Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:54 PM UTC

PDB ID	:	1JMU / pdb_00001jmu
Title	:	Crystal Structure of the Reovirus mu1/sigma3 Complex
Authors	:	Liemann, S.; Nibert, M.L.; Harrison, S.C.
Deposited on	:	2001-07-20
Resolution	:	2.80 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:

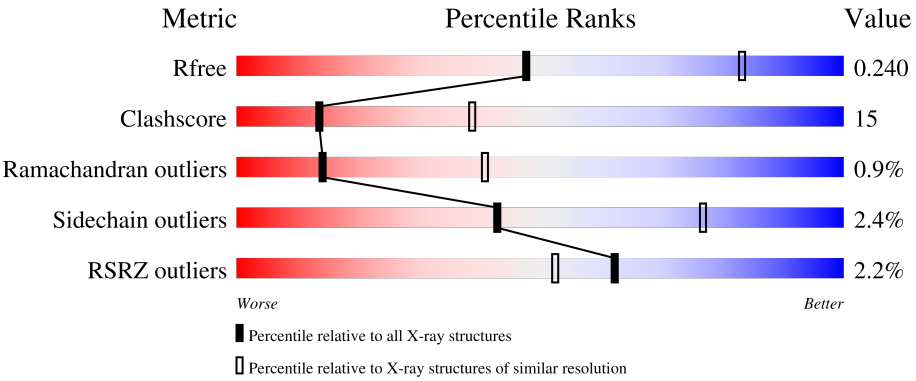
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 (i)

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

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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% 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	41	46% 32% • 20%
1	C	41	51% 27% • 20%
1	E	41	46% 32% • 20%
2	B	666	2% 62% 27% • 9%
2	D	666	4% 62% 27% • 9%

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Mol	Chain	Length	Quality of chain
2	F	666	2% 61% 27% 9%
3	G	366	1% 71% 27%
3	H	366	1% 73% 25%
3	I	366	1% 73% 26%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 23657 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 PROTEIN MU-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	33	Total	C	N	O	S	0	0	0
			230	141	37	51	1			
1	C	33	Total	C	N	O	S	0	0	0
			230	141	37	51	1			
1	E	33	Total	C	N	O	S	0	0	0
			230	141	37	51	1			

- Molecule 2 is a protein called PROTEIN MU-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	608	Total	C	N	O	S	0	0	0
			4641	2950	770	903	18			
2	D	608	Total	C	N	O	S	0	0	0
			4641	2950	770	903	18			
2	F	608	Total	C	N	O	S	0	0	0
			4641	2950	770	903	18			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	272	PRO	LEU	SEE REMARK 999	UNP P11077
B	284	LYS	ARG	SEE REMARK 999	UNP P11077
B	344	LEU	PRO	SEE REMARK 999	UNP P11077
B	359	PHE	LEU	SEE REMARK 999	UNP P11077
D	272	PRO	LEU	SEE REMARK 999	UNP P11077
D	284	LYS	ARG	SEE REMARK 999	UNP P11077
D	344	LEU	PRO	SEE REMARK 999	UNP P11077
D	359	PHE	LEU	SEE REMARK 999	UNP P11077
F	272	PRO	LEU	SEE REMARK 999	UNP P11077
F	284	LYS	ARG	SEE REMARK 999	UNP P11077
F	344	LEU	PRO	SEE REMARK 999	UNP P11077
F	359	PHE	LEU	SEE REMARK 999	UNP P11077

- Molecule 3 is a protein called SIGMA 3 PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	366	Total	C	N	O	S	0	0	0
			2888	1820	508	532	28			
3	H	366	Total	C	N	O	S	0	0	0
			2888	1820	508	532	28			
3	I	366	Total	C	N	O	S	0	0	0
			2888	1820	508	532	28			

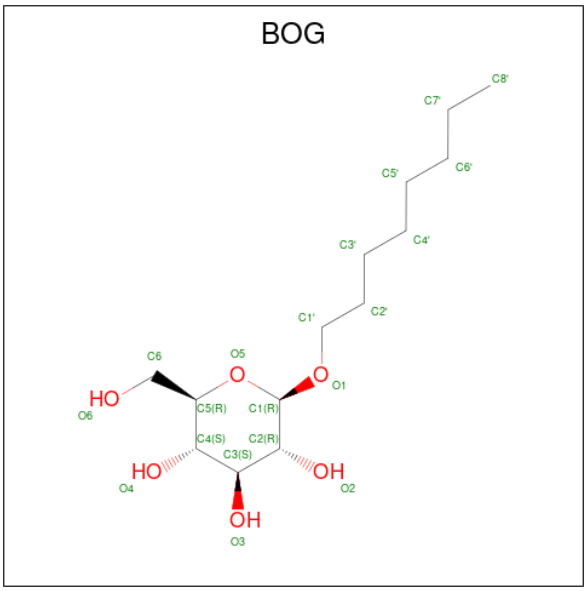
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	104	CYS	ALA	engineered mutation	UNP Q86292
G	325	ASN	ASP	SEE REMARK 999	UNP Q86292
H	104	CYS	ALA	engineered mutation	UNP Q86292
H	325	ASN	ASP	SEE REMARK 999	UNP Q86292
I	104	CYS	ALA	engineered mutation	UNP Q86292
I	325	ASN	ASP	SEE REMARK 999	UNP Q86292

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

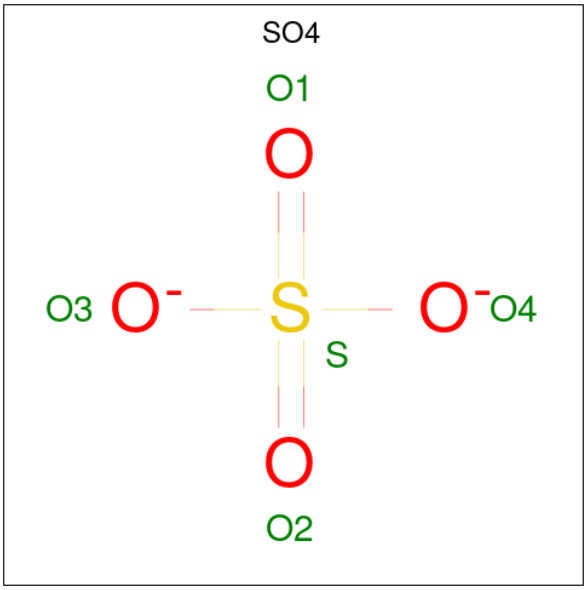
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		

- Molecule 5 is octyl beta-D-glucopyranoside (CCD ID: BOG) (formula: $C_{14}H_{28}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 20 14 6	0	0
5	D	1	Total C O 20 14 6	0	0
5	F	1	Total C O 20 14 6	0	0

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total O S 5 4 1	0	0
6	D	1	Total O S 5 4 1	0	0
6	F	1	Total O S 5 4 1	0	0
6	G	1	Total O S 5 4 1	0	0
6	G	1	Total O S 5 4 1	0	0
6	H	1	Total O S 5 4 1	0	0
6	H	1	Total O S 5 4 1	0	0
6	I	1	Total O S 5 4 1	0	0
6	I	1	Total O S 5 4 1	0	0

- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	G	1	Total Zn 1 1	0	0
7	H	1	Total Zn 1 1	0	0
7	I	1	Total Zn 1 1	0	0

- Molecule 8 is water.

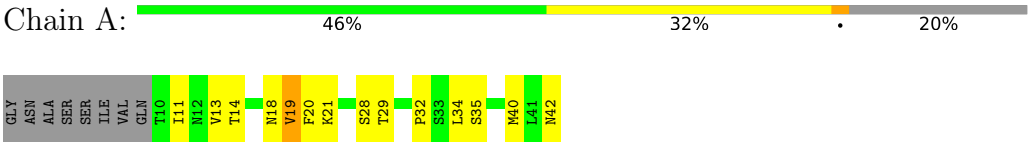
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	5	Total O 5 5	0	0
8	B	42	Total O 42 42	0	0
8	C	2	Total O 2 2	0	0
8	D	46	Total O 46 46	0	0
8	E	1	Total O 1 1	0	0
8	F	56	Total O 56 56	0	0
8	G	41	Total O 41 41	0	0
8	H	45	Total O 45 45	0	0
8	I	33	Total O 33 33	0	0

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 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.

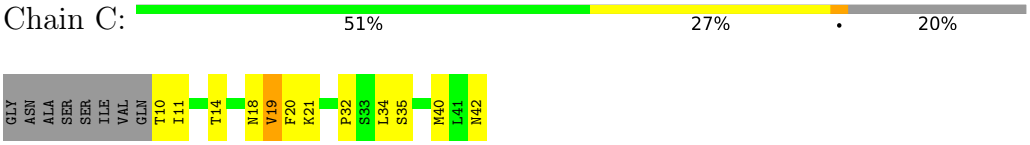
• Molecule 1: PROTEIN MU-1

Chain A:



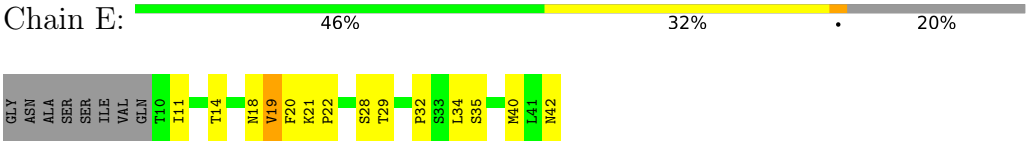
• Molecule 1: PROTEIN MU-1

Chain C:



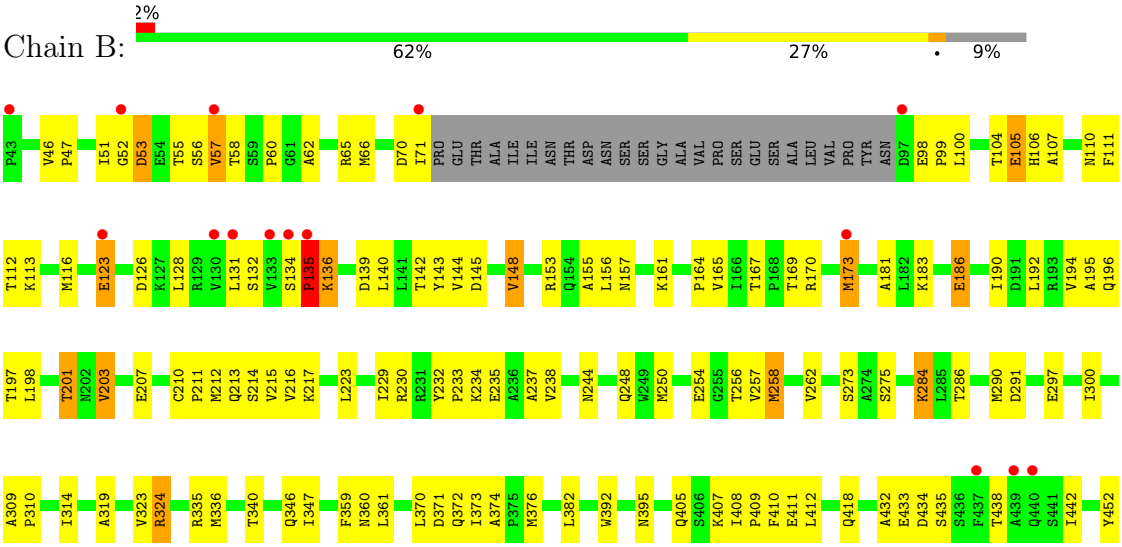
• Molecule 1: PROTEIN MU-1

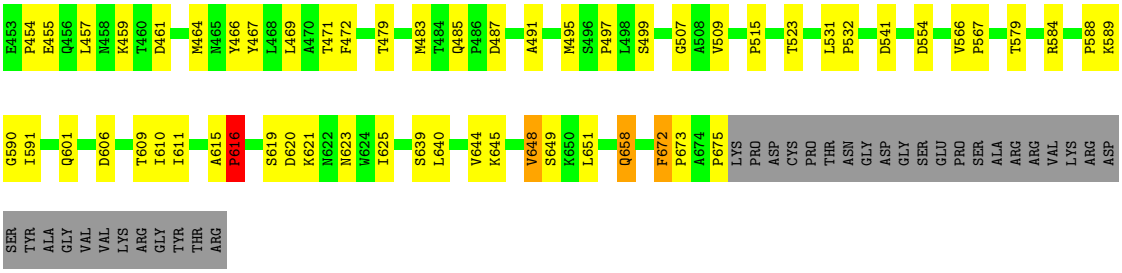
Chain E:



