	6.1
2	B	1463	ILE	6.0
4	D	1929	ILE	5.8
2	B	1476	GLU	5.8
2	B	1467	ARG	5.3

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Mol	Chain	Res	Type	RSRZ
2	B	1462	THR	5.2
4	D	1930	ASN	5.2
2	B	1577	GLN	5.1
1	A	1011	VAL	4.9
1	A	1088	THR	4.8
2	B	1477	VAL	4.6
2	B	1444	TYR	4.3
2	B	1439	ASN	4.3
1	A	1015	LYS	4.2
2	B	1466	GLY	4.1
4	D	1931	TYR	4.1
1	A	1012	GLU	4.1
2	B	1441	SER	4.1
2	B	1478	GLY	4.0
1	A	1207	ASP	4.0
1	A	1007	GLU	3.9
1	A	1089	GLY	3.9
1	A	1208	ASP	3.9
1	A	1210	GLU	3.5
1	A	1209	ALA	3.2
2	B	1576	PRO	3.2
1	A	1206	HIS	3.2
4	D	1968	ASN	3.0
2	B	1309	TYR	2.9
2	B	1435	HIS	2.7
1	A	1090	ILE	2.7
1	A	1087	ALA	2.6
4	D	1946	SER	2.5
4	D	1933	LYS	2.5
1	A	1086	ASP	2.4
2	B	1442	VAL	2.4
1	A	1094	ARG	2.4
2	B	1447	THR	2.3
3	C	1782	THR	2.3
3	C	1781	TYR	2.3
3	C	1836	GLU	2.2
4	D	1959	LEU	2.1
1	A	1091	ASP	2.1
1	A	1095	GLU	2.0
4	D	1941	ALA	2.0
1	A	1093	HIS	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](#)

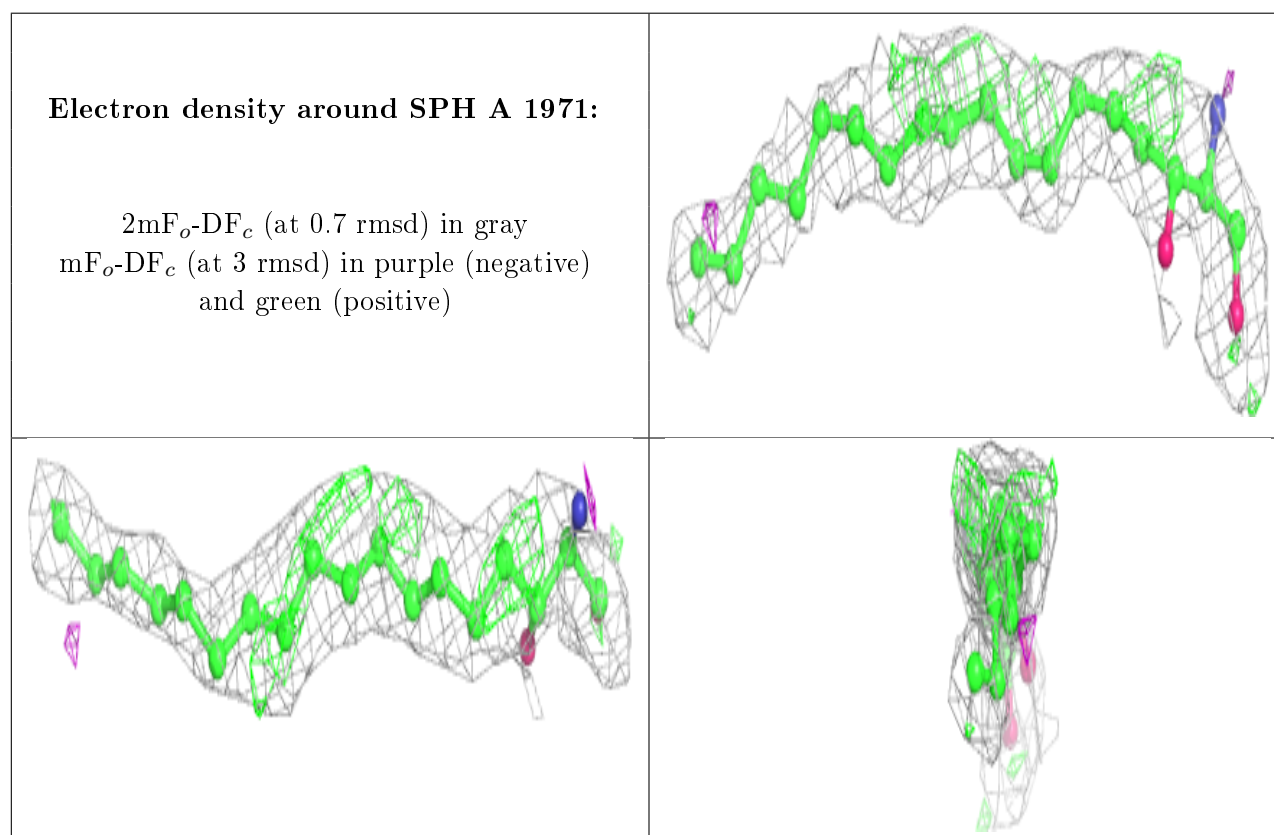
There are no carbohydrates in this entry.

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. 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(\AA^2)	Q<0.9
5	SPH	A	1971	21/21	0.81	0.26	22,31,43,46	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.