



Full wwPDB EM Validation Report ⓘ

Mar 12, 2026 – 09:18 AM UTC

PDB ID : 3EPF / pdb_00003epf
EMDB ID : EMD-1563
Title : CryoEM structure of poliovirus receptor bound to poliovirus type 2
Authors : Zhang, P.; Mueller, S.; Morais, M.C.; Bator, C.M.; Bowman, V.D.; Hafenstein, S.; Wimmer, E.; Rossmann, M.G.
Deposited on : 2008-09-29
Resolution : 9.00 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>
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:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

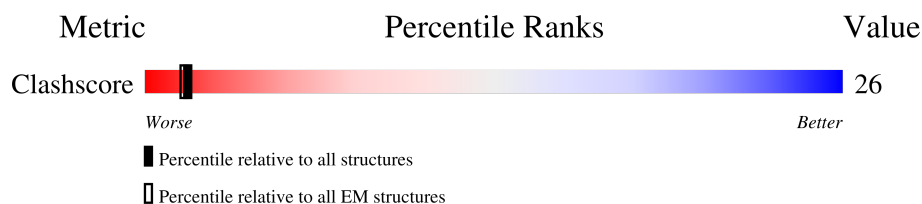
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 9.00 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)	EM structures (#Entries)
Clashscore	229148	23984

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	R	213	 41% 54% .
2	1	278	 72% 25% .
3	2	262	 82% 17% .
4	4	68	 76% 24%
5	3	235	 87% 11% .

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8461 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Poliovirus receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	213	Total	C	N	O	S	0	0
			1638	1038	281	310	9		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	105	ASP	ASN	engineered mutation	UNP P15151
R	120	SER	ASN	engineered mutation	UNP P15151
R	188	GLN	ASN	engineered mutation	UNP P15151
R	218	GLN	ASN	engineered mutation	UNP P15151
R	237	SER	ASN	engineered mutation	UNP P15151

- Molecule 2 is a protein called Protein VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	272	Total	C	N	O	S	0	0
			2129	1361	363	400	5		

- Molecule 3 is a protein called Protein VP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	262	Total	C	N	O	S	0	0
			2042	1298	346	384	14		

There is a discrepancy between the modelled and reference sequences:

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

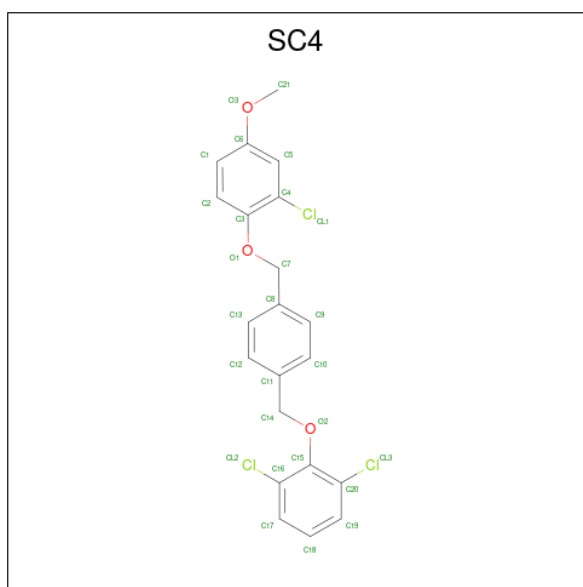
- Molecule 4 is a protein called Protein VP4.

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

- Molecule 5 is a protein called Protein VP3.

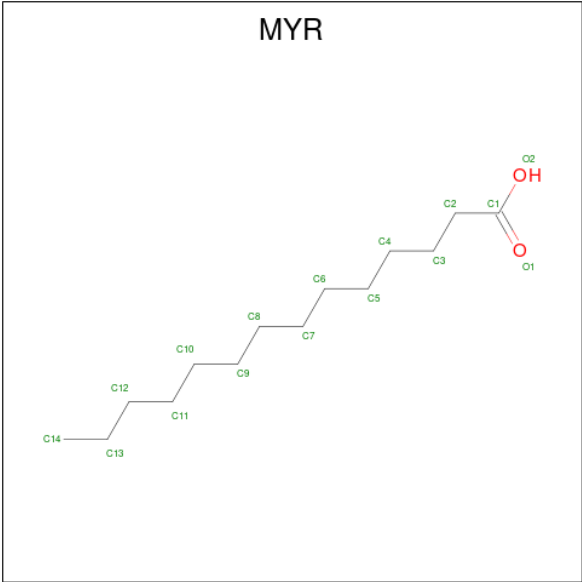
Mol	Chain	Residues	Atoms					AltConf	Trace
5	3	235	Total	C	N	O	S	0	0
			1825	1156	303	349	17		

- Molecule 6 is 1[2-CHLORO-4-METHOXY-PHENYL-OXYMETHYL]-4-[2,6-DICHLORO-PHENYL-OXYMETHYL]-BENZENE (CCD ID: SC4) (formula: C₂₁H₁₇Cl₃O₃).



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

- Molecule 7 is MYRISTIC ACID (CCD ID: MYR) (formula: C₁₄H₂₈O₂).



Mol	Chain	Residues	Atoms			AltConf
7	4	1	Total	C	O	0
			11	10	1	

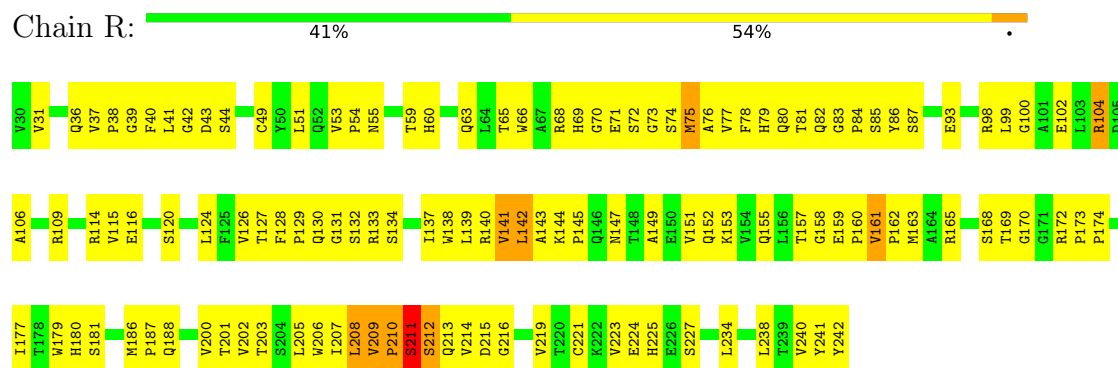
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		AltConf
8	1	136	Total	O	0
			136	136	
8	2	95	Total	O	0
			95	95	
8	4	25	Total	O	0
			25	25	
8	3	15	Total	O	0
			15	15	

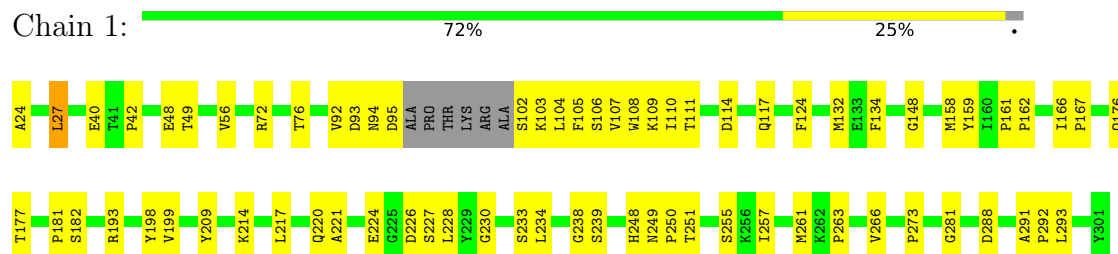
3 Residue-property plots

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.

