



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:17 PM UTC

PDB ID : 1DCH / pdb_00001dch
Title : CRYSTAL STRUCTURE OF DCOH, A BIFUNCTIONAL, PROTEIN-BINDING TRANSCRIPTION COACTIVATOR
Authors : Endrizzi, J.A.; Cronk, J.D.; Wang, W.; Crabtree, G.R.; Alber, T.
Deposited on : 1995-01-24
Resolution : 3.00 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

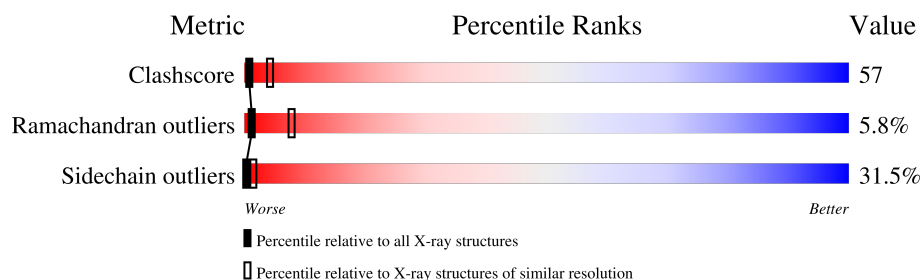
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	104	20% 37% 32% 7% 5%
1	B	104	19% 40% 28% 8% 5%
1	C	104	24% 38% 24% 9% 5%
1	D	104	18% 43% 27% 7% 5%
1	E	104	24% 37% 28% 7% 5%
1	F	104	19% 48% 19% 9% 5%
1	G	104	20% 44% 20% 11% 5%
1	H	104	22% 36% 28% 10% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	200	-	-	X	-
2	SO4	F	200	-	-	X	-
2	SO4	G	200	-	-	X	-

2 Entry composition

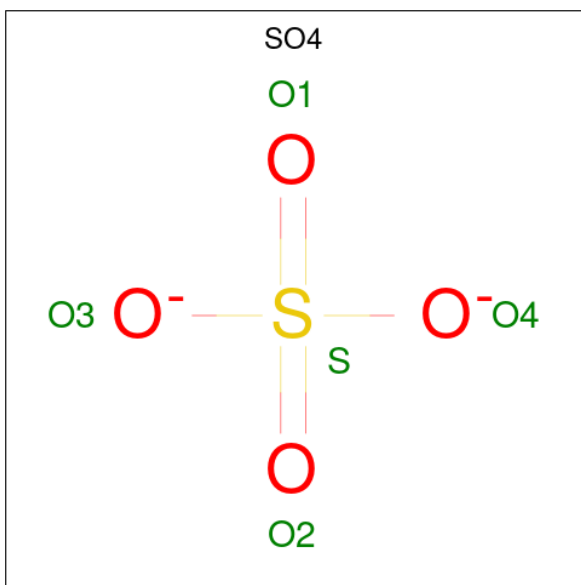
There are 2 unique types of molecules in this entry. The entry contains 6494 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 DCOH (DIMERIZATION COFACTOR OF HNF-1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	99	Total	C	N	O	S	0	0	0
			806	512	145	146	3			
1	B	99	Total	C	N	O	S	0	0	0
			806	512	145	146	3			
1	C	99	Total	C	N	O	S	0	0	0
			810	514	146	147	3			
1	D	99	Total	C	N	O	S	0	0	0
			803	511	146	143	3			
1	E	99	Total	C	N	O	S	0	0	0
			802	510	146	143	3			
1	F	99	Total	C	N	O	S	0	0	0
			807	513	146	145	3			
1	G	99	Total	C	N	O	S	0	0	0
			810	514	146	147	3			
1	H	99	Total	C	N	O	S	0	0	0
			810	514	146	147	3			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		

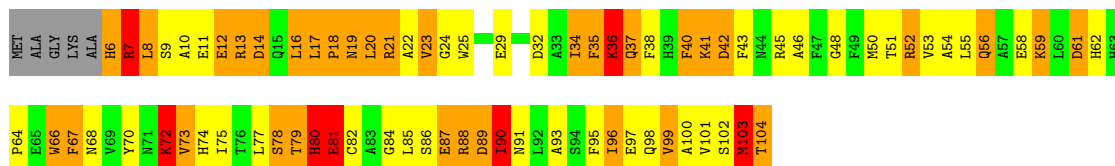
3 Residue-property plots

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.

Note EDS was not executed.

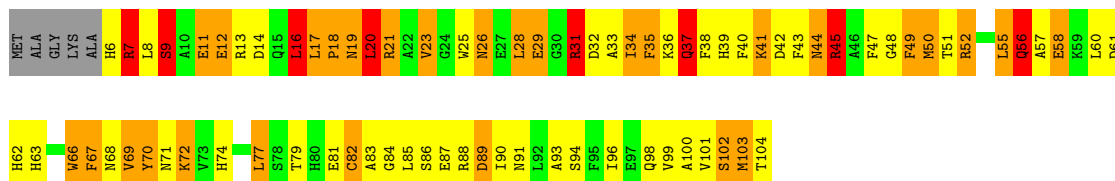
• Molecule 1: DCOH (DIMERIZATION COFACTOR OF HNF-1)

Chain A: 



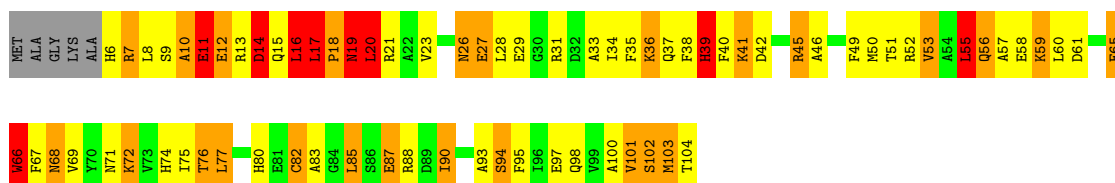
• Molecule 1: DCOH (DIMERIZATION COFACTOR OF HNF-1)

Chain B: 



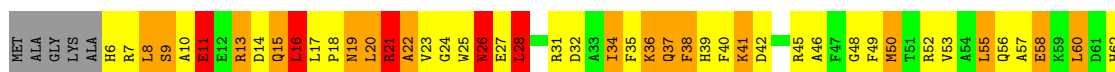
• Molecule 1: DCOH (DIMERIZATION COFACTOR OF HNF-1)

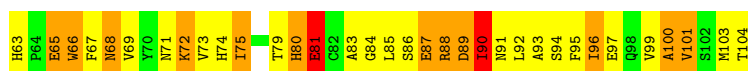
Chain C: 



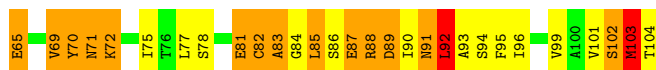
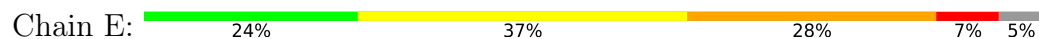
• Molecule 1: DCOH (DIMERIZATION COFACTOR OF HNF-1)

Chain D: 

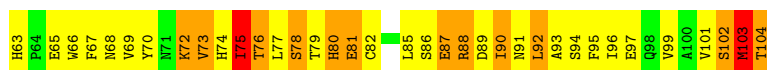
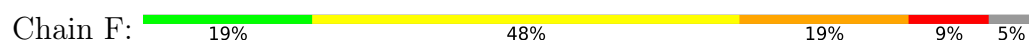




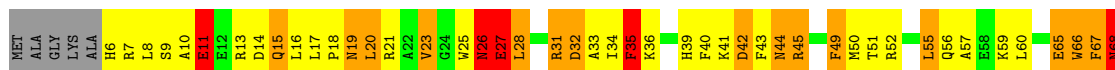
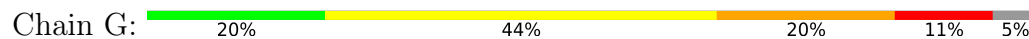
- Molecule 1: DCOH (DIMERIZATION COFACTOR OF HNF-1)



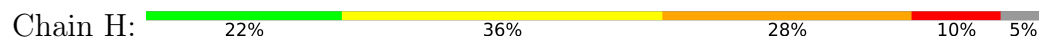
- Molecule 1: DCOH (DIMERIZATION COFACTOR OF HNF-1)



- Molecule 1: DCOH (DIMERIZATION COFACTOR OF HNF-1)



- Molecule 1: DCOH (DIMERIZATION COFACTOR OF HNF-1)



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	105.65Å 105.65Å 196.23Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	6.00 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-3.00)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.184 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6494	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	1.59	9/825 (1.1%)	1.99	30/1114 (2.7%)
1	B	1.54	4/825 (0.5%)	2.09	29/1114 (2.6%)
1	C	1.45	4/829 (0.5%)	2.12	26/1119 (2.3%)
1	D	1.50	5/822 (0.6%)	2.09	26/1110 (2.3%)
1	E	1.51	6/821 (0.7%)	2.06	23/1109 (2.1%)
1	F	1.50	3/826 (0.4%)	1.99	21/1115 (1.9%)
1	G	1.36	3/829 (0.4%)	2.11	30/1119 (2.7%)
1	H	1.54	9/829 (1.1%)	2.08	31/1119 (2.8%)
All	All	1.50	43/6606 (0.7%)	2.07	216/8919 (2.4%)

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	A	0	1
1	C	1	1
1	D	0	1
1	F	0	1
1	G	0	3
1	H	0	3
All	All	1	10

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	100	ALA	C-N	13.65	1.48	1.34
1	B	11	GLU	C-N	-9.39	1.22	1.33
1	E	70	TYR	CA-C	-6.87	1.47	1.52
1	H	34	ILE	CA-C	-6.84	1.44	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	11	GLU	CD-OE1	6.66	1.38	1.25
1	E	81	GLU	CD-OE1	6.60	1.37	1.25
1	H	27	GLU	CD-OE2	6.59	1.37	1.25
1	G	81	GLU	CD-OE1	6.48	1.37	1.25
1	A	12	GLU	CA-C	-6.22	1.45	1.52
1	A	21	ARG	NE-CZ	6.18	1.39	1.33
1	D	80	HIS	CG-ND1	6.13	1.45	1.38
1	H	14	ASP	N-CA	-6.08	1.38	1.46
1	C	87	GLU	CD-OE1	6.08	1.36	1.25
1	G	11	GLU	CD-OE1	6.07	1.36	1.25
1	B	87	GLU	CD-OE1	6.05	1.36	1.25
1	E	14	ASP	CA-C	6.03	1.60	1.52
1	H	81	GLU	CD-OE2	5.84	1.36	1.25
1	H	80	HIS	CG-ND1	5.79	1.44	1.38
1	F	74	HIS	CA-C	-5.78	1.45	1.52
1	A	11	GLU	CD-OE1	5.65	1.36	1.25
1	F	46	ALA	CA-C	-5.65	1.45	1.52
1	D	21	ARG	NE-CZ	5.64	1.39	1.33
1	H	12	GLU	CD-OE1	5.64	1.36	1.25
1	D	16	LEU	CA-C	5.60	1.59	1.52
1	A	14	ASP	CG-OD1	5.54	1.35	1.25
1	H	29	GLU	CD-OE2	5.51	1.35	1.25
1	E	71	ASN	N-CA	-5.49	1.39	1.46
1	E	52	ARG	CA-C	-5.30	1.46	1.52
1	B	12	GLU	CD-OE2	5.28	1.35	1.25
1	A	29	GLU	CD-OE2	5.24	1.35	1.25
1	A	80	HIS	CE1-NE2	5.23	1.37	1.32
1	F	80	HIS	CE1-NE2	5.22	1.37	1.32
1	E	13	ARG	N-CA	-5.22	1.39	1.46
1	G	27	GLU	CD-OE2	5.08	1.35	1.25
1	H	87	GLU	CD-OE2	5.06	1.34	1.25
1	A	67	PHE	CA-C	-5.06	1.46	1.52
1	A	81	GLU	CD-OE2	5.06	1.34	1.25
1	C	12	GLU	CD-OE2	5.05	1.34	1.25
1	H	11	GLU	CD-OE1	5.05	1.34	1.25
1	D	81	GLU	CD-OE1	5.04	1.34	1.25
1	B	14	ASP	CG-OD2	5.03	1.34	1.25
1	C	66	TRP	CA-C	-5.01	1.46	1.52
1	D	80	HIS	CE1-NE2	5.01	1.37	1.32