• Molecule 2: PROTEIN MU-1

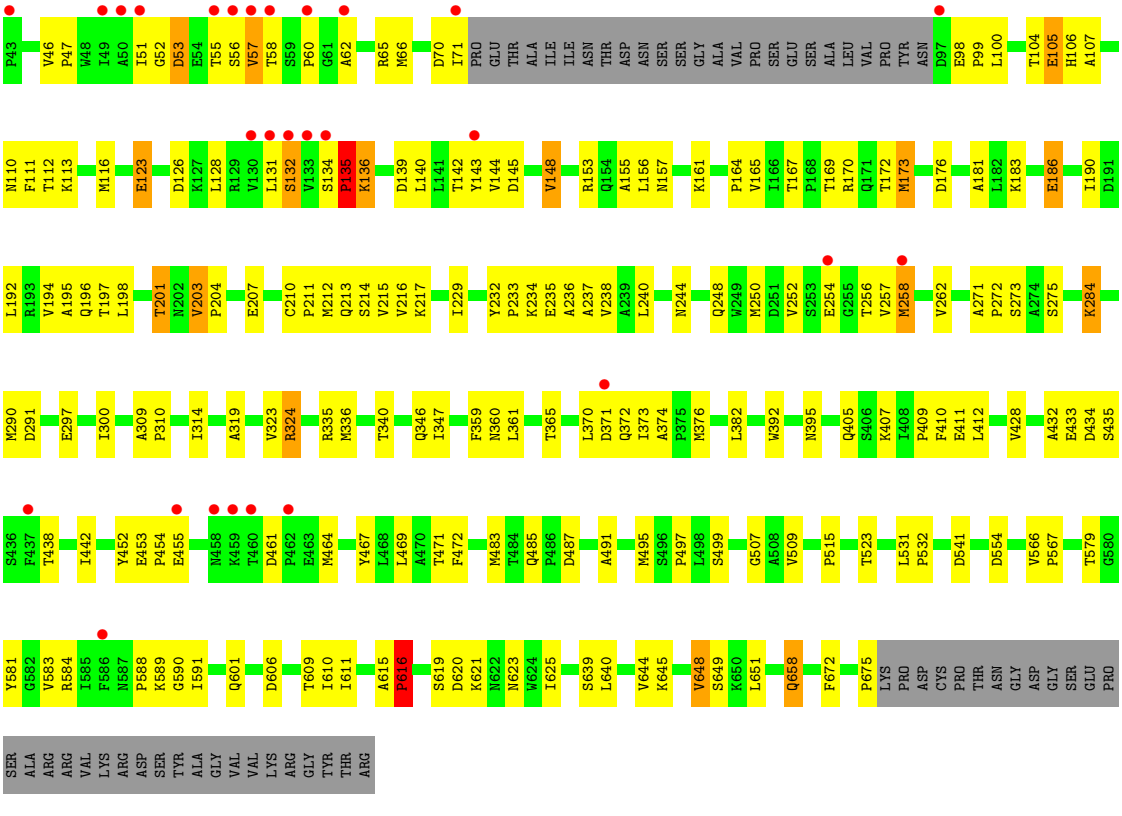
Chain B:





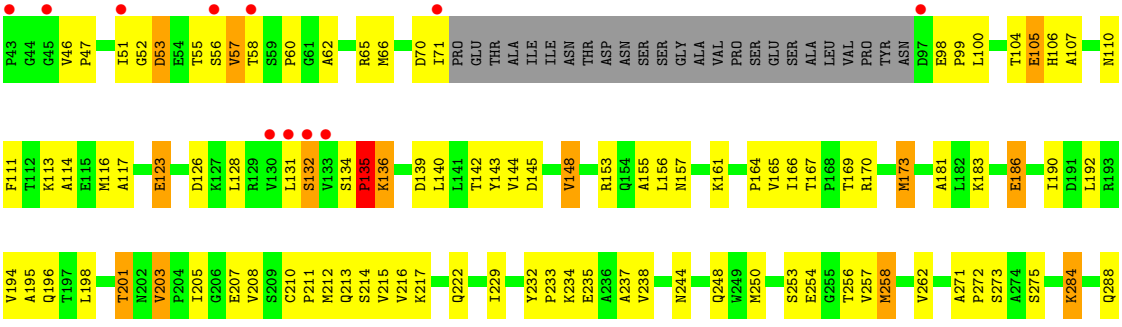
• Molecule 2: PROTEIN MU-1

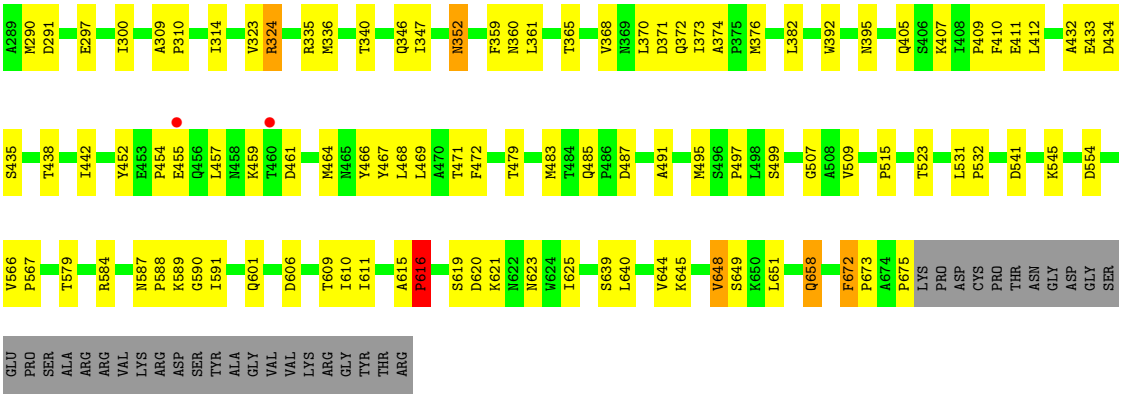
Chain D:



• Molecule 2: PROTEIN MU-1

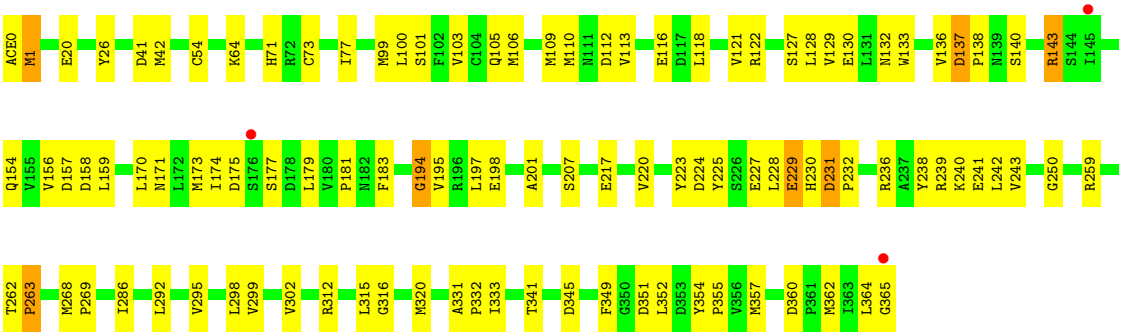
Chain F:





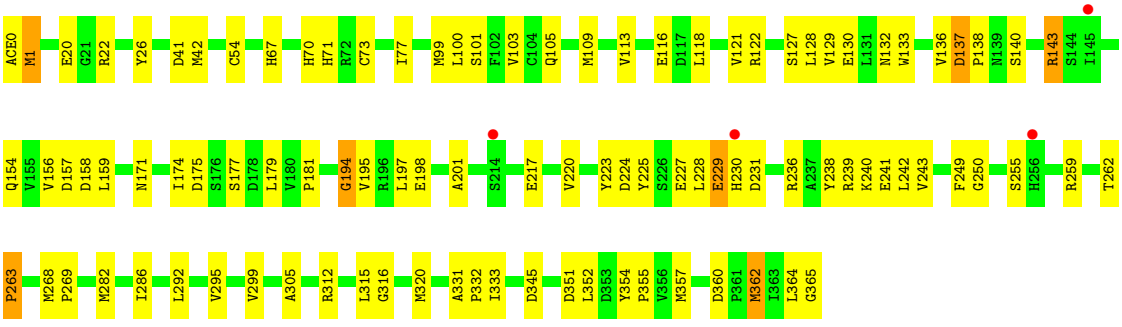
• Molecule 3: SIGMA 3 PROTEIN

Chain G:



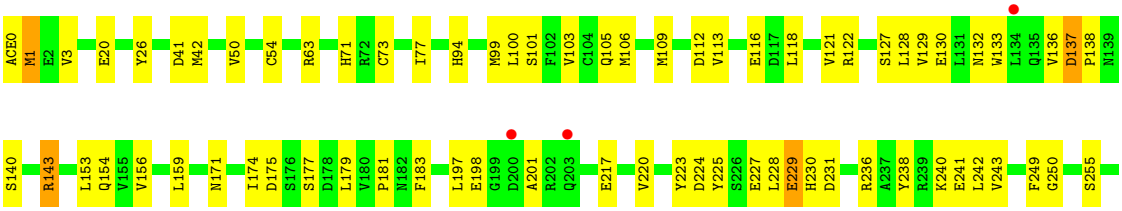
• Molecule 3: SIGMA 3 PROTEIN

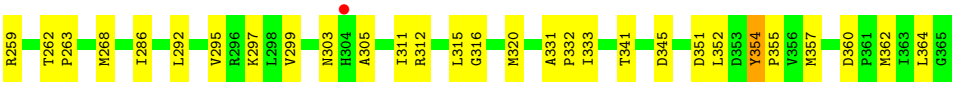
Chain H:



• Molecule 3: SIGMA 3 PROTEIN

Chain I:




R259
T262
P263
M268
I286
L292
V295
R296
K297
L298
V299
N303
H304
A305
I311
R312
L315
G316
M320
A331
P332
I333
T341
D345
D351
L352
D353
Y354
P355
V356
M357
D360
P361
M362
I363
L364
G365

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	180.29Å 184.94Å 284.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.00 – 2.80 35.00 – 2.81	Depositor EDS
% Data completeness (in resolution range)	93.6 (35.00-2.80) 93.6 (35.00-2.81)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.87 (at 2.81Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.216 , 0.241 0.216 , 0.240	Depositor DCC
R_{free} test set	5422 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	49.0	Xtriage
Anisotropy	0.838	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 39.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.006 for k,h,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	23657	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.39% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACE, ZN, SO4, CL, BOG

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	0.48	0/233	1.02	1/317 (0.3%)
1	C	0.47	0/233	1.00	1/317 (0.3%)
1	E	0.41	0/233	1.01	1/317 (0.3%)
2	B	0.55	2/4737 (0.0%)	0.96	18/6466 (0.3%)
2	D	0.55	2/4737 (0.0%)	0.96	16/6466 (0.2%)
2	F	0.55	2/4737 (0.0%)	0.97	20/6466 (0.3%)
3	G	0.51	0/2958	0.95	11/4007 (0.3%)
3	H	0.51	0/2958	0.96	13/4007 (0.3%)
3	I	0.49	0/2958	0.97	15/4007 (0.4%)
All	All	0.53	6/23784 (0.0%)	0.96	96/32370 (0.3%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	258	MET	SD-CE	6.07	1.94	1.79
2	F	173	MET	SD-CE	5.44	1.93	1.79
2	F	116	MET	SD-CE	5.25	1.92	1.79
2	D	173	MET	SD-CE	5.24	1.92	1.79
2	B	173	MET	SD-CE	5.16	1.92	1.79
2	D	258	MET	SD-CE	5.06	1.92	1.79