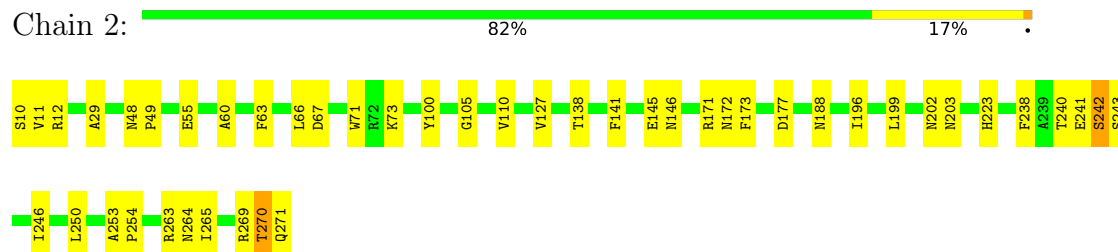
• Molecule 1: Poliovirus receptor



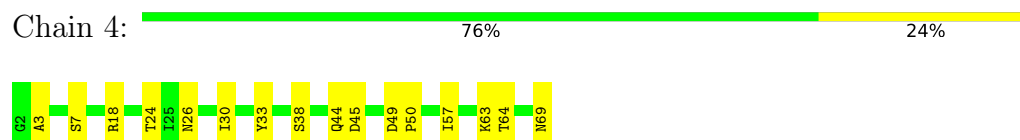
• Molecule 2: Protein VP1



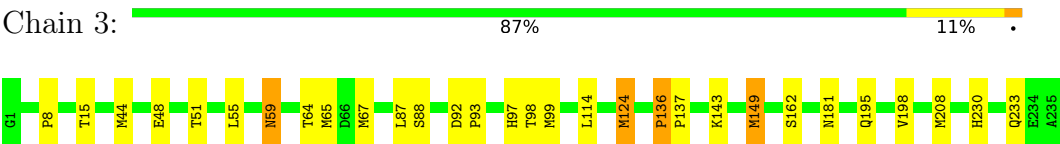
• Molecule 3: Protein VP2



• Molecule 4: Protein VP4



● Molecule 5: Protein VP3



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	Not provided	
Resolution determination method	Not provided	
CTF correction method	Not provided	
Microscope	FEI/PHILIPS CM300FEG/T	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	1236	Depositor
Maximum defocus (nm)	2745	Depositor
Magnification	47000	Depositor
Image detector	KODAK SO-163 FILM	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	R	0.60	1/1678 (0.1%)	1.10	11/2289 (0.5%)
2	1	0.55	0/2193	1.00	12/2996 (0.4%)
3	2	0.54	0/2098	1.00	14/2863 (0.5%)
4	4	0.60	0/527	0.99	1/713 (0.1%)
5	3	0.60	3/1869 (0.2%)	0.90	6/2549 (0.2%)
All	All	0.57	4/8365 (0.0%)	1.00	44/11410 (0.4%)

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	R	1	6
2	1	0	1
All	All	1	7

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	3	124	MET	SD-CE	7.62	1.98	1.79
5	3	149	MET	SD-CE	-7.45	1.60	1.79
1	R	211	SER	C-N	-6.04	1.25	1.33
5	3	136	PRO	CA-C	5.29	1.54	1.51

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	211	SER	O-C-N	-10.91	109.01	123.19
1	R	209	VAL	CA-C-N	10.24	132.64	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	209	VAL	C-N-CA	10.24	132.64	119.84
1	R	37	VAL	N-CA-C	9.04	118.03	107.73
2	1	266	VAL	N-CA-C	8.54	120.83	109.21
2	1	288	ASP	N-CA-C	8.51	127.06	110.56
3	2	177	ASP	N-CA-C	8.13	119.77	111.07
2	1	124	PHE	N-CA-C	-7.88	103.64	113.18
2	1	199	VAL	N-CA-C	7.30	119.16	112.29
3	2	242	SER	N-CA-C	-7.19	103.44	111.71
1	R	104	ARG	N-CA-C	7.00	120.28	108.23
1	R	53	VAL	N-CA-C	6.92	114.40	107.55
3	2	127	VAL	N-CA-C	6.67	115.33	107.73
3	2	12	ARG	N-CA-C	6.61	121.43	113.23
1	R	161	VAL	N-CA-C	6.36	122.62	108.88
3	2	29	ALA	N-CA-C	-6.13	103.08	110.44
2	1	117	GLN	N-CA-C	6.12	117.62	111.07
4	4	44	GLN	N-CA-C	-6.12	101.08	109.71
1	R	75	MET	N-CA-C	6.05	119.38	108.48
3	2	55	GLU	CA-C-N	6.03	126.46	119.47
3	2	55	GLU	C-N-CA	6.03	126.46	119.47
3	2	223	HIS	N-CA-C	5.80	118.56	108.76
3	2	202	ASN	N-CA-C	5.77	118.18	109.41
2	1	281	GLY	CA-C-N	5.74	125.36	119.56
2	1	281	GLY	C-N-CA	5.74	125.36	119.56
2	1	291	ALA	CA-C-N	5.69	125.22	119.19
2	1	291	ALA	C-N-CA	5.69	125.22	119.19
5	3	162	SER	N-CA-C	5.64	118.20	111.71
3	2	105	GLY	N-CA-C	-5.61	102.87	112.64
2	1	103	LYS	N-CA-C	5.57	122.66	110.80
5	3	59	ASN	N-CA-C	5.50	117.98	111.33
3	2	270	THR	N-CA-C	5.47	118.00	109.52
2	1	56	VAL	N-CA-C	-5.47	101.89	108.45
1	R	208	LEU	CA-C-N	5.46	131.52	121.70
1	R	208	LEU	C-N-CA	5.46	131.52	121.70
3	2	199	LEU	N-CA-C	5.43	118.70	111.75
5	3	98	THR	N-CA-C	-5.39	103.58	110.53
3	2	203	ASN	CB-CA-C	-5.37	98.89	109.67
3	2	265	ILE	N-CA-C	5.31	116.44	109.58
5	3	88	SER	CA-C-N	5.28	125.59	119.47
5	3	88	SER	C-N-CA	5.28	125.59	119.47
5	3	55	LEU	N-CA-C	5.13	117.78	111.82
1	R	209	VAL	N-CA-C	5.09	125.25	111.00
2	1	27	LEU	N-CA-C	-5.03	103.21	110.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	R	143	ALA	CA