All (216) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	69	VAL	CA-C-N	-15.02	102.98	121.90
1	E	69	VAL	C-N-CA	-15.02	102.98	121.90
1	C	19	ASN	CA-CB-CG	-10.96	101.64	112.60
1	G	68	ASN	CA-CB-CG	10.79	123.39	112.60
1	D	89	ASP	CA-CB-CG	-10.34	102.26	112.60
1	A	100	ALA	CA-C-N	-9.91	105.44	121.19
1	A	100	ALA	C-N-CA	-9.91	105.44	121.19
1	H	69	VAL	CA-C-N	-9.64	104.48	122.60
1	H	69	VAL	C-N-CA	-9.64	104.48	122.60
1	B	14	ASP	N-CA-CB	9.58	124.43	110.06
1	F	19	ASN	N-CA-CB	9.57	124.33	110.16
1	F	11	GLU	N-CA-CB	9.07	123.22	110.07
1	D	26	ASN	CA-CB-CG	-8.66	103.94	112.60
1	G	57	ALA	N-CA-C	-8.63	101.84	111.07
1	G	35	PHE	CA-CB-CG	-8.44	105.36	113.80
1	H	54	ALA	CA-C-N	8.39	131.87	120.54
1	H	54	ALA	C-N-CA	8.39	131.87	120.54
1	H	69	VAL	N-CA-CB	8.35	125.00	111.23
1	H	23	VAL	N-CA-C	8.29	120.08	112.29
1	B	11	GLU	O-C-N	8.27	130.93	122.08
1	B	99	VAL	N-CA-CB	8.26	119.99	110.65
1	C	6	HIS	CA-C-N	-8.09	110.78	122.19
1	C	6	HIS	C-N-CA	-8.09	110.78	122.19
1	H	91	ASN	N-CA-CB	-7.99	98.33	110.16
1	B	7	ARG	CA-C-N	-7.97	110.97	122.77
1	B	7	ARG	C-N-CA	-7.97	110.97	122.77
1	B	69	VAL	N-CA-CB	7.83	124.15	111.23
1	A	17	LEU	N-CA-C	7.74	123.99	113.77
1	D	11	GLU	N-CA-CB	7.74	122.14	110.22
1	F	34	ILE	CB-CA-C	7.69	124.02	110.71
1	A	59	LYS	N-CA-CB	7.66	121.35	109.94
1	C	10	ALA	N-CA-CB	7.61	121.60	110.26
1	G	44	ASN	CA-C-N	7.57	130.43	120.28
1	G	44	ASN	C-N-CA	7.57	130.43	120.28
1	F	7	ARG	CD-NE-CZ	-7.50	113.90	124.40
1	C	17	LEU	N-CA-C	7.46	126.31	109.81
1	F	37	GLN	N-CA-CB	-7.45	98.16	110.68
1	H	14	ASP	CA-CB-CG	7.41	120.01	112.60
1	D	38	PHE	CA-CB-CG	7.39	121.19	113.80
1	B	16	LEU	CA-C-N	7.32	128.76	120.06
1	B	16	LEU	C-N-CA	7.32	128.76	120.06
1	C	36	LYS	CA-C-N	-7.26	112.49	122.95
1	C	36	LYS	C-N-CA	-7.26	112.49	122.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	19	ASN	N-CA-CB	-7.18	98.35	110.49
1	G	42	ASP	CA-CB-CG	7.13	119.73	112.60
1	H	33	ALA	CA-C-N	-7.10	113.94	123.10
1	H	33	ALA	C-N-CA	-7.10	113.94	123.10
1	B	35	PHE	CA-C-O	-7.05	113.71	121.33
1	G	98	GLN	N-CA-CB	7.01	120.64	110.20
1	C	29	GLU	N-CA-CB	7.00	121.08	110.30
1	F	92	LEU	N-CA-C	-6.98	102.87	113.89
1	D	87	GLU	N-CA-C	-6.95	102.27	111.24
1	D	65	GLU	CA-C-N	-6.88	110.81	122.92
1	D	65	GLU	C-N-CA	-6.88	110.81	122.92
1	G	90	ILE	CA-C-N	6.87	129.97	120.63
1	G	90	ILE	C-N-CA	6.87	129.97	120.63
1	F	7	ARG	N-CA-CB	6.85	122.07	110.49
1	G	26	ASN	CB-CA-C	-6.81	98.73	109.84
1	A	72	LYS	N-CA-CB	6.81	122.02	110.71
1	H	86	SER	CA-C-O	-6.80	113.66	121.68
1	D	50	MET	CA-C-N	6.78	129.37	120.28
1	D	50	MET	C-N-CA	6.78	129.37	120.28
1	C	39	HIS	CA-CB-CG	-6.71	107.09	113.80
1	A	12	GLU	O-C-N	6.63	129.80	122.11
1	H	55	LEU	CA-C-N	6.63	129.16	120.28
1	H	55	LEU	C-N-CA	6.63	129.16	120.28
1	F	61	ASP	CA-C-N	6.62	132.04	122.44
1	F	61	ASP	C-N-CA	6.62	132.04	122.44
1	D	75	ILE	N-CA-C	6.56	117.35	108.17
1	B	56	GLN	N-CA-C	6.55	118.22	111.14
1	E	89	ASP	CA-CB-CG	-6.54	106.06	112.60
1	D	21	ARG	N-CA-CB	6.54	120.43	109.78
1	C	14	ASP	CB-CA-C	6.50	122.73	109.67
1	G	32	ASP	CA-CB-CG	-6.47	106.12	112.60
1	A	79	THR	N-CA-C	6.45	119.83	110.28
1	C	45	ARG	CA-C-N	6.45	128.92	120.28
1	C	45	ARG	C-N-CA	6.45	128.92	120.28
1	C	27	GLU	N-CA-C	6.43	119.80	110.28
1	D	101	VAL	N-CA-CB	6.43	118.80	110.57
1	G	20	LEU	O-C-N	6.40	128.66	122.07
1	C	80	HIS	CA-CB-CG	-6.37	107.43	113.80
1	H	71	ASN	CA-CB-CG	-6.37	106.23	112.60
1	E	65	GLU	CA-C-N	-6.35	110.76	121.75
1	E	65	GLU	C-N-CA	-6.35	110.76	121.75
1	D	60	LEU	N-CA-CB	6.33	120.23	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	14	ASP	CB-CA-C	6.30	123.61	110.32
1	E	63	HIS	N-CA-C	6.28	119.41	110.24
1	G	96	ILE	CB-CA-C	-6.28	103.67	111.70
1	D	68	ASN	CA-CB-CG	6.26	118.86	112.60
1	D	34	ILE	CA-C-N	-6.23	112.35	122.82
1	D	34	ILE	C-N-CA	-6.23	112.35	122.82
1	G	83	ALA	CA-C-N	-6.22	117.37	122.16
1	G	83	ALA	C-N-CA	-6.22	117.37	122.16
1	G	91	ASN	CA-CB-CG	-6.21	106.39	112.60
1	E	13	ARG	N-CA-CB	-6.16	100.07	110.49
1	H	56	GLN	CB-CA-C	-6.15	100.58	110.79
1	D	26	ASN	CA-C-N	-6.15	114.02	122.93
1	D	26	ASN	C-N-CA	-6.15	114.02	122.93
1	G	103	MET	N-CA-CB	6.13	120.85	110.49
1	H	49	PHE	CA-CB-CG	6.13	119.93	113.80
1	E	13	ARG	CD-NE-CZ	-6.10	115.86	124.40
1	E	91	ASN	CA-CB-CG	-6.09	106.50	112.60
1	D	20	LEU	N-CA-CB	6.08	119.13	110.13
1	D	81	GLU	N-CA-C	-6.07	104.58	111.14
1	A	23	VAL	N-CA-C	6.02	118.79	112.83
1	C	57	ALA	CA-C-N	6.01	129.84	120.82
1	C	57	ALA	C-N-CA	6.01	129.84	120.82
1	E	38	PHE	N-CA-C	6.01	118.77	110.35
1	H	10	ALA	N-CA-C	-6.00	104.68	112.23
1	C	76	THR	CB-CA-C	-5.99	100.21	110.16
1	E	65	GLU	O-C-N	-5.98	115.76	122.93
1	C	20	LEU	N-CA-CB	5.97	118.99	110.16
1	A	35	PHE	N-CA-CB	-5.92	101.59	110.60
1	H	9	SER	CA-C-N	-5.91	110.64	120.68
1	H	9	SER	C-N-CA	-5.91	110.64	120.68
1	A	19	ASN	CA-CB-CG	5.88	118.47	112.60
1	F	13	ARG	N-CA-C	-5.78	104.98	111.28
1	H	66	TRP	CA-CB-CG	5.77	124.57	113.60
1	A	24	GLY	CA-C-N	-5.75	113.38	121.72
1	A	24	GLY	C-N-CA	-5.75	113.38	121.72
1	A	6	HIS	N-CA-CB	5.74	120.25	110.50
1	F	87	GLU	N-CA-CB	5.74	119.47	109.72
1	D	95	PHE	N-CA-C	-5.73	105.12	111.36
1	G	26	ASN	CA-C-N	-5.71	113.48	121.99
1	G	26	ASN	C-N-CA	-5.71	113.48	121.99
1	B	39	HIS	N-CA-CB	-5.70	101.19	110.59
1	E	48	GLY	N-CA-C	-5.68	105.92	112.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	25	TRP	N-CA-CB	5.67	119.01	109.94
1	B	56	GLN	N-CA-CB	5.64	118.25	110.07
1	E	92	LEU	CB-CA-C	5.63	119.10	109.24
1	A	88	ARG	O-C-N	5.60	127.91	122.09
1	G	76	THR	CA-C-O	-5.58	114.24	120.66
1	A	91	ASN	CB-CA-C	-5.56	102.40	110.96
1	B	14	ASP	CA-C-N	-5.54	111.45	120.71
1	B	14	ASP	C-N-CA	-5.54	111.45	120.71
1	A	100	ALA	O-C-N	5.54	128.70	122.22
1	H	102	SER	N-CA-C	5.54	119.77	111.96
1	C	7	ARG	O-C-N	-5.53	116.91	123.22
1	E	26	ASN	N-CA-CB	-5.53	101.15	110.49
1	C	87	GLU	N-CA-CB	5.53	118.43	110.20
1	F	76	THR	CB-CA-C	-5.50	101.03	110.16
1	E	52	ARG	CB-CA-C	-5.50	101.51	110.85
1	B	20	LEU	N-CA-C	-5.50	105.19	111.07
1	B	31	ARG	CB-CA-C	5.45	120.81	110.51
1	B	9	SER	CB-CA-C	-5.45	99.58	110.42
1	C	80	HIS	N-CA-C	5.44	117.97	111.71
1	H	68	ASN	CA-CB-CG	5.44	118.04	112.60
1	B	61	ASP	N-CA-C	5.44	119.08	111.74
1	A	48	GLY	N-CA-C	-5.43	106.21	112.73
1	C	68	ASN	CA-CB-CG	5.43	118.03	112.60
1	E	52	ARG	N-CA-C	-5.41	105.46	111.36
1	B	89	ASP	CB-CA-C	-5.40	102.40	110.88
1	F	72	LYS	CB-CA-C	-5.40	101.83	110.14
1	F	75	ILE	N-CA-C	5.39	115.66	108.11
1	C	45	ARG	CD-NE-CZ	-5.39	116.86	124.40
1	A	10	ALA	N-CA-C	-5.39	105.41	111.28
1	G	10	ALA	CA-C-N	5.38	127.95	120.63
1	G	10	ALA	C-N-CA	5.38	127.95	120.63
1	G	49	PHE	CA-CB-CG	5.38	119.18	113.80
1	G	101	VAL	CB-CA-C	-5.38	104.97	112.02
1	E	23	VAL	N-CA-C	5.36	118.14	112.83
1	E	14	ASP	CA-CB-CG	5.35	117.95	112.60
1	A	61	ASP	CA-C-N	5.35	130.50	122.47
1	A	61	ASP	C-N-CA	5.35	130.50	122.47
1	A	103	MET	CB-CA-C	5.33	119.60	111.76
1	F	73	VAL	O-C-N	-5.33	117.44	122.98
1	E	103	MET	CB-CA-C	-5.32	99.83	110.42
1	G	26	ASN	CA-CB-CG	-5.31	107.29	112.60
1	F	80	HIS	CA-CB-CG	-5.28	108.52	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	13	ARG	CA-C-O	5.28	126.36	120.82
1	A	25	TRP	N-CA-CB	5.27	118.46	109.87
1	C	55	LEU	CA-C-N	5.26	127.78	120.63
1	C	55	LEU	C-N-CA	5.26	127.78	120.63
1	F	26	ASN	CA-CB-CG	5.23	117.83	112.60
1	B	67	PHE	CA-C-N	-5.22	114.70	122.74
1	B	67	PHE	C-N-CA	-5.22	114.70	122.74
1	B	70	TYR	N-CA-C	-5.21	106.06	112.72
1	D	69	VAL	CA-C-N	-5.20	111.60	121.54
1	D	69	VAL	C-N-CA	-5.20	111.60	121.54
1	H	34	ILE	N-CA-CB	5.20	120.83	111.21
1	A	40	PHE	CA-CB-CG	-5.19	108.61	113.80
1	H	64	PRO	CB-CA-C	-5.18	104.17	110.95
1	A	58	GLU	CB-CA-C	-5.17	102.10	110.79
1	E	69	VAL	O-C-N	-5.17	116.11	122.57
1	B	37	GLN	CA-C-O	-5.17	114.87	120.81
1	E	46	ALA	CA-C-O	-5.15	115.39	120.70
1	A	64	PRO	O-C-N	5.15	128.95	123.23
1	D	28	LEU	N-CA-C	5.15	117.95	109.76
1	F	74	HIS	CA-C-O	-5.13	113.97	120.28
1	A	68	ASN	CA-CB-CG	5.12	117.72	112.60
1	A	90	ILE	CA-C-N	5.12	127.40	120.65
1	A	90	ILE	C-N-CA	5.12	127.40	120.65
1	H	78	SER	CA-C-O	-5.11	115.68	121.25
1	H	91	ASN	N-CA-C	5.11	116.93	111.36
1	G	11	GLU	O-C-N	5.10	127.54	122.03
1	E	71	ASN	CA-C-O	-5.10	113.94	119.95
1	F	11	GLU	N-CA-C	5.10	116.64	111.14
1	E	26	ASN	OD1-CG-ND2	5.09	127.69	122.60
1	G	91	ASN	CB-CA-C	-5.08	103.07	110.95
1	B	37	GLN	CA-C-N	5.08	130.79	122.81
1	B	37	GLN	C-N-CA	5.08	130.79	122.81
1	H	70	TYR	CB-CA-C	5.08	118.72	110.24
1	B	44	ASN	N-CA-C	-5.06	105.65	111.07
1	B	45	ARG	CA-C-N	5.04	127.98	120.31
1	B	45	ARG	C-N-CA	5.04	127.98	120.31
1	A	59	LYS	CB-CA-C	5.04	118.88	110.81
1	H	61	ASP	CA-CB-CG	5.04	117.64	112.60
1	D	11	GLU	O-C-N	5.03	128.10	122.22
1	B	33	ALA	N-CA-CB	-5.02	102.44	110.77
1	A	20	LEU	O-C-N	5.01	127.23	122.07
1	G	98	GLN	CA-C-N	5.01	126.96	120.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	98	GLN	C-N-CA	5.01	126.96	120.70
1	D	19	ASN	CA-CB-CG	5.00	117.61	112.60
1	F	25	TRP	CA-C-N	-5.00	114.07	123.03
1	F	25	TRP	C-N-CA	-5.00	114.07	123.03
1	G	19	ASN	CA-CB-CG	-5.00	107.60	112.60

