Full wwPDB X-ray Structure Validation Report ⓘ

Apr 10, 2023 – 11:28 PM EDT

PDB ID	:	2PLV
Title	:	STRUCTURAL FACTORS THAT CONTROL CONFORMATIONAL TRANSITIONS AND SEROTYPE SPECIFICITY IN TYPE 3 POLIOVIRUS
Authors	:	Filman, D.J.; Hogle, J.M.
Deposited on	:	1989-10-17
Resolution	:	2.88 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

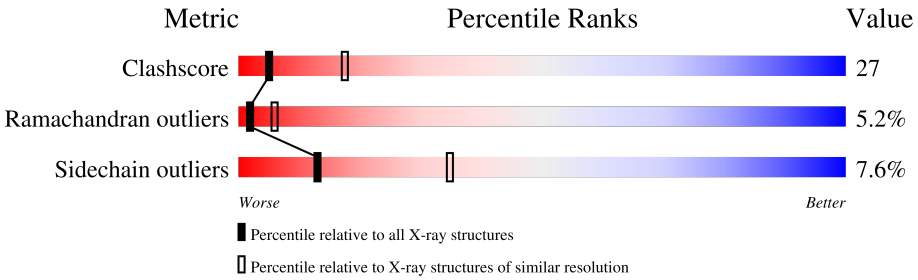
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.88 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	2947 (2.90-2.86)
Ramachandran outliers	138981	2868 (2.90-2.86)
Sidechain outliers	138945	2871 (2.90-2.86)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	1	302	53% 33% 8% • 5%
2	2	272	54% 35% 8% ••
3	3	238	47% 42% 7% ••
4	4	68	37% 38% 16% • 7%

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	1	0	X	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 7162 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 HUMAN POLIOVIRUS TYPE 1 (SUBUNIT VP1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	288	Total	C	N	O	S	0	0	0
			2251	1431	383	432	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	8	SER	ARG	conflict	UNP P03300
1	9	SER	GLU	conflict	UNP P03300

- Molecule 2 is a protein called HUMAN POLIOVIRUS TYPE 1 (SUBUNIT VP2).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	268	Total	C	N	O	S	0	0	0
			2085	1317	358	396	14			

- Molecule 3 is a protein called HUMAN POLIOVIRUS TYPE 1 (SUBUNIT VP3).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	235	Total	C	N	O	S	0	0	0
			1834	1169	299	349	17			

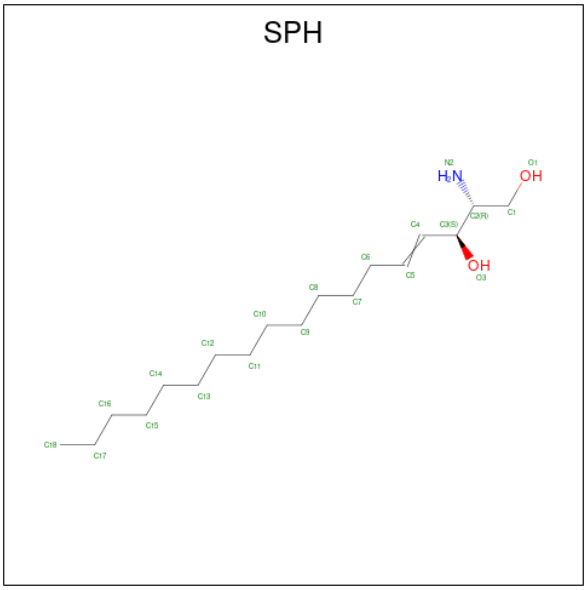
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	123	SER	PHE	conflict	UNP P03300

- Molecule 4 is a protein called HUMAN POLIOVIRUS TYPE 1 (SUBUNIT VP4).

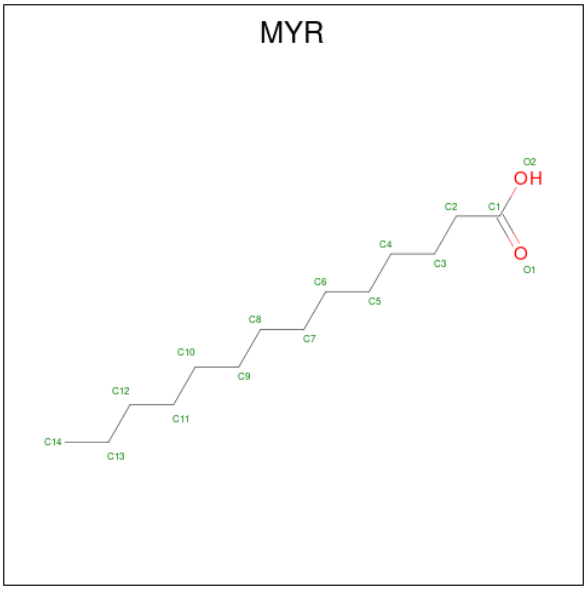
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	4	63	Total	C	N	O	S	0	0	1
			477	293	82	101	1			

- Molecule 5 is SPHINGOSINE (three-letter code: SPH) (formula: $C_{18}H_{37}NO_2$).



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

- Molecule 6 is MYRISTIC ACID (three-letter code: MYR) (formula: $C_{14}H_{28}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	4	1	15	14	1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	1	159	Total O 159 159	0	0
7	2	149	Total O 149 149	0	0
7	3	129	Total O 129 129	0	0
7	4	42	Total O 42 42	0	0

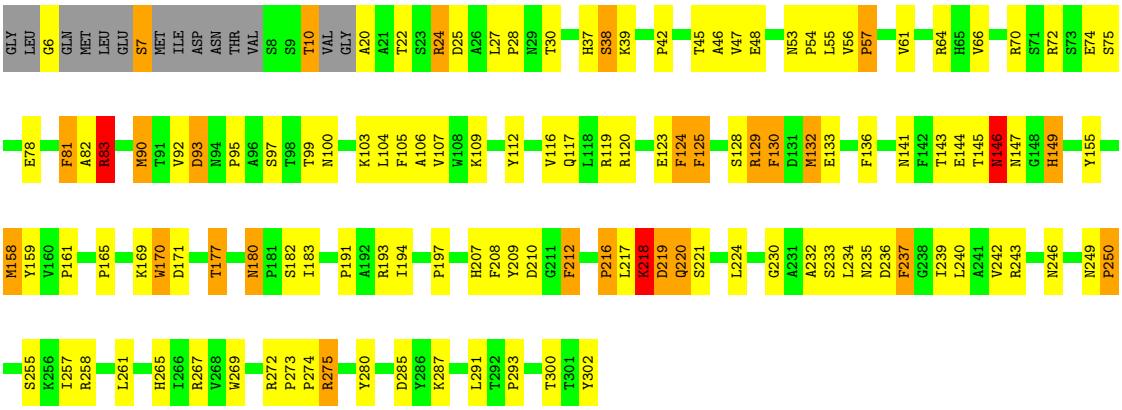
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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. 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. 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.

Note EDS was not executed.