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1	198	TYR	Sidechain
1	R	141	VAL	Peptide
1	R	142	LEU	Peptide
1	R	210	PRO	Peptide
1	R	211	SER	Peptide
1	R	212	SER	Mainchain
1	R	213	GLN	Peptide

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	R	1638	0	1617	327	0
2	1	2129	0	2068	161	0
3	2	2042	0	1969	37	0
4	4	518	0	495	12	0
5	3	1825	0	1800	57	0
6	1	27	0	17	3	0
7	4	11	0	16	0	0
8	1	136	0	0	8	0
8	2	95	0	0	1	0
8	3	15	0	0	1	0
8	4	25	0	0	1	0
All	All	8461	0	7982	422	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 26.

All (422) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:130:GLN:CG	2:1:106:SER:HA	1.13	1.55
1:R:130:GLN:CG	2:1:106:SER:CA	1.86	1.54
1:R:115:VAL:HG11	1:R:142:LEU:CD1	1.28	1.53
1:R:130:GLN:NE2	2:1:105:PHE:CE1	1.76	1.52
1:R:115:VAL:CG1	1:R:142:LEU:HD11	1.03	1.50
1:R:130:GLN:CB	2:1:106:SER:HA	1.38	1.49
1:R:115:VAL:CG1	1:R:142:LEU:CD1	1.79	1.48
1:R:130:GLN:HG3	2:1:106:SER:CA	1.42	1.43
1:R:128:PHE:HE2	2:1:108:TRP:NE1	1.17	1.41
1:R:83:GLY:CA	2:1:226:ASP:O	1.70	1.37
1:R:41:LEU:CB	1:R:143:ALA:HB3	1.59	1.33
1:R:41:LEU:HB3	1:R:143:ALA:CB	1.60	1.31
1:R:128:PHE:CE2	2:1:108:TRP:NE1	2.02	1.25
1:R:99:LEU:HG	2:1:226:ASP:OD2	1.37	1.24
1:R:128:PHE:CE1	2:1:114:ASP:OD1	1.69	1.22
1:R:132:SER:OG	2:1:107:VAL:HG11	1.39	1.22
1:R:130:GLN:HB2	2:1:106:SER:CA	1.72	1.20
1:R:130:GLN:HG2	2:1:106:SER:C	1.66	1.20
1:R:40:PHE:CZ	1:R:144:LYS:HB3	1.79	1.18
1:R:128:PHE:CD2	8:1:397:HOH:O	1.65	1.18
1:R:130:GLN:CA	2:1:107:VAL:H	1.58	1.16
1:R:162:PRO:HD2	1:R:163:MET:HA	1.30	1.14
1:R:128:PHE:CG	8:1:397:HOH:O	1.65	1.14
1:R:99:LEU:CG	2:1:226:ASP:OD2	1.94	1.13
1:R:161:VAL:HB	1:R:163:MET:HB2	1.21	1.13
1:R:43:ASP:HB2	1:R:44:SER:CA	1.79	1.12
1:R:83:GLY:HA3	2:1:226:ASP:C	1.74	1.12
1:R:130:GLN:HB2	2:1:106:SER:CB	1.79	1.12
1:R:130:GLN:HA	2:1:107:VAL:H	0.95	1.10
1:R:115:VAL:HG13	1:R:142:LEU:HD12	1.34	1.09
1:R:132:SER:OG	2:1:107:VAL:CG1	1.99	1.08
1:R:82:GLN:HB2	2:1:228:LEU:H	1.16	1.08
1:R:142:LEU:O	1:R:173:PRO:CD	2.01	1.08
1:R:115:VAL:HG13	1:R:142:LEU:CD1	1.68	1.07
1:R:43:ASP:CB	1:R:44:SER:HA	1.85	1.06
1:R:82:GLN:CB	2:1:228:LEU:H	1.68	1.06
1:R:73:GLY:N	5:3:97:HIS:NE2	2.05	1.05
1:R:116:GLU:CD	5:3:59:ASN:ND2	2.16	1.04
1:R:130:GLN:HA	2:1:107:VAL:N	1.71	1.04
1:R:130:GLN:HG3	2:1:106:SER:N	1.71	1.04
1:R:129:PRO:O	2:1:107:VAL:O	1.76	1.04
1:R:98:ARG:HD3	1:R:104:ARG:HH21	1.21	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:132:SER:CB	2:1:166:ILE:HD13	1.89	1.03
1:R:79:HIS:CD2	2:1:234:LEU:HD12	1.94	1.02
1:R:116:GLU:CD	5:3:59:ASN:HD21	1.66	1.01
1:R:98:ARG:HD3	1:R:104:ARG:NH2	1.75	1.01
1:R:130:GLN:HG2	2:1:107:VAL:N	1.74	1.01
1:R:83:GLY:N	2:1:227:SER:HA	1.74	1.01
1:R:130:GLN:CB	2:1:106:SER:CA	2.16	1.01
1:R:132:SER:HB3	2:1:166:ILE:HD13	1.40	0.99
1:R:54:PRO:HA	1:R:55:ASN:HB2	1.43	0.99
1:R:132:SER:CB	2:1:107:VAL:HG11	1.92	0.99
1:R:82:GLN:CB	2:1:228:LEU:N	2.26	0.99
1:R:177:ILE:HD12	1:R:205:LEU:HB2	1.45	0.99
1:R:130:GLN:CG	2:1:106:SER:C	2.27	0.97
1:R:83:GLY:HA3	2:1:226:ASP:O	0.80	0.97
1:R:73:GLY:CA	5:3:97:HIS:NE2	2.28	0.97
1:R:73:GLY:HA3	5:3:97:HIS:CD2	2.00	0.96
1:R:128:PHE:CE2	8:1:397:HOH:O	1.96	0.96
1:R:40:PHE:CZ	1:R:144:LYS:CB	2.47	0.96
1:R:82:GLN:HB3	2:1:228:LEU:N	1.82	0.95
1:R:130:GLN:HB2	2:1:106:SER:HA	1.32	0.95
1:R:116:GLU:HA	5:3:59:ASN:ND2	1.81	0.95
1:R:143:ALA:O	1:R:225:HIS:NE2	1.99	0.94
1:R:128:PHE:CD1	8:1:397:HOH:O	1.93	0.94
1:R:116:GLU:CG	5:3:59:ASN:HD21	1.80	0.94
1:R:73:GLY:HA3	5:3:97:HIS:NE2	1.82	0.94
1:R:130:GLN:HG3	2:1:105:PHE:C	1.94	0.92
1:R:68:ARG:HD2	1:R:76:ALA:HB3	1.52	0.92
1:R:79:HIS:HD2	2:1:234:LEU:HD12	1.30	0.90
1:R:83:GLY:H	2:1:227:SER:HA	1.32	0.90
1:R:142:LEU:O	1:R:173:PRO:HD3	1.71	0.90
1:R:40:PHE:HZ	1:R:144:LYS:HB3	1.33	0.90
1:R:86:TYR:CE1	2:1:224:GLU:OE1	2.25	0.89
1:R:162:PRO:CD	1:R:163:MET:HA	2.03	0.88
1:R:141:VAL:HG13	1:R:142:LEU:N	1.89	0.88
1:R:43:ASP:HB2	1:R:44:SER:HA	0.91	0.87