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	17	LEU	CA

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	103	MET	Peptide
1	C	11	GLU	Mainchain
1	D	81	GLU	Mainchain
1	F	34	ILE	Mainchain
1	G	26	ASN	Mainchain
1	G	35	PHE	Sidechain
1	G	70	TYR	Mainchain
1	H	14	ASP	Mainchain
1	H	70	TYR	Sidechain
1	H	80	HIS	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	806	0	771	115	0
1	B	806	0	771	102	0
1	C	810	0	777	89	0
1	D	803	0	771	84	0
1	E	802	0	769	106	0
1	F	807	0	775	96	0
1	G	810	0	777	88	0
1	H	810	0	777	91	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	5	0	0	2	0
2	B	5	0	0	1	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	1	0
2	F	5	0	0	3	0
2	G	5	0	0	2	0
2	H	5	0	0	1	0
All	All	6494	0	6188	729	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 57.

All (729) 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:E:8:LEU:HD21	1:E:90:ILE:HD11	1.20	1.15
1:D:34:ILE:HG23	1:D:85:LEU:HD11	1.23	1.14
1:A:8:LEU:HB3	1:A:13:ARG:HB3	1.26	1.14
1:E:8:LEU:HB3	1:E:13:ARG:HD2	1.27	1.09
1:A:45:ARG:HG2	1:A:103:MET:HG2	1.37	1.04
1:B:19:ASN:H	1:B:19:ASN:ND2	1.50	1.00
1:H:28:LEU:HD12	1:H:33:ALA:HB3	1.44	0.99
1:E:19:ASN:H	1:E:19:ASN:ND2	1.53	0.98
1:C:19:ASN:ND2	1:C:19:ASN:H	1.52	0.96
1:A:37:GLN:HE22	1:A:72:LYS:HB2	1.27	0.96
1:H:19:ASN:H	1:H:19:ASN:HD22	1.15	0.93
1:A:103:MET:HE2	1:C:52:ARG:HD2	1.49	0.93
1:F:19:ASN:H	1:F:19:ASN:HD22	1.14	0.91
1:B:19:ASN:H	1:B:19:ASN:HD22	0.91	0.90
1:C:56:GLN:HG2	1:C:95:PHE:CD2	2.06	0.90
1:E:19:ASN:H	1:E:19:ASN:HD22	1.14	0.89
1:H:56:GLN:HE22	1:H:60:LEU:HD21	1.37	0.89
1:C:17:LEU:HB3	1:C:21:ARG:HD2	1.53	0.88
1:F:103:MET:N	1:F:103:MET:HE2	1.89	0.88
1:A:62:HIS:HB2	1:A:88:ARG:HD3	1.55	0.87
1:B:19:ASN:HD22	1:B:19:ASN:N	1.71	0.87
1:C:35:PHE:CZ	1:C:74:HIS:HB3	2.10	0.87
1:H:12:GLU:HA	1:H:15:GLN:HE21	1.40	0.87
1:F:61:ASP:HB2	1:G:59:LYS:NZ	1.91	0.86
1:D:6:HIS:O	1:D:86:SER:HA	1.75	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:19:ASN:H	1:H:19:ASN:ND2	1.69	0.85
1:C:95:PHE:HA	1:C:98:GLN:NE2	1.91	0.84
1:G:28:LEU:HD23	1:G:35:PHE:CD1	2.12	0.83
1:H:12:GLU:HA	1:H:15:GLN:NE2	1.95	0.82
1:H:62:HIS:ND1	1:H:88:ARG:HG3	1.94	0.82
1:A:16:LEU:C	1:A:18:PRO:HD2	2.04	0.81
1:H:28:LEU:HD12	1:H:33:ALA:CB	2.12	0.80
1:C:19:ASN:ND2	1:C:19:ASN:N	2.29	0.80
1:A:7:ARG:HG2	1:A:7:ARG:HH11	1.45	0.80
1:F:19:ASN:HD22	1:F:19:ASN:N	1.78	0.80
1:G:26:ASN:HB2	1:G:35:PHE:CE1	2.16	0.80
1:H:66:TRP:HE3	1:H:75:ILE:HD11	1.47	0.80
1:E:28:LEU:HD12	1:E:33:ALA:HB3	1.64	0.79
1:F:20:LEU:HD21	1:F:93:ALA:CB	2.12	0.79
1:D:34:ILE:HG23	1:D:85:LEU:CD1	2.08	0.79
1:D:8:LEU:CD2	1:D:90:ILE:HD13	2.13	0.78
1:C:95:PHE:HA	1:C:98:GLN:HE22	1.45	0.78
1:D:11:GLU:HG2	1:D:15:GLN:NE2	1.98	0.78
1:B:32:ASP:HB3	1:B:84:GLY:HA2	1.66	0.77
1:G:49:PHE:HD1	1:G:99:VAL:HG12	1.49	0.77
1:A:8:LEU:HB3	1:A:13:ARG:CB	2.13	0.77
1:D:37:GLN:HE21	1:D:74:HIS:HB2	1.49	0.77
1:C:56:GLN:HE22	1:C:59:LYS:HE2	1.49	0.77
1:F:6:HIS:CB	1:F:86:SER:HB2	2.15	0.77
1:A:6:HIS:HA	1:A:87:GLU:OE2	1.86	0.76
1:D:9:SER:O	1:D:13:ARG:HG2	1.85	0.76
1:F:28:LEU:HD22	1:F:33:ALA:HB3	1.68	0.76
1:G:19:ASN:O	1:G:23:VAL:HG23	1.85	0.75
1:A:37:GLN:HB2	1:A:74:HIS:CD2	2.21	0.75
1:C:17:LEU:HD23	1:C:17:LEU:N	2.01	0.75
1:F:58:GLU:OE1	1:F:58:GLU:HA	1.87	0.75
1:B:101:VAL:HG23	1:B:102:SER:H	1.52	0.75
1:C:56:GLN:HA	1:C:56:GLN:NE2	2.02	0.75
1:E:95:PHE:CE2	1:E:99:VAL:HG21	2.22	0.75
1:H:52:ARG:HH11	1:H:103:MET:HE1	1.51	0.75
1:B:19:ASN:ND2	1:B:19:ASN:N	2.29	0.74
1:C:10:ALA:HB1	1:C:14:ASP:OD2	1.87	0.74
1:B:94:SER:O	1:B:98:GLN:HG2	1.88	0.74
1:C:13:ARG:HG3	1:C:13:ARG:HH11	1.52	0.74
1:C:56:GLN:HG2	1:C:95:PHE:CE2	2.22	0.74
1:C:51:THR:O	1:C:55:LEU:HD12	1.87	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:45:ARG:HG3	1:G:103:MET:CG	2.19	0.73
1:H:56:GLN:HG3	1:H:95:PHE:CD2	2.24	0.73
1:G:28:LEU:HD11	1:G:31:ARG:HD3	1.71	0.73
1:C:16:LEU:N	1:C:16:LEU:HD23	2.03	0.72
1:D:16:LEU:C	1:D:18:PRO:HD2	2.14	0.72
1:G:45:ARG:HG3	1:G:103:MET:HG2	1.69	0.72
1:G:92:LEU:O	1:G:96:ILE:HG12	1.89	0.72
1:A:103:MET:HE2	1:C:52:ARG:CD	2.20	0.72
1:E:88:ARG:HA	1:E:91:ASN:HB3	1.72	0.72
1:A:87:GLU:H	1:A:87:GLU:CD	1.95	0.72
1:G:32:ASP:HB3	1:G:84:GLY:HA2	1.71	0.72
1:F:55:LEU:HD23	1:G:55:LEU:HB3	1.72	0.72
1:D:37:GLN:NE2	1:D:74:HIS:HB2	2.05	0.72
1:A:8:LEU:HG	1:A:85:LEU:O	1.90	0.71
1:G:13:ARG:HB3	1:G:17:LEU:HD12	1.72	0.71
1:C:93:ALA:O	1:C:97:GLU:HB2	1.90	0.71
1:H:62:HIS:CE1	1:H:88:ARG:HG3	2.25	0.71
1:A:59:LYS:HE2	1:D:58:GLU:O	1.90	0.71
1:A:17:LEU:O	1:A:21:ARG:HG3	1.90	0.71
1:E:101:VAL:O	1:E:103:MET:N	2.23	0.71
1:A:52:ARG:NH2	1:C:45:ARG:HG3	2.05	0.71
1:F:20:LEU:HD21	1:F:93:ALA:HB3	1.71	0.70
1:F:87:GLU:O	1:F:91:ASN:HB2	1.91	0.70
1:F:49:PHE:CE1	1:F:96:ILE:HG23	2.26	0.70
1:H:39:HIS:CE1	1:H:72:LYS:HG2	2.26	0.70
1:C:46:ALA:O	1:C:50:MET:HG3	1.89	0.70
1:B:55:LEU:HD23	1:C:58:GLU:HG3	1.73	0.70
1:G:101:VAL:HG12	1:G:102:SER:N	2.07	0.70
1:B:37:GLN:HE22	1:B:72:LYS:HB3	1.57	0.70
1:B:12:GLU:O	1:B:16:LEU:HB2	1.92	0.70
1:C:23:VAL:HG11	1:C:97:GLU:CD	2.17	0.70
1:F:31:ARG:NH2	1:F:65:GLU:OE2	2.24	0.70
1:A:80:HIS:ND1	2:A:200:SO4:O1	2.25	0.70
1:E:69:VAL:HG13	1:F:65:GLU:HG2	1.73	0.70
1:B:8:LEU:O	1:B:9:SER:O	2.10	0.69
1:B:16:LEU:C	1:B:18:PRO:HD2	2.17	0.69
1:D:19:ASN:O	1:D:22:ALA:HB3	1.93	0.69
1:E:19:ASN:HD22	1:E:19:ASN:N	1.90	0.69
1:H:19:ASN:ND2	1:H:19:ASN:N	2.38	0.69
1:A:45:ARG:HG2	1:A:103:MET:CG	2.19	0.69
1:E:16:LEU:C	1:E:18:PRO:HD2	2.17	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:28:LEU:HD12	1:G:31:ARG:HG3	1.72	0.69
1:H:52:ARG:NH1	1:H:103:MET:HE1	2.08	0.69
1:E:87:GLU:O	1:E:91:ASN:HB2	1.92	0.69
1:C:17:LEU:HD22	1:C:20:LEU:HD12	1.73	0.68
1:D:17:LEU:N	1:D:18:PRO:HD2	2.08	0.68
1:G:28:LEU:CD1	1:G:31:ARG:HD3	2.23	0.68
1:F:25:TRP:CD2	1:F:36:LYS:HB2	2.29	0.68
1:H:103:MET:N	1:H:103:MET:HE2	2.08	0.68
1:A:7:ARG:HD2	1:A:7:ARG:C	2.19	0.68
1:B:101:VAL:HG23	1:B:102:SER:N	2.09	0.68
1:B:28:LEU:N	1:B:28:LEU:HD23	2.09	0.68
1:H:66:TRP:CE3	1:H:75:ILE:HD11	2.28	0.68
1:C:56:GLN:HA	1:C:56:GLN:HE21	1.59	0.67
1:C:23:VAL:HG11	1:C:97:GLU:OE2	1.94	0.67
1:G:66:TRP:H	1:G:66:TRP:CD1	2.13	0.67
1:A:34:ILE:HG23	1:A:85:LEU:HD11	1.75	0.67
1:B:37:GLN:NE2	1:B:38:PHE:O	2.28	0.67
1:E:11:GLU:O	1:E:14:ASP:HB3	1.93	0.67
1:D:11:GLU:O	1:D:15:GLN:N	2.27	0.67
1:D:14:ASP:O	1:D:18:PRO:HG3	1.94	0.67
1:D:86:SER:OG	1:D:88:ARG:HB2	1.95	0.67
1:H:92:LEU:O	1:H:96:ILE:HG13	1.93	0.67
1:B:52:ARG:HD2	1:D:48:GLY:HA3	1.76	0.67
1:E:32:ASP:OD2	1:E:84:GLY:HA3	1.94	0.67
1:E:13:ARG:O	1:E:15:GLN:N	2.28	0.67
1:G:80:HIS:HB3	2:G:200:SO4:O3	1.95	0.66
1:G:32:ASP:HB3	1:G:84:GLY:CA	2.24	0.66
1:D:41:LYS:HG3	1:D:41:LYS:O	1.93	0.66
1:G:68:ASN:C	1:G:68:ASN:HD22	2.04	0.66
1:E:15:GLN:C	1:E:18:PRO:HD2	2.20	0.66
1:A:34:ILE:HG23	1:A:85:LEU:CD1	2.25	0.66
1:F:56:GLN:HA	1:F:56:GLN:NE2	2.10	0.66
1:B:7:ARG:NE	1:B:82:CYS:O	2.29	0.66
1:A:8:LEU:HD13	1:A:13:ARG:HB2	1.78	0.66
1:A:62:HIS:NE2	1:A:89:ASP:OD1	2.28	0.65
1:B:55:LEU:HD23	1:C:58:GLU:CG	2.26	0.65
1:C:37:GLN:OE1	1:C:74:HIS:NE2	2.30	0.65
1:A:85:LEU:HD12	1:A:89:ASP:OD2	1.97	0.65
1:D:21:ARG:HH12	1:D:27:GLU:HB2	1.61	0.65
1:D:36:LYS:HG3	1:D:37:GLN:N	2.11	0.65
1:F:41:LYS:HB3	1:F:45:ARG:HE	1.62	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:40:PHE:O	1:E:71:ASN:HB2	1.98	0.64
1:F:12:GLU:HA	1:F:15:GLN:CD	2.22	0.64
1:F:61:ASP:HB2	1:G:59:LYS:HZ2	1.62	0.64
1:C:8:LEU:O	1:C:13:ARG:NH1	2.30	0.64
1:E:19:ASN:ND2	1:E:19:ASN:N	2.33	0.64
1:G:36:LYS:NZ	1:G:97:GLU:OE2	2.30	0.64
1:G:28:LEU:CD1	1:G:31:ARG:HG3	2.27	0.64
1:E:28:LEU:HA	1:E:35:PHE:HE1	1.63	0.64
1:H:9:SER:OG	1:H:12:GLU:N	2.28	0.64
1:E:77:LEU:HD22	1:E:92:LEU:HD23	1.80	0.63
1:G:21:ARG:NH2	1:G:27:GLU:OE2	2.29	0.63
1:B:71:ASN:OD1	1:B:72:LYS:HE3	1.99	0.63
1:G:68:ASN:HD22	1:G:69:VAL:N	1.96	0.63
1:A:17:LEU:N	1:A:18:PRO:HD2	2.11	0.63
1:G:11:GLU:O	1:G:14:ASP:N	2.30	0.63
1:D:79:THR:HG21	1:D:88:ARG:HB2	1.80	0.63
1:C:23:VAL:HG12	1:C:36:LYS:NZ	2.13	0.62
1:H:79:THR:O	1:H:83:ALA:N	2.30	0.62
1:A:79:THR:N	1:A:84:GLY:O	2.31	0.62
1:B:58:GLU:HA	1:B:58:GLU:OE1	1.99	0.62
1:F:7:ARG:HD2	1:F:82:CYS:O	1.98	0.62
