



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:01 AM UTC

PDB ID : 2CG8 / pdb_00002cg8
Title : The bifunctional dihydroneopterin aldolase 6-hydroxymethyl-7,8- dihydropterin synthase from *Streptococcus pneumoniae*
Authors : Garcon, A.; Levy, C.; Derrick, J.P.
Deposited on : 2006-02-28
Resolution : 2.90 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
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

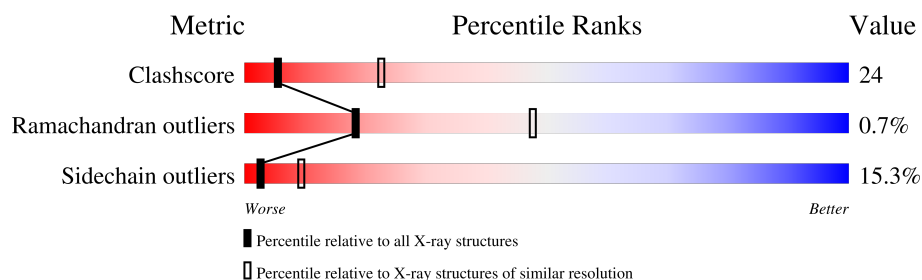
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)

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	270	39% 31% 16% • 11%
1	B	270	38% 37% 12% 5% 8%
1	C	270	38% 35% 16% • 8%
1	D	270	45% 31% 12% • 8%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7968 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 DIHYDRONEOPTERIN ALDOLASE 6-HYDROXYMETHYL-7,8-DIHYDROPTERIN SYNTHASE.

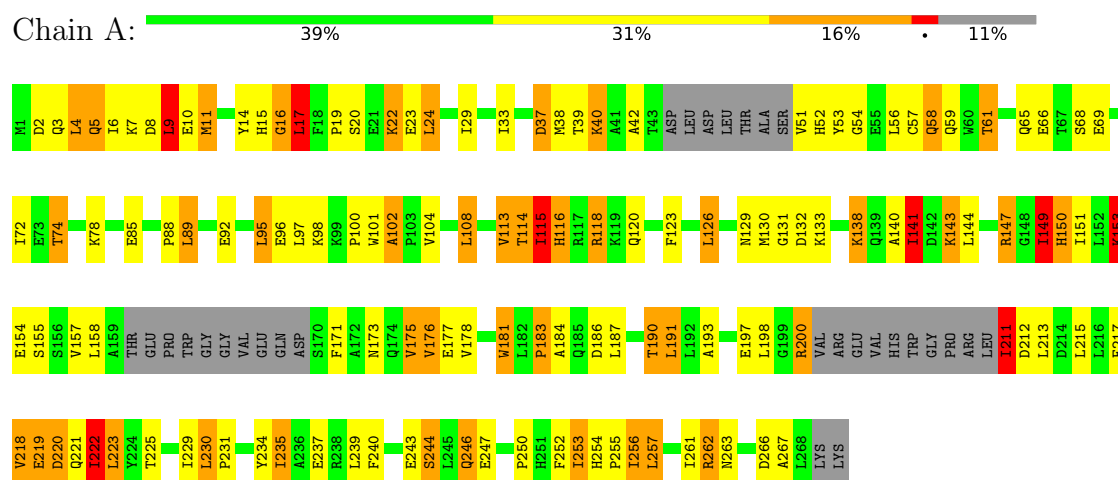
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	241	Total	C	N	O	S	0	0	1
			1953	1263	321	362	7			
1	B	248	Total	C	N	O	S	0	0	1
			2006	1293	331	375	7			
1	C	249	Total	C	N	O	S	0	0	1
			2011	1299	329	376	7			
1	D	248	Total	C	N	O	S	0	0	2
			1998	1289	331	371	7			

3 Residue-property plots

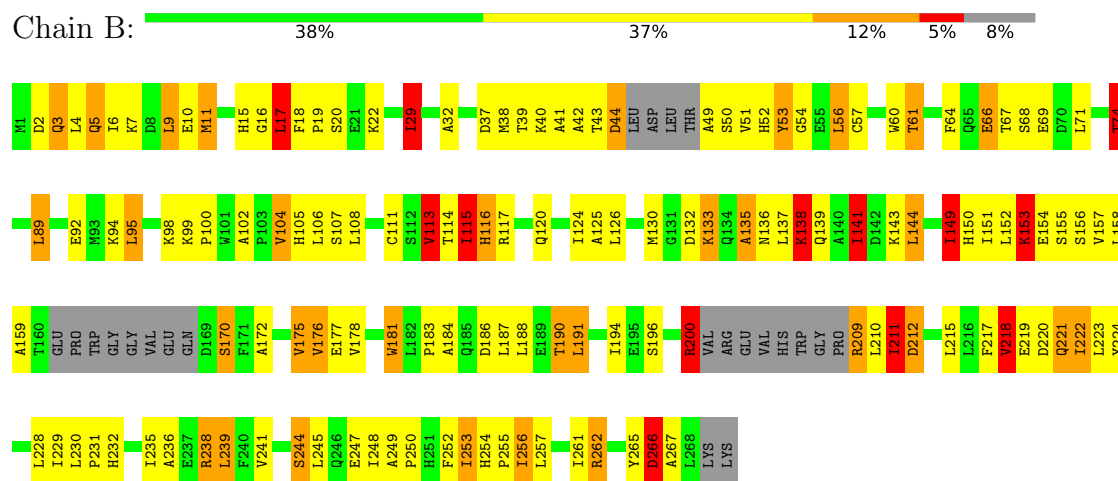
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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.

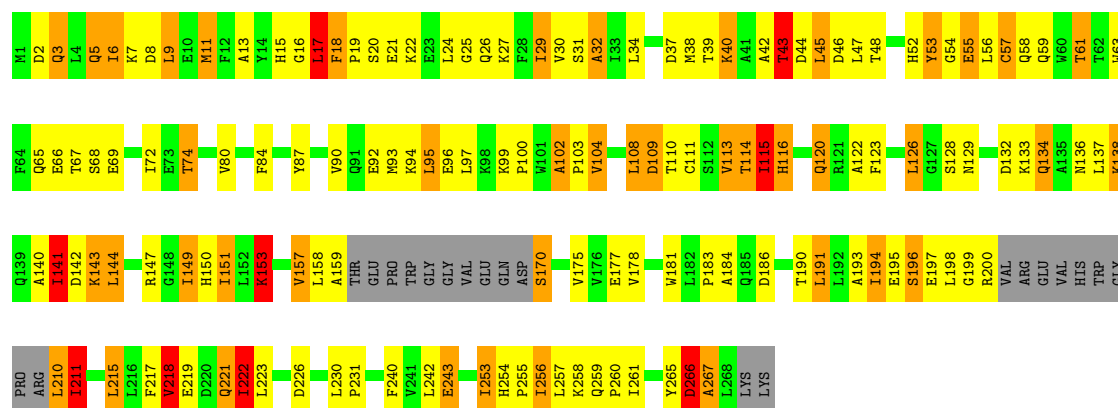
- Molecule 1: DIHYDRONEOPTERIN ALDOLASE 6-HYDROXYMETHYL-7,8-DIHYDROPTERIN SYNTHASE