1:R:128:PHE:CZ	2:1:111:THR:CG2	2.58	0.87
1:R:128:PHE:CD2	2:1:108:TRP:CD1	2.63	0.86
1:R:128:PHE:O	2:1:108:TRP:HA	1.74	0.86
1:R:99:LEU:CD1	2:1:226:ASP:OD2	2.24	0.85
1:R:130:GLN:HG3	2:1:106:SER:HA	0.93	0.85
1:R:141:VAL:HG13	1:R:142:LEU:HB2	1.56	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:40:PHE:HZ	1:R:144:LYS:CB	1.85	0.85
1:R:128:PHE:CE2	2:1:108:TRP:CD1	2.63	0.85
1:R:130:GLN:NE2	2:1:105:PHE:HE1	1.44	0.85
1:R:141:VAL:HG13	1:R:142:LEU:CB	2.07	0.84
1:R:82:GLN:NE2	2:1:228:LEU:HD13	1.19	0.84
2:1:24:ALA:HB2	2:1:76:THR:HG21	1.58	0.84
3:2:11:VAL:HA	8:4:145:HOH:O	1.78	0.84
1:R:128:PHE:HE1	2:1:114:ASP:OD1	1.55	0.84
1:R:81:THR:N	2:1:234:LEU:HD11	1.93	0.83
1:R:81:THR:N	2:1:234:LEU:CD1	2.41	0.83
1:R:81:THR:HG21	2:1:234:LEU:HA	1.60	0.83
1:R:116:GLU:OE1	5:3:59:ASN:ND2	2.11	0.82
2:1:176:GLN:HE22	5:3:233:GLN:NE2	1.77	0.82
1:R:54:PRO:CA	1:R:55:ASN:HB2	2.11	0.81
1:R:142:LEU:O	1:R:173:PRO:CG	2.28	0.80
2:1:148:GLY:HA3	2:1:251:THR:HG23	1.63	0.80
1:R:79:HIS:CD2	2:1:234:LEU:CD1	2.65	0.80
1:R:130:GLN:HB2	2:1:106:SER:HB3	1.61	0.80
1:R:142:LEU:HD23	1:R:172:ARG:HG2	1.63	0.80
1:R:130:GLN:CB	2:1:107:VAL:H	1.94	0.79
2:1:233:SER:HB3	8:3:244:HOH:O	1.82	0.79
1:R:129:PRO:C	2:1:107:VAL:O	2.25	0.79
1:R:128:PHE:CZ	8:1:397:HOH:O	2.22	0.78
1:R:130:GLN:CG	2:1:107:VAL:N	2.44	0.78
1:R:81:THR:CG2	2:1:234:LEU:HA	2.10	0.77
1:R:81:THR:H	2:1:234:LEU:HD11	1.48	0.76
1:R:215:ASP:O	1:R:238:LEU:HB3	1.85	0.76
3:2:263:ARG:HG2	5:3:136:PRO:HD2	1.68	0.76
3:2:48:ASN:HB3	3:2:49:PRO:HD3	1.66	0.76
1:R:63:GLN:HG2	1:R:81:THR:HA	1.69	0.75
1:R:130:GLN:HE21	2:1:107:VAL:HG23	1.51	0.75
1:R:82:GLN:HE22	2:1:228:LEU:CD1	1.46	0.75
1:R:173:PRO:HG2	1:R:225:HIS:HE1	1.52	0.74
1:R:41:LEU:CA	1:R:143:ALA:HB3	2.17	0.74
1:R:86:TYR:HE1	2:1:224:GLU:OE1	1.71	0.74
1:R:130:GLN:NE2	2:1:105:PHE:CZ	2.53	0.73
1:R:72:SER:C	5:3:97:HIS:NE2	2.46	0.73
1:R:99:LEU:HD12	2:1:226:ASP:OD2	1.87	0.73
1:R:130:GLN:NE2	2:1:105:PHE:CD1	2.53	0.73
1:R:130:GLN:HE21	2:1:105:PHE:HE1	1.15	0.73
1:R:82:GLN:NE2	2:1:228:LEU:HD12	1.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:3:51:THR:HG21	5:3:99:MET:H	1.53	0.72
1:R:100:GLY:CA	3:2:138:THR:HG21	2.19	0.72
1:R:80:GLN:HG2	1:R:98:ARG:HG2	1.71	0.72
2:1:177:THR:HG21	2:1:182:SER:OG	1.89	0.72
1:R:142:LEU:CD2	1:R:172:ARG:HG2	2.20	0.71
1:R:130:GLN:CB	2:1:107:VAL:N	2.52	0.71
1:R:41:LEU:HB3	1:R:143:ALA:HB3	0.77	0.71
1:R:165:ARG:HG3	1:R:206:TRP:HB3	1.73	0.71
1:R:130:GLN:CA	2:1:107:VAL:N	2.42	0.71
1:R:82:GLN:HE21	2:1:228:LEU:CD1	1.36	0.71
1:R:128:PHE:HB3	1:R:129:PRO:HD3	1.70	0.71
1:R:132:SER:HB2	2:1:107:VAL:HG11	1.73	0.71
1:R:124:LEU:HA	1:R:134:SER:HB2	1.73	0.70
1:R:128:PHE:HZ	2:1:111:THR:CG2	2.04	0.70
1:R:141:VAL:HG11	1:R:142:LEU:HD13	1.72	0.70
1:R:40:PHE:HZ	1:R:144:LYS:CD	2.05	0.70
1:R:40:PHE:HZ	1:R:144:LYS:HD3	1.56	0.70
1:R:116:GLU:CA	5:3:59:ASN:ND2	2.55	0.70
1:R:40:PHE:CE1	1:R:227:SER:OG	2.44	0.70
1:R:68:ARG:HD2	1:R:76:ALA:CB	2.21	0.70
1:R:104:ARG:HD2	1:R:106:ALA:HB2	1.74	0.69
2:1:109:LYS:HA	2:1:239:SER:HB3	1.73	0.69
1:R:130:GLN:HG3	2:1:105:PHE:O	1.90	0.69
1:R:141:VAL:HG13	1:R:142:LEU:CA	2.22	0.69
1:R:116:GLU:CA	5:3:59:ASN:HD21	2.05	0.69
1:R:132:SER:OG	2:1:107:VAL:HG12	1.92	0.69
1:R:128:PHE:CZ	2:1:111:THR:HG21	2.26	0.69
1:R:100:GLY:HA2	3:2:138:THR:HG21	1.75	0.68
1:R:85:SER:HA	2:1:214:LYS:HZ3	1.58	0.68
1:R:116:GLU:HA	5:3:59:ASN:HD21	1.55	0.68
1:R:82:GLN:HE22	2:1:228:LEU:HD11	1.00	0.67
1:R:40:PHE:CE1	1:R:227:SER:CB	2.77	0.67
1:R:128:PHE:CE1	8:1:397:HOH:O	2.20	0.67
1:R:173:PRO:HG2	1:R:225:HIS:CE1	2.30	0.67
1:R:142:LEU:HD23	1:R:172:ARG:CG	2.24	0.67
1:R:143:ALA:O	1:R:225:HIS:CE1	2.47	0.67
1:R:82:GLN:HB2	2:1:228:LEU:N	1.97	0.67
1:R:98:ARG:HG3	1:R:99:LEU:H	1.60	0.66
1:R:130:GLN:CD	2:1:105:PHE:CE1	2.71	0.66
3:2:145:GLU:OE2	3:2:269:ARG:HD2	1.94	0.66