1:F:10:ALA:HA	1:F:13:ARG:HG3	1.80	0.62
1:F:37:GLN:HG3	1:F:37:GLN:O	2.00	0.62
1:A:62:HIS:CB	1:A:88:ARG:HD3	2.28	0.62
1:F:17:LEU:HD13	1:F:34:ILE:HD11	1.82	0.61
1:E:20:LEU:HD11	1:E:93:ALA:HB3	1.82	0.61
1:A:81:GLU:HB2	2:A:200:SO4:O4	2.01	0.61
1:B:79:THR:HB	1:B:82:CYS:SG	2.40	0.61
1:A:8:LEU:CD1	1:A:13:ARG:HB2	2.31	0.61
1:A:54:ALA:HB1	1:B:43:PHE:CZ	2.34	0.61
1:H:45:ARG:HD2	1:H:104:THR:C	2.26	0.61
1:A:46:ALA:O	1:A:50:MET:HG3	2.00	0.60
1:A:101:VAL:HG11	1:E:21:ARG:HB3	1.83	0.60
1:E:42:ASP:OD1	1:E:45:ARG:HB2	2.01	0.60
1:F:25:TRP:CE3	1:F:36:LYS:HB2	2.36	0.60
1:H:15:GLN:O	1:H:18:PRO:HD2	2.00	0.60
1:H:77:LEU:HD21	1:H:92:LEU:HD23	1.83	0.60
1:B:44:ASN:ND2	1:D:55:LEU:HB3	2.16	0.60
1:F:8:LEU:HB3	1:F:13:ARG:HE	1.65	0.60
1:H:7:ARG:HG3	1:H:8:LEU:H	1.66	0.60
1:A:8:LEU:HD13	1:A:13:ARG:CB	2.32	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:103:MET:HE2	1:F:103:MET:CA	2.29	0.60
1:H:56:GLN:NE2	1:H:60:LEU:HD21	2.13	0.60
1:A:6:HIS:HA	1:A:87:GLU:CD	2.26	0.60
1:A:62:HIS:CD2	1:A:88:ARG:HD2	2.36	0.60
1:G:20:LEU:O	1:G:23:VAL:N	2.31	0.60
1:F:8:LEU:CD2	1:F:90:ILE:HD11	2.32	0.60
1:H:67:PHE:CE1	1:H:69:VAL:HG23	2.36	0.60
1:A:41:LYS:HE3	1:A:45:ARG:HH12	1.66	0.60
1:H:56:GLN:HE22	1:H:60:LEU:CD2	2.10	0.59
1:C:9:SER:O	1:C:13:ARG:HG3	2.02	0.59
1:H:99:VAL:HG13	1:H:103:MET:HE3	1.83	0.59
1:B:36:LYS:HD3	1:B:38:PHE:CZ	2.36	0.59
1:G:56:GLN:HA	1:G:59:LYS:HB3	1.85	0.59
1:C:17:LEU:CD2	1:C:90:ILE:HD11	2.32	0.59
1:C:35:PHE:CE1	1:C:74:HIS:HB3	2.38	0.59
1:G:16:LEU:HB3	1:G:90:ILE:HD12	1.84	0.59
1:H:79:THR:HG23	2:H:200:SO4:O1	2.03	0.59
1:B:25:TRP:CZ3	1:B:77:LEU:HD12	2.37	0.59
1:D:26:ASN:HB3	1:D:35:PHE:CE1	2.38	0.59
1:E:35:PHE:HA	1:E:75:ILE:O	2.01	0.59
1:F:8:LEU:HD21	1:F:90:ILE:HD11	1.83	0.59
1:A:13:ARG:HH22	1:A:32:ASP:CG	2.10	0.59
1:A:66:TRP:HA	1:A:74:HIS:O	2.03	0.59
1:B:36:LYS:HD3	1:B:38:PHE:CE1	2.38	0.59
1:C:8:LEU:HD23	1:C:8:LEU:N	2.17	0.58
1:E:17:LEU:HD12	1:E:17:LEU:N	2.16	0.58
1:H:45:ARG:NH1	1:H:104:THR:HB	2.18	0.58
1:C:95:PHE:CA	1:C:98:GLN:HE22	2.16	0.58
1:A:37:GLN:HE22	1:A:72:LYS:CB	2.08	0.58
1:D:8:LEU:O	1:D:13:ARG:HD2	2.04	0.58
1:F:17:LEU:CD1	1:F:34:ILE:HD11	2.33	0.58
1:E:8:LEU:HD22	1:E:85:LEU:HB3	1.86	0.58
1:E:60:LEU:N	1:E:60:LEU:HD23	2.17	0.58
1:H:102:SER:OG	1:H:103:MET:HE2	2.03	0.58
1:G:28:LEU:HD23	1:G:35:PHE:HD1	1.63	0.58
1:D:89:ASP:OD1	1:D:89:ASP:N	2.37	0.58
1:D:79:THR:CG2	1:D:88:ARG:HB2	2.34	0.58
1:F:49:PHE:CZ	1:F:96:ILE:HG23	2.38	0.58
1:D:15:GLN:O	1:D:18:PRO:HG2	2.04	0.58
1:F:51:THR:O	1:F:54:ALA:N	2.36	0.58
1:B:17:LEU:N	1:B:18:PRO:HD2	2.18	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:13:ARG:C	1:E:15:GLN:H	2.12	0.57
1:G:19:ASN:HD22	1:G:19:ASN:H	1.52	0.57
1:H:28:LEU:CD1	1:H:33:ALA:HB3	2.28	0.57
1:B:26:ASN:O	1:B:35:PHE:N	2.37	0.57
1:B:36:LYS:O	1:B:36:LYS:HG2	2.03	0.57
1:C:17:LEU:HD22	1:C:20:LEU:CD1	2.33	0.57
1:C:53:VAL:HG22	1:C:66:TRP:CH2	2.40	0.57
1:B:101:VAL:O	1:B:104:THR:HG23	2.05	0.57
1:A:7:ARG:HH11	1:A:7:ARG:CG	2.14	0.57
1:F:55:LEU:CD2	1:G:55:LEU:HB3	2.34	0.57
1:A:95:PHE:CE1	1:A:99:VAL:HG21	2.39	0.57
1:E:41:LYS:HZ2	1:E:45:ARG:HH22	1.52	0.56
1:E:33:ALA:HB1	1:E:77:LEU:O	2.05	0.56
1:F:8:LEU:HB3	1:F:13:ARG:NE	2.20	0.56
1:A:34:ILE:HG21	1:A:85:LEU:HD21	1.86	0.56
1:A:62:HIS:HD2	1:A:88:ARG:HD2	1.69	0.56
1:A:7:ARG:NE	1:A:32:ASP:OD2	2.38	0.56
1:A:43:PHE:HB2	1:A:70:TYR:CD1	2.40	0.56
1:F:42:ASP:OD1	1:F:45:ARG:HG3	2.06	0.56
1:B:56:GLN:O	1:B:56:GLN:HG3	2.05	0.56
1:D:11:GLU:HG2	1:D:15:GLN:HE21	1.66	0.56
1:E:18:PRO:O	1:E:21:ARG:N	2.39	0.56
1:A:41:LYS:HB3	1:A:45:ARG:NH1	2.21	0.56
1:B:31:ARG:HG2	1:B:32:ASP:N	2.21	0.56
1:D:8:LEU:HD21	1:D:16:LEU:HD13	1.88	0.56
1:F:19:ASN:N	1:F:19:ASN:ND2	2.53	0.56
1:H:36:LYS:HD2	1:H:38:PHE:CE2	2.41	0.56
1:E:18:PRO:HA	1:E:21:ARG:HB2	1.87	0.56
1:H:86:SER:OG	1:H:88:ARG:HG2	2.06	0.56
1:G:14:ASP:O	1:G:18:PRO:HG3	2.06	0.55
1:C:16:LEU:HB3	1:C:90:ILE:CD1	2.36	0.55
1:D:31:ARG:HH22	1:D:65:GLU:CD	2.12	0.55
1:E:8:LEU:CD2	1:E:90:ILE:HD11	2.13	0.55
1:F:17:LEU:HB2	1:F:21:ARG:NH2	2.20	0.55
1:F:34:ILE:O	1:F:76:THR:HA	2.07	0.55
1:A:54:ALA:HB1	1:B:43:PHE:HZ	1.72	0.55
1:D:7:ARG:NE	1:D:32:ASP:OD2	2.40	0.55
1:C:41:LYS:HG2	1:C:45:ARG:NH2	2.20	0.55
1:F:42:ASP:OD1	1:F:42:ASP:N	2.37	0.55
1:B:45:ARG:HG3	1:D:52:ARG:NH2	2.21	0.55
1:E:8:LEU:HD23	1:E:13:ARG:HG3	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:34:ILE:HD12	1:F:85:LEU:HD11	1.88	0.55
1:H:17:LEU:HD13	1:H:27:GLU:OE2	2.06	0.55
1:A:53:VAL:HG11	1:A:66:TRP:CZ3	2.41	0.55
1:D:37:GLN:HG3	1:D:38:PHE:N	2.11	0.55
1:A:35:PHE:O	1:A:36:LYS:HB2	2.07	0.55
1:F:93:ALA:O	1:F:97:GLU:HB2	2.07	0.55
1:H:103:MET:HE2	1:H:103:MET:H	1.71	0.55
1:E:25:TRP:CE3	1:E:34:ILE:HD12	2.41	0.55
1:A:77:LEU:HB3	1:A:89:ASP:HB3	1.88	0.54
1:A:18:PRO:O	1:A:21:ARG:N	2.40	0.54
1:E:9:SER:O	1:E:13:ARG:HB2	2.07	0.54
1:A:53:VAL:HG11	1:A:66:TRP:HZ3	1.73	0.54
1:D:8:LEU:HD23	1:D:90:ILE:HD13	1.86	0.54
1:D:79:THR:OG1	1:D:86:SER:HB3	2.07	0.54
1:F:61:ASP:HB2	1:G:59:LYS:HZ1	1.70	0.54
1:G:35:PHE:CD2	1:G:74:HIS:CE1	2.96	0.54
1:H:10:ALA:O	1:H:14:ASP:HB3	2.08	0.54
1:B:58:GLU:CG	1:C:55:LEU:HD23	2.37	0.54
1:B:88:ARG:O	1:B:91:ASN:OD1	2.25	0.54
1:D:8:LEU:HD21	1:D:16:LEU:CD1	2.38	0.54
1:E:77:LEU:CD2	1:E:92:LEU:HD23	2.38	0.54
1:A:56:GLN:NE2	1:A:95:PHE:CD2	2.73	0.54
1:B:67:PHE:CE2	1:B:69:VAL:CG2	2.91	0.54
1:E:27:GLU:N	1:E:34:ILE:HG22	2.23	0.54
1:F:12:GLU:HA	1:F:15:GLN:HG3	1.89	0.54
1:E:15:GLN:O	1:E:18:PRO:HG2	2.08	0.54
1:B:51:THR:HG22	1:B:55:LEU:HD12	1.88	0.54
1:H:45:ARG:HH11	1:H:104:THR:HB	1.73	0.54
1:C:56:GLN:HE21	1:C:56:GLN:CA	2.21	0.53
1:D:36:LYS:N	1:D:75:ILE:O	2.39	0.53
1:F:16:LEU:C	1:F:18:PRO:HD2	2.33	0.53
1:A:9:SER:OG	1:A:12:GLU:OE1	2.26	0.53
1:A:37:GLN:NE2	1:A:72:LYS:HB2	2.09	0.53
1:A:45:ARG:HD3	1:A:104:THR:HA	1.90	0.53
1:A:77:LEU:O	1:A:78:SER:HB2	2.07	0.53
1:B:17:LEU:HD13	1:B:90:ILE:HD11	1.90	0.53
1:C:11:GLU:O	1:C:15:GLN:HG2	2.08	0.53
1:H:39:HIS:NE2	1:H:72:LYS:HG2	2.23	0.53
1:C:9:SER:OG	1:C:12:GLU:HG3	2.08	0.53
1:C:18:PRO:HA	1:C:21:ARG:HD3	1.91	0.53
1:D:87:GLU:O	1:D:90:ILE:N	2.41	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:LEU:HB2	1:A:13:ARG:NE	2.23	0.53
1:F:102:SER:C	1:F:103:MET:HE2	2.34	0.53
1:C:18:PRO:O	1:C:21:ARG:N	2.41	0.53
1:H:13:ARG:NH2	1:H:32:ASP:OD2	2.40	0.53
1:E:43:PHE:HB2	1:E:70:TYR:CE1	2.44	0.53
1:H:43:PHE:HD1	1:H:70:TYR:O	1.92	0.53
1:A:8:LEU:HB2	1:A:13:ARG:HE	1.74	0.53
1:A:42:ASP:OD1	1:A:45:ARG:HB2	2.09	0.53
1:A:19:ASN:HD22	1:E:23:VAL:CG2	2.21	0.52
1:A:62:HIS:CD2	1:A:88:ARG:HG2	2.44	0.52
1:H:99:VAL:CG1	1:H:103:MET:HE3	2.38	0.52
1:A:17:LEU:HB2	1:A:21:ARG:CZ	2.40	0.52
1:B:8:LEU:HG	1:B:85:LEU:O	2.09	0.52
1:D:37:GLN:HA	1:D:74:HIS:HA	1.90	0.52
1:E:62:HIS:NE2	1:E:89:ASP:OD1	2.36	0.52
1:E:63:HIS:CE1	1:F:70:TYR:CD1	2.97	0.52
1:H:21:ARG:HE	1:H:27:GLU:CD	2.16	0.52
1:B:37:GLN:HE21	1:B:38:PHE:C	2.18	0.52
1:B:79:THR:CB	1:B:86:SER:HB3	2.39	0.52
1:D:28:LEU:HD12	1:D:35:PHE:CD1	2.44	0.52
1:C:13:ARG:HG3	1:C:13:ARG:NH1	2.21	0.52
1:D:21:ARG:O	1:D:24:GLY:N	2.38	0.52
1:E:16:LEU:O	1:E:19:ASN:ND2	2.43	0.52
1:A:6:HIS:O	1:A:8:LEU:N	2.43	0.52
1:A:62:HIS:CD2	1:A:88:ARG:CD	2.93	0.52
1:F:80:HIS:N	2:F:200:SO4:O1	2.31	0.52
1:E:32:ASP:HB3	1:E:84:GLY:CA	2.40	0.52
1:F:79:THR:HG23	2:F:200:SO4:O3	2.09	0.52
1:D:8:LEU:HD22	1:D:90:ILE:HD13	1.90	0.52
1:B:67:PHE:CE2	1:B:69:VAL:HG23	2.45	0.52
1:C:40:PHE:N	1:C:40:PHE:CD1	2.78	0.52
1:G:19:ASN:H	1:G:19:ASN:ND2	2.08	0.52
1:H:13:ARG:O	1:H:17:LEU:N	2.41	0.52
1:H:93:ALA:O	1:H:97:GLU:HG2	2.10	0.51
1:A:23:VAL:HG12	1:A:36:LYS:NZ	2.25	0.51
1:H:42:ASP:C	1:H:71:ASN:HB3	2.34	0.51
1:B:32:ASP:HB3	1:B:84:GLY:CA	2.38	0.51
1:C:26:ASN:O	1:C:34:ILE:HA	2.09	0.51
1:D:8:LEU:HD23	1:D:90:ILE:CD1	2.41	0.51
1:E:26:ASN:C	1:E:34:ILE:HG22	2.35	0.51
1:G:18:PRO:O	1:G:21:ARG:HB2	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:87:GLU:O	1:H:91:ASN:HB2	2.10	0.51
1:C:35:PHE:HZ	1:C:74:HIS:CD2	2.29	0.51
1:A:18:PRO:O	1:A:22:ALA:N	2.38	0.51
1:C:75:ILE:CG2	1:C:77:LEU:HD21	2.41	0.51
1:B:56:GLN:HG2	1:B:60:LEU:HD12	1.91	0.51