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	20	GLU	N-CA-C	-8.47	101.63	114.16
3	I	20	GLU	N-CA-C	-8.12	102.14	114.16
2	B	134	SER	CA-C-N	8.09	129.96	119.84
2	B	134	SER	C-N-CA	8.09	129.96	119.84
2	D	134	SER	CA-C-N	8.06	129.91	119.84
2	D	134	SER	C-N-CA	8.06	129.91	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	20	GLU	N-CA-C	-8.04	102.27	114.16
2	F	134	SER	CA-C-N	7.87	129.67	119.84
2	F	134	SER	C-N-CA	7.87	129.67	119.84
3	H	231	ASP	CA-C-N	7.20	126.45	118.97
3	H	231	ASP	C-N-CA	7.20	126.45	118.97
2	B	53	ASP	N-CA-C	7.08	120.30	108.20
2	F	53	ASP	N-CA-C	7.02	120.21	108.20
2	D	53	ASP	N-CA-C	6.94	120.07	108.20
3	I	243	VAL	N-CA-C	6.83	117.45	110.82
3	H	250	GLY	N-CA-C	-6.68	105.22	112.04
3	G	231	ASP	CA-C-N	6.58	125.81	118.97
3	G	231	ASP	C-N-CA	6.58	125.81	118.97
2	F	672	PHE	CA-C-N	6.41	126.44	119.90
2	F	672	PHE	C-N-CA	6.41	126.44	119.90
3	G	250	GLY	N-CA-C	-6.35	105.56	112.04
3	I	231	ASP	CA-C-N	6.22	125.44	118.97
3	I	231	ASP	C-N-CA	6.22	125.44	118.97
3	H	41	ASP	N-CA-C	-6.22	106.23	113.88
3	G	243	VAL	N-CA-C	6.17	116.81	110.82
2	D	297	GLU	CA-C-N	6.14	126.32	119.32
2	D	297	GLU	C-N-CA	6.14	126.32	119.32
3	G	41	ASP	N-CA-C	-6.06	106.43	113.88
3	I	250	GLY	N-CA-C	-6.05	105.87	112.04
2	D	672	PHE	CA-C-N	6.04	126.06	119.90
2	D	672	PHE	C-N-CA	6.04	126.06	119.90
2	F	203	VAL	CA-C-N	6.03	126.19	119.32
2	F	203	VAL	C-N-CA	6.03	126.19	119.32
3	I	41	ASP	N-CA-C	-6.00	106.49	113.88
2	B	203	VAL	CA-C-N	5.97	126.13	119.32
2	B	203	VAL	C-N-CA	5.97	126.13	119.32
2	F	297	GLU	CA-C-N	5.97	126.13	119.32
2	F	297	GLU	C-N-CA	5.97	126.13	119.32
2	B	672	PHE	CA-C-N	5.93	125.95	119.90
2	B	672	PHE	C-N-CA	5.93	125.95	119.90
3	H	243	VAL	N-CA-C	5.92	117.46	111.00
3	H	137	ASP	CA-C-N	5.81	126.21	119.47
3	H	137	ASP	C-N-CA	5.81	126.21	119.47
3	I	262	THR	N-CA-C	-5.74	103.53	110.13
3	I	305	ALA	N-CA-C	5.74	119.46	112.23
3	H	262	THR	N-CA-C	-5.72	103.55	110.13
2	B	297	GLU	CA-C-N	5.70	125.82	119.32
2	B	297	GLU	C-N-CA	5.70	125.82	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	352	LEU	N-CA-C	5.65	120.28	113.17
2	D	523	THR	N-CA-C	-5.64	102.80	110.36
2	D	203	VAL	CA-C-N	5.64	125.75	119.32
2	D	203	VAL	C-N-CA	5.64	125.75	119.32
2	B	523	THR	N-CA-C	-5.63	102.82	110.36
3	G	137	ASP	CA-C-N	5.60	125.97	119.47
3	G	137	ASP	C-N-CA	5.60	125.97	119.47
2	D	554	ASP	N-CA-C	5.59	117.84	108.73
2	F	523	THR	N-CA-C	-5.59	102.87	110.36
2	D	273	SER	N-CA-C	-5.55	101.79	110.17
3	G	262	THR	N-CA-C	-5.52	103.78	110.13
2	F	507	GLY	N-CA-C	5.52	121.26	114.69
2	B	507	GLY	N-CA-C	5.51	121.25	114.69
2	D	258	MET	N-CA-C	5.50	116.64	108.60
2	F	273	SER	N-CA-C	-5.46	101.93	110.17
3	I	137	ASP	CA-C-N	5.46	125.80	119.47
3	I	137	ASP	C-N-CA	5.46	125.80	119.47
2	F	258	MET	N-CA-C	5.45	116.55	108.60
3	H	362	MET	N-CA-C	5.39	116.72	108.42
2	B	132	SER	N-CA-C	-5.37	106.23	112.89
2	F	554	ASP	N-CA-C	5.36	117.47	108.73
3	I	352	LEU	N-CA-C	5.36	119.92	113.17
2	D	132	SER	N-CA-C	-5.35	106.25	112.89
2	D	148	VAL	N-CA-C	5.34	116.17	108.48
2	D	507	GLY	N-CA-C	5.33	121.04	114.69
3	G	352	LEU	N-CA-C	5.33	119.89	113.17
3	I	50	VAL	N-CA-C	5.31	116.62	108.71
2	B	148	VAL	N-CA-C	5.31	116.12	108.48
2	F	545	LYS	N-CA-C	-5.29	105.68	111.82
1	E	19	VAL	N-CA-C	5.25	115.68	108.12
2	F	132	SER	N-CA-C	-5.25	106.39	112.89
1	A	19	VAL	N-CA-C	5.21	115.63	108.12
3	I	354	TYR	CA-C-N	5.19	125.17	120.03
3	I	354	TYR	C-N-CA	5.19	125.17	120.03
2	B	273	SER	N-CA-C	-5.19	102.34	110.17
1	C	19	VAL	N-CA-C	5.17	115.57	108.12
2	F	479	THR	CA-C-N	5.16	125.46	119.47
2	F	479	THR	C-N-CA	5.16	125.46	119.47
2	B	479	THR	CA-C-N	5.16	125.45	119.47
2	B	479	THR	C-N-CA	5.16	125.45	119.47
2	B	258	MET	N-CA-C	5.15	116.12	108.60
2	F	222	GLN	N-CA-C	5.12	120.39	114.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	207	SER	N-CA-C	-5.12	106.55	112.89
2	B	554	ASP	N-CA-C	5.12	117.07	108.73
3	H	305	ALA	N-CA-C	5.11	119.59	112.90
2	F	148	VAL	N-CA-C	5.08	115.79	108.48
3	H	255	SER	N-CA-C	5.02	117.43	109.50
3	I	255	SER	N-CA-C	5.02	117.43	109.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	230	0	227	17	0
1	C	230	0	227	15	0
1	E	230	0	227	16	0
2	B	4641	0	4673	169	0
2	D	4641	0	4673	166	0
2	F	4641	0	4673	174	0
3	G	2888	0	2814	70	0
3	H	2888	0	2814	67	0
3	I	2888	0	2814	68	0
4	A	1	0	0	0	0
5	B	20	0	28	2	0
5	D	20	0	28	1	0
5	F	20	0	28	1	0
6	B	5	0	0	0	0
6	D	5	0	0	0	0
6	F	5	0	0	0	0
6	G	10	0	0	0	0
6	H	10	0	0	0	0
6	I	10	0	0	0	0
7	G	1	0	0	0	0
7	H	1	0	0	0	0
7	I	1	0	0	0	0
8	A	5	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	42	0	0	0	0
8	C	2	0	0	0	0
8	D	46	0	0	0	0
8	E	1	0	0	0	0
8	F	56	0	0	3	0
8	G	41	0	0	0	0
8	H	45	0	0	1	0
8	I	33	0	0	2	0
All	All	23657	0	23226	682	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 15.