1:R:132:SER:HB3	2:1:166:ILE:CD1	2.23	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:82:GLN:HE21	2:1:228:LEU:HD12	1.06	0.66
1:R:128:PHE:HD2	2:1:108:TRP:CD1	2.10	0.66
1:R:59:THR:HG23	1:R:127:THR:HG23	1.78	0.66
1:R:240:VAL:O	1:R:241:TYR:HD2	1.79	0.66
2:1:102:SER:O	2:1:104:LEU:N	2.29	0.65
1:R:157:THR:OG1	1:R:158:GLY:HA2	1.97	0.65
1:R:40:PHE:CZ	1:R:144:LYS:HD3	2.32	0.65
1:R:141:VAL:HG11	1:R:142:LEU:CD1	2.26	0.65
1:R:141:VAL:CG1	1:R:142:LEU:CD1	2.75	0.65
1:R:40:PHE:HE1	1:R:227:SER:OG	1.80	0.65
1:R:84:PRO:O	2:1:214:LYS:NZ	2.30	0.65
2:1:158:MET:SD	2:1:177:THR:HG23	2.36	0.65
1:R:128:PHE:HD2	2:1:108:TRP:HD1	1.43	0.64
1:R:99:LEU:CB	2:1:226:ASP:OD2	2.45	0.64
1:R:159:GLU:N	1:R:160:PRO:HD3	2.13	0.64
1:R:40:PHE:HE1	1:R:227:SER:CB	2.10	0.64
1:R:215:ASP:O	1:R:238:LEU:CB	2.45	0.64
1:R:73:GLY:CA	5:3:97:HIS:CD2	2.76	0.64
1:R:116:GLU:HA	5:3:59:ASN:CG	2.22	0.64
1:R:133:ARG:HB2	2:1:167:PRO:O	1.98	0.64
1:R:83:GLY:CA	2:1:227:SER:HA	2.28	0.63
1:R:149:ALA:HB2	1:R:234:LEU:HD12	1.81	0.63
2:1:132:MET:HG2	2:1:261:MET:HE3	1.81	0.63
1:R:81:THR:N	2:1:234:LEU:HD13	2.11	0.62
1:R:142:LEU:O	1:R:173:PRO:HG3	1.99	0.62
1:R:141:VAL:CG1	1:R:142:LEU:N	2.59	0.62
2:1:132:MET:HE1	6:1:999:SC4:H71	1.81	0.62
1:R:100:GLY:HA2	3:2:138:THR:CG2	2.30	0.62
1:R:132:SER:HB2	2:1:166:ILE:HD13	1.79	0.62
1:R:130:GLN:NE2	2:1:107:VAL:HG23	2.14	0.62
1:R:66:TRP:HB2	1:R:78:PHE:HB3	1.81	0.61
1:R:82:GLN:NE2	2:1:228:LEU:CD1	0.78	0.61
1:R:99:LEU:HD23	3:2:141:PHE:CE1	2.35	0.61
1:R:139:LEU:HD22	1:R:140:ARG:HG3	1.80	0.61
1:R:162:PRO:HD3	1:R:208:LEU:H	1.66	0.60
1:R:215:ASP:HB3	1:R:216:GLY:CA	2.30	0.60
1:R:151:VAL:HA	1:R:163:MET:O	2.01	0.60
5:3:65:MET:HA	5:3:65:MET:HE2	1.84	0.60
1:R:162:PRO:HD3	1:R:209:VAL:O	2.02	0.59
1:R:128:PHE:CZ	2:1:111:THR:HG22	2.35	0.59
1:R:141:VAL:CG2	1:R:142:LEU:HD12	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:3:64:THR:O	5:3:67:MET:HG2	2.03	0.59
1:R:142:LEU:O	1:R:173:PRO:HD2	2.01	0.59
1:R:181:SER:HB3	1:R:219:VAL:HG23	1.85	0.59
1:R:82:GLN:NE2	2:1:228:LEU:HD11	0.65	0.59
1:R:41:LEU:HB3	1:R:143:ALA:CA	2.29	0.58
1:R:131:GLY:H	2:1:107:VAL:HB	1.67	0.58
2:1:27:LEU:HD21	2:1:72:ARG:HG3	1.85	0.58
2:1:132:MET:CG	2:1:261:MET:HE3	2.33	0.58
1:R:68:ARG:HG2	1:R:70:GLY:HA3	1.85	0.58
3:2:110:VAL:HG22	3:2:250:LEU:HD12	1.86	0.58
1:R:215:ASP:HB3	1:R:216:GLY:HA2	1.85	0.58
1:R:75:MET:O	5:3:93:PRO:HD3	2.04	0.58
1:R:163:MET:HE3	1:R:206:TRP:HB2	1.86	0.58
1:R:214:VAL:HG22	1:R:215:ASP:H	1.67	0.58
5:3:198:VAL:HG11	5:3:208:MET:CE	2.34	0.58
1:R:116:GLU:CB	5:3:59:ASN:HD21	2.16	0.57
2:1:132:MET:HE1	6:1:999:SC4:C7	2.34	0.57
1:R:41:LEU:CA	1:R:143:ALA:CB	2.81	0.57
1:R:151:VAL:HG21	1:R:238:LEU:HA	1.86	0.57
4:4:18:ARG:HG3	4:4:24:THR:HG21	1.87	0.57
1:R:188:GLN:HB3	1:R:208:LEU:O	2.03	0.57
1:R:116:GLU:CD	5:3:59:ASN:CG	2.72	0.57
3:2:60:ALA:O	3:2:254:PRO:HG2	2.04	0.57
3:2:66:LEU:HD12	3:2:250:LEU:HD23	1.86	0.57
1:R:172:ARG:HA	1:R:201:THR:H	1.70	0.57
3:2:100:TYR:CE1	5:3:137:PRO:HG2	2.40	0.57
3:2:73:LYS:HE2	3:2:242:SER:HA	1.87	0.56
1:R:65:THR:HB	1:R:124:LEU:HG	1.86	0.56
1:R:98:ARG:C	1:R:100:GLY:H	2.13	0.56
1:R:128:PHE:CE1	2:1:111:THR:HG21	2.40	0.56
2:1:132:MET:SD	2:1:261:MET:HE3	2.44	0.56
1:R:131:GLY:HA2	1:R:133:ARG:HD3	1.86	0.56
2:1:24:ALA:HB2	2:1:76:THR:CG2	2.33	0.56
1:R:41:LEU:C	1:R:143:ALA:CB	2.79	0.56
1:R:141:VAL:CG1	1:R:142:LEU:HD12	2.35	0.56
1:R:161:VAL:HB	1:R:163:MET:CB	2.14	0.56
2:1:93:ASP:C	2:1:95:ASP:H	2.14	0.56
1:R:82:GLN:HB3	2:1:228:LEU:CA	2.31	0.56
1:R:141:VAL:CG1	1:R:142:LEU:HB2	2.34	0.56
3:2:263:ARG:HD3	5:3:136:PRO:O	2.06	0.56
2:1:249:ASN:OD1	2:1:250:PRO:HD2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:40:PHE:CZ	1:R:144:LYS:HB2	2.41	0.55
1:R:85:SER:HA	2:1:214:LYS:NZ	2.21	0.55
1:R:42:GLY:N	1:R:43:ASP:HA	2.22	0.55
1:R:81:THR:HG21	2:1:234:LEU:CA	2.33	0.55
1:R:130:GLN:HG2	2:1:107:VAL:HG23	1.87	0.55
3:2:270:THR:O	3:2:271:GLN:HG2	2.07	0.54
1:R:100:GLY:HA3	3:2:138:THR:HG21	1.89	0.54