1:C:17:LEU:HD23	1:C:90:ILE:HD11	1.92	0.51
1:G:93:ALA:HA	1:G:96:ILE:HG13	1.92	0.51
1:A:16:LEU:O	1:A:18:PRO:HD2	2.10	0.51
1:F:27:GLU:HG3	1:F:34:ILE:CD1	2.41	0.51
1:F:92:LEU:O	1:F:96:ILE:HG13	2.11	0.51
1:H:8:LEU:HG	1:H:12:GLU:HB3	1.93	0.51
1:E:56:GLN:HG3	1:E:95:PHE:CZ	2.46	0.50
1:A:19:ASN:O	1:A:22:ALA:HB3	2.11	0.50
1:D:80:HIS:C	1:D:83:ALA:H	2.18	0.50
1:G:43:PHE:CD2	1:H:63:HIS:CD2	2.99	0.50
1:D:46:ALA:O	1:D:50:MET:HG3	2.11	0.50
1:E:20:LEU:HD11	1:E:93:ALA:CB	2.42	0.50
1:D:71:ASN:OD1	1:D:71:ASN:N	2.45	0.50
1:B:44:ASN:HD21	1:D:55:LEU:HB3	1.75	0.50
1:F:8:LEU:HD21	1:F:90:ILE:CD1	2.42	0.50
1:G:34:ILE:HG12	1:G:85:LEU:HD21	1.93	0.50
1:A:17:LEU:HB2	1:A:21:ARG:NH2	2.27	0.50
1:B:29:GLU:O	1:B:29:GLU:HG2	2.10	0.50
1:G:17:LEU:N	1:G:18:PRO:CD	2.74	0.50
1:A:95:PHE:O	1:A:99:VAL:HG23	2.11	0.50
1:C:94:SER:O	1:C:97:GLU:HB3	2.11	0.50
1:F:38:PHE:O	1:F:72:LYS:HA	2.12	0.50
1:D:57:ALA:HB1	1:D:63:HIS:HA	1.92	0.50
1:H:17:LEU:N	1:H:18:PRO:HD2	2.27	0.50
1:A:13:ARG:O	1:A:17:LEU:HD12	2.11	0.50
1:B:37:GLN:HB2	1:B:74:HIS:CE1	2.47	0.50
1:B:56:GLN:CG	1:B:60:LEU:HD12	2.41	0.50
1:E:27:GLU:HA	1:E:33:ALA:O	2.12	0.50
1:H:32:ASP:HB3	1:H:84:GLY:HA2	1.94	0.50
1:A:86:SER:OG	1:A:88:ARG:HB3	2.12	0.49
1:E:17:LEU:N	1:E:18:PRO:HD2	2.26	0.49
1:E:52:ARG:HB3	1:G:44:ASN:OD1	2.12	0.49
1:F:12:GLU:HA	1:F:15:GLN:CG	2.41	0.49
1:F:35:PHE:HA	1:F:75:ILE:O	2.11	0.49
1:B:25:TRP:CE3	1:B:34:ILE:HD12	2.47	0.49
1:B:28:LEU:HD21	1:B:35:PHE:HB2	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:56:GLN:HB2	1:C:95:PHE:CZ	2.48	0.49
1:G:43:PHE:CD2	1:H:63:HIS:HD2	2.31	0.49
1:E:56:GLN:HG3	1:E:95:PHE:CE2	2.47	0.49
1:A:35:PHE:CG	1:A:36:LYS:N	2.80	0.49
1:E:40:PHE:O	1:E:71:ASN:ND2	2.45	0.49
1:F:17:LEU:CB	1:F:21:ARG:NH2	2.76	0.49
1:H:103:MET:H	1:H:103:MET:CE	2.25	0.49
1:B:6:HIS:O	1:B:82:CYS:HB3	2.13	0.49
1:B:37:GLN:OE1	1:B:74:HIS:NE2	2.40	0.49
1:D:36:LYS:O	1:D:75:ILE:N	2.30	0.49
1:F:80:HIS:C	1:F:80:HIS:CD2	2.91	0.49
1:A:97:GLU:HA	1:A:97:GLU:OE1	2.12	0.49
1:A:43:PHE:CD2	1:B:63:HIS:NE2	2.80	0.49
1:B:11:GLU:HG2	1:B:12:GLU:N	2.27	0.49
1:D:89:ASP:O	1:D:93:ALA:N	2.41	0.49
1:B:58:GLU:HG2	1:C:55:LEU:CD2	2.43	0.49
1:E:43:PHE:CD2	1:F:63:HIS:CD2	3.01	0.49
1:E:55:LEU:HD23	1:H:55:LEU:HD12	1.95	0.49
1:F:85:LEU:HD23	1:F:89:ASP:HB2	1.94	0.49
1:H:9:SER:OG	1:H:12:GLU:HB2	2.12	0.49
1:C:67:PHE:CZ	1:C:69:VAL:CG2	2.95	0.49
1:G:66:TRP:CD1	1:G:66:TRP:N	2.76	0.49
1:F:26:ASN:O	1:F:34:ILE:HG13	2.13	0.49
1:C:56:GLN:NE2	1:C:56:GLN:CA	2.75	0.48
1:D:31:ARG:NH2	1:D:65:GLU:OE2	2.29	0.48
1:E:38:PHE:CD1	1:E:38:PHE:N	2.77	0.48
1:G:49:PHE:CD1	1:G:99:VAL:HG12	2.40	0.48
1:H:71:ASN:OD1	1:H:71:ASN:N	2.42	0.48
1:B:8:LEU:C	1:B:9:SER:O	2.55	0.48
1:E:28:LEU:HG	1:E:35:PHE:CD1	2.48	0.48
1:G:7:ARG:HA	1:G:85:LEU:O	2.13	0.48
1:G:17:LEU:N	1:G:18:PRO:HD3	2.28	0.48
1:G:42:ASP:OD1	1:G:45:ARG:HB2	2.13	0.48
1:G:43:PHE:CG	1:H:63:HIS:CD2	3.01	0.48
1:A:102:SER:O	1:C:102:SER:HB2	2.14	0.48
1:C:45:ARG:HG2	1:C:103:MET:HG3	1.96	0.48
1:E:39:HIS:HD2	1:E:72:LYS:CD	2.27	0.48
1:D:49:PHE:HD1	1:D:99:VAL:HG12	1.79	0.48
1:D:92:LEU:O	1:D:96:ILE:HB	2.13	0.48
1:E:20:LEU:CD1	1:E:93:ALA:CB	2.92	0.48
1:H:16:LEU:C	1:H:18:PRO:HD2	2.38	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:GLN:CB	1:C:74:HIS:CD2	2.97	0.48
1:D:62:HIS:CE1	1:D:79:THR:HG22	2.48	0.48
1:E:41:LYS:NZ	1:E:45:ARG:NH2	2.62	0.48
1:F:40:PHE:HE2	1:F:73:VAL:HG23	1.79	0.48
1:H:7:ARG:HG3	1:H:8:LEU:N	2.29	0.48
1:H:66:TRP:HE3	1:H:75:ILE:CD1	2.24	0.48
1:B:66:TRP:CD1	1:B:66:TRP:N	2.79	0.48
1:D:20:LEU:C	1:D:25:TRP:HB2	2.39	0.48
1:F:26:ASN:O	1:F:34:ILE:HA	2.14	0.48
1:A:16:LEU:HD13	1:A:90:ILE:HG21	1.96	0.47
1:A:41:LYS:CB	1:A:45:ARG:NH1	2.77	0.47
1:E:82:CYS:O	1:E:83:ALA:HB3	2.14	0.47
1:A:9:SER:O	1:A:13:ARG:HD2	2.14	0.47
1:B:41:LYS:HE3	1:B:45:ARG:NH1	2.29	0.47
1:B:25:TRP:O	1:B:26:ASN:ND2	2.47	0.47
1:E:36:LYS:HB3	1:E:38:PHE:CE1	2.50	0.47
1:A:40:PHE:N	1:A:40:PHE:CD1	2.82	0.47
1:D:62:HIS:CE1	1:D:79:THR:CG2	2.98	0.47
1:E:17:LEU:N	1:E:17:LEU:CD1	2.77	0.47
1:E:45:ARG:HG2	1:E:103:MET:HG2	1.97	0.47
1:F:21:ARG:C	1:F:23:VAL:H	2.21	0.47
1:A:62:HIS:HB2	1:A:88:ARG:CD	2.37	0.47
1:B:67:PHE:HE2	1:B:69:VAL:CG2	2.26	0.47
1:C:23:VAL:HG12	1:C:36:LYS:HZ1	1.79	0.47
1:C:53:VAL:CG2	1:C:66:TRP:CZ3	2.97	0.47
1:C:68:ASN:HA	1:C:72:LYS:O	2.14	0.47
1:D:87:GLU:O	1:D:89:ASP:N	2.47	0.47
1:H:17:LEU:N	1:H:18:PRO:CD	2.77	0.47
1:D:79:THR:HG21	1:D:88:ARG:CB	2.44	0.47
1:E:45:ARG:HG2	1:E:103:MET:CG	2.45	0.47
1:G:88:ARG:NH1	2:G:200:SO4:O4	2.48	0.47
1:B:67:PHE:HE2	1:B:69:VAL:HG23	1.79	0.47
1:C:28:LEU:N	1:C:33:ALA:O	2.46	0.47
1:C:82:CYS:O	1:C:83:ALA:HB3	2.15	0.47
1:D:9:SER:C	1:D:13:ARG:HG2	2.39	0.47
1:D:20:LEU:O	1:D:25:TRP:HB2	2.15	0.47
1:D:72:LYS:HD3	1:D:72:LYS:H	1.78	0.47
1:H:45:ARG:HH11	1:H:104:THR:CB	2.28	0.47
1:B:82:CYS:O	1:B:83:ALA:HB3	2.15	0.47
1:B:57:ALA:HB1	1:B:63:HIS:HA	1.97	0.47
1:D:68:ASN:HD22	1:D:73:VAL:HG22	1.80	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:ILE:O	1:A:34:ILE:HG12	2.14	0.47
1:B:26:ASN:HD22	1:B:26:ASN:HA	1.36	0.47
1:B:37:GLN:CD	1:B:74:HIS:NE2	2.73	0.47
1:E:31:ARG:HH22	1:E:65:GLU:CD	2.21	0.47
1:B:13:ARG:NH2	1:B:32:ASP:OD1	2.47	0.46
1:F:56:GLN:HA	1:F:56:GLN:HE21	1.80	0.46
1:F:77:LEU:CD2	1:F:92:LEU:HD23	2.45	0.46
1:E:70:TYR:CE1	1:F:63:HIS:CE1	3.03	0.46
1:G:25:TRP:CD2	1:G:36:LYS:HB2	2.51	0.46
1:E:15:GLN:HG2	1:E:16:LEU:HD23	1.96	0.46
1:F:95:PHE:O	1:F:99:VAL:HG23	2.14	0.46
1:G:87:GLU:O	1:G:90:ILE:HB	2.15	0.46
1:A:54:ALA:HB1	1:B:43:PHE:CE2	2.51	0.46
1:C:28:LEU:HA	1:C:28:LEU:HD23	1.53	0.46
1:C:65:GLU:HG3	1:C:76:THR:HB	1.97	0.46
1:F:49:PHE:CZ	1:F:96:ILE:CG2	2.98	0.46
1:G:8:LEU:HB2	1:G:13:ARG:HG3	1.97	0.46
1:H:78:SER:OG	1:H:79:THR:N	2.48	0.46
1:A:17:LEU:HB3	1:A:21:ARG:NE	2.30	0.46
1:A:17:LEU:C	1:A:21:ARG:HG3	2.40	0.46
1:E:13:ARG:NH2	1:E:32:ASP:OD1	2.48	0.46
1:F:6:HIS:O	1:F:7:ARG:HB2	2.16	0.46
1:G:92:LEU:O	1:G:92:LEU:HD12	2.15	0.46
1:F:28:LEU:HD11	1:F:35:PHE:HB2	1.98	0.46
1:G:60:LEU:HD23	1:G:60:LEU:HA	1.68	0.46
1:H:77:LEU:CD2	1:H:92:LEU:HD23	2.45	0.46
1:C:13:ARG:HH11	1:C:13:ARG:CG	2.20	0.46
1:C:17:LEU:CB	1:C:21:ARG:HD2	2.36	0.46
1:F:12:GLU:CA	1:F:15:GLN:HG3	2.46	0.46
1:G:40:PHE:O	1:G:71:ASN:ND2	2.49	0.46
1:G:74:HIS:C	1:G:74:HIS:CD2	2.93	0.46
1:A:43:PHE:CD2	1:B:63:HIS:CD2	3.03	0.46
1:D:17:LEU:N	1:D:18:PRO:CD	2.78	0.46
1:D:53:VAL:HG11	1:D:96:ILE:HD11	1.98	0.46
1:E:31:ARG:CG	1:E:32:ASP:N	2.79	0.46
1:E:39:HIS:CD2	1:E:72:LYS:CG	2.98	0.46
1:G:79:THR:OG1	1:G:86:SER:HB3	2.16	0.46
1:G:87:GLU:O	1:G:91:ASN:HB2	2.15	0.46
1:E:8:LEU:HA	1:E:8:LEU:HD12	1.44	0.46
1:E:41:LYS:HD3	1:E:45:ARG:NH2	2.31	0.46
1:F:17:LEU:N	1:F:18:PRO:CD	2.79	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:9:SER:C	1:G:13:ARG:HD2	2.41	0.46
1:H:103:MET:H	1:H:103:MET:HG2	1.23	0.46
1:E:15:GLN:CG	1:E:16:LEU:N	2.76	0.46
1:E:55:LEU:HD23	1:H:55:LEU:HA	1.98	0.46
1:F:12:GLU:HA	1:F:15:GLN:OE1	2.16	0.46
1:F:96:ILE:O	1:F:96:ILE:HG22	2.16	0.46
1:C:53:VAL:CG2	1:C:66:TRP:CH2	3.00	0.45
1:F:45:ARG:HB3	1:F:103:MET:HG3	1.98	0.45
1:G:66:TRP:H	1:G:66:TRP:HD1	1.62	0.45
1:H:45:ARG:HD3	1:H:104:THR:H	1.81	0.45
1:A:7:ARG:HG2	1:A:7:ARG:NH1	2.24	0.45
1:A:86:SER:HB2	1:A:87:GLU:OE2	2.17	0.45
1:A:95:PHE:CE1	1:A:99:VAL:CG2	2.99	0.45
1:D:21:ARG:HA	1:D:25:TRP:O	2.16	0.45
1:G:82:CYS:O	1:G:83:ALA:HB2	2.16	0.45
1:H:7:ARG:CG	1:H:8:LEU:N	2.78	0.45
1:E:24:GLY:HA3	1:E:36:LYS:HE3	1.97	0.45
1:E:32:ASP:HB3	1:E:84:GLY:HA2	1.98	0.45
1:H:11:GLU:O	1:H:15:GLN:N	2.49	0.45
1:H:49:PHE:HB2	1:H:103:MET:HG3	1.97	0.45
1:B:52:ARG:HE	1:B:52:ARG:HB3	1.49	0.45
1:C:56:GLN:CG	1:C:95:PHE:CE2	2.97	0.45
1:G:79:THR:HG22	1:G:80:HIS:N	2.30	0.45
1:H:56:GLN:CG	1:H:95:PHE:CE2	2.99	0.45
1:E:62:HIS:CD2	1:E:88:ARG:HG2	2.51	0.45
1:E:95:PHE:CE2	1:E:99:VAL:CG2	2.97	0.45
1:H:15:GLN:HE21	1:H:15:GLN:HB2	1.30	0.45
1:A:34:ILE:CG2	1:A:85:LEU:CD2	2.94	0.45
1:B:49:PHE:N	1:B:103:MET:HE3	2.32	0.45
1:C:49:PHE:O	1:C:53:VAL:HG13	2.16	0.45
1:C:101:VAL:O	1:C:101:VAL:HG13	2.16	0.45
1:E:17:LEU:N	1:E:18:PRO:CD	2.80	0.45
1:E:43:PHE:CD2	1:F:63:HIS:NE2	2.84	0.45