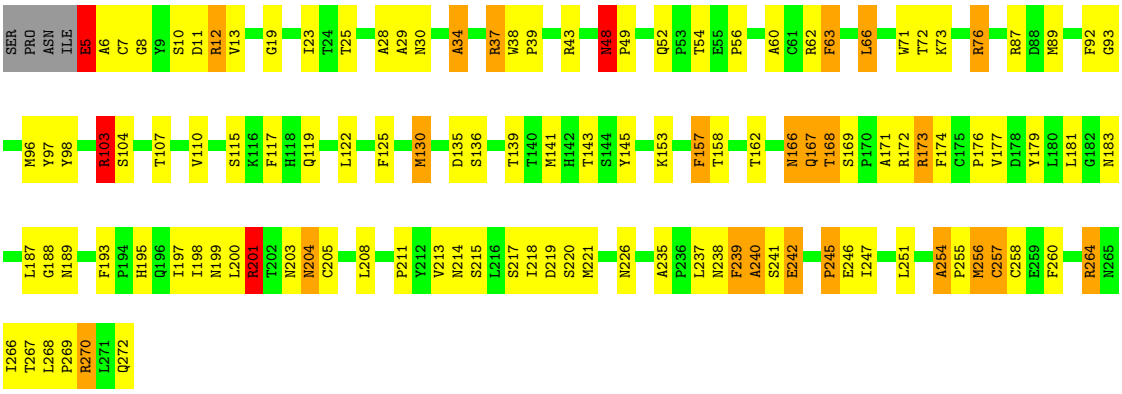
• Molecule 1: HUMAN POLIOVIRUS TYPE 1 (SUBUNIT VP1)

Chain 1:



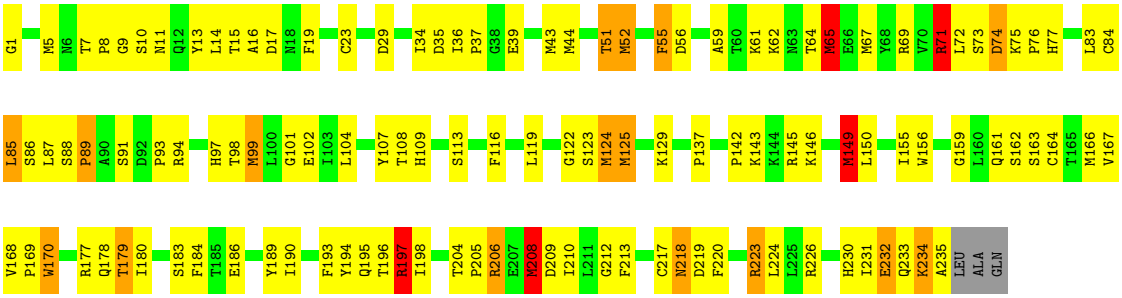
• Molecule 2: HUMAN POLIOVIRUS TYPE 1 (SUBUNIT VP2)

Chain 2:



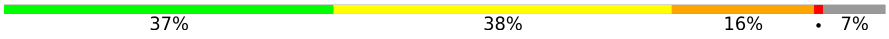
• Molecule 3: HUMAN POLIOVIRUS TYPE 1 (SUBUNIT VP3)

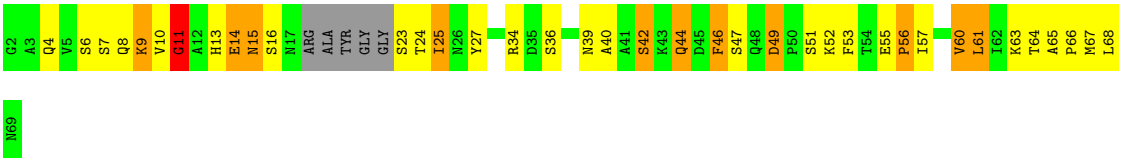
Chain 3:



• Molecule 4: HUMAN POLIOVIRUS TYPE 1 (SUBUNIT VP4)

Chain 4:





4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	322.94Å 358.04Å 380.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.88	Depositor
% Data completeness (in resolution range)	72.6 ((Not available)-2.88)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REAL-SPACE REFINEMENT	Depositor
R, R_{free}	0.200 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7162	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SPH, 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	1.94	3/2313 (0.1%)	2.09	34/3160 (1.1%)
2	2	1.95	8/2142 (0.4%)	2.10	38/2928 (1.3%)
3	3	1.92	6/1881 (0.3%)	2.07	33/2562 (1.3%)
4	4	1.95	5/484 (1.0%)	2.11	11/653 (1.7%)
All	All	1.94	22/6820 (0.3%)	2.09	116/9303 (1.2%)

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	6	GLY	N-CA	10.41	1.61	1.46
3	3	1	GLY	N-CA	9.08	1.59	1.46
1	1	20	ALA	N-CA	7.87	1.62	1.46
4	4	23	SER	N-CA	7.71	1.61	1.46
4	4	14	GLU	CD-OE2	6.58	1.32	1.25
2	2	5	GLU	N-CA	5.83	1.58	1.46
4	4	47	SER	C-N	-5.45	1.21	1.34
4	4	11	GLY	N-CA	5.35	1.54	1.46
2	2	19	GLY	N-CA	5.34	1.54	1.46
2	2	245	PRO	C-N	-5.26	1.22	1.34
4	4	14	GLU	N-CA	5.23	1.56	1.46
1	1	93	ASP	C-N	-5.22	1.22	1.34
2	2	93	GLY	N-CA	5.18	1.53	1.46
2	2	30	ASN	C-N	-5.16	1.22	1.34
2	2	188	GLY	N-CA	5.13	1.53	1.46
3	3	159	GLY	N-CA	5.11	1.53	1.46
2	2	19	GLY	CA-C	5.10	1.60	1.51
3	3	9	GLY	N-CA	5.09	1.53	1.46
3	3	101	GLY	N-CA	5.09	1.53	1.46
3	3	9	GLY	CA-C	5.07	1.59	1.51
3	3	122	GLY	N-CA	5.07	1.53	1.46
2	2	235	ALA	C-N	-5.03	1.24	1.34