1:R:120:SER:HB3	1:R:138:TRP:CG	2.43	0.54
2:1:132:MET:HG2	2:1:261:MET:CE	2.37	0.54
1:R:41:LEU:HD22	1:R:42:GLY:H	1.72	0.54
1:R:147:ASN:ND2	1:R:223:VAL:HG21	2.23	0.54
1:R:99:LEU:HD23	3:2:171:ARG:CZ	2.36	0.54
1:R:99:LEU:HB3	2:1:226:ASP:OD2	2.07	0.54
1:R:73:GLY:HA3	5:3:97:HIS:CE1	2.43	0.54
1:R:152:GLN:O	1:R:163:MET:HB3	2.08	0.54
1:R:75:MET:HE1	5:3:92:ASP:OD2	1.65	0.54
1:R:80:GLN:CG	1:R:98:ARG:HG2	2.38	0.53
2:1:40:GLU:HB3	4:4:64:THR:HB	1.91	0.53
1:R:36:GLN:NE2	1:R:137:ILE:HG13	2.23	0.53
1:R:40:PHE:CE1	1:R:227:SER:HB3	2.43	0.53
1:R:41:LEU:H	1:R:143:ALA:HB2	1.73	0.53
3:2:241:GLU:N	3:2:241:GLU:CD	2.66	0.53
1:R:49:CYS:HB2	1:R:66:TRP:HZ2	1.73	0.53
1:R:87:SER:OG	5:3:181:ASN:ND2	2.42	0.53
1:R:132:SER:HB2	2:1:166:ILE:HG21	1.90	0.53
1:R:127:THR:HG22	1:R:129:PRO:HD2	1.91	0.53
2:1:217:LEU:O	2:1:220:GLN:HG2	2.09	0.53
1:R:130:GLN:HA	2:1:107:VAL:CA	2.38	0.52
2:1:193:ARG:NH1	5:3:8:PRO:HG2	2.23	0.52
1:R:41:LEU:C	1:R:143:ALA:HB3	2.33	0.52
1:R:80:GLN:O	1:R:98:ARG:NH2	2.42	0.52
2:1:176:GLN:HE22	5:3:233:GLN:HE22	1.54	0.52
1:R:73:GLY:N	1:R:74:SER:HA	2.25	0.52
3:2:172:ASN:ND2	3:2:173:PHE:H	2.07	0.52
1:R:43:ASP:CB	1:R:44:SER:CA	2.66	0.51
2:1:209:TYR:O	2:1:230:GLY:HA2	2.11	0.51
3:2:10:SER:HB2	4:4:69:ASN:O	2.10	0.51
1:R:40:PHE:CE1	1:R:144:LYS:HB2	2.46	0.51
3:2:241:GLU:HB3	3:2:243:SER:O	2.11	0.51
1:R:71:GLU:OE1	5:3:97:HIS:CG	2.63	0.51
2:1:273:PRO:HB3	3:2:188:ASN:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:169:THR:HA	1:R:202:VAL:HG23	1.93	0.50
1:R:158:GLY:HA3	1:R:159:GLU:HB3	1.94	0.49
1:R:187:PRO:O	1:R:188:GLN:HG3	2.11	0.49
8:1:348:HOH:O	5:3:15:THR:HG23	2.11	0.49
1:R:93:GLU:HB3	1:R:109:ARG:HB3	1.92	0.49
1:R:98:ARG:CD	1:R:104:ARG:NH2	2.64	0.49
3:2:63:PHE:CD1	3:2:253:ALA:HB2	2.47	0.49
1:R:155:GLN:NE2	1:R:212:SER:H	2.10	0.49
5:3:149:MET:O	5:3:149:MET:HG2	2.13	0.49
1:R:81:THR:HG23	2:1:234:LEU:HA	1.88	0.49
5:3:198:VAL:HG11	5:3:208:MET:HE1	1.95	0.49
1:R:100:GLY:CA	3:2:138:THR:CG2	2.87	0.49
2:1:182:SER:H	5:3:15:THR:CG2	2.25	0.49
1:R:102:GLU:HG3	1:R:104:ARG:NH1	2.28	0.49
1:R:71:GLU:OE1	5:3:97:HIS:CD2	2.66	0.48
1:R:114:ARG:CD	5:3:59:ASN:HD22	2.26	0.48
1:R:180:HIS:HA	1:R:186:MET:HG3	1.96	0.48
1:R:241:TYR:HA	1:R:242:TYR:C	2.37	0.48
2:1:49:THR:O	4:4:57:ILE:HD11	2.13	0.48
2:1:158:MET:SD	2:1:177:THR:CG2	3.02	0.48
1:R:60:HIS:O	1:R:128:PHE:N	2.26	0.48
1:R:84:PRO:C	2:1:214:LYS:NZ	2.71	0.48
3:2:146:ASN:HB3	3:2:172:ASN:ND2	2.29	0.48
2:1:221:ALA:O	2:1:224:GLU:HB2	2.13	0.48
1:R:99:LEU:CD2	3:2:141:PHE:CE1	2.97	0.48
1:R:145:PRO:HA	1:R:170:GLY:O	2.12	0.48
1:R:240:VAL:O	1:R:241:TYR:CD2	2.64	0.48
2:1:261:MET:HE1	2:1:263:PRO:HG3	1.96	0.48
1:R:40:PHE:CE1	1:R:144:LYS:CB	2.96	0.47
3:2:11:VAL:HG23	4:4:69:ASN:HB3	1.94	0.47
2:1:273:PRO:HB3	3:2:188:ASN:CB	2.44	0.47
1:R:179:TRP:CZ3	1:R:219:VAL:HG22	2.49	0.47
2:1:193:ARG:CZ	5:3:8:PRO:HG2	2.44	0.47
1:R:54:PRO:CA	1:R:55:ASN:CB	2.87	0.47
1:R:141:VAL:HG13	1:R:142:LEU:CD1	2.44	0.47
1:R:224:GLU:O	1:R:225:HIS:CB	2.62	0.47
2:1:159:TYR:CE2	2:1:161:PRO:HG3	2.49	0.47
2:1:181:PRO:HA	5:3:15:THR:HG22	1.97	0.47
1:R:98:ARG:O	1:R:99:LEU:HD22	2.15	0.47
1:R:104:ARG:HD3	1:R:104:ARG:HA	1.57	0.47
1:R:170:GLY:HA2	1:R:200:VAL:HG13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:257:ILE:N	2:1:257:ILE:HD12	2.29	0.47
1:R:73:GLY:CA	5:3:97:HIS:CE1	2.98	0.47
1:R:152:GLN:HB2	1:R:153:LYS:HA	1.97	0.47
2:1:48:GLU:HA	3:2:196:ILE:HB	1.95	0.46
1:R:141:VAL:CG1	1:R:142:LEU:HD13	2.40	0.46
1:R:186:MET:O	1:R:188:GLN:N	2.48	0.46
2:1:132:MET:HE1	6:1:999:SC4:C8	2.46	0.46
1:R:115:VAL:HG13	1:R:141:VAL:HG21	1.98	0.46
1:R:188:GLN:O	1:R:207:ILE:HG22	2.16	0.46
3:2:71:TRP:CE3	3:2:246:ILE:HD11	2.50	0.46
1:R:40:PHE:HD1	1:R:227:SER:HG	1.48	0.46
2:1:94:ASN:OD1	2:1:248:HIS:HB3	2.16	0.46
2:1:176:GLN:HE22	5:3:233:GLN:HE21	1.58	0.46
1:R:38:PRO:HA	1:R:39:GLY:HA3	1.66	0.45