1:E:88:ARG:HA	1:E:91:ASN:CB	2.44	0.45
1:F:8:LEU:HD13	1:F:86:SER:HA	1.97	0.45
1:F:12:GLU:C	1:F:15:GLN:HG3	2.41	0.45
1:E:20:LEU:HD13	1:E:93:ALA:HB1	1.99	0.45
1:F:17:LEU:N	1:F:18:PRO:HD2	2.32	0.45
1:H:82:CYS:O	1:H:83:ALA:HB3	2.16	0.45
1:A:38:PHE:CD1	1:A:38:PHE:N	2.81	0.45
1:A:53:VAL:CG1	1:A:66:TRP:CZ3	3.00	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:8:LEU:HA	1:D:8:LEU:HD12	1.29	0.45
1:E:17:LEU:O	1:E:21:ARG:N	2.40	0.45
1:F:17:LEU:HD11	1:F:34:ILE:CD1	2.47	0.45
1:F:77:LEU:O	1:F:78:SER:HB2	2.16	0.45
1:G:79:THR:CG2	1:G:80:HIS:N	2.79	0.45
1:H:51:THR:HG22	1:H:51:THR:O	2.16	0.45
1:B:20:LEU:HD21	1:B:93:ALA:HB3	1.99	0.45
1:B:37:GLN:CD	1:B:74:HIS:HE2	2.24	0.45
1:B:41:LYS:HE3	1:B:45:ARG:HH12	1.82	0.45
1:E:96:ILE:O	1:E:96:ILE:HG22	2.17	0.45
1:H:9:SER:O	1:H:13:ARG:HG3	2.17	0.45
1:B:8:LEU:CD1	1:B:90:ILE:HG13	2.46	0.45
1:G:69:VAL:HG13	1:H:65:GLU:HB3	1.99	0.45
1:G:82:CYS:SG	1:G:83:ALA:N	2.88	0.45
1:A:41:LYS:CE	1:A:45:ARG:HH12	2.30	0.44
1:A:67:PHE:O	1:A:73:VAL:HA	2.17	0.44
1:A:87:GLU:CD	1:A:87:GLU:N	2.72	0.44
1:B:20:LEU:HD12	1:B:20:LEU:HA	1.78	0.44
1:B:41:LYS:HE3	1:B:45:ARG:NH2	2.32	0.44
1:C:98:GLN:O	1:C:101:VAL:N	2.41	0.44
1:F:103:MET:HB3	1:F:104:THR:H	1.31	0.44
1:A:17:LEU:CB	1:A:21:ARG:CZ	2.96	0.44
1:B:25:TRP:CZ3	1:B:77:LEU:CD1	3.00	0.44
1:E:20:LEU:O	1:E:23:VAL:HG12	2.17	0.44
1:F:33:ALA:HB1	1:F:76:THR:HG23	2.00	0.44
1:H:33:ALA:HB1	1:H:76:THR:HG22	1.99	0.44
1:F:88:ARG:H	1:F:88:ARG:HG2	1.27	0.44
1:G:39:HIS:ND1	1:G:39:HIS:C	2.75	0.44
1:H:62:HIS:CE1	1:H:88:ARG:CG	2.99	0.44
1:F:66:TRP:N	1:F:66:TRP:CD1	2.82	0.44
1:H:35:PHE:HA	1:H:75:ILE:O	2.18	0.44
1:A:23:VAL:HG12	1:A:23:VAL:O	2.16	0.44
1:B:86:SER:OG	1:B:88:ARG:HB2	2.16	0.44
1:G:28:LEU:HD11	1:G:33:ALA:HB3	1.99	0.44
1:B:70:TYR:CD2	1:B:71:ASN:ND2	2.86	0.44
1:F:8:LEU:CD2	1:F:90:ILE:CD1	2.96	0.44
1:G:7:ARG:HG3	1:G:82:CYS:HB2	2.00	0.44
1:E:30:GLY:O	1:E:31:ARG:HB3	2.17	0.44
1:H:57:ALA:O	1:H:61:ASP:N	2.51	0.44
1:D:99:VAL:O	1:D:101:VAL:N	2.51	0.44
1:B:8:LEU:HD11	1:B:90:ILE:HG13	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:LEU:HA	1:B:17:LEU:HD12	1.65	0.43
1:F:77:LEU:HD22	1:F:92:LEU:HD23	1.99	0.43
1:D:28:LEU:HD13	1:D:35:PHE:HB3	1.99	0.43
1:H:28:LEU:HD23	1:H:28:LEU:HA	1.82	0.43
1:F:8:LEU:HD22	1:F:85:LEU:HB3	1.99	0.43
1:G:13:ARG:NH2	1:G:32:ASP:OD2	2.51	0.43
1:G:87:GLU:H	1:G:87:GLU:HG2	1.58	0.43
1:C:23:VAL:HG12	1:C:36:LYS:HZ2	1.81	0.43
1:C:35:PHE:CZ	1:C:74:HIS:CD2	3.06	0.43
1:C:36:LYS:HE2	1:C:38:PHE:CE2	2.53	0.43
1:E:86:SER:C	1:E:88:ARG:H	2.25	0.43
1:G:11:GLU:O	1:G:15:GLN:N	2.51	0.43
1:A:20:LEU:HD23	1:A:20:LEU:HA	1.70	0.43
1:D:91:ASN:H	1:D:91:ASN:HD22	1.66	0.43
1:E:20:LEU:HD23	1:E:20:LEU:HA	1.72	0.43
1:B:58:GLU:O	1:C:59:LYS:HG3	2.18	0.43
1:C:98:GLN:C	1:C:100:ALA:N	2.76	0.43
1:E:8:LEU:HD22	1:E:85:LEU:HD12	2.01	0.43
1:G:32:ASP:O	1:G:78:SER:HB2	2.18	0.43
1:B:101:VAL:CG2	1:B:102:SER:H	2.27	0.43
1:C:39:HIS:CD2	1:C:71:ASN:ND2	2.87	0.43
1:G:8:LEU:H	1:G:8:LEU:HG	1.65	0.43
1:G:27:GLU:HA	1:G:34:ILE:HG22	2.00	0.43
1:B:79:THR:OG1	1:B:86:SER:HB3	2.18	0.43
1:G:79:THR:N	1:G:89:ASP:OD2	2.52	0.43
1:A:23:VAL:HG12	1:A:36:LYS:HZ1	1.82	0.43
1:B:16:LEU:HG	1:B:90:ILE:HG21	2.01	0.43
1:D:11:GLU:HG2	1:D:15:GLN:HE22	1.80	0.42
1:D:56:GLN:HG3	1:D:60:LEU:HD21	1.99	0.42
1:E:28:LEU:CD1	1:E:33:ALA:HB3	2.43	0.42
1:E:72:LYS:HB2	1:E:72:LYS:HE3	1.38	0.42
1:F:79:THR:HA	2:F:200:SO4:O1	2.19	0.42
1:G:67:PHE:CD1	1:G:67:PHE:C	2.97	0.42
1:B:17:LEU:N	1:B:18:PRO:CD	2.83	0.42
1:C:53:VAL:HG22	1:C:66:TRP:CZ3	2.54	0.42
1:A:34:ILE:HG21	1:A:34:ILE:HD12	1.75	0.42
1:B:49:PHE:HB2	1:B:103:MET:HG3	2.02	0.42
1:B:58:GLU:HG2	1:C:55:LEU:HD23	2.01	0.42
1:C:45:ARG:HG2	1:C:103:MET:CG	2.48	0.42
1:C:94:SER:O	1:C:98:GLN:OE1	2.37	0.42
1:E:21:ARG:NH2	1:E:27:GLU:OE2	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:49:PHE:HE1	1:F:96:ILE:HG23	1.77	0.42
1:F:57:ALA:O	1:F:61:ASP:N	2.52	0.42
1:A:34:ILE:CG2	1:A:85:LEU:CD1	2.95	0.42
1:C:85:LEU:HA	1:C:85:LEU:HD12	1.58	0.42
1:E:55:LEU:HD23	1:H:55:LEU:CD1	2.50	0.42
1:H:103:MET:N	1:H:103:MET:CE	2.80	0.42
1:A:18:PRO:O	1:A:21:ARG:HB2	2.20	0.42
1:C:67:PHE:CD1	1:C:67:PHE:C	2.96	0.42
1:D:35:PHE:CD1	1:D:35:PHE:N	2.88	0.42
1:D:91:ASN:H	1:D:91:ASN:ND2	2.18	0.42
1:E:62:HIS:HD2	1:E:88:ARG:O	2.03	0.42
1:H:35:PHE:CG	1:H:36:LYS:N	2.87	0.42
1:A:32:ASP:O	1:A:78:SER:OG	2.31	0.42
1:E:12:GLU:O	1:E:15:GLN:HB3	2.20	0.42
1:G:51:THR:O	1:G:55:LEU:HD23	2.19	0.42
1:H:8:LEU:HD12	1:H:8:LEU:HA	1.38	0.42
1:H:56:GLN:CG	1:H:95:PHE:CD2	3.00	0.42
1:A:13:ARG:NH2	1:A:32:ASP:OD2	2.44	0.42
1:B:42:ASP:OD1	1:B:45:ARG:HB2	2.20	0.42
1:B:62:HIS:ND1	2:B:200:SO4:O2	2.41	0.42
1:D:94:SER:HA	1:D:97:GLU:HB2	2.01	0.42
1:G:87:GLU:O	1:G:91:ASN:N	2.48	0.42
1:D:49:PHE:HD1	1:D:99:VAL:CG1	2.33	0.42
1:E:26:ASN:O	1:E:35:PHE:CE1	2.73	0.42
1:E:36:LYS:HD2	1:E:38:PHE:CZ	2.54	0.42
1:G:19:ASN:ND2	1:G:19:ASN:N	2.65	0.42
1:A:34:ILE:CG2	1:A:85:LEU:HD21	2.48	0.42
1:B:101:VAL:CG2	1:B:102:SER:N	2.80	0.42
1:B:48:GLY:HA3	1:D:52:ARG:CG	2.50	0.42
1:F:17:LEU:CD1	1:F:34:ILE:CD1	2.97	0.42
1:A:95:PHE:CD1	1:A:95:PHE:C	2.98	0.41
1:A:99:VAL:C	1:A:101:VAL:N	2.78	0.41
1:F:99:VAL:O	1:F:103:MET:HE3	2.20	0.41
1:H:98:GLN:HE21	1:H:98:GLN:C	2.27	0.41
1:B:21:ARG:CG	1:B:21:ARG:HH11	2.33	0.41
1:B:40:PHE:O	1:B:71:ASN:HB2	2.20	0.41
1:D:15:GLN:HE21	1:D:15:GLN:HB3	1.65	0.41
1:B:28:LEU:CD2	1:B:35:PHE:CB	2.98	0.41
1:B:41:LYS:HE3	1:B:45:ARG:HH22	1.85	0.41
1:H:25:TRP:NE1	1:H:97:GLU:OE2	2.46	0.41
1:A:13:ARG:NH2	1:A:32:ASP:OD1	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:ALA:HA	1:A:96:ILE:HG13	2.01	0.41
1:D:39:HIS:CD2	1:D:40:PHE:O	2.73	0.41
1:E:20:LEU:CD1	1:E:93:ALA:HB1	2.50	0.41
1:F:56:GLN:HE21	1:F:56:GLN:CA	2.31	0.41
1:G:15:GLN:HE21	1:G:15:GLN:HB3	1.46	0.41
1:G:27:GLU:HA	1:G:34:ILE:HA	2.03	0.41
1:A:99:VAL:O	1:A:102:SER:HB2	2.20	0.41
1:E:16:LEU:HD12	1:E:90:ILE:HD12	2.03	0.41
1:F:21:ARG:C	1:F:23:VAL:N	2.78	0.41
1:G:77:LEU:CD2	1:G:92:LEU:HD23	2.50	0.41
1:A:14:ASP:O	1:A:18:PRO:HD3	2.21	0.41
1:A:34:ILE:HG23	1:A:85:LEU:HD13	2.02	0.41
1:G:45:ARG:HH11	1:G:45:ARG:HD2	1.75	0.41
1:B:62:HIS:NE2	1:B:89:ASP:OD1	2.54	0.41
1:C:95:PHE:CD1	1:C:95:PHE:C	2.98	0.41
1:D:38:PHE:CE2	1:D:100:ALA:HB2	2.56	0.41
1:D:75:ILE:CD1	1:D:96:ILE:CD1	2.99	0.41
1:C:67:PHE:HB2	1:D:67:PHE:HD1	1.85	0.41
1:F:68:ASN:HA	1:F:72:LYS:O	2.19	0.41
1:H:32:ASP:HB3	1:H:84:GLY:CA	2.51	0.41
1:B:13:ARG:O	1:B:17:LEU:N	2.53	0.41
1:E:32:ASP:O	1:E:84:GLY:HA2	2.21	0.41
1:E:35:PHE:CD1	1:E:35:PHE:N	2.88	0.41
1:F:67:PHE:CD1	1:F:67:PHE:C	2.98	0.41
1:H:67:PHE:CZ	1:H:69:VAL:CG2	3.04	0.41
1:B:56:GLN:C	1:B:58:GLU:N	2.78	0.41
1:D:13:ARG:HG2	1:D:13:ARG:H	1.53	0.41
1:H:35:PHE:O	1:H:36:LYS:HB2	2.21	0.41
1:A:7:ARG:HB2	1:A:82:CYS:HB2	2.03	0.40
1:D:66:TRP:CD1	1:D:66:TRP:H	2.39	0.40
1:F:17:LEU:CB	1:F:21:ARG:HH21	2.33	0.40
1:G:35:PHE:CD2	1:G:35:PHE:C	2.99	0.40
1:G:65:GLU:HG3	1:G:76:THR:HB	2.03	0.40
1:A:62:HIS:CD2	1:A:88:ARG:CG	3.04	0.40
1:B:21:ARG:HH11	1:B:21:ARG:HG2	1.86	0.40
1:B:47:PHE:HA	1:B:50:MET:HB2	2.03	0.40
1:D:25:TRP:HE1	1:D:97:GLU:HG2	1.87	0.40
1:E:62:HIS:ND1	2:E:200:SO4:O4	2.55	0.40
1:C:12:GLU:C	1:C:14:ASP:N	2.79	0.40
1:C:37:GLN:HB3	1:C:74:HIS:CD2	2.56	0.40
1:D:32:ASP:HB3	1:D:84:GLY:HA2	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:13:ARG:HB3	1:E:14:ASP:H	1.52	0.40
1:E:92:LEU:O	1:E:96:ILE:HG13	2.21	0.40
1:G:35:PHE:HB2	1:G:75:ILE:O	2.21	0.40
1:C:53:VAL:HG22	1:C:66:TRP:HH2	1.86	0.40
1:E:32:ASP:HB3	1:E:84:GLY:HA3	2.02	0.40
1:G:6:HIS:N	1:G:82:CYS:HB3	2.36	0.40
1:G:42:ASP:OD1	1:G:45:ARG:NE	2.54	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	97/104 (93%)	76 (78%)	16 (16%)	5 (5%)	1	9
1	B	97/104 (93%)	77 (79%)	15 (16%)	5 (5%)	1	9
1	C	97/104 (93%)	71 (73%)	22 (23%)	4 (4%)	2	13
1	D	97/104 (93%)	78 (80%)	13 (13%)	6 (6%)	1	6
1	E	97/104 (93%)	75 (77%)	13 (13%)	9 (9%)	0	2
1	F	97/104 (93%)	78 (80%)	11 (11%)	8 (8%)	0	3
1	G	97/104 (93%)	82 (84%)	11 (11%)	4 (4%)	2	13
1	H	97/104 (93%)	82 (84%)	11 (11%)	4 (4%)	2	13
All	All	776/832 (93%)	619 (80%)	112 (14%)	45 (6%)	1	8