All (682) 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:66:MET:HE1	2:B:144:VAL:HG11	1.18	1.13
2:F:66:MET:HE1	2:F:144:VAL:HG11	1.18	1.11
2:D:66:MET:HE1	2:D:144:VAL:HG11	1.17	1.07
3:H:109:MET:HE2	3:H:129:VAL:HG13	1.37	1.06
2:D:153:ARG:HH11	2:D:153:ARG:HB2	1.24	1.03
1:E:42:ASN:HB3	2:F:104:THR:HG21	1.42	1.00
3:G:109:MET:HE2	3:G:129:VAL:HG13	1.39	1.00
3:I:109:MET:HE2	3:I:129:VAL:HG13	1.43	0.99
1:C:42:ASN:HB3	2:D:104:THR:HG21	1.44	0.97
2:F:579:THR:HA	2:F:584:ARG:HH22	1.30	0.97
1:A:42:ASN:HB3	2:B:104:THR:HG21	1.46	0.96
3:G:171:ASN:HD22	3:G:259:ARG:HH11	1.02	0.96
2:F:153:ARG:HB2	2:F:153:ARG:HH11	1.30	0.96
2:B:153:ARG:HB2	2:B:153:ARG:HH11	1.28	0.95
3:G:171:ASN:HD22	3:G:259:ARG:NH1	1.65	0.93
2:D:471:THR:HG22	2:D:472:PHE:H	1.32	0.93
3:H:171:ASN:HD22	3:H:259:ARG:HH11	1.06	0.93
2:B:579:THR:HA	2:B:584:ARG:HH22	1.31	0.93
3:I:171:ASN:HD22	3:I:259:ARG:HH11	1.07	0.92
3:H:171:ASN:HD22	3:H:259:ARG:NH1	1.68	0.92
2:D:579:THR:HA	2:D:584:ARG:HH22	1.35	0.92
2:B:471:THR:HG22	2:B:472:PHE:H	1.31	0.90
3:I:171:ASN:HD22	3:I:259:ARG:NH1	1.69	0.90
2:B:66:MET:HE3	2:B:71:ILE:HD11	1.52	0.90
2:B:435:SER:HB3	2:B:442:ILE:HB	1.54	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:644:VAL:HG22	2:D:186:GLU:HG2	1.52	0.89
3:G:171:ASN:ND2	3:G:259:ARG:HH11	1.70	0.89
2:B:186:GLU:HG2	2:F:644:VAL:HG22	1.54	0.88
2:F:471:THR:HG22	2:F:472:PHE:H	1.36	0.88
2:D:153:ARG:HB2	2:D:153:ARG:NH1	1.87	0.88
2:B:153:ARG:HB2	2:B:153:ARG:NH1	1.90	0.87
2:F:66:MET:HE3	2:F:71:ILE:HD11	1.56	0.87
2:D:644:VAL:HG22	2:F:186:GLU:HG2	1.56	0.86
2:D:435:SER:HB3	2:D:442:ILE:HB	1.56	0.86
3:H:171:ASN:ND2	3:H:259:ARG:HH11	1.73	0.85
3:I:171:ASN:ND2	3:I:259:ARG:HH11	1.75	0.85
2:F:435:SER:HB3	2:F:442:ILE:HB	1.59	0.84
2:D:66:MET:HE3	2:D:71:ILE:HD11	1.59	0.83
2:F:153:ARG:HB2	2:F:153:ARG:NH1	1.94	0.81
2:D:336:MET:HE2	3:H:333:ILE:HD13	1.65	0.79
2:B:131:LEU:HD21	2:B:135:PRO:HD3	1.66	0.78
2:F:495:MET:HE1	2:F:531:LEU:HD22	1.67	0.77
2:D:382:LEU:HD23	2:D:491:ALA:HB2	1.67	0.76
2:F:372:GLN:O	2:F:509:VAL:HG23	1.86	0.75
2:D:471:THR:HG22	2:D:472:PHE:N	2.02	0.75
2:D:66:MET:CE	2:D:144:VAL:HG11	2.09	0.74
2:D:131:LEU:HD21	2:D:135:PRO:HD3	1.67	0.74
2:B:471:THR:HG22	2:B:472:PHE:N	2.02	0.73
2:B:579:THR:HA	2:B:584:ARG:NH2	2.04	0.73
2:D:372:GLN:O	2:D:509:VAL:HG23	1.88	0.73
2:F:131:LEU:HD21	2:F:135:PRO:HD3	1.67	0.73
3:G:362:MET:HE3	3:G:364:LEU:HD23	1.70	0.73
2:B:382:LEU:HD23	2:B:491:ALA:HB2	1.71	0.73
2:B:495:MET:HE1	2:B:531:LEU:HD22	1.71	0.73
2:F:579:THR:HA	2:F:584:ARG:NH2	2.02	0.72
3:H:362:MET:HE3	3:H:364:LEU:HD23	1.71	0.72
2:F:382:LEU:HD23	2:F:491:ALA:HB2	1.70	0.71
2:D:495:MET:HE1	2:D:531:LEU:HD22	1.70	0.71
2:F:70:ASP:C	2:F:71:ILE:HD12	2.14	0.71
3:G:109:MET:CE	3:G:129:VAL:HG13	2.19	0.71
3:G:143:ARG:HG2	3:G:143:ARG:HH11	1.55	0.71
2:B:70:ASP:C	2:B:71:ILE:HD12	2.15	0.71
2:B:66:MET:CE	2:B:144:VAL:HG11	2.11	0.71
2:D:70:ASP:C	2:D:71:ILE:HD12	2.16	0.71
3:I:362:MET:HE3	3:I:364:LEU:HD23	1.73	0.70
2:B:372:GLN:O	2:B:509:VAL:HG23	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:42:ASN:HB3	2:F:104:THR:CG2	2.21	0.70
3:H:143:ARG:HG2	3:H:143:ARG:HH11	1.57	0.70
2:D:579:THR:HA	2:D:584:ARG:NH2	2.07	0.69
2:D:46:VAL:HG11	2:D:65:ARG:NE	2.08	0.69
3:I:109:MET:HE1	3:I:130:GLU:O	1.92	0.69
2:F:471:THR:HG22	2:F:472:PHE:N	2.06	0.68
2:B:566:VAL:HG11	2:D:194:VAL:HG13	1.75	0.67
3:H:109:MET:CE	3:H:129:VAL:HG13	2.21	0.67
3:G:118:LEU:O	3:G:122:ARG:HG2	1.94	0.67
1:E:18:ASN:HB3	2:F:212:MET:HG2	1.77	0.67
2:F:46:VAL:HG11	2:F:65:ARG:CD	2.25	0.67
1:E:42:ASN:CB	2:F:104:THR:HG21	2.23	0.67
3:I:143:ARG:HG2	3:I:143:ARG:HH11	1.60	0.67
2:B:46:VAL:HG11	2:B:65:ARG:CD	2.25	0.66
1:C:18:ASN:HB3	2:D:212:MET:HG2	1.76	0.66
1:A:18:ASN:HB3	2:B:212:MET:HG2	1.77	0.66
2:D:46:VAL:HG11	2:D:65:ARG:CD	2.25	0.66
1:C:42:ASN:HB3	2:D:104:THR:CG2	2.24	0.66
2:B:46:VAL:HG11	2:B:65:ARG:NE	2.11	0.66
2:F:46:VAL:HG11	2:F:65:ARG:NE	2.11	0.66
2:B:376:MET:HG2	2:B:495:MET:HE3	1.78	0.65
2:D:60:PRO:HG2	2:D:153:ARG:HH12	1.62	0.65
2:F:212:MET:HE2	2:F:216:VAL:HG23	1.78	0.65
2:D:213:GLN:O	2:D:217:LYS:HG2	1.97	0.65
2:F:395:ASN:HB2	2:F:432:ALA:HB3	1.78	0.65
2:D:66:MET:HE1	2:D:144:VAL:CG1	2.11	0.64
2:F:66:MET:CE	2:F:144:VAL:HG11	2.11	0.64
2:F:376:MET:HG2	2:F:495:MET:HE3	1.79	0.64
3:I:109:MET:CE	3:I:129:VAL:HG13	2.23	0.64
2:B:212:MET:HE2	2:B:216:VAL:HG23	1.80	0.64
2:F:213:GLN:O	2:F:217:LYS:HG2	1.97	0.64
2:B:371:ASP:O	2:B:372:GLN:HB2	1.96	0.64
2:D:336:MET:HE2	3:H:333:ILE:CD1	2.28	0.64
3:H:118:LEU:O	3:H:122:ARG:HG2	1.98	0.64
2:B:336:MET:HE2	3:G:333:ILE:HD13	1.78	0.63
2:B:213:GLN:O	2:B:217:LYS:HG2	1.97	0.63
2:B:53:ASP:HB3	2:B:56:SER:OG	1.98	0.63
2:D:53:ASP:HB3	2:D:56:SER:OG	1.99	0.63
2:B:212:MET:HE3	2:B:215:VAL:HB	1.80	0.63
2:D:212:MET:HE2	2:D:216:VAL:HG23	1.79	0.63
2:D:395:ASN:HB2	2:D:432:ALA:HB3	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:109:MET:HE1	3:H:130:GLU:O	1.97	0.63
2:F:212:MET:HE3	2:F:215:VAL:HB	1.80	0.63
2:B:588:PRO:HD2	2:B:591:ILE:HD12	1.81	0.63
1:C:42:ASN:CB	2:D:104:THR:HG21	2.25	0.62
3:G:299:VAL:HG13	3:G:320:MET:HG2	1.80	0.62
2:F:409:PRO:HD2	2:F:412:LEU:HD12	1.81	0.62
3:H:22:ARG:NH1	8:H:704:HOH:O	2.32	0.62
2:D:60:PRO:HG2	2:D:153:ARG:NH1	2.13	0.62
2:D:371:ASP:O	2:D:372:GLN:HB2	2.00	0.62
2:F:60:PRO:HG2	2:F:153:ARG:HH12	1.64	0.62
2:F:53:ASP:HB3	2:F:56:SER:OG	1.99	0.62
3:G:109:MET:HE1	3:G:130:GLU:O	1.99	0.62
2:B:194:VAL:HG13	2:F:566:VAL:HG11	1.80	0.62
2:D:140:LEU:N	2:D:140:LEU:HD12	2.15	0.62
2:F:371:ASP:O	2:F:372:GLN:HB2	2.00	0.61
3:I:118:LEU:O	3:I:122:ARG:HG2	2.00	0.61
1:A:42:ASN:HB3	2:B:104:THR:CG2	2.25	0.61
2:D:471:THR:CG2	2:D:472:PHE:H	2.11	0.61
2:D:376:MET:HG2	2:D:495:MET:HE3	1.81	0.61
3:I:299:VAL:HG13	3:I:320:MET:HG2	1.82	0.61
2:D:405:GLN:HB3	2:D:464:MET:CE	2.30	0.61
2:B:60:PRO:HG2	2:B:153:ARG:HH12	1.65	0.61
2:D:140:LEU:HD12	2:D:140:LEU:H	1.66	0.61
3:I:113:VAL:HG11	3:I:128:LEU:HD11	1.82	0.61
2:D:212:MET:HE3	2:D:215:VAL:HB	1.82	0.61
2:B:284:LYS:HD3	2:F:291:ASP:OD1	2.01	0.60
2:F:405:GLN:HB3	2:F:464:MET:CE	2.31	0.60
2:F:60:PRO:HG2	2:F:153:ARG:NH1	2.16	0.60
2:B:346:GLN:HG2	2:B:360:ASN:OD1	2.02	0.60
2:B:395:ASN:HB2	2:B:432:ALA:HB3	1.82	0.60
3:H:236:ARG:HE	3:H:240:LYS:HD2	1.67	0.60
3:G:236:ARG:HE	3:G:240:LYS:HD2	1.66	0.60
2:D:324:ARG:NH1	2:D:487:ASP:OD1	2.35	0.59
2:F:588:PRO:HD2	2:F:591:ILE:HD12	1.83	0.59
2:D:346:GLN:HG2	2:D:360:ASN:OD1	2.02	0.59
2:F:66:MET:HE1	2:F:144:VAL:CG1	2.13	0.59
2:D:258:MET:SD	2:F:99:PRO:HG3	2.41	0.59
1:A:18:ASN:HB2	8:A:603:HOH:O	2.01	0.59
2:B:60:PRO:HG2	2:B:153:ARG:NH1	2.16	0.59
3:G:132:ASN:HA	3:G:360:ASP:OD1	2.02	0.59
2:D:566:VAL:HG11	2:F:194:VAL:HG13	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:99:PRO:HG3	2:F:258:MET:SD	2.43	0.59
2:B:183:LYS:O	2:B:186:GLU:HB2	2.03	0.59
1:A:42:ASN:CB	2:B:104:THR:HG21	2.27	0.59
2:B:405:GLN:HB3	2:B:464:MET:CE	2.33	0.59
2:B:66:MET:HE1	2:B:144:VAL:CG1	2.12	0.58
3:H:113:VAL:HG11	3:H:128:LEU:HD11	1.85	0.58
1:C:14:THR:HG22	1:C:14:THR:O	2.02	0.58
2:F:405:GLN:HB3	2:F:464:MET:HE1	1.86	0.58
2:D:588:PRO:HD2	2:D:591:ILE:HD12	1.85	0.58
2:F:183:LYS:O	2:F:186:GLU:HB2	2.04	0.58
2:B:140:LEU:N	2:B:140:LEU:HD12	2.18	0.58
2:F:140:LEU:N	2:F:140:LEU:HD12	2.19	0.58
1:A:14:THR:O	1:A:14:THR:HG22	2.01	0.58
2:D:347:ILE:HD11	2:D:359:PHE:CE1	2.39	0.58
1:E:14:THR:HG22	1:E:14:THR:O	2.02	0.58
2:B:471:THR:CG2	2:B:472:PHE:H	2.11	0.57
2:F:335:ARG:HD2	2:F:411:GLU:OE2	2.04	0.57
2:B:235:GLU:OE1	2:B:235:GLU:N	2.37	0.57
2:F:46:VAL:HG11	2:F:65:ARG:HD2	1.87	0.57
2:B:46:VAL:HG11	2:B:65:ARG:HD2	1.86	0.57
2:B:411:GLU:CD	2:B:411:GLU:H	2.12	0.57
2:D:405:GLN:HB3	2:D:464:MET:HE1	1.85	0.57
2:B:153:ARG:HD3	2:F:132:SER:O	2.05	0.57
2:D:284:LYS:HA	2:D:284:LYS:HE3	1.86	0.57
2:F:235:GLU:N	2:F:235:GLU:OE1	2.38	0.57
2:F:347:ILE:HD11	2:F:359:PHE:CE1	2.40	0.57
3:I:132:ASN:HA	3:I:360:ASP:OD1	2.05	0.57
2:D:46:VAL:HG11	2:D:65:ARG:CZ	2.34	0.57
3:G:113:VAL:HG11	3:G:128:LEU:HD11	1.86	0.57
2:D:409:PRO:HD2	2:D:412:LEU:HD12	1.86	0.56
2:F:346:GLN:HG2	2:F:360:ASN:OD1	2.05	0.56
3:H:132:ASN:HA	3:H:360:ASP:OD1	2.04	0.56
3:H:223:TYR:OH	3:H:351:ASP:HB3	2.05	0.56
2:F:237:ALA:HA	5:F:709:BOG:H8'1	1.88	0.56
2:F:411:GLU:CD	2:F:411:GLU:H	2.13	0.56
3:G:223:TYR:OH	3:G:351:ASP:HB3	2.05	0.56
2:D:183:LYS:O	2:D:186:GLU:HB2	2.05	0.56
2:F:324:ARG:NH1	2:F:487:ASP:OD1	2.37	0.56
2:F:347:ILE:HD11	2:F:359:PHE:CZ	2.39	0.56
2:D:347:ILE:HD11	2:D:359:PHE:CZ	2.40	0.56
2:B:347:ILE:HD11	2:B:359:PHE:CE1	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:335:ARG:HD2	2:B:411:GLU:OE2	2.05	0.56
2:B:409:PRO:HD2	2:B:412:LEU:HD12	1.86	0.56
2:D:411:GLU:CD	2:D:411:GLU:H	2.14	0.56
2:B:140:LEU:HD12	2:B:140:LEU:H	1.70	0.56
2:B:284:LYS:HE3	2:B:284:LYS:HA	1.87	0.56
2:B:347:ILE:HD11	2:B:359:PHE:CZ	2.40	0.56
2:F:100:LEU:HD23	2:F:167:THR:HG22	1.88	0.56
2:B:407:LYS:HE2	2:B:461:ASP:OD1	2.06	0.55
2:F:471:THR:CG2	2:F:472:PHE:H	2.15	0.55
2:D:100:LEU:HD13	2:D:165:VAL:HG11	1.88	0.55
2:D:340:THR:O	2:D:340:THR:HG22	2.06	0.55
2:D:309:ALA:HB3	2:D:310:PRO:HD3	1.89	0.55
2:D:46:VAL:HG11	2:D:65:ARG:HD2	1.87	0.55
2:D:235:GLU:OE1	2:D:235:GLU:N	2.39	0.55
1:E:11:ILE:O	2:F:234:LYS:HE3	2.06	0.55
3:H:299:VAL:HG13	3:H:320:MET:HG2	1.89	0.55
2:B:309:ALA:HB3	2:B:310:PRO:HD3	1.88	0.55
2:B:499:SER:HA	2:D:601:GLN:HB3	1.87	0.55
2:D:335:ARG:HD2	2:D:411:GLU:OE2	2.07	0.55
3:I:223:TYR:OH	3:I:351:ASP:HB3	2.06	0.55
2:D:140:LEU:HB3	2:D:170:ARG:HD3	1.89	0.55
3:I:236:ARG:HE	3:I:240:LYS:HD2	1.70	0.55
2:B:340:THR:HG22	2:B:340:THR:O	2.05	0.55
2:F:309:ALA:HB3	2:F:310:PRO:HD3	1.89	0.55
2:B:324:ARG:NH1	2:B:487:ASP:OD1	2.40	0.54
2:D:145:ASP:OD2	2:D:161:LYS:HG2	2.07	0.54
3:H:241:GLU:O	3:H:242:LEU:HD23	2.06	0.54
2:F:140:LEU:HD12	2:F:140:LEU:H	1.70	0.54
3:I:1:MET:HE2	3:I:71:HIS:HB3	1.89	0.54
2:B:123:GLU:HG3	2:B:238:VAL:HG11	1.89	0.54
3:H:101:SER:O	3:H:105:GLN:HG3	2.07	0.54
2:B:433:GLU:HG2	2:B:434:ASP:H	1.72	0.54
3:I:241:GLU:O	3:I:242:LEU:HD23	2.08	0.54
2:D:237:ALA:HA	5:D:709:BOG:H8'1	1.89	0.54
2:B:336:MET:HE2	3:G:333:ILE:CD1	2.38	0.54
2:D:291:ASP:OD1	2:F:284:LYS:HD3	2.08	0.54
3:H:174:ILE:HD13	3:H:181:PRO:HG3	1.90	0.54
1:C:11:ILE:O	2:D:234:LYS:HE3	2.08	0.54
2:F:46:VAL:HG11	2:F:65:ARG:CZ	2.38	0.53
2:F:340:THR:O	2:F:340:THR:HG22	2.07	0.53
3:H:137:ASP:N	3:H:138:PRO:HD3	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:113:LYS:HE2	1:E:40:MET:O	2.08	0.53
2:F:148:VAL:O	2:F:155:ALA:HA	2.09	0.53
2:B:275:SER:HA	2:B:651:LEU:CD1	2.39	0.53
2:D:407:LYS:HE2	2:D:461:ASP:OD1	2.07	0.53
2:F:66:MET:CE	2:F:71:ILE:HD11	2.33	0.53
2:F:123:GLU:HG3	2:F:238:VAL:HG11	1.90	0.53
2:F:284:LYS:HE3	2:F:284:LYS:HA	1.89	0.53
2:F:275:SER:HA	2:F:651:LEU:CD1	2.39	0.53
3:G:174:ILE:HD13	3:G:181:PRO:HG3	1.89	0.53
1:A:11:ILE:O	2:B:234:LYS:HE3	2.08	0.53
2:B:46:VAL:HG11	2:B:65:ARG:CZ	2.38	0.53
2:B:405:GLN:HB3	2:B:464:MET:HE1	1.91	0.53
2:D:433:GLU:HG2	2:D:434:ASP:H	1.74	0.53
2:B:136:LYS:O	2:B:139:ASP:HB2	2.08	0.53
2:B:237:ALA:HA	5:B:709:BOG:H8'1	1.89	0.53
2:F:248:GLN:HE21	2:F:257:VAL:HG12	1.74	0.53
2:B:66:MET:CE	2:B:71:ILE:HD11	2.33	0.52
2:B:291:ASP:OD1	2:D:284:LYS:HD3	2.08	0.52
2:F:213:GLN:OE1	2:F:675:PRO:HD2	2.09	0.52
3:I:177:SER:HB2	3:I:179:LEU:HG	1.91	0.52
2:D:123:GLU:HG3	2:D:238:VAL:HG11	1.91	0.52
2:D:452:TYR:CE2	2:D:454:PRO:HG3	2.44	0.52
2:F:407:LYS:HE2	2:F:461:ASP:OD1	2.10	0.52
2:F:452:TYR:CE2	2:F:454:PRO:HG3	2.43	0.52
3:G:177:SER:HB2	3:G:179:LEU:HG	1.90	0.52
3:I:198:GLU:HG3	3:I:355:PRO:HB2	1.91	0.52
3:G:1:MET:HE2	3:G:71:HIS:HB3	1.91	0.52
3:I:101:SER:O	3:I:105:GLN:HG3	2.10	0.52
2:B:248:GLN:HE21	2:B:257:VAL:HG12	1.75	0.52
2:D:248:GLN:HE21	2:D:257:VAL:HG12	1.75	0.52
2:F:100:LEU:HD13	2:F:165:VAL:HG11	1.92	0.52
2:F:192:LEU:O	2:F:196:GLN:HG3	2.10	0.52
2:B:192:LEU:O	2:B:196:GLN:HG3	2.09	0.52
2:B:145:ASP:OD2	2:B:161:LYS:HG2	2.10	0.52
2:B:340:THR:HG21	3:G:341:THR:HB	1.92	0.52
2:D:232:TYR:N	2:D:233:PRO:HD3	2.25	0.52
2:F:131:LEU:HD13	2:F:181:ALA:HB2	1.92	0.52
2:F:373:ILE:O	2:F:374:ALA:HB3	2.10	0.52
3:I:3:VAL:HA	8:I:711:HOH:O	2.10	0.52
2:F:433:GLU:HG2	2:F:434:ASP:H	1.74	0.51
2:B:100:LEU:HD23	2:B:167:THR:HG22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:66:MET:CE	2:D:71:ILE:HD11	2.35	0.51
2:D:100:LEU:HD23	2:D:167:THR:HG22	1.91	0.51
2:F:275:SER:C	2:F:651:LEU:HD11	2.35	0.51
3:I:174:ILE:HD13	3:I:181:PRO:HG3	1.91	0.51
3:I:137:ASP:OD2	3:I:140:SER:HB3	2.10	0.51
3:H:177:SER:HB2	3:H:179:LEU:HG	1.92	0.51
2:B:136:LYS:NZ	2:D:157:ASN:O	2.44	0.51
2:D:275:SER:HA	2:D:651:LEU:CD1	2.40	0.51
3:G:241:GLU:O	3:G:242:LEU:HD23	2.11	0.51
2:D:428:VAL:HG11	8:F:713:HOH:O	2.11	0.51
2:F:140:LEU:HB3	2:F:170:ARG:HD3	1.93	0.51
3:G:143:ARG:HH11	3:G:143:ARG:CG	2.23	0.51
2:B:410:PHE:HB2	2:B:467:TYR:CE1	2.45	0.51
1:A:40:MET:O	2:F:113:LYS:HE2	2.11	0.51
2:B:100:LEU:HD13	2:B:165:VAL:HG11	1.92	0.51
2:F:145:ASP:OD2	2:F:161:LYS:HG2	2.12	0.51
2:F:352:ASN:HB3	3:G:64:LYS:HA	1.92	0.51
3:G:101:SER:O	3:G:105:GLN:HG3	2.10	0.51
2:B:213:GLN:OE1	2:B:675:PRO:HD2	2.11	0.50
2:D:136:LYS:O	2:D:139:ASP:HB2	2.11	0.50
2:B:131:LEU:HD13	2:B:181:ALA:HB2	1.93	0.50
2:B:275:SER:C	2:B:651:LEU:HD11	2.37	0.50
3:H:198:GLU:HG3	3:H:355:PRO:HB2	1.93	0.50
2:D:58:THR:O	2:D:156:LEU:HD21	2.11	0.50
3:G:137:ASP:N	3:G:138:PRO:HD3	2.25	0.50
3:H:229:GLU:HG2	3:H:230:HIS:N	2.26	0.50
2:D:131:LEU:HD13	2:D:181:ALA:HB2	1.93	0.50
2:B:232:TYR:N	2:B:233:PRO:HD3	2.27	0.50
2:B:452:TYR:CE2	2:B:454:PRO:HG3	2.46	0.50
1:C:34:LEU:HB3	2:D:110:ASN:HD22	1.76	0.50
2:B:148:VAL:O	2:B:155:ALA:HA	2.10	0.50
2:D:148:VAL:O	2:D:155:ALA:HA	2.11	0.50
2:D:192:LEU:O	2:D:196:GLN:HG3	2.12	0.50
3:G:198:GLU:HG3	3:G:355:PRO:HB2	1.93	0.50
3:I:137:ASP:N	3:I:138:PRO:HD3	2.26	0.49
2:D:373:ILE:O	2:D:374:ALA:HB3	2.11	0.49
2:B:373:ILE:O	2:B:374:ALA:HB3	2.10	0.49
2:D:132:SER:O	2:F:153:ARG:HD3	2.12	0.49
3:H:1:MET:HE2	3:H:71:HIS:HB3	1.95	0.49
2:F:71:ILE:HD12	2:F:71:ILE:N	2.28	0.49
3:H:99:MET:O	3:H:103:VAL:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:250:MET:CB	2:B:257:VAL:HG22	2.42	0.49
2:B:601:GLN:HB3	2:F:499:SER:HA	1.93	0.49
2:D:131:LEU:HD23	2:D:131:LEU:O	2.13	0.49
2:F:610:ILE:HG13	2:F:611:ILE:HG23	1.94	0.49
3:G:136:VAL:O	3:G:143:ARG:HD3	2.13	0.49
3:H:137:ASP:OD2	3:H:140:SER:HB3	2.13	0.49
1:A:34:LEU:HB3	2:B:110:ASN:HD22	1.77	0.49
2:B:433:GLU:CG	2:B:434:ASP:H	2.25	0.49
1:E:34:LEU:HB3	2:F:110:ASN:HD22	1.77	0.49
2:B:123:GLU:HG3	2:B:238:VAL:CG1	2.43	0.49
2:B:567:PRO:HG3	2:D:197:THR:HB	1.94	0.49
2:F:51:ILE:HG22	2:F:62:ALA:O	2.12	0.49
2:F:232:TYR:N	2:F:233:PRO:HD3	2.26	0.49
2:F:136:LYS:O	2:F:139:ASP:HB2	2.11	0.49
2:F:143:TYR:N	8:F:736:HOH:O	2.37	0.49
2:F:250:MET:CB	2:F:257:VAL:HG22	2.42	0.49
3:H:122:ARG:CD	3:H:177:SER:HB3	2.43	0.49
2:B:113:LYS:HE2	1:C:40:MET:O	2.12	0.48
2:D:250:MET:CB	2:D:257:VAL:HG22	2.43	0.48
2:F:410:PHE:HB2	2:F:467:TYR:CE1	2.48	0.48
2:F:314:ILE:HD11	2:F:541:ASP:HB2	1.95	0.48
3:I:122:ARG:CD	3:I:177:SER:HB3	2.43	0.48
2:D:589:LYS:HG3	2:D:590:GLY:N	2.29	0.48
2:B:198:LEU:CD1	2:F:566:VAL:HB	2.44	0.48
2:D:100:LEU:HB3	2:D:165:VAL:CG1	2.44	0.48
2:B:644:VAL:HG22	2:D:186:GLU:CG	2.35	0.48
3:H:143:ARG:HH11	3:H:143:ARG:CG	2.24	0.48
2:B:290:MET:HE1	1:C:32:PRO:HB2	1.95	0.48
2:B:314:ILE:HD11	2:B:541:ASP:HB2	1.96	0.48
2:D:410:PHE:HB2	2:D:467:TYR:CE1	2.47	0.48
2:F:566:VAL:CG2	2:F:567:PRO:HD3	2.43	0.48
3:I:113:VAL:CG1	3:I:128:LEU:HD11	2.43	0.48