1:R:161:VAL:HG12	1:R:208:LEU:HB2	1.97	0.45
5:3:44:MET:HA	5:3:44:MET:HE2	1.98	0.45
2:1:110:ILE:HG13	2:1:239:SER:HA	1.99	0.45
1:R:210:PRO:HB2	1:R:211:SER:H	1.68	0.45
2:1:176:GLN:NE2	5:3:233:GLN:NE2	2.55	0.45
5:3:87:LEU:HD11	5:3:114:LEU:HD12	1.98	0.45
1:R:157:THR:OG1	1:R:158:GLY:CA	2.64	0.44
4:4:57:ILE:HD13	4:4:57:ILE:HA	1.78	0.44
1:R:81:THR:HG21	2:1:234:LEU:HD23	0.45	0.44
1:R:130:GLN:CB	2:1:106:SER:C	2.75	0.44
1:R:172:ARG:O	1:R:174:PRO:HD3	2.17	0.44
1:R:207:ILE:HA	1:R:208:LEU:HB3	2.00	0.44
1:R:31:VAL:HG12	1:R:51:LEU:HD11	1.98	0.44
1:R:162:PRO:HB2	1:R:238:LEU:HG	2.00	0.44
1:R:41:LEU:CB	1:R:143:ALA:CB	2.48	0.44
1:R:73:GLY:HA2	5:3:230:HIS:NE2	2.32	0.44
3:2:238:PHE:O	3:2:240:THR:N	2.51	0.44
1:R:177:ILE:HG22	1:R:223:VAL:HG22	2.00	0.44
1:R:114:ARG:HD3	5:3:59:ASN:HD22	1.83	0.44
1:R:130:GLN:HE22	1:R:133:ARG:HD2	1.82	0.44
1:R:141:VAL:HG21	1:R:142:LEU:HD12	2.00	0.44
4:4:33:TYR:HB2	4:4:38:SER:HB2	2.00	0.44
1:R:65:THR:HA	1:R:78:PHE:O	2.18	0.43
1:R:83:GLY:C	2:1:226:ASP:O	2.52	0.43
2:1:134:PHE:O	2:1:193:ARG:HA	2.19	0.43
1:R:130:GLN:CG	2:1:105:PHE:O	2.64	0.43
1:R:162:PRO:CD	1:R:208:LEU:H	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:82:GLN:O	1:R:98:ARG:HG3	2.18	0.43
3:2:110:VAL:HG22	3:2:250:LEU:CD1	2.47	0.43
3:2:263:ARG:NH1	5:3:137:PRO:O	2.52	0.43
2:1:102:SER:C	2:1:104:LEU:H	2.24	0.43
3:2:67:ASP:N	8:2:336:HOH:O	2.51	0.43
3:2:241:GLU:C	3:2:243:SER:N	2.74	0.43
1:R:40:PHE:HZ	1:R:144:LYS:CG	2.31	0.42
1:R:116:GLU:OE2	5:3:59:ASN:OD1	2.37	0.42
4:4:7:SER:HA	4:4:26:ASN:HA	2.01	0.42
2:1:42:PRO:HA	4:4:63:LYS:O	2.18	0.42
1:R:69:HIS:N	1:R:70:GLY:HA3	2.33	0.42
1:R:31:VAL:HG11	1:R:134:SER:HA	2.01	0.42
1:R:132:SER:HB2	2:1:166:ILE:CG2	2.49	0.42
1:R:75:MET:CE	5:3:92:ASP:OD2	2.40	0.42
1:R:144:LYS:HG3	1:R:145:PRO:N	2.34	0.42
3:2:263:ARG:HB2	3:2:264:ASN:H	1.68	0.42
1:R:128:PHE:HB3	1:R:129:PRO:CD	2.43	0.42
2:1:92:VAL:HG23	2:1:255:SER:HB2	2.02	0.42
4:4:49:ASP:HA	4:4:50:PRO:HD3	1.85	0.42
1:R:81:THR:HA	2:1:234:LEU:HD22	1.63	0.42
1:R:128:PHE:HE2	2:1:108:TRP:HE1	0.48	0.42
2:1:148:GLY:HA3	2:1:251:THR:CG2	2.43	0.42
1:R:142:LEU:HD23	1:R:172:ARG:CB	2.50	0.42
5:3:195:GLN:OE1	5:3:195:GLN:HA	2.20	0.41
1:R:71:GLU:OE1	5:3:97:HIS:CE1	2.73	0.41
1:R:144:LYS:CG	1:R:145:PRO:N	2.83	0.41
1:R:168:SER:HB3	1:R:203:THR:HG23	2.01	0.41
1:R:98:ARG:CG	1:R:99:LEU:H	2.24	0.41
1:R:85:SER:CA	2:1:214:LYS:NZ	2.84	0.41
8:1:348:HOH:O	5:3:15:THR:CG2	2.67	0.41
1:R:157:THR:CB	1:R:158:GLY:HA2	2.50	0.41
1:R:159:GLU:H	1:R:160:PRO:HD3	1.82	0.41
2:1:24:ALA:HB3	4:4:45:ASP:O	2.21	0.41
3:2:141:PHE:CE2	3:2:171:ARG:HG2	2.56	0.41
1:R:76:ALA:H	1:R:77:VAL:HG23	1.85	0.41
1:R:161:VAL:HA	1:R:162:PRO:HD3	1.94	0.41
4:4:3:ALA:HA	4:4:30:ILE:HG12	2.01	0.41
5:3:44:MET:O	5:3:48:GLU:HG3	2.20	0.41
5:3:124:MET:O	5:3:124:MET:HG3	2.18	0.41
1:R:41:LEU:O	1:R:143:ALA:CB	2.69	0.41
1:R:40:PHE:CZ	1:R:144:LYS:CD	2.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:126:VAL:HA	1:R:132:SER:HA	2.03	0.41
1:R:186:MET:H	1:R:187:PRO:CD	2.34	0.41
1:R:221:CYS:HB3	1:R:234:LEU:HG	2.02	0.41
2:1:162:PRO:HD3	2:1:238:GLY:CA	2.50	0.41
5:3:143:LYS:HA	5:3:143:LYS:HD3	1.75	0.41
2:1:94:ASN:O	2:1:95:ASP:HB2	2.21	0.40
2:1:292:PRO:HG2	2:1:293:LEU:HD12	2.02	0.40
1:R:116:GLU:CG	5:3:59:ASN:ND2	2.62	0.40
1:R:139:LEU:HB3	1:R:140:ARG:H	1.57	0.40
1:R:157:THR:HG21	1:R:211:SER:OG	2.22	0.40
1:R:80:GLN:CD	1:R:98:ARG:HG2	2.46	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
6	SC4	1	999	-	29,29,29	1.40	5 (17%)	39,39,39	1.41	5 (12%)
7	MYR	4	1	4	9,10,15	0.60	0	8,9,15	0.52	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	SC4	1	999	-	-	0/12/12/12	0/3/3/3
7	MYR	4	1	4	-	6/8/8/13	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	1	999	SC4	C5-C6	3.55	1.44	1.39
6	1	999	SC4	C18-C19	2.61	1.43	1.38
6	1	999	SC4	C15-C16	2.44	1.45	1.41
6	1	999	SC4	C18-C17	2.36	1.42	1.38
6	1	999	SC4	C3-C4	2.14	1.43	1.39