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	3	197	ARG	NE-CZ-NH2	7.72	124.16	120.30
2	2	264	ARG	NE-CZ-NH2	7.67	124.14	120.30
1	1	267	ARG	NE-CZ-NH2	7.65	124.12	120.30
3	3	223	ARG	NE-CZ-NH2	7.57	124.08	120.30
3	3	69	ARG	NE-CZ-NH2	7.55	124.08	120.30
1	1	64	ARG	NE-CZ-NH2	7.52	124.06	120.30
2	2	201	ARG	NE-CZ-NH2	7.50	124.05	120.30
2	2	103	ARG	NE-CZ-NH2	7.50	124.05	120.30
2	2	43	ARG	NE-CZ-NH2	7.49	124.05	120.30
1	1	129	ARG	NE-CZ-NH2	7.49	124.05	120.30
1	1	275	ARG	NE-CZ-NH2	7.46	124.03	120.30
1	1	120	ARG	NE-CZ-NH2	7.46	124.03	120.30
1	1	193	ARG	NE-CZ-NH2	7.46	124.03	120.30
2	2	176	PRO	CA-N-CD	-7.46	101.06	111.50
4	4	34	ARG	NE-CZ-NH2	7.45	124.03	120.30
3	3	145	ARG	NE-CZ-NH2	7.44	124.02	120.30
1	1	243	ARG	NE-CZ-NH2	7.43	124.02	120.30
3	3	206	ARG	NE-CZ-NH2	7.43	124.01	120.30
3	3	177	ARG	NE-CZ-NH2	7.42	124.01	120.30
1	1	272	ARG	NE-CZ-NH2	7.41	124.00	120.30
2	2	12	ARG	NE-CZ-NH2	7.41	124.00	120.30
1	1	72	ARG	NE-CZ-NH2	7.40	124.00	120.30
2	2	62	ARG	NE-CZ-NH2	7.39	124.00	120.30
2	2	76	ARG	NE-CZ-NH2	7.39	124.00	120.30
3	3	226	ARG	NE-CZ-NH2	7.39	124.00	120.30
1	1	70	ARG	NE-CZ-NH2	7.37	123.99	120.30
1	1	119	ARG	NE-CZ-NH2	7.37	123.98	120.30
3	3	71	ARG	NE-CZ-NH2	7.37	123.98	120.30
2	2	270	ARG	NE-CZ-NH2	7.35	123.97	120.30
2	2	172	ARG	NE-CZ-NH2	7.34	123.97	120.30
1	1	24	ARG	NE-CZ-NH2	7.31	123.96	120.30
2	2	37	ARG	NE-CZ-NH2	7.31	123.96	120.30
1	1	258	ARG	NE-CZ-NH2	7.31	123.95	120.30
3	3	94	ARG	NE-CZ-NH2	7.30	123.95	120.30
2	2	173	ARG	NE-CZ-NH2	7.29	123.94	120.30
2	2	87	ARG	NE-CZ-NH2	7.29	123.94	120.30
1	1	83	ARG	NE-CZ-NH2	7.22	123.91	120.30
1	1	146	ASN	CB-CA-C	-6.76	96.88	110.40
1	1	130	PHE	N-CA-C	6.61	128.84	111.00
2	2	193	PHE	CB-CA-C	-6.57	97.26	110.40
2	2	174	PHE	CB-CA-C	-6.34	97.72	110.40
3	3	166	MET	CG-SD-CE	6.30	110.28	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	125	PHE	N-CA-C	6.27	127.93	111.00
2	2	204	ASN	CB-CA-C	-6.25	97.90	110.40
3	3	44	MET	CG-SD-CE	6.23	110.17	100.20
3	3	65	MET	CG-SD-CE	6.23	110.16	100.20
2	2	89	MET	CG-SD-CE	6.21	110.14	100.20
3	3	125	MET	CG-SD-CE	6.21	110.13	100.20
3	3	67	MET	CG-SD-CE	6.18	110.09	100.20
3	3	19	PHE	CB-CA-C	-6.18	98.04	110.40
3	3	193	PHE	CB-CA-C	-6.18	98.04	110.40
3	3	124	MET	CG-SD-CE	6.16	110.05	100.20
4	4	8	GLN	O-C-N	6.15	132.54	122.70
2	2	96	MET	CG-SD-CE	6.14	110.02	100.20
2	2	130	MET	CG-SD-CE	6.14	110.02	100.20
1	1	158	MET	CG-SD-CE	6.13	110.01	100.20
3	3	149	MET	CG-SD-CE	6.12	110.00	100.20
1	1	90	MET	CG-SD-CE	6.11	109.98	100.20
3	3	99	MET	CG-SD-CE	6.11	109.98	100.20
2	2	221	MET	CG-SD-CE	6.11	109.97	100.20
3	3	208	MET	CG-SD-CE	6.11	109.97	100.20
3	3	52	MET	CG-SD-CE	6.10	109.97	100.20
2	2	256	MET	CG-SD-CE	6.09	109.95	100.20
3	3	5	MET	CG-SD-CE	6.09	109.95	100.20
3	3	43	MET	CG-SD-CE	6.09	109.95	100.20
2	2	141	MET	CG-SD-CE	6.08	109.92	100.20
2	2	260	PHE	N-CA-C	6.07	127.39	111.00
2	2	63	PHE	N-CA-C	6.01	127.24	111.00
1	1	136	PHE	N-CA-C	6.01	127.23	111.00
4	4	67	MET	CG-SD-CE	6.00	109.81	100.20
1	1	132	MET	CG-SD-CE	5.98	109.76	100.20
1	1	237	PHE	N-CA-C	5.89	126.90	111.00
2	2	125	PHE	CB-CA-C	-5.87	98.65	110.40
4	4	25	ILE	O-C-N	5.79	131.97	122.70
1	1	130	PHE	CB-CA-C	-5.74	98.92	110.40
2	2	203	ASN	N-CA-C	5.60	126.13	111.00
1	1	7	SER	O-C-N	5.56	131.60	122.70
3	3	213	PHE	CB-CA-C	-5.55	99.30	110.40
1	1	212	PHE	CB-CA-C	-5.54	99.31	110.40
1	1	141	ASN	O-C-N	5.53	131.55	122.70
3	3	232	GLU	O-C-N	5.52	131.53	122.70
4	4	46	PHE	N-CA-C	5.50	125.85	111.00
1	1	125	PHE	CB-CA-C	-5.46	99.47	110.40
1	1	124	PHE	CA-C-N	-5.42	105.28	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	4	46	PHE	CB-CA-C	-5.40	99.60	110.40
4	4	53	PHE	CB-CA-C	-5.40	99.60	110.40
3	3	55	PHE	N-CA-C	5.39	125.54	111.00
4	4	47	SER	O-C-N	5.38	131.32	122.70
3	3	220	PHE	CB-CA-C	-5.38	99.64	110.40
2	2	174	PHE	N-CA-C	5.31	125.34	111.00
3	3	220	PHE	N-CA-C	5.28	125.26	111.00
2	2	157	PHE	CB-CA-C	-5.28	99.84	110.40
2	2	247	ILE	O-C-N	5.28	131.13	121.10
1	1	272	ARG	O-C-N	5.27	131.12	121.10
1	1	208	PHE	CB-CA-C	-5.26	99.89	110.40
2	2	239	PHE	N-CA-C	5.26	125.19	111.00
3	3	19	PHE	N-CA-C	5.25	125.18	111.00
3	3	55	PHE	CB-CA-C	-5.24	99.92	110.40
4	4	40	ALA	O-C-N	5.21	131.04	122.70
2	2	183	ASN	N-CA-C	5.21	125.07	111.00
2	2	246	GLU	O-C-N	5.18	130.98	122.70
2	2	63	PHE	CB-CA-C	-5.17	100.05	110.40
1	1	218	LYS	CB-CA-C	-5.15	100.09	110.40
3	3	193	PHE	N-CA-C	5.15	124.91	111.00
3	3	184	PHE	CB-CA-C	-5.12	100.16	110.40
3	3	116	PHE	CB-CA-C	-5.11	100.17	110.40
1	1	237	PHE	CB-CA-C	-5.10	100.21	110.40
2	2	260	PHE	CB-CA-C	-5.09	100.22	110.40
2	2	254	ALA	O-C-N	5.09	130.77	121.10
2	2	92	PHE	CB-CA-C	-5.08	100.24	110.40
1	1	180	ASN	CB-CA-C	-5.07	100.25	110.40
1	1	81	PHE	CB-CA-C	-5.05	100.31	110.40
1	1	243	ARG	O-C-N	5.04	130.77	122.70
4	4	39	ASN	CB-CA-C	-5.04	100.31	110.40
2	2	193	PHE	O-C-N	5.04	130.68	121.10
4	4	44	GLN	O-C-N	5.01	130.72	122.70

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	1	2251	0	2197	125	0
2	2	2085	0	2000	106	0
3	3	1834	0	1816	120	0
4	4	477	0	457	41	0
5	1	21	0	36	26	0
6	4	15	0	27	1	0
7	1	159	0	0	7	0
7	2	149	0	0	4	0
7	3	129	0	0	12	0
7	4	42	0	0	6	0
All	All	7162	0	6533	359	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 27.