2:B:157:ASN:O	2:F:136:LYS:NZ	2.38	0.48
2:D:250:MET:HA	2:D:257:VAL:HG22	1.96	0.48
2:D:300:ILE:O	2:D:515:PRO:HG2	2.13	0.48
3:G:354:TYR:N	3:G:354:TYR:CD1	2.81	0.48
2:D:275:SER:C	2:D:651:LEU:HD11	2.39	0.48
2:D:433:GLU:CG	2:D:434:ASP:H	2.27	0.48
2:D:453:GLU:OE1	3:I:63:ARG:NH2	2.42	0.48
3:I:354:TYR:CD1	3:I:354:TYR:N	2.82	0.48
2:F:123:GLU:HG3	2:F:238:VAL:CG1	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:648:VAL:CG2	2:F:649:SER:N	2.77	0.47
2:B:589:LYS:HG3	2:B:590:GLY:N	2.28	0.47
3:G:71:HIS:NE2	3:G:73:CYS:HB2	2.29	0.47
2:B:250:MET:HB2	2:B:257:VAL:HG22	1.96	0.47
2:B:371:ASP:O	2:B:372:GLN:CB	2.62	0.47
3:H:121:VAL:HG21	3:H:128:LEU:HD13	1.95	0.47
3:I:143:ARG:HH11	3:I:143:ARG:CG	2.26	0.47
3:I:268:MET:HE3	3:I:286:ILE:HG12	1.97	0.47
2:B:258:MET:SD	2:D:99:PRO:HG3	2.55	0.47
2:F:250:MET:HB2	2:F:257:VAL:HG22	1.96	0.47
2:F:589:LYS:HG3	2:F:590:GLY:N	2.29	0.47
3:G:99:MET:O	3:G:103:VAL:HG23	2.14	0.47
2:B:71:ILE:HD12	2:B:71:ILE:N	2.29	0.47
3:G:154:GLN:O	3:G:156:VAL:HG23	2.14	0.47
3:G:239:ARG:HD2	3:G:365:GLY:OXT	2.15	0.47
2:B:143:TYR:CE2	2:B:164:PRO:HG3	2.50	0.47
2:B:254:GLU:C	2:B:256:THR:N	2.73	0.47
2:B:566:VAL:CG2	2:B:567:PRO:HD3	2.45	0.47
3:I:136:VAL:O	3:I:143:ARG:HD3	2.14	0.47
2:B:58:THR:O	2:B:156:LEU:HD21	2.14	0.47
2:B:105:GLU:HG2	2:B:106:HIS:N	2.30	0.47
2:D:65:ARG:HH11	2:D:65:ARG:HB3	1.79	0.47
2:F:55:THR:C	2:F:57:VAL:H	2.22	0.47
2:F:300:ILE:O	2:F:515:PRO:HG2	2.14	0.47
3:H:0:ACE:O	3:H:1:MET:CB	2.63	0.47
3:H:225:TYR:O	3:H:228:LEU:HB3	2.15	0.47
2:D:213:GLN:OE1	2:D:675:PRO:HD2	2.15	0.47
2:F:336:MET:HE2	3:I:333:ILE:HD13	1.96	0.47
2:B:324:ARG:NH2	2:B:485:GLN:OE1	2.48	0.47
2:D:123:GLU:HG3	2:D:238:VAL:CG1	2.45	0.47
2:F:620:ASP:HB3	2:F:623:ASN:ND2	2.31	0.47
8:A:604:HOH:O	2:B:213:GLN:HG2	2.14	0.46
2:D:190:ILE:O	2:D:194:VAL:HG23	2.15	0.46
2:F:58:THR:O	2:F:156:LEU:HD21	2.15	0.46
3:I:99:MET:O	3:I:103:VAL:HG23	2.15	0.46
2:D:621:LYS:O	2:D:625:ILE:HG13	2.16	0.46
2:B:611:ILE:C	2:B:611:ILE:HD12	2.40	0.46
3:G:116:GLU:CD	3:G:116:GLU:H	2.24	0.46
3:H:292:LEU:O	3:H:295:VAL:HG22	2.15	0.46
3:I:292:LEU:O	3:I:295:VAL:HG22	2.15	0.46
2:B:610:ILE:HG13	2:B:611:ILE:HG23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:126:ASP:C	2:D:128:LEU:H	2.24	0.46
2:F:105:GLU:HG2	2:F:106:HIS:N	2.31	0.46
3:G:312:ARG:HD2	3:G:316:GLY:O	2.16	0.46
3:H:136:VAL:O	3:H:143:ARG:HD3	2.15	0.46
3:H:312:ARG:HD2	3:H:316:GLY:O	2.15	0.46
2:D:319:ALA:HB3	2:D:532:PRO:HG3	1.98	0.46
3:H:0:ACE:O	3:H:1:MET:HB3	2.15	0.46
2:B:55:THR:C	2:B:57:VAL:H	2.23	0.46
2:F:324:ARG:HD3	8:F:759:HOH:O	2.16	0.46
2:F:606:ASP:O	2:F:609:THR:HG23	2.15	0.46
3:G:225:TYR:O	3:G:228:LEU:HB3	2.15	0.46
2:D:126:ASP:C	2:D:128:LEU:N	2.74	0.46
2:D:143:TYR:CE2	2:D:164:PRO:HG3	2.50	0.46
2:F:433:GLU:CG	2:F:434:ASP:H	2.29	0.46
3:G:54:CYS:HA	3:G:77:ILE:HG12	1.98	0.46
2:B:71:ILE:HG21	2:B:142:THR:HG21	1.98	0.46
2:B:190:ILE:O	2:B:194:VAL:HG23	2.16	0.46
2:D:254:GLU:C	2:D:256:THR:N	2.74	0.46
2:F:340:THR:HG21	3:I:341:THR:HB	1.96	0.46
3:G:229:GLU:HG2	3:G:230:HIS:N	2.30	0.46
3:H:239:ARG:HD2	3:H:365:GLY:OXT	2.16	0.46
2:D:405:GLN:HB3	2:D:464:MET:HE3	1.98	0.46
2:F:212:MET:HE3	2:F:212:MET:O	2.15	0.46
3:G:1:MET:O	3:G:1:MET:HG2	2.16	0.46
3:I:229:GLU:HG2	3:I:230:HIS:N	2.31	0.46
2:D:566:VAL:CG2	2:D:567:PRO:HD3	2.45	0.46
3:G:231:ASP:HA	3:G:232:PRO:HD3	1.75	0.46
2:D:314:ILE:HD11	2:D:541:ASP:HB2	1.97	0.45
2:D:611:ILE:C	2:D:611:ILE:HD12	2.42	0.45
2:F:143:TYR:CE2	2:F:164:PRO:HG3	2.50	0.45
3:H:113:VAL:CG1	3:H:128:LEU:HD11	2.45	0.45
2:B:250:MET:HA	2:B:257:VAL:HG22	1.97	0.45
2:D:98:GLU:OE2	2:D:169:THR:HB	2.17	0.45
2:B:319:ALA:HB3	2:B:532:PRO:HG3	1.99	0.45
2:F:65:ARG:HH11	2:F:65:ARG:HB3	1.82	0.45
2:B:639:SER:O	2:B:640:LEU:C	2.59	0.45
2:D:55:THR:C	2:D:57:VAL:H	2.24	0.45
2:D:648:VAL:CG2	2:D:649:SER:N	2.80	0.45
2:F:71:ILE:HG21	2:F:142:THR:HG21	1.97	0.45
2:F:370:LEU:O	2:F:373:ILE:HG12	2.16	0.45
3:I:225:TYR:O	3:I:228:LEU:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:105:GLU:HG2	2:D:106:HIS:N	2.31	0.45
2:D:203:VAL:CG2	2:D:658:GLN:HA	2.46	0.45
3:G:133:TRP:HB2	3:G:220:VAL:HB	1.99	0.45
3:G:137:ASP:OD2	3:G:140:SER:HB3	2.16	0.45
2:B:140:LEU:HB3	2:B:170:ARG:HD3	1.97	0.45
2:F:131:LEU:O	2:F:131:LEU:HD23	2.16	0.45
2:F:250:MET:HA	2:F:257:VAL:HG22	1.99	0.45
3:I:133:TRP:HB2	3:I:220:VAL:HB	1.98	0.45
2:B:100:LEU:HB3	2:B:165:VAL:CG1	2.46	0.45
2:B:606:ASP:O	2:B:609:THR:HG23	2.17	0.45
2:D:51:ILE:HG22	2:D:62:ALA:O	2.17	0.45
1:E:21:LYS:HD3	2:F:207:GLU:OE1	2.17	0.45
2:F:190:ILE:O	2:F:194:VAL:HG23	2.17	0.45
2:F:324:ARG:NH2	2:F:485:GLN:OE1	2.49	0.45
2:B:405:GLN:HB3	2:B:464:MET:HE3	1.97	0.45
2:D:250:MET:HB2	2:D:257:VAL:HG22	1.98	0.45
2:D:610:ILE:HG13	2:D:611:ILE:HG23	1.98	0.45
3:G:292:LEU:O	3:G:295:VAL:HG22	2.17	0.45
2:B:201:THR:CG2	2:B:244:ASN:ND2	2.80	0.45
2:B:223:LEU:O	2:F:589:LYS:HE3	2.17	0.45
3:G:113:VAL:CG1	3:G:128:LEU:HD11	2.47	0.45
3:I:116:GLU:CD	3:I:116:GLU:H	2.24	0.45
3:I:312:ARG:HD2	3:I:316:GLY:O	2.16	0.45
2:B:51:ILE:HG22	2:B:62:ALA:O	2.17	0.45
2:D:639:SER:O	2:D:640:LEU:C	2.60	0.45
3:G:121:VAL:HG21	3:G:128:LEU:HD13	1.98	0.45
3:G:238:TYR:CE1	3:G:242:LEU:HD12	2.52	0.45
3:I:297:LYS:HB2	8:I:716:HOH:O	2.17	0.45
2:F:442:ILE:HG23	2:F:442:ILE:O	2.17	0.44
3:I:71:HIS:NE2	3:I:73:CYS:HB2	2.31	0.44
2:D:71:ILE:HD12	2:D:71:ILE:N	2.31	0.44
2:D:371:ASP:O	2:D:372:GLN:CB	2.64	0.44
2:F:98:GLU:OE2	2:F:169:THR:HB	2.17	0.44
2:F:405:GLN:HB3	2:F:464:MET:HE3	1.99	0.44
3:G:122:ARG:CD	3:G:177:SER:HB3	2.47	0.44
3:G:242:LEU:O	3:G:349:PHE:HB2	2.18	0.44
1:A:18:ASN:CB	2:B:212:MET:HG2	2.45	0.44
2:B:212:MET:HE3	2:B:212:MET:O	2.17	0.44
2:F:254:GLU:C	2:F:256:THR:N	2.74	0.44
2:B:211:PRO:O	2:B:214:SER:N	2.50	0.44
2:B:620:ASP:HB3	2:B:623:ASN:ND2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:606:ASP:O	2:D:609:THR:HG23	2.18	0.44
3:G:315:LEU:N	3:G:315:LEU:HD22	2.32	0.44
2:B:621:LYS:O	2:B:625:ILE:HG13	2.17	0.44
2:D:201:THR:CG2	2:D:244:ASN:ND2	2.80	0.44
3:H:26:TYR:CD2	3:H:26:TYR:C	2.95	0.44
3:H:54:CYS:HA	3:H:77:ILE:HG12	1.99	0.44
3:H:224:ASP:HB2	3:H:357:MET:CG	2.47	0.44
3:I:154:GLN:O	3:I:156:VAL:HG23	2.17	0.44
2:B:47:PRO:HB2	2:B:66:MET:HB3	1.99	0.44
2:B:370:LEU:O	2:B:373:ILE:HG12	2.18	0.44
2:D:324:ARG:NH2	2:D:485:GLN:OE1	2.51	0.44
1:E:19:VAL:HB	2:F:248:GLN:HB2	1.99	0.44
3:I:54:CYS:HA	3:I:77:ILE:HG12	1.99	0.44
2:D:195:ALA:HB2	2:D:229:ILE:CD1	2.48	0.44
2:D:499:SER:HA	2:F:601:GLN:HB3	1.99	0.44
2:F:126:ASP:C	2:F:128:LEU:N	2.75	0.44
2:D:136:LYS:NZ	2:F:157:ASN:O	2.46	0.44
2:F:100:LEU:HB3	2:F:165:VAL:CG1	2.48	0.44
2:F:126:ASP:C	2:F:128:LEU:H	2.25	0.44
3:H:268:MET:HE3	3:H:286:ILE:HG12	1.99	0.44
3:H:354:TYR:N	3:H:354:TYR:CD1	2.85	0.44
2:B:126:ASP:C	2:B:128:LEU:N	2.75	0.43
2:D:620:ASP:HB3	2:D:623:ASN:ND2	2.32	0.43
2:F:47:PRO:HB2	2:F:66:MET:HB3	1.99	0.43
3:G:354:TYR:HB3	3:G:355:PRO:HD2	1.99	0.43
3:H:133:TRP:HB2	3:H:220:VAL:HB	1.99	0.43
2:B:107:ALA:O	2:B:111:PHE:HD1	2.02	0.43
1:C:10:THR:O	2:D:252:VAL:HG23	2.18	0.43
3:G:268:MET:HE3	3:G:286:ILE:HG12	1.99	0.43
3:H:71:HIS:NE2	3:H:73:CYS:HB2	2.32	0.43
2:D:566:VAL:N	2:D:567:PRO:CD	2.82	0.43
2:D:615:ALA:O	2:D:616:PRO:C	2.62	0.43
1:E:18:ASN:CB	2:F:212:MET:HG2	2.46	0.43
2:F:648:VAL:HG23	2:F:649:SER:N	2.33	0.43
3:H:249:PHE:CD2	3:H:259:ARG:HG2	2.53	0.43
3:I:26:TYR:CD2	3:I:26:TYR:C	2.97	0.43
2:B:203:VAL:CG2	2:B:658:GLN:HA	2.48	0.43
2:B:392:TRP:CE3	2:B:483:MET:HB2	2.54	0.43
2:D:172:THR:HG22	2:D:176:ASP:OD2	2.18	0.43
2:D:370:LEU:O	2:D:373:ILE:HG12	2.18	0.43
3:H:354:TYR:HB3	3:H:355:PRO:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:65:ARG:HH11	2:B:65:ARG:HB3	1.83	0.43
2:B:198:LEU:HD12	2:F:566:VAL:HB	2.01	0.43
2:B:452:TYR:HE1	2:B:457:LEU:HD12	1.84	0.43
2:F:203:VAL:CG2	2:F:658:GLN:HA	2.49	0.43
1:A:19:VAL:HB	2:B:248:GLN:HB2	2.00	0.43
2:B:300:ILE:O	2:B:515:PRO:HG2	2.18	0.43
1:C:18:ASN:CB	2:D:212:MET:HG2	2.44	0.43
2:D:107:ALA:O	2:D:111:PHE:HD1	2.00	0.43
2:F:361:LEU:HD21	2:F:469:LEU:HD22	2.00	0.43
2:F:566:VAL:HG23	2:F:567:PRO:HD3	1.99	0.43
3:I:113:VAL:HG21	3:I:128:LEU:HG	2.00	0.43
1:A:28:SER:O	1:A:29:THR:HG23	2.19	0.43
2:B:98:GLU:OE2	2:B:169:THR:HB	2.18	0.43
2:B:131:LEU:HD23	2:B:131:LEU:O	2.17	0.43
2:F:639:SER:O	2:F:640:LEU:C	2.60	0.43
3:I:227:GLU:HG3	3:I:354:TYR:CD2	2.53	0.43
3:I:315:LEU:N	3:I:315:LEU:HD22	2.34	0.43
2:B:615:ALA:O	2:B:619:SER:HB2	2.19	0.43
2:D:153:ARG:HH11	2:D:153:ARG:CB	2.12	0.43
2:D:361:LEU:HD21	2:D:469:LEU:HD22	1.99	0.43
2:F:361:LEU:HD22	2:F:365:THR:HG21	2.00	0.43
3:H:197:LEU:HD13	3:H:201:ALA:O	2.18	0.43
3:I:133:TRP:HA	3:I:136:VAL:HG23	1.99	0.43
3:I:354:TYR:HB3	3:I:355:PRO:HD2	2.01	0.43
2:B:126:ASP:C	2:B:128:LEU:H	2.26	0.43
2:F:392:TRP:CE3	2:F:483:MET:HB2	2.54	0.43
3:G:100:LEU:HD22	3:G:159:LEU:HD12	2.00	0.43
3:H:238:TYR:CE1	3:H:242:LEU:HD12	2.53	0.43
3:I:0:ACE:O	3:I:1:MET:CB	2.67	0.43
2:B:361:LEU:HD21	2:B:469:LEU:HD22	2.01	0.42
2:D:271:ALA:HA	2:D:272:PRO:HD3	1.86	0.42
2:D:566:VAL:HB	2:F:198:LEU:CD1	2.49	0.42
3:G:224:ASP:HB2	3:G:357:MET:CG	2.49	0.42
3:G:295:VAL:O	3:G:299:VAL:HG23	2.19	0.42
3:H:100:LEU:HD22	3:H:159:LEU:HD12	2.00	0.42
3:H:295:VAL:O	3:H:299:VAL:HG23	2.19	0.42
2:B:112:THR:HG22	2:B:116:MET:HE2	2.02	0.42
2:F:611:ILE:HD12	2:F:611:ILE:C	2.44	0.42
3:G:194:GLY:O	3:G:195:VAL:C	2.62	0.42
3:G:197:LEU:HD13	3:G:201:ALA:O	2.19	0.42
3:I:109:MET:HE1	3:I:130:GLU:C	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:408:ILE:HD12	2:B:418:GLN:HB3	2.00	0.42
2:B:566:VAL:N	2:B:567:PRO:CD	2.82	0.42
2:D:71:ILE:HG21	2:D:142:THR:HG21	2.01	0.42
1:E:22:PRO:HD2	2:F:208:VAL:HG23	2.02	0.42
2:F:371:ASP:O	2:F:372:GLN:CB	2.64	0.42
2:F:459:LYS:HA	2:F:466:TYR:OH	2.19	0.42
3:G:113:VAL:HG21	3:G:128:LEU:HG	2.02	0.42
3:H:1:MET:O	3:H:1:MET:HG2	2.19	0.42
3:I:26:TYR:CD2	3:I:42:MET:HE2	2.53	0.42
1:A:32:PRO:HB2	2:F:290:MET:HE1	2.01	0.42
2:D:615:ALA:O	2:D:619:SER:HB2	2.19	0.42
3:G:227:GLU:HG3	3:G:354:TYR:CD2	2.54	0.42
3:G:227:GLU:HG3	3:G:354:TYR:HD2	1.85	0.42
3:H:113:VAL:HG21	3:H:128:LEU:HG	2.01	0.42
3:H:331:ALA:HB3	3:H:332:PRO:HD3	2.01	0.42
3:I:121:VAL:HG21	3:I:128:LEU:HD13	2.01	0.42
3:I:227:GLU:HG3	3:I:354:TYR:HD2	1.85	0.42
2:D:47:PRO:HB2	2:D:66:MET:HB3	2.00	0.42
1:E:28:SER:O	1:E:29:THR:HG23	2.18	0.42
2:F:253:SER:HB3	2:F:254:GLU:OE2	2.19	0.42
3:G:106:MET:HE2	3:G:183:PHE:CE2	2.55	0.42
2:F:46:VAL:HA	2:F:47:PRO:HD3	1.90	0.42
2:F:205:ILE:O	2:F:658:GLN:HG3	2.19	0.42
2:F:566:VAL:N	2:F:567:PRO:CD	2.83	0.42
2:F:621:LYS:O	2:F:625:ILE:HG13	2.19	0.42
3:I:238:TYR:CE1	3:I:242:LEU:HD12	2.53	0.42
2:B:46:VAL:HG13	2:B:47:PRO:HD2	2.01	0.42
3:H:315:LEU:HD22	3:H:315:LEU:N	2.34	0.42
3:G:170:LEU:HA	3:G:173:MET:HE3	2.02	0.42
3:G:263:PRO:HG3	3:G:269:PRO:HG3	2.02	0.42
2:B:46:VAL:HG13	2:B:47:PRO:CD	2.50	0.42
2:B:201:THR:CG2	2:B:201:THR:O	2.68	0.42
2:F:497:PRO:HG3	2:F:532:PRO:HB2	2.01	0.42
2:F:672:PHE:N	2:F:673:PRO:HD3	2.34	0.42
3:G:26:TYR:CD2	3:G:26:TYR:C	2.96	0.42
1:C:19:VAL:HB	2:D:248:GLN:HB2	2.02	0.42
2:D:581:TYR:O	3:H:70:HIS:HA	2.19	0.42
2:F:201:THR:CG2	2:F:244:ASN:ND2	2.83	0.42
2:F:615:ALA:O	2:F:616:PRO:C	2.63	0.41
2:F:615:ALA:O	2:F:619:SER:HB2	2.20	0.41
3:I:224:ASP:HB2	3:I:357:MET:CG	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:PHE:HB3	2:B:210:CYS:O	2.19	0.41
2:B:195:ALA:HB2	2:B:229:ILE:CD1	2.49	0.41
2:B:197:THR:HB	2:F:567:PRO:HG3	2.02	0.41
1:C:21:LYS:HD3	2:D:207:GLU:OE1	2.20	0.41
2:F:143:TYR:N	2:F:143:TYR:CD1	2.88	0.41
2:F:271:ALA:HA	2:F:272:PRO:HD3	1.85	0.41
3:G:331:ALA:HB3	3:G:332:PRO:HD3	2.02	0.41
3:I:106:MET:HE2	3:I:183:PHE:CE2	2.55	0.41
1:A:21:LYS:HD3	2:B:207:GLU:OE1	2.20	0.41
2:B:153:ARG:HH11	2:B:153:ARG:CB	2.15	0.41
2:D:211:PRO:O	2:D:214:SER:N	2.53	0.41
2:F:284:LYS:O	2:F:288:GLN:HG3	2.21	0.41
3:H:26:TYR:CD2	3:H:42:MET:HE2	2.55	0.41
3:H:99:MET:HB2	3:H:282:MET:HE1	2.01	0.41
3:H:157:ASP:O	3:H:158:ASP:HB2	2.21	0.41
3:I:1:MET:O	3:I:1:MET:HG2	2.20	0.41
1:A:35:SER:O	2:B:106:HIS:HE1	2.02	0.41
1:C:20:PHE:HB3	2:D:210:CYS:O	2.21	0.41
2:D:212:MET:HE3	2:D:212:MET:O	2.20	0.41
2:F:620:ASP:OD2	3:I:1:MET:HA	2.21	0.41
3:I:100:LEU:HD22	3:I:159:LEU:HD12	2.01	0.41
3:I:197:LEU:HD13	3:I:201:ALA:O	2.19	0.41
2:D:203:VAL:HA	2:D:204:PRO:HD3	1.88	0.41
2:D:566:VAL:HG23	2:D:567:PRO:HD3	2.02	0.41
2:F:165:VAL:HG12	2:F:166:ILE:N	2.36	0.41
2:F:587:ASN:HA	2:F:588:PRO:HD3	1.89	0.41
3:H:154:GLN:O	3:H:156:VAL:HG23	2.20	0.41
3:H:263:PRO:HG3	3:H:269:PRO:HG3	2.02	0.41
3:I:0:ACE:O	3:I:1:MET:HB3	2.20	0.41
3:H:116:GLU:H	3:H:116:GLU:CD	2.27	0.41
3:I:249:PHE:CD2	3:I:259:ARG:HG2	2.56	0.41
2:B:230:ARG:HH11	2:B:230:ARG:HG2	1.86	0.41
2:F:123:GLU:HG3	2:F:238:VAL:HB	2.03	0.41
2:B:131:LEU:HD21	2:B:135:PRO:CD	2.44	0.41
2:B:615:ALA:O	2:B:616:PRO:C	2.63	0.41
2:B:672:PHE:N	2:B:673:PRO:HD3	2.35	0.41
2:D:46:VAL:HG13	2:D:47:PRO:HD2	2.02	0.41
2:D:290:MET:HE1	1:E:32:PRO:HB2	2.02	0.41
2:D:497:PRO:HG3	2:D:532:PRO:HB2	2.03	0.41
2:F:452:TYR:HE1	2:F:457:LEU:HD12	1.86	0.41
3:G:0:ACE:O	3:G:1:MET:CB	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:26:TYR:CD2	3:G:42:MET:HE2	2.56	0.41
3:H:227:GLU:HG3	3:H:354:TYR:CD2	2.56	0.41
2:B:254:GLU:C	2:B:256:THR:H	2.28	0.41
2:B:497:PRO:HG3	2:B:532:PRO:HB2	2.03	0.41
1:C:35:SER:H	2:D:110:ASN:ND2	2.18	0.41
2:D:361:LEU:HD22	2:D:365:THR:HG21	2.03	0.41
1:E:20:PHE:HB3	2:F:210:CYS:O	2.21	0.41
2:F:195:ALA:HB2	2:F:229:ILE:CD1	2.51	0.41
3:H:194:GLY:O	3:H:195:VAL:C	2.64	0.41
3:H:227:GLU:HG3	3:H:354:TYR:HD2	1.86	0.41
1:A:13:VAL:HG11	5:B:709:BOG:H5'1	2.03	0.40
2:B:143:TYR:CD1	2:B:143:TYR:N	2.89	0.40
2:B:648:VAL:CG2	2:B:649:SER:N	2.83	0.40
2:D:198:LEU:HD12	2:D:198:LEU:HA	1.88	0.40
2:F:46:VAL:HG13	2:F:47:PRO:HD2	2.04	0.40
3:G:110:MET:O	3:G:110:MET:HE3	2.21	0.40
3:G:127:SER:HA	3:G:364:LEU:HB3	2.02	0.40
3:G:298:LEU:O	3:G:302:VAL:HG23	2.21	0.40
3:I:303:ASN:HD22	3:I:311:ILE:HD13	1.87	0.40
2:D:112:THR:HG22	2:D:116:MET:HE2	2.03	0.40
2:D:583:VAL:HG21	3:H:67:HIS:HB3	2.03	0.40
2:D:648:VAL:HG23	2:D:649:SER:N	2.35	0.40
2:F:107:ALA:O	2:F:111:PHE:HD1	2.03	0.40
2:B:286:THR:O	2:B:290:MET:HG3	2.22	0.40
1:E:35:SER:O	2:F:106:HIS:HE1	2.04	0.40
2:F:368:VAL:HB	2:F:468:LEU:HB3	2.02	0.40
3:I:303:ASN:HD22	3:I:303:ASN:HA	1.69	0.40
3:I:331:ALA:HB3	3:I:332:PRO:HD3	2.03	0.40
2:B:212:MET:HE2	2:B:216:VAL:CG2	2.49	0.40
2:B:566:VAL:HG23	2:B:567:PRO:HD3	2.03	0.40
2:F:114:ALA:O	2:F:117:ALA:HB3	2.21	0.40
3:H:127:SER:HA	3:H:364:LEU:HB3	2.03	0.40
3:I:94:HIS:CE1	3:I:153:LEU:HD23	2.56	0.40
3:I:127:SER:HA	3:I:364:LEU:HB3	2.03	0.40
2:B:459:LYS:HA	2:B:466:TYR:OH	2.21	0.40
2:D:46:VAL:HG13	2:D:47:PRO:CD	2.52	0.40
2:D:236:ALA:O	2:D:240:LEU:HG	2.22	0.40
2:D:254:GLU:O	2:D:256:THR:N	2.55	0.40
2:D:392:TRP:CE3	2:D:483:MET:HB2	2.57	0.40
2:F:211:PRO:O	2:F:214:SER:N	2.53	0.40
3:G:143:ARG:CG	3:G:143:ARG:NH1	2.81	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:157:ASP:O	3:G:158:ASP:HB2	2.22	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	31/41 (76%)	28 (90%)	3 (10%)	0	100	100
1	C	31/41 (76%)	28 (90%)	3 (10%)	0	100	100
1	E	31/41 (76%)	27 (87%)	4 (13%)	0	100	100
2	B	604/666 (91%)	560 (93%)	38 (6%)	6 (1%)	12	38
2	D	604/666 (91%)	561 (93%)	37 (6%)	6 (1%)	12	38
2	F	604/666 (91%)	561 (93%)	36 (6%)	7 (1%)	10	34
3	G	364/366 (100%)	336 (92%)	25 (7%)	3 (1%)	16	44
3	H	364/366 (100%)	336 (92%)	25 (7%)	3 (1%)	16	44
3	I	364/366 (100%)	336 (92%)	26 (7%)	2 (0%)	24	55
All	All	2997/3219 (93%)	2773 (92%)	197 (7%)	27 (1%)	14	41