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	1	999	SC4	O1-C3-C4	4.62	121.89	116.39
6	1	999	SC4	C21-O3-C6	2.83	123.56	117.50
6	1	999	SC4	O1-C3-C2	-2.73	117.99	123.95
6	1	999	SC4	C15-C16-CL2	2.41	121.58	118.40
6	1	999	SC4	C15-C20-CL3	2.29	121.42	118.40

There are no chirality outliers.

All (6) torsion outliers are listed below:

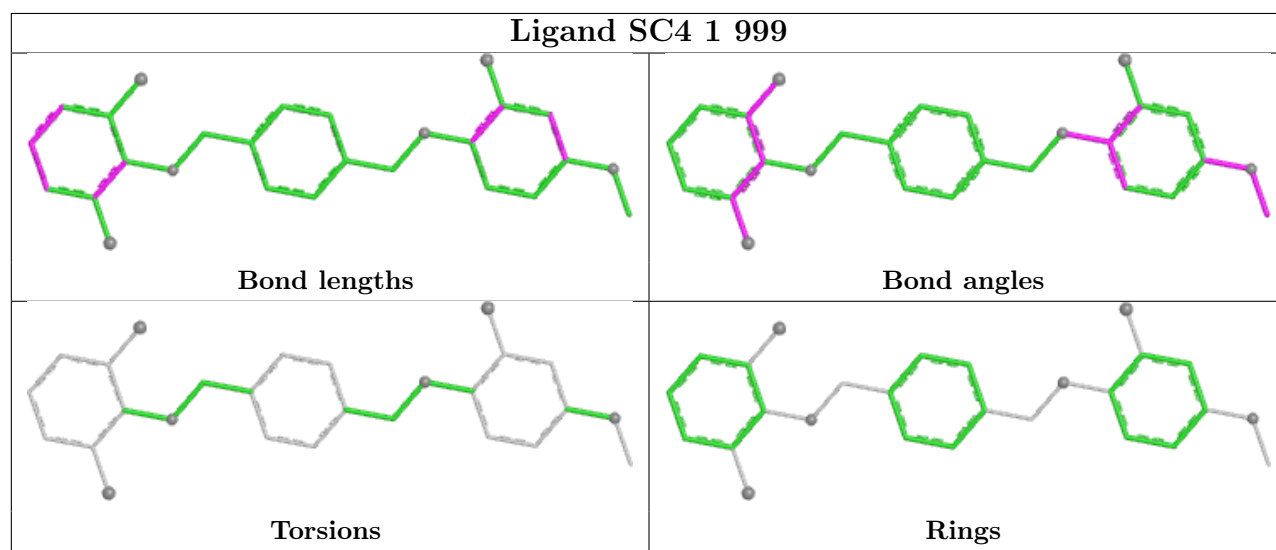
Mol	Chain	Res	Type	Atoms
7	4	1	MYR	O1-C1-C2-C3
7	4	1	MYR	C1-C2-C3-C4
7	4	1	MYR	C6-C7-C8-C9
7	4	1	MYR	C5-C6-C7-C8
7	4	1	MYR	C4-C5-C6-C7
7	4	1	MYR	C7-C8-C9-C10

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	1	999	SC4	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 Map visualisation

This section contains visualisations of the EMDB entry EMD-1563. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis ⓘ

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.