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	ARG
1	A	78	SER
1	B	9	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	17	LEU
1	D	10	ALA
1	D	88	ARG
1	E	12	GLU
1	E	13	ARG
1	E	14	ASP
1	E	78	SER
1	F	7	ARG
1	G	83	ALA
1	G	103	MET
1	A	36	LYS
1	B	23	VAL
1	C	16	LEU
1	D	8	LEU
1	D	100	ALA
1	E	8	LEU
1	E	10	ALA
1	E	103	MET
1	F	78	SER
1	F	81	GLU
1	G	82	CYS
1	H	7	ARG
1	A	18	PRO
1	B	100	ALA
1	D	22	ALA
1	E	102	SER
1	F	8	LEU
1	F	52	ARG
1	F	103	MET
1	H	15	GLN
1	E	83	ALA
1	H	69	VAL
1	H	81	GLU
1	A	8	LEU
1	F	51	THR
1	B	18	PRO
1	B	103	MET
1	C	19	ASN
1	C	18	PRO
1	D	90	ILE
1	F	69	VAL
1	G	69	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	84/88 (96%)	57 (68%)	27 (32%)	0	1
1	B	84/88 (96%)	55 (66%)	29 (34%)	0	1
1	C	85/88 (97%)	53 (62%)	32 (38%)	0	1
1	D	83/88 (94%)	60 (72%)	23 (28%)	0	2
1	E	83/88 (94%)	55 (66%)	28 (34%)	0	1
1	F	84/88 (96%)	61 (73%)	23 (27%)	0	2
1	G	85/88 (97%)	60 (71%)	25 (29%)	0	2
1	H	85/88 (97%)	60 (71%)	25 (29%)	0	2
All	All	673/704 (96%)	461 (68%)	212 (32%)	0	1