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	616	PRO
2	D	616	PRO
2	F	616	PRO
3	G	1	MET
3	H	1	MET
3	I	1	MET
2	B	135	PRO

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Mol	Chain	Res	Type
2	D	135	PRO
2	D	136	LYS
2	F	135	PRO
2	B	136	LYS
2	D	52	GLY
2	F	52	GLY
2	F	136	LYS
2	B	52	GLY
2	D	186	GLU
2	D	323	VAL
2	B	186	GLU
2	B	323	VAL
2	F	186	GLU
2	F	352	ASN
2	F	323	VAL
3	G	263	PRO
3	H	263	PRO
3	I	263	PRO
3	G	194	GLY
3	H	194	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	A	28/34 (82%)	28 (100%)	0	100	100
1	C	28/34 (82%)	28 (100%)	0	100	100
1	E	28/34 (82%)	28 (100%)	0	100	100
2	B	513/561 (91%)	498 (97%)	15 (3%)	37	73
2	D	513/561 (91%)	498 (97%)	15 (3%)	37	73
2	F	513/561 (91%)	498 (97%)	15 (3%)	37	73
3	G	317/317 (100%)	311 (98%)	6 (2%)	50	81
3	H	317/317 (100%)	312 (98%)	5 (2%)	55	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	I	317/317 (100%)	311 (98%)	6 (2%)	50 81
All	All	2574/2736 (94%)	2512 (98%)	62 (2%)	43 77