All (359) 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)
2:2:5:GLU:CG	2:2:7:CYS:HB3	1.58	1.32
3:3:124:MET:HG3	7:3:320:HOH:O	1.32	1.23
1:1:132:MET:CE	5:1:0:SPH:H81	1.69	1.23
1:1:177:THR:HG21	1:1:182:SER:OG	1.40	1.21
3:3:124:MET:CG	7:3:320:HOH:O	1.83	1.17
2:2:5:GLU:CG	2:2:7:CYS:CB	2.25	1.14
1:1:237:PHE:CE2	5:1:0:SPH:H71	1.82	1.14
2:2:5:GLU:HG2	2:2:7:CYS:HB3	1.19	1.11
2:2:179:TYR:HA	3:3:65:MET:HE2	1.24	1.10
1:1:149:HIS:HE1	7:1:303:HOH:O	1.35	1.08
2:2:48:ASN:HB3	2:2:49:PRO:HD3	1.18	1.08
3:3:167:VAL:O	3:3:169:PRO:HD3	1.56	1.05
2:2:48:ASN:HB3	2:2:49:PRO:CD	1.85	1.04
1:1:132:MET:HE1	5:1:0:SPH:C8	1.87	1.04
2:2:179:TYR:CA	3:3:65:MET:HE2	1.90	1.01
2:2:179:TYR:HA	3:3:65:MET:CE	1.90	1.00
2:2:5:GLU:HG3	2:2:7:CYS:CB	1.90	0.99
2:2:37:ARG:O	2:2:211:PRO:HG3	1.64	0.97
2:2:187:LEU:HD22	3:3:65:MET:CE	1.96	0.94
2:2:5:GLU:HG3	2:2:7:CYS:HB3	1.41	0.94
2:2:5:GLU:OE2	2:2:7:CYS:HB2	1.66	0.94
1:1:149:HIS:CE1	7:1:303:HOH:O	2.15	0.93
2:2:5:GLU:HG3	2:2:7:CYS:CA	1.99	0.93
3:3:83:LEU:HD12	3:3:83:LEU:O	1.69	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:132:MET:HE1	5:1:0:SPH:H81	0.93	0.92
2:2:5:GLU:CD	2:2:7:CYS:H	1.72	0.92
1:1:22:THR:HG22	1:1:24:ARG:H	1.32	0.92
1:1:56:VAL:HB	1:1:57:PRO:HD2	1.52	0.91
1:1:112:TYR:HE2	5:1:0:SPH:HO3	0.92	0.90
2:2:168:THR:CG2	2:2:169:SER:N	2.36	0.88
3:3:71:ARG:NH1	3:3:209:ASP:OD2	2.07	0.87
2:2:267:THR:O	2:2:269:PRO:HD3	1.75	0.86
2:2:270:ARG:O	2:2:270:ARG:HG2	1.73	0.86
2:2:168:THR:HG22	2:2:169:SER:N	1.90	0.86
1:1:144:GLU:O	1:1:146:ASN:N	2.09	0.84
1:1:144:GLU:C	1:1:146:ASN:H	1.79	0.83
1:1:237:PHE:CE2	5:1:0:SPH:C7	2.61	0.83
3:3:232:GLU:OE1	3:3:234:LYS:HG2	1.78	0.83
2:2:166:ASN:O	2:2:166:ASN:OD1	1.97	0.83
3:3:149:MET:HE2	3:3:150:LEU:HD23	1.61	0.83
2:2:34:ALA:HB3	2:2:211:PRO:HD2	1.61	0.82
1:1:191:PRO:HG2	3:3:13:TYR:HB2	1.61	0.82
2:2:5:GLU:HG3	2:2:7:CYS:N	1.93	0.81
4:4:14:GLU:HG2	4:4:16:SER:HB2	1.63	0.81
1:1:158:MET:SD	1:1:177:THR:HG23	2.22	0.80
2:2:5:GLU:HG2	2:2:7:CYS:CB	2.04	0.79
1:1:218:LYS:HD2	7:2:417:HOH:O	1.82	0.79
1:1:27:LEU:HB3	1:1:28:PRO:HD2	1.66	0.78
1:1:219:ASP:O	1:1:219:ASP:OD2	2.01	0.78
4:4:14:GLU:HG2	4:4:16:SER:H	1.50	0.77
1:1:237:PHE:CZ	5:1:0:SPH:H71	2.20	0.77
4:4:14:GLU:HG3	7:4:84:HOH:O	1.85	0.76
3:3:7:THR:HB	3:3:8:PRO:HD2	1.67	0.75
2:2:242:GLU:OE2	2:2:242:GLU:N	2.19	0.74
3:3:149:MET:CE	3:3:150:LEU:CD2	2.65	0.74
1:1:22:THR:HG22	1:1:24:ARG:N	2.03	0.74
4:4:14:GLU:HG2	4:4:16:SER:N	2.03	0.73
2:2:5:GLU:CG	2:2:7:CYS:H	2.02	0.73
2:2:5:GLU:OE1	2:2:5:GLU:CA	2.38	0.72
3:3:210:ILE:O	3:3:210:ILE:HG13	1.89	0.72
1:1:112:TYR:HE2	5:1:0:SPH:O3	1.71	0.72
4:4:14:GLU:CG	4:4:16:SER:HB2	2.19	0.72
3:3:74:ASP:HA	3:3:198:ILE:O	1.89	0.71
1:1:109:LYS:HA	1:1:239:ILE:HG22	1.71	0.71
3:3:232:GLU:OE1	3:3:234:LYS:CG	2.39	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:38:TRP:CD1	2:2:39:PRO:HD2	2.26	0.71
2:2:168:THR:HG22	2:2:169:SER:H	1.54	0.70
2:2:34:ALA:HB3	2:2:211:PRO:CD	2.22	0.70
3:3:71:ARG:HB2	3:3:71:ARG:CZ	2.19	0.70
3:3:97:HIS:CE1	3:3:230:HIS:ND1	2.60	0.70
3:3:97:HIS:CE1	7:3:246:HOH:O	2.45	0.70
4:4:10:VAL:HG12	4:4:13:HIS:CE1	2.27	0.70
3:3:234:LYS:O	3:3:235:ALA:HB3	1.91	0.70
3:3:71:ARG:HH12	3:3:209:ASP:CG	1.95	0.69
4:4:42:SER:OG	4:4:44:GLN:HB2	1.92	0.69
2:2:5:GLU:OE1	2:2:5:GLU:HA	1.91	0.69
2:2:12:ARG:HA	2:2:28:ALA:O	1.93	0.69
3:3:196:THR:O	3:3:197:ARG:HB3	1.93	0.69
4:4:10:VAL:CG2	4:4:25:ILE:HD12	2.22	0.69
1:1:132:MET:CE	5:1:0:SPH:C8	2.58	0.69
3:3:97:HIS:ND1	7:3:246:HOH:O	2.25	0.69
3:3:234:LYS:O	3:3:235:ALA:CB	2.40	0.69
4:4:65:ALA:HB1	4:4:66:PRO:HD2	1.73	0.69
3:3:149:MET:CE	3:3:150:LEU:HD23	2.24	0.68
4:4:14:GLU:C	4:4:16:SER:H	1.94	0.68
1:1:103:LYS:HD3	1:1:170:TRP:CD2	2.27	0.68
4:4:61:LEU:O	4:4:61:LEU:HG	1.93	0.68
2:2:5:GLU:OE1	2:2:6:ALA:N	2.27	0.68
3:3:195:GLN:OE1	3:3:195:GLN:HA	1.92	0.68
2:2:110:VAL:HG22	2:2:251:LEU:HD12	1.77	0.67
2:2:5:GLU:CG	2:2:7:CYS:N	2.58	0.67