All (212) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ARG
1	A	13	ARG
1	A	16	LEU
1	A	34	ILE
1	A	36	LYS
1	A	37	GLN
1	A	41	LYS
1	A	42	ASP
1	A	51	THR
1	A	52	ARG
1	A	55	LEU
1	A	56	GLN
1	A	61	ASP
1	A	66	TRP
1	A	72	LYS
1	A	73	VAL
1	A	75	ILE
1	A	80	HIS
1	A	81	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	87	GLU
1	A	89	ASP
1	A	90	ILE
1	A	96	ILE
1	A	98	GLN
1	A	99	VAL
1	A	103	MET
1	A	104	THR
1	B	7	ARG
1	B	16	LEU
1	B	17	LEU
1	B	19	ASN
1	B	20	LEU
1	B	21	ARG
1	B	23	VAL
1	B	26	ASN
1	B	28	LEU
1	B	29	GLU
1	B	31	ARG
1	B	34	ILE
1	B	37	GLN
1	B	41	LYS
1	B	45	ARG
1	B	49	PHE
1	B	50	MET
1	B	52	ARG
1	B	55	LEU
1	B	56	GLN
1	B	58	GLU
1	B	66	TRP
1	B	68	ASN
1	B	72	LYS
1	B	77	LEU
1	B	81	GLU
1	B	82	CYS
1	B	96	ILE
1	B	102	SER
1	C	7	ARG
1	C	11	GLU
1	C	14	ASP
1	C	16	LEU
1	C	17	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	20	LEU
1	C	26	ASN
1	C	27	GLU
1	C	31	ARG
1	C	39	HIS
1	C	41	LYS
1	C	42	ASP
1	C	53	VAL
1	C	55	LEU
1	C	56	GLN
1	C	59	LYS
1	C	60	LEU
1	C	61	ASP
1	C	65	GLU
1	C	66	TRP
1	C	72	LYS
1	C	77	LEU
1	C	82	CYS
1	C	85	LEU
1	C	87	GLU
1	C	88	ARG
1	C	90	ILE
1	C	94	SER
1	C	101	VAL
1	C	102	SER
1	C	103	MET
1	C	104	THR
1	D	9	SER
1	D	11	GLU
1	D	13	ARG
1	D	15	GLN
1	D	16	LEU
1	D	21	ARG
1	D	23	VAL
1	D	26	ASN
1	D	28	LEU
1	D	36	LYS
1	D	37	GLN
1	D	41	LYS
1	D	42	ASP
1	D	45	ARG
1	D	55	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	58	GLU
1	D	66	TRP
1	D	72	LYS
1	D	81	GLU
1	D	90	ILE
1	D	96	ILE
1	D	103	MET
1	D	104	THR
1	E	7	ARG
1	E	8	LEU
1	E	9	SER
1	E	15	GLN
1	E	19	ASN
1	E	21	ARG
1	E	23	VAL
1	E	26	ASN
1	E	27	GLU
1	E	29	GLU
1	E	31	ARG
1	E	34	ILE
1	E	36	LYS
1	E	41	LYS
1	E	45	ARG
1	E	56	GLN
1	E	59	LYS
1	E	72	LYS
1	E	81	GLU
1	E	82	CYS
1	E	85	LEU
1	E	87	GLU
1	E	88	ARG
1	E	92	LEU
1	E	94	SER
1	E	102	SER
1	E	103	MET
1	E	104	THR
1	F	8	LEU
1	F	9	SER
1	F	11	GLU
1	F	13	ARG
1	F	15	GLN
1	F	19	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	20	LEU
1	F	26	ASN
1	F	28	LEU
1	F	29	GLU
1	F	34	ILE
1	F	37	GLN
1	F	58	GLU
1	F	59	LYS
1	F	75	ILE
1	F	81	GLU
1	F	88	ARG
1	F	90	ILE
1	F	94	SER
1	F	101	VAL
1	F	102	SER
1	F	103	MET
1	F	104	THR
1	G	11	GLU
1	G	15	GLN
1	G	23	VAL
1	G	27	GLU
1	G	28	LEU
1	G	31	ARG
1	G	41	LYS
1	G	45	ARG
1	G	50	MET
1	G	52	ARG
1	G	55	LEU
1	G	65	GLU
1	G	66	TRP
1	G	67	PHE
1	G	68	ASN
1	G	69	VAL
1	G	72	LYS
1	G	76	THR
1	G	78	SER
1	G	86	SER
1	G	96	ILE
1	G	98	GLN
1	G	101	VAL
1	G	103	MET
1	G	104	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	8	LEU
1	H	12	GLU
1	H	14	ASP
1	H	15	GLN
1	H	19	ASN
1	H	21	ARG
1	H	31	ARG
1	H	36	LYS
1	H	37	GLN
1	H	41	LYS
1	H	56	GLN
1	H	60	LEU
1	H	66	TRP
1	H	68	ASN
1	H	69	VAL
1	H	75	ILE
1	H	79	THR
1	H	80	HIS
1	H	88	ARG
1	H	91	ASN
1	H	96	ILE
1	H	98	GLN
1	H	102	SER
1	H	103	MET
1	H	104	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	ASN
1	A	37	GLN
1	A	74	HIS
1	A	98	GLN
1	B	19	ASN
1	B	26	ASN
1	C	19	ASN
1	C	26	ASN
1	C	39	HIS
1	C	56	GLN
1	C	91	ASN
1	C	98	GLN
1	D	15	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	26	ASN
1	D	37	GLN
1	D	39	HIS
1	D	62	HIS
1	D	80	HIS
1	D	91	ASN
1	E	19	ASN
1	E	26	ASN
1	E	56	GLN
1	E	91	ASN
1	F	15	GLN
1	F	19	ASN
1	F	56	GLN
1	F	80	HIS
1	G	15	GLN
1	G	19	ASN
1	G	56	GLN
1	G	68	ASN
1	G	74	HIS
1	G	91	ASN
1	H	15	GLN
1	H	19	ASN
1	H	26	ASN
1	H	56	GLN
1	H	63	HIS
1	H	98	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

8 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	$\# Z > 2$
2	SO4	D	200	-	4,4,4	0.84	0	6,6,6	0.33	0
2	SO4	C	200	-	4,4,4	0.88	0	6,6,6	0.39	0
2	SO4	B	200	-	4,4,4	0.97	0	6,6,6	0.37	0
2	SO4	F	200	-	4,4,4	0.71	0	6,6,6	0.19	0
2	SO4	E	200	-	4,4,4	0.99	0	6,6,6	0.22	0
2	SO4	G	200	-	4,4,4	0.65	0	6,6,6	0.35	0
2	SO4	H	200	-	4,4,4	0.94	0	6,6,6	0.50	0
2	SO4	A	200	-	4,4,4	0.68	0	6,6,6	0.35	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	200	SO4	1	0
2	F	200	SO4	3	0
2	E	200	SO4	1	0
2	G	200	SO4	2	0
2	H	200	SO4	1	0
2	A	200	SO4	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.