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	57	VAL
2	B	105	GLU
2	B	123	GLU
2	B	135	PRO
2	B	173	MET
2	B	201	THR
2	B	262	VAL
2	B	284	LYS
2	B	324	ARG
2	B	438	THR
2	B	455	GLU
2	B	616	PRO
2	B	645	LYS
2	B	648	VAL
2	B	658	GLN
2	D	57	VAL
2	D	105	GLU
2	D	123	GLU
2	D	135	PRO
2	D	173	MET
2	D	201	THR
2	D	262	VAL
2	D	284	LYS
2	D	324	ARG
2	D	438	THR
2	D	455	GLU
2	D	616	PRO
2	D	645	LYS
2	D	648	VAL
2	D	658	GLN
2	F	57	VAL
2	F	105	GLU
2	F	123	GLU
2	F	135	PRO
2	F	173	MET
2	F	201	THR

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Mol	Chain	Res	Type
2	F	262	VAL
2	F	284	LYS
2	F	324	ARG
2	F	438	THR
2	F	455	GLU
2	F	616	PRO
2	F	645	LYS
2	F	648	VAL
2	F	658	GLN
3	G	112	ASP
3	G	143	ARG
3	G	175	ASP
3	G	217	GLU
3	G	229	GLU
3	G	345	ASP
3	H	143	ARG
3	H	175	ASP
3	H	217	GLU
3	H	229	GLU
3	H	345	ASP
3	I	112	ASP
3	I	143	ARG
3	I	175	ASP
3	I	217	GLU
3	I	229	GLU
3	I	345	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	106	HIS
2	B	110	ASN
2	B	171	GLN
2	B	248	GLN
2	B	346	GLN
2	B	358	HIS
2	B	369	ASN
2	B	528	ASN
2	B	571	GLN
2	B	658	GLN
2	D	106	HIS
2	D	110	ASN

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Mol	Chain	Res	Type
2	D	248	GLN
2	D	346	GLN
2	D	358	HIS
2	D	369	ASN
2	D	465	ASN
2	D	528	ASN
2	D	569	GLN
2	D	571	GLN
2	D	658	GLN
2	F	106	HIS
2	F	110	ASN
2	F	248	GLN
2	F	346	GLN
2	F	358	HIS
2	F	369	ASN
2	F	571	GLN
2	F	658	GLN
3	G	7	ASN
3	G	70	HIS
3	G	105	GLN
3	G	111	ASN
3	G	132	ASN
3	G	154	GLN
3	G	171	ASN
3	G	303	ASN
3	G	329	GLN
3	H	7	ASN
3	H	111	ASN
3	H	132	ASN
3	H	154	GLN
3	H	171	ASN
3	H	329	GLN
3	I	7	ASN
3	I	111	ASN
3	I	132	ASN
3	I	154	GLN
3	I	171	ASN
3	I	256	HIS
3	I	303	ASN
3	I	329	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 for Mogul analysis.

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	SO4	G	504	-	4,4,4	0.63	0	6,6,6	0.13	0
5	BOG	F	709	-	20,20,20	1.48	5 (25%)	25,25,25	0.69	0
6	SO4	B	710	-	4,4,4	0.50	0	6,6,6	0.18	0
6	SO4	D	710	-	4,4,4	0.53	0	6,6,6	0.10	0
6	SO4	I	509	-	4,4,4	0.64	0	6,6,6	0.11	0
6	SO4	H	508	-	4,4,4	0.67	0	6,6,6	0.14	0
5	BOG	D	709	-	20,20,20	1.40	4 (20%)	25,25,25	0.68	0
6	SO4	G	507	-	4,4,4	0.64	0	6,6,6	0.12	0
6	SO4	H	505	-	4,4,4	0.72	0	6,6,6	0.12	0
5	BOG	B	709	-	20,20,20	1.42	3 (15%)	25,25,25	0.70	0
6	SO4	F	710	-	4,4,4	0.51	0	6,6,6	0.14	0
6	SO4	I	506	-	4,4,4	0.71	0	6,6,6	0.11	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
5	BOG	B	709	-	-	2/11/31/31	0/1/1/1
5	BOG	D	709	-	-	2/11/31/31	0/1/1/1
5	BOG	F	709	-	-	2/11/31/31	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	709	BOG	O5-C1	3.37	1.50	1.41
5	D	709	BOG	O5-C1	3.36	1.50	1.41
5	B	709	BOG	O5-C1	3.16	1.50	1.41
5	B	709	BOG	O1-C1	3.04	1.45	1.40
5	F	709	BOG	C4-C5	2.89	1.59	1.53
5	D	709	BOG	O1-C1	2.72	1.44	1.40
5	F	709	BOG	O1-C1	2.70	1.44	1.40
5	D	709	BOG	C4-C5	2.58	1.58	1.53
5	B	709	BOG	C4-C5	2.54	1.58	1.53
5	F	709	BOG	C4-C3	2.17	1.58	1.52
5	F	709	BOG	C1-C2	2.11	1.58	1.52
5	D	709	BOG	C4-C3	2.01	1.57	1.52

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	709	BOG	O1-C1'-C2'-C3'
5	F	709	BOG	O1-C1'-C2'-C3'
5	F	709	BOG	C3'-C4'-C5'-C6'
5	D	709	BOG	O1-C1'-C2'-C3'
5	D	709	BOG	C3'-C4'-C5'-C6'
5	B	709	BOG	C3'-C4'-C5'-C6'

There are no ring outliers.