3:3:124:MET:HG2	7:3:320:HOH:O	1.64	0.67
3:3:97:HIS:CE1	3:3:230:HIS:CE1	2.83	0.67
4:4:14:GLU:CD	4:4:16:SER:HB2	2.15	0.66
1:1:233:SER:HB2	7:1:410:HOH:O	1.95	0.66
1:1:47:VAL:HG22	3:3:119:LEU:HD13	1.78	0.65
2:2:48:ASN:CB	2:2:49:PRO:CD	2.65	0.65
1:1:159:TYR:HB2	5:1:0:SPH:H162	1.79	0.65
1:1:22:THR:HB	1:1:25:ASP:OD1	1.97	0.64
2:2:38:TRP:CG	2:2:39:PRO:HD2	2.32	0.64
1:1:90:MET:CE	1:1:240:LEU:O	2.46	0.64
1:1:159:TYR:O	1:1:161:PRO:HD3	1.98	0.64
2:2:143:THR:HG23	2:2:173:ARG:HA	1.79	0.64
1:1:237:PHE:CZ	5:1:0:SPH:H4	2.33	0.64
1:1:90:MET:HE1	1:1:240:LEU:O	1.99	0.63
3:3:149:MET:HE2	3:3:150:LEU:CD2	2.26	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:187:LEU:HD22	3:3:65:MET:SD	2.39	0.63
2:2:187:LEU:HD22	3:3:65:MET:HE3	1.79	0.63
4:4:60:VAL:HG12	4:4:60:VAL:O	1.98	0.63
3:3:85:LEU:HD22	3:3:86:SER:N	2.13	0.62
1:1:177:THR:CG2	1:1:182:SER:OG	2.33	0.62
7:3:366:HOH:O	4:4:46:PHE:HB2	1.99	0.62
1:1:103:LYS:HD3	1:1:170:TRP:CG	2.34	0.62
3:3:85:LEU:CD2	3:3:86:SER:N	2.62	0.62
1:1:237:PHE:CE2	5:1:0:SPH:C4	2.83	0.61
3:3:77:HIS:HE1	3:3:194:TYR:O	1.83	0.61
4:4:55:GLU:N	4:4:56:PRO:HD3	2.15	0.61
3:3:74:ASP:HB2	7:3:296:HOH:O	2.01	0.61
1:1:92:VAL:HG12	1:1:106:ALA:H	1.66	0.61
3:3:75:LYS:HB2	3:3:76:PRO:HD2	1.81	0.61
1:1:218:LYS:O	1:1:220:GLN:N	2.34	0.61
1:1:133:GLU:O	1:1:133:GLU:HG2	2.01	0.61
2:2:63:PHE:CD1	2:2:254:ALA:HB2	2.36	0.61
4:4:57:ILE:HD11	4:4:61:LEU:HB3	1.81	0.61
1:1:128:SER:HB3	1:1:207:HIS:CE1	2.35	0.60
4:4:10:VAL:HG21	4:4:25:ILE:HD12	1.82	0.60
1:1:249:ASN:CG	1:1:250:PRO:HD2	2.22	0.60
5:1:0:SPH:H3	7:1:361:HOH:O	2.02	0.60
1:1:104:LEU:O	1:1:104:LEU:HG	2.02	0.59
2:2:5:GLU:CD	2:2:7:CYS:CB	2.71	0.59
2:2:5:GLU:CD	2:2:7:CYS:HB2	2.22	0.59
3:3:83:LEU:HD12	3:3:83:LEU:C	2.22	0.59
2:2:267:THR:HG22	2:2:269:PRO:HD3	1.84	0.59
2:2:5:GLU:C	2:2:7:CYS:N	2.57	0.58
2:2:239:PHE:CD2	2:2:240:ALA:N	2.71	0.58
4:4:42:SER:C	4:4:44:GLN:H	2.07	0.58
2:2:25:THR:HG23	2:2:25:THR:O	2.04	0.58
3:3:87:LEU:HD13	3:3:190:ILE:HD11	1.86	0.58
3:3:77:HIS:CE1	3:3:194:TYR:O	2.57	0.58
3:3:208:MET:HE2	3:3:208:MET:H	1.68	0.58
4:4:15:ASN:N	7:4:84:HOH:O	2.21	0.58
2:2:195:HIS:HA	2:2:208:LEU:HD21	1.87	0.57
4:4:10:VAL:CG1	4:4:13:HIS:CE1	2.87	0.57
1:1:218:LYS:C	1:1:220:GLN:H	2.08	0.57
1:1:45:THR:OG1	1:1:46:ALA:N	2.38	0.57
3:3:88:SER:HB3	3:3:91:SER:OG	2.03	0.57
1:1:300:THR:HA	3:3:84:CYS:H	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:218:ASN:HD22	3:3:219:ASP:N	2.04	0.56
2:2:187:LEU:HD22	3:3:65:MET:HE1	1.82	0.56
2:2:166:ASN:OD1	2:2:168:THR:HG22	2.06	0.56
2:2:5:GLU:CD	2:2:7:CYS:N	2.53	0.56
1:1:47:VAL:CG2	3:3:119:LEU:HD13	2.36	0.56
1:1:216:PRO:HG2	2:2:145:TYR:CD1	2.41	0.55
4:4:42:SER:HG	4:4:44:GLN:HB2	1.70	0.55
3:3:149:MET:HE1	3:3:150:LEU:CD2	2.35	0.55
3:3:204:THR:CG2	3:3:205:PRO:HD2	2.36	0.55
1:1:237:PHE:CD2	5:1:0:SPH:H71	2.40	0.55
4:4:14:GLU:HG2	4:4:16:SER:CB	2.36	0.54
1:1:83:ARG:HG2	7:3:258:HOH:O	2.06	0.54
3:3:34:ILE:O	3:3:36:ILE:N	2.39	0.54
1:1:237:PHE:CD2	5:1:0:SPH:C7	2.91	0.54
2:2:60:ALA:O	2:2:255:PRO:HG2	2.08	0.53
1:1:38:SER:OG	1:1:39:LYS:N	2.41	0.53
1:1:105:PHE:CD1	1:1:105:PHE:O	2.62	0.53
3:3:55:PHE:HE1	3:3:212:GLY:HA3	1.73	0.53
3:3:149:MET:HE1	3:3:150:LEU:HG	1.90	0.53
2:2:110:VAL:HG22	2:2:251:LEU:CD1	2.39	0.53
3:3:73:SER:HA	3:3:208:MET:CE	2.38	0.53
4:4:10:VAL:HG11	4:4:13:HIS:ND1	2.23	0.53
2:2:179:TYR:N	3:3:65:MET:HE2	2.22	0.53
2:2:256:MET:O	2:2:258:CYS:N	2.41	0.53
3:3:104:LEU:O	3:3:179:THR:HG21	2.08	0.53
1:1:48:GLU:OE2	3:3:162:SER:OG	2.22	0.53
1:1:112:TYR:CD2	5:1:0:SPH:H5	2.43	0.53
1:1:99:THR:CG2	7:1:352:HOH:O	2.56	0.52
1:1:218:LYS:HD3	2:2:268:LEU:HB3	1.91	0.52
1:1:74:GLU:OE1	3:3:224:LEU:N	2.39	0.52
1:1:280:TYR:HB3	1:1:285:ASP:O	2.09	0.52
1:1:133:GLU:HG2	7:1:369:HOH:O	2.08	0.52
2:2:136:SER:OG	2:2:139:THR:HG22	2.10	0.52
3:3:107:TYR:O	3:3:179:THR:HG21	2.08	0.52
1:1:183:ILE:HD11	1:1:194:ILE:HG12	1.91	0.52
1:1:209:TYR:O	1:1:230:GLY:HA2	2.10	0.52
2:2:98:TYR:CE1	2:2:266:ILE:HD12	2.45	0.52
2:2:122:LEU:HB2	2:2:198:ILE:HB	1.90	0.52
3:3:178:GLN:C	3:3:180:ILE:H	2.14	0.52
2:2:13:VAL:HA	2:2:25:THR:O	2.10	0.51
1:1:158:MET:SD	1:1:177:THR:CG2	2.96	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:144:GLU:C	1:1:146:ASN:N	2.50	0.51
1:1:302:TYR:CE2	3:3:189:TYR:HB3	2.46	0.51
1:1:112:TYR:HD2	5:1:0:SPH:H5	1.76	0.51
3:3:83:LEU:O	3:3:83:LEU:CD1	2.50	0.51
1:1:149:HIS:HB3	7:1:309:HOH:O	2.11	0.51
3:3:51:THR:HB	7:3:277:HOH:O	2.11	0.51
1:1:22:THR:CG2	1:1:24:ARG:H	2.16	0.51
4:4:13:HIS:CD2	4:4:13:HIS:H	2.27	0.50
1:1:95:PRO:HD2	1:1:103:LYS:HG3	1.93	0.50
4:4:10:VAL:CG1	4:4:13:HIS:ND1	2.74	0.50
4:4:24:THR:HG23	4:4:24:THR:O	2.10	0.50
1:1:218:LYS:C	1:1:220:GLN:N	2.65	0.50
3:3:14:LEU:O	3:3:16:ALA:N	2.44	0.50
4:4:55:GLU:N	4:4:56:PRO:CD	2.74	0.50
1:1:75:SER:HA	3:3:107:TYR:OH	2.11	0.49
1:1:261:LEU:C	1:1:261:LEU:HD23	2.31	0.49
2:2:187:LEU:CD2	3:3:65:MET:CE	2.82	0.49
3:3:89:PRO:HB2	3:3:104:LEU:CD2	2.41	0.49
1:1:237:PHE:HZ	5:1:0:SPH:H4	1.77	0.49
2:2:219:ASP:CG	2:2:220:SER:H	2.15	0.49
1:1:27:LEU:HB3	1:1:28:PRO:CD	2.40	0.49
1:1:130:PHE:O	1:1:130:PHE:CD1	2.66	0.49
2:2:198:ILE:HG22	2:2:198:ILE:O	2.11	0.49
3:3:87:LEU:HD13	3:3:190:ILE:CD1	2.43	0.49
3:3:155:ILE:HG22	3:3:155:ILE:O	2.13	0.49
3:3:13:TYR:C	3:3:13:TYR:CD2	2.86	0.49
3:3:129:LYS:O	3:3:195:GLN:HB3	2.11	0.49
1:1:81:PHE:O	1:1:83:ARG:N	2.34	0.49
3:3:89:PRO:HB2	3:3:104:LEU:HD23	1.95	0.49
1:1:237:PHE:CZ	5:1:0:SPH:C4	2.96	0.49
2:2:110:VAL:O	2:2:205:CYS:HB2	2.13	0.49
2:2:213:VAL:O	2:2:214:ASN:HB2	2.12	0.49
3:3:149:MET:O	3:3:149:MET:HG2	2.02	0.49
1:1:159:TYR:CB	5:1:0:SPH:H162	2.42	0.48
3:3:14:LEU:O	3:3:14:LEU:HG	2.13	0.48
1:1:48:GLU:HA	2:2:197:ILE:HB	1.94	0.48
2:2:66:LEU:N	2:2:66:LEU:HD23	2.29	0.48
3:3:85:LEU:CD2	3:3:85:LEU:C	2.82	0.48
4:4:10:VAL:HG22	4:4:25:ILE:HD12	1.93	0.48
3:3:109:HIS:HB2	3:3:223:ARG:HG2	1.95	0.48
1:1:78:GLU:OE1	1:1:265:HIS:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:14:GLU:C	4:4:16:SER:N	2.64	0.48
1:1:56:VAL:HB	1:1:57:PRO:CD	2.36	0.48
2:2:76:ARG:HB2	2:2:157:PHE:O	2.14	0.48
3:3:183:SER:O	3:3:186:GLU:HG2	2.13	0.48
1:1:103:LYS:NZ	1:1:246:ASN:O	2.47	0.48
3:3:56:ASP:OD1	3:3:61:LYS:HE3	2.14	0.48
2:2:213:VAL:HG22	3:3:37:PRO:HG2	1.95	0.47
3:3:156:TRP:CD1	3:3:164:CYS:HB2	2.49	0.47
4:4:27:TYR:OH	7:4:86:HOH:O	2.20	0.47
1:1:83:ARG:CG	7:3:258:HOH:O	2.62	0.47
1:1:169:LYS:O	1:1:171:ASP:N	2.46	0.47
2:2:267:THR:C	2:2:269:PRO:HD3	2.33	0.47
1:1:30:THR:HB	1:1:66:VAL:HB	1.95	0.47
1:1:105:PHE:O	1:1:105:PHE:CG	2.67	0.47
2:2:97:TYR:CE1	2:2:269:PRO:HG3	2.50	0.47
1:1:291:LEU:C	1:1:293:PRO:HD3	2.35	0.47
1:1:237:PHE:HE2	5:1:0:SPH:C4	2.26	0.47
2:2:204:ASN:ND2	7:2:381:HOH:O	2.30	0.47
3:3:231:ILE:HG13	3:3:232:GLU:N	2.30	0.46
1:1:233:SER:O	1:1:235:ASN:N	2.48	0.46
2:2:5:GLU:C	2:2:7:CYS:H	2.18	0.46
3:3:233:GLN:O	3:3:235:ALA:N	2.47	0.46
1:1:10:THR:OG1	4:4:4:GLN:OE1	2.33	0.46
3:3:73:SER:C	3:3:75:LYS:H	2.18	0.46
3:3:149:MET:HE1	3:3:150:LEU:CG	2.46	0.46
1:1:124:PHE:CE1	1:1:274:PRO:HG3	2.50	0.46
2:2:71:TRP:CD1	2:2:72:THR:N	2.84	0.46
2:2:214:ASN:OD1	2:2:215:SER:N	2.48	0.46
1:1:169:LYS:C	1:1:171:ASP:H	2.19	0.46
1:1:197:PRO:HD3	3:3:23:CYS:SG	2.56	0.46
3:3:85:LEU:HD22	3:3:85:LEU:C	2.36	0.46
1:1:90:MET:CE	1:1:242:VAL:HG23	2.45	0.46
1:1:169:LYS:C	1:1:171:ASP:N	2.69	0.46
3:3:149:MET:CE	3:3:150:LEU:HG	2.46	0.46
2:2:54:THR:O	2:2:56:PRO:HD3	2.16	0.46
4:4:9:LYS:N	7:4:70:HOH:O	2.49	0.46
1:1:128:SER:HB3	1:1:207:HIS:NE2	2.31	0.46
2:2:168:THR:HG23	2:2:169:SER:N	2.26	0.46
4:4:14:GLU:O	4:4:16:SER:N	2.48	0.46
2:2:107:THR:O	2:2:107:THR:HG22	2.16	0.45
3:3:156:TRP:CD1	3:3:156:TRP:C	2.89	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:159:TYR:CG	5:1:0:SPH:H142	2.51	0.45
3:3:85:LEU:HD23	3:3:86:SER:N	2.31	0.45
4:4:65:ALA:HB1	4:4:66:PRO:CD	2.45	0.45
1:1:107:VAL:O	1:1:107:VAL:HG12	2.17	0.45