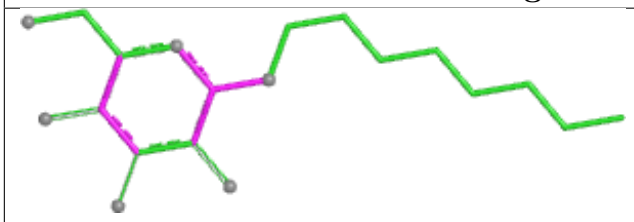
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	709	BOG	1	0
5	D	709	BOG	1	0
5	B	709	BOG	2	0

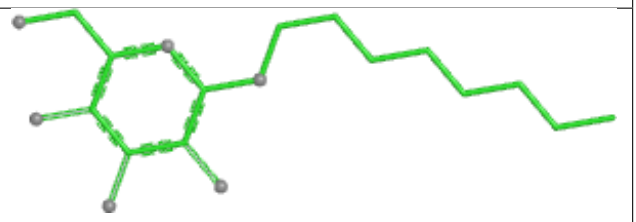
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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.

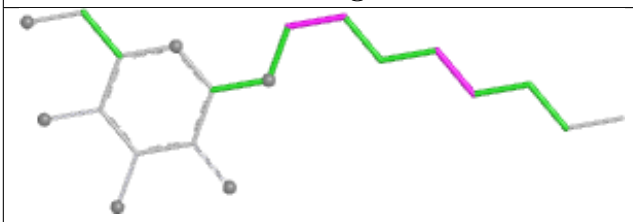
Ligand BOG F 709



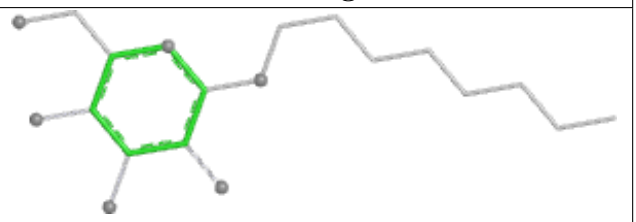
Bond lengths



Bond angles

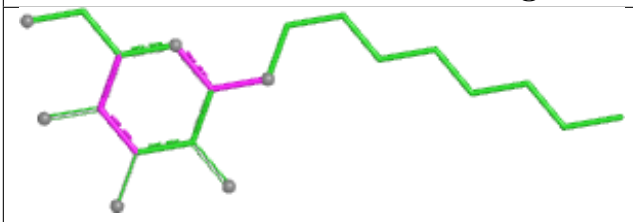


Torsions

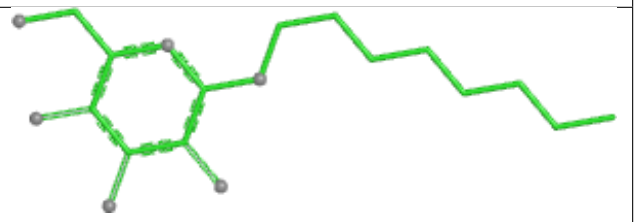


Rings

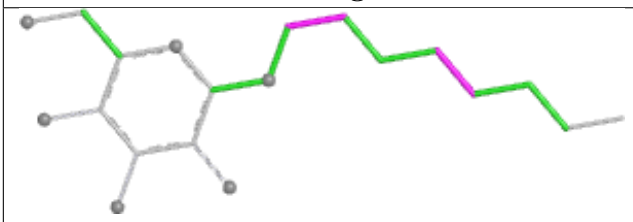
Ligand BOG D 709



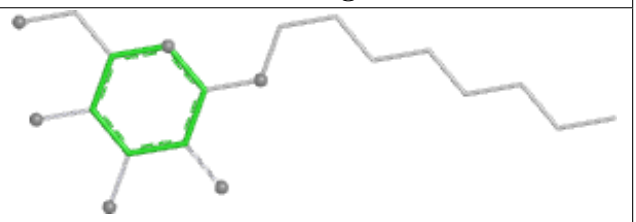
Bond lengths



Bond angles

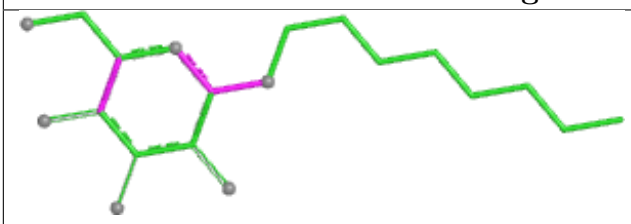


Torsions

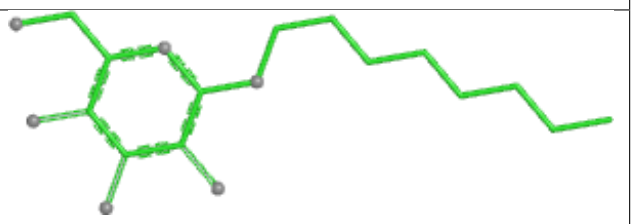


Rings

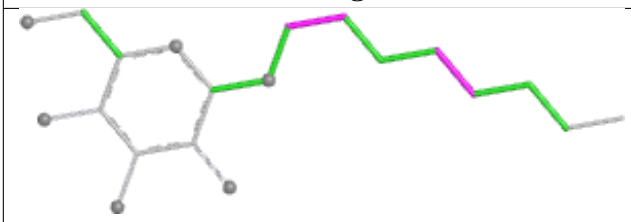
Ligand BOG B 709



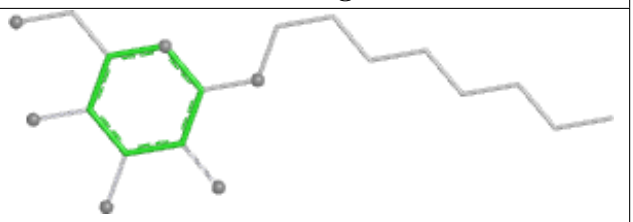
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	33/41 (80%)	0.47	0 100 100	51, 59, 71, 73	0
1	C	33/41 (80%)	0.29	0 100 100	52, 58, 70, 72	0
1	E	33/41 (80%)	0.28	0 100 100	53, 60, 70, 73	0
2	B	608/666 (91%)	0.11	15 (2%) 58 48	32, 50, 87, 126	0
2	D	608/666 (91%)	0.13	28 (4%) 37 29	32, 50, 87, 125	0
2	F	608/666 (91%)	0.10	13 (2%) 63 54	33, 50, 87, 125	0
3	G	365/366 (99%)	0.09	3 (0%) 82 75	34, 52, 84, 115	0
3	H	365/366 (99%)	0.18	4 (1%) 78 70	34, 52, 84, 114	0
3	I	365/366 (99%)	0.13	4 (1%) 78 70	36, 53, 84, 115	0
All	All	3018/3219 (93%)	0.13	67 (2%) 62 52	32, 51, 86, 126	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	131	LEU	4.6
2	D	133	VAL	4.3
2	B	439	ALA	4.3
2	D	43	PRO	4.2
2	B	133	VAL	4.1
2	B	43	PRO	3.8
2	F	133	VAL	3.6
2	D	55	THR	3.5
2	D	58	THR	3.4
2	F	51	ILE	3.4
2	B	71	ILE	3.4
2	D	130	VAL	3.3
2	D	455	GLU	3.2
2	D	51	ILE	3.1
2	D	56	SER	3.1

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Mol	Chain	Res	Type	RSRZ
2	B	440	GLN	3.0
2	D	458	ASN	3.0
3	G	145	ILE	2.9
3	I	203	GLN	2.9
2	D	460	THR	2.9
2	F	58	THR	2.9
3	I	200	ASP	2.8
2	D	131	LEU	2.8
2	D	437	PHE	2.8
2	F	455	GLU	2.8
2	F	71	ILE	2.8
2	F	45	GLY	2.8
3	I	134	LEU	2.7
2	B	131	LEU	2.7
2	B	130	VAL	2.7
3	H	214	SER	2.6
2	F	43	PRO	2.6
2	F	460	THR	2.6
3	I	304	HIS	2.5
2	D	50	ALA	2.4
2	B	97	ASP	2.4
2	D	62	ALA	2.4
2	B	57	VAL	2.4
2	D	71	ILE	2.3
2	D	57	VAL	2.3
2	D	586	PHE	2.3
3	H	145	ILE	2.3
2	D	258	MET	2.3
2	D	254	GLU	2.3
3	H	256	HIS	2.3
2	D	97	ASP	2.2
2	B	52	GLY	2.2
2	B	134	SER	2.2
2	F	56	SER	2.2
3	G	365	GLY	2.2
2	B	173	MET	2.2
3	G	176	SER	2.2
3	H	230	HIS	2.1
2	D	462	PRO	2.1
2	F	130	VAL	2.1
2	D	49	ILE	2.1
2	F	132	SER	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	437	PHE	2.1
2	B	135	PRO	2.1
2	D	371	ASP	2.1
2	D	143	TYR	2.1
2	D	132	SER	2.0
2	D	134	SER	2.0
2	B	123	GLU	2.0
2	D	459	LYS	2.0
2	D	60	PRO	2.0
2	F	97	ASP	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 oligosaccharides 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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	SO4	I	506	5/5	0.77	0.24	114,114,114,114	0
5	BOG	F	709	20/20	0.80	0.21	70,91,94,95	0
6	SO4	I	509	5/5	0.82	0.15	101,101,102,102	0
5	BOG	B	709	20/20	0.83	0.19	70,91,94,94	0
6	SO4	G	504	5/5	0.83	0.13	112,112,112,112	0
6	SO4	H	508	5/5	0.84	0.21	100,101,101,102	0
6	SO4	G	507	5/5	0.84	0.14	100,101,101,101	0
6	SO4	H	505	5/5	0.84	0.14	114,114,114,115	0
6	SO4	B	710	5/5	0.86	0.11	69,69,70,71	0
5	BOG	D	709	20/20	0.90	0.15	68,89,92,93	0
6	SO4	D	710	5/5	0.90	0.09	69,69,70,70	0
4	CL	A	601	1/1	0.91	0.28	76,76,76,76	0
6	SO4	F	710	5/5	0.92	0.09	70,71,71,72	0

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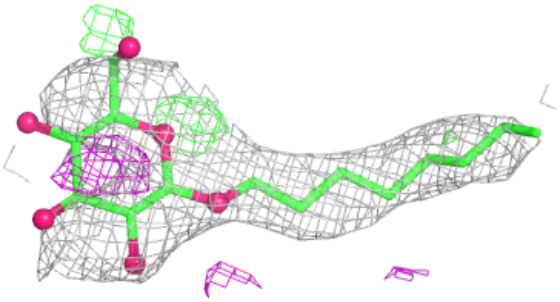
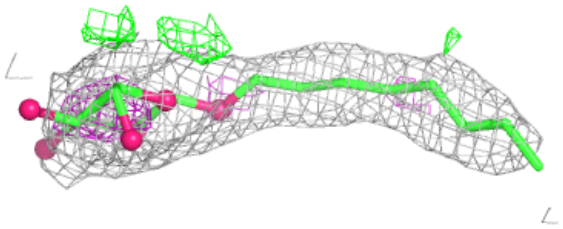
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	ZN	I	701	1/1	0.99	0.02	52,52,52,52	0
7	ZN	H	703	1/1	1.00	0.03	45,45,45,45	0
7	ZN	G	702	1/1	1.00	0.01	39,39,39,39	0

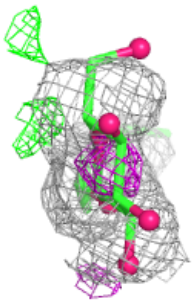
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around BOG F 709:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

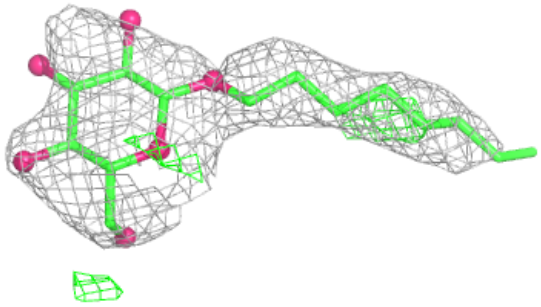


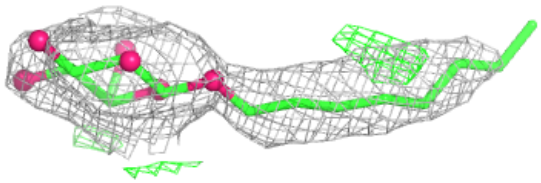


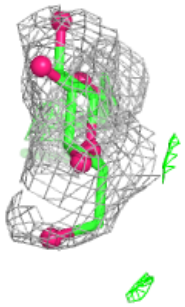


Electron density around BOG B 709:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

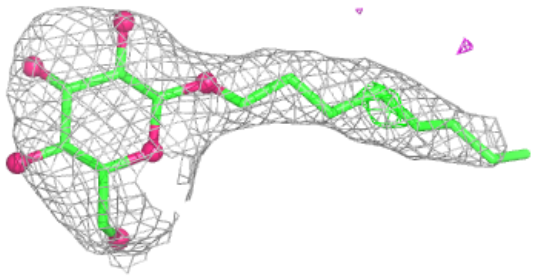


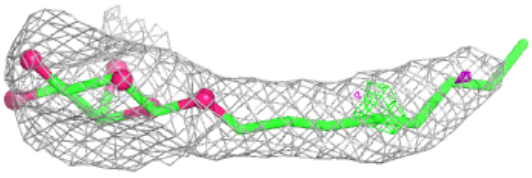


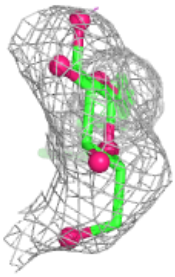


Electron density around BOG D 709:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.