4:4:49:ASP:OD1	4:4:51:SER:HB2	2.17	0.45
3:3:62:LYS:O	3:3:64:THR:HG23	2.17	0.45
2:2:239:PHE:O	2:2:240:ALA:C	2.55	0.45
2:2:256:MET:O	2:2:257:CYS:C	2.55	0.45
3:3:196:THR:O	3:3:197:ARG:CB	2.63	0.45
1:1:81:PHE:C	1:1:83:ARG:H	2.17	0.44
1:1:116:VAL:H	3:3:233:GLN:NE2	2.16	0.44
2:2:187:LEU:CD2	3:3:65:MET:HE1	2.46	0.44
4:4:61:LEU:HA	7:4:108:HOH:O	2.16	0.44
1:1:233:SER:C	1:1:235:ASN:N	2.69	0.44
2:2:71:TRP:CD1	2:2:71:TRP:C	2.88	0.44
1:1:218:LYS:HB2	1:1:219:ASP:H	1.49	0.44
2:2:267:THR:O	2:2:269:PRO:CD	2.58	0.44
3:3:170:TRP:O	3:3:170:TRP:CG	2.71	0.44
2:2:158:THR:O	2:2:177:VAL:HA	2.18	0.44
2:2:226:ASN:ND2	7:2:342:HOH:O	2.48	0.44
3:3:51:THR:HG21	3:3:99:MET:H	1.82	0.44
3:3:87:LEU:HG	3:3:87:LEU:O	2.17	0.44
1:1:105:PHE:CD1	1:1:105:PHE:C	2.91	0.43
1:1:155:TYR:N	1:1:155:TYR:CD2	2.87	0.43
2:2:5:GLU:OE1	2:2:5:GLU:C	2.55	0.43
3:3:195:GLN:OE1	3:3:195:GLN:CA	2.64	0.43
1:1:274:PRO:HG2	3:3:102:GLU:HG3	2.00	0.43
2:2:219:ASP:OD1	2:2:220:SER:N	2.37	0.43
2:2:256:MET:C	2:2:258:CYS:N	2.71	0.43
3:3:190:ILE:O	3:3:190:ILE:HG22	2.18	0.43
3:3:233:GLN:O	3:3:233:GLN:HG2	2.19	0.43
1:1:212:PHE:CD1	1:1:212:PHE:N	2.87	0.43
2:2:29:ALA:HA	4:4:68:LEU:HD21	2.00	0.43
6:4:1:MYR:H101	6:4:1:MYR:H71	1.66	0.43
1:1:177:THR:HG22	1:1:180:ASN:HB2	2.01	0.42
2:2:166:ASN:O	2:2:168:THR:N	2.51	0.42
3:3:10:SER:O	3:3:11:ASN:HB2	2.19	0.42
1:1:116:VAL:CG2	3:3:233:GLN:HB2	2.49	0.42
2:2:12:ARG:NH1	7:2:278:HOH:O	2.51	0.42
2:2:135:ASP:OD2	2:2:171:ALA:HB3	2.19	0.42
1:1:53:ASN:C	1:1:55:LEU:H	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:204:THR:HG23	3:3:205:PRO:HD2	2.00	0.42
4:4:42:SER:C	4:4:44:GLN:N	2.72	0.42
2:2:199:ASN:O	2:2:201:ARG:N	2.52	0.42
1:1:273:PRO:HB3	2:2:189:ASN:HB2	2.01	0.42
1:1:37:HIS:CD2	1:1:37:HIS:O	2.73	0.42
1:1:93:ASP:OD2	1:1:93:ASP:C	2.58	0.42
1:1:237:PHE:CG	5:1:0:SPH:H92	2.55	0.42
2:2:71:TRP:CE2	2:2:237:LEU:HB2	2.55	0.42
3:3:196:THR:OG1	3:3:197:ARG:N	2.50	0.42
1:1:24:ARG:O	1:1:24:ARG:HG3	2.20	0.42
2:2:198:ILE:HD13	2:2:205:CYS:HA	2.01	0.42
3:3:142:PRO:HD3	7:3:325:HOH:O	2.19	0.42
1:1:132:MET:CE	5:1:0:SPH:C10	2.98	0.41
2:2:5:GLU:HG3	2:2:8:GLY:N	2.34	0.41
2:2:104:SER:HB2	2:2:258:CYS:HB2	2.03	0.41
2:2:117:PHE:CE1	3:3:125:MET:HG3	2.55	0.41
1:1:57:PRO:HA	3:3:167:VAL:HG11	2.03	0.41
1:1:123:GLU:C	1:1:125:PHE:H	2.22	0.41
2:2:5:GLU:O	2:2:7:CYS:N	2.53	0.41
3:3:7:THR:HB	3:3:8:PRO:CD	2.45	0.41
3:3:14:LEU:HB3	3:3:17:ASP:HB3	2.02	0.41
4:4:11:GLY:HA3	7:4:78:HOH:O	2.19	0.41
3:3:98:THR:O	3:3:99:MET:C	2.59	0.41
3:3:113:SER:O	3:3:217:CYS:HB2	2.19	0.41
1:1:217:LEU:O	1:1:218:LYS:C	2.59	0.41
3:3:108:THR:HB	3:3:224:LEU:HB3	2.02	0.41
1:1:132:MET:CE	5:1:0:SPH:H101	2.51	0.41
3:3:233:GLN:O	3:3:234:LYS:C	2.59	0.41
1:1:257:ILE:HD12	1:1:257:ILE:N	2.36	0.41
1:1:116:VAL:HG22	3:3:233:GLN:HB2	2.01	0.41
2:2:23:ILE:HD12	2:2:63:PHE:CZ	2.56	0.41
2:2:181:LEU:HG	2:2:181:LEU:O	2.21	0.41
3:3:232:GLU:HG2	7:3:363:HOH:O	2.21	0.41
1:1:116:VAL:HG23	1:1:117:GLN:N	2.36	0.40
2:2:71:TRP:HD1	2:2:72:THR:N	2.19	0.40
2:2:103:ARG:HB3	2:2:218:ILE:HG13	2.03	0.40
3:3:71:ARG:HG3	3:3:72:LEU:N	2.36	0.40
3:3:149:MET:CE	3:3:150:LEU:CG	2.98	0.40
1:1:57:PRO:O	1:1:61:VAL:HG22	2.21	0.40
1:1:269:TRP:CD1	3:3:39:GLU:HB2	2.57	0.40
2:2:242:GLU:O	2:2:245:PRO:HD3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:68:LEU:HD23	4:4:68:LEU:HA	1.91	0.40
3:3:74:ASP:CG	3:3:206:ARG:HE	2.22	0.40
1:1:56:VAL:CB	1:1:57:PRO:HD2	2.33	0.40
1:1:237:PHE:CG	5:1:0:SPH:C9	3.04	0.40
3:3:34:ILE:HD13	3:3:34:ILE:HG21	1.86	0.40
1:1:42:PRO:HA	4:4:63:LYS:O	2.22	0.40
2:2:119:GLN:HG2	3:3:123:SER:N	2.36	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	1	284/302 (94%)	225 (79%)	43 (15%)	16 (6%)	2 5
2	2	266/272 (98%)	222 (84%)	36 (14%)	8 (3%)	4 15
3	3	233/238 (98%)	180 (77%)	38 (16%)	15 (6%)	1 3
4	4	59/68 (87%)	47 (80%)	7 (12%)	5 (8%)	1 2
All	All	842/880 (96%)	674 (80%)	124 (15%)	44 (5%)	2 6

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	82	ALA
1	1	145	THR
1	1	219	ASP
2	2	200	LEU
2	2	257	CYS
3	3	15	THR
3	3	29	ASP
3	3	35	ASP

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Mol	Chain	Res	Type
3	3	137	PRO
3	3	197	ARG
1	1	146	ASN
1	1	170	TRP
1	1	234	LEU
1	1	236	ASP
2	2	130	MET
2	2	167	GLN
3	3	170	TRP
3	3	179	THR
3	3	234	LYS
4	4	15	ASN
1	1	210	ASP
1	1	232	ALA
2	2	240	ALA
3	3	168	VAL
1	1	54	PRO
1	1	57	PRO
1	1	165	PRO
1	1	218	LYS
1	1	275	ARG
2	2	48	ASN
2	2	166	ASN
3	3	65	MET
4	4	60	VAL
1	1	216	PRO
2	2	34	ALA
3	3	59	ALA
3	3	74	ASP
3	3	89	PRO
3	3	161	GLN
4	4	9	LYS
4	4	56	PRO
1	1	250	PRO
3	3	93	PRO
4	4	11	GLY

5.3.2 Protein sidechains (i)

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	249/261 (95%)	232 (93%)	17 (7%)	16 40
2	2	228/232 (98%)	208 (91%)	20 (9%)	10 28
3	3	210/212 (99%)	199 (95%)	11 (5%)	23 53
4	4	54/57 (95%)	46 (85%)	8 (15%)	3 8
All	All	741/762 (97%)	685 (92%)	56 (8%)	13 35

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	7	SER
1	1	10	THR
1	1	38	SER
1	1	83	ARG
1	1	97	SER
1	1	100	ASN
1	1	129	ARG
1	1	143	THR
1	1	146	ASN
1	1	147	ASN
1	1	149	HIS
1	1	177	THR
1	1	220	GLN
1	1	221	SER
1	1	224	LEU
1	1	255	SER
1	1	287	LYS
2	2	5	GLU
2	2	10	SER
2	2	11	ASP
2	2	48	ASN
2	2	52	GLN
2	2	66	LEU
2	2	73	LYS
2	2	103	ARG
2	2	115	SER
2	2	153	LYS
2	2	162	THR
2	2	167	GLN
2	2	168	THR

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Mol	Chain	Res	Type
2	2	201	ARG
2	2	217	SER
2	2	238	ASN
2	2	241	SER
2	2	242	GLU
2	2	264	ARG
2	2	272	GLN
3	3	51	THR
3	3	52	MET
3	3	71	ARG
3	3	85	LEU
3	3	143	LYS
3	3	146	LYS
3	3	149	MET
3	3	163	SER
3	3	197	ARG
3	3	208	MET
3	3	218	ASN
4	4	6	SER
4	4	7	SER
4	4	36	SER
4	4	42	SER
4	4	49	ASP
4	4	52	LYS
4	4	61	LEU
4	4	64	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
2	2	48	ASN
2	2	165	ASN
3	3	218	ASN
3	3	233	GLN
4	4	13	HIS
4	4	31	ASN
4	4	39	ASN

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 monosaccharides 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	MYR	4	1	4	14,14,15	0.51	0	13,13,15	1.14	1 (7%)
5	SPH	1	0	-	19,20,20	1.38	2 (10%)	18,21,21	1.65	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
6	MYR	4	1	4	-	7/11/12/13	-
5	SPH	1	0	-	2/2/2/4	12/21/21/21	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	1	0	SPH	C4-C5	5.13	1.53	1.31
5	1	0	SPH	C3-C4	2.01	1.53	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	1	0	SPH	C3-C4-C5	-5.51	112.51	124.79
5	1	0	SPH	C6-C5-C4	-2.69	113.37	125.39
6	4	1	MYR	O1-C1-C2	-2.27	112.00	126.89

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	1	0	SPH	C2
5	1	0	SPH	C3

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	1	0	SPH	O1-C1-C2-N2
5	1	0	SPH	O1-C1-C2-C3
5	1	0	SPH	C1-C2-C3-O3
5	1	0	SPH	C1-C2-C3-C4
5	1	0	SPH	N2-C2-C3-C4
5	1	0	SPH	C2-C3-C4-C5
5	1	0	SPH	O3-C3-C4-C5
6	4	1	MYR	C7-C8-C9-C10
6	4	1	MYR	C10-C11-C12-C13
6	4	1	MYR	C5-C6-C7-C8
6	4	1	MYR	C6-C7-C8-C9
5	1	0	SPH	C11-C12-C13-C14
6	4	1	MYR	C11-C12-C13-C14
5	1	0	SPH	C4-C5-C6-C7
6	4	1	MYR	C9-C10-C11-C12
6	4	1	MYR	C1-C2-C3-C4
5	1	0	SPH	C7-C8-C9-C10
5	1	0	SPH	C10-C11-C12-C13
5	1	0	SPH	N2-C2-C3-O3

There are no ring outliers.

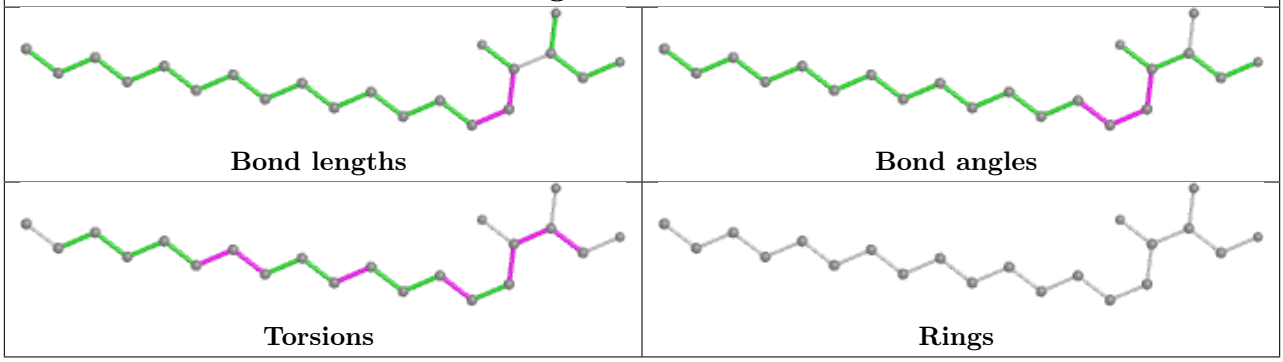
2 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	4	1	MYR	1	0
5	1	0	SPH	26	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 then 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.

Ligand SPH 1 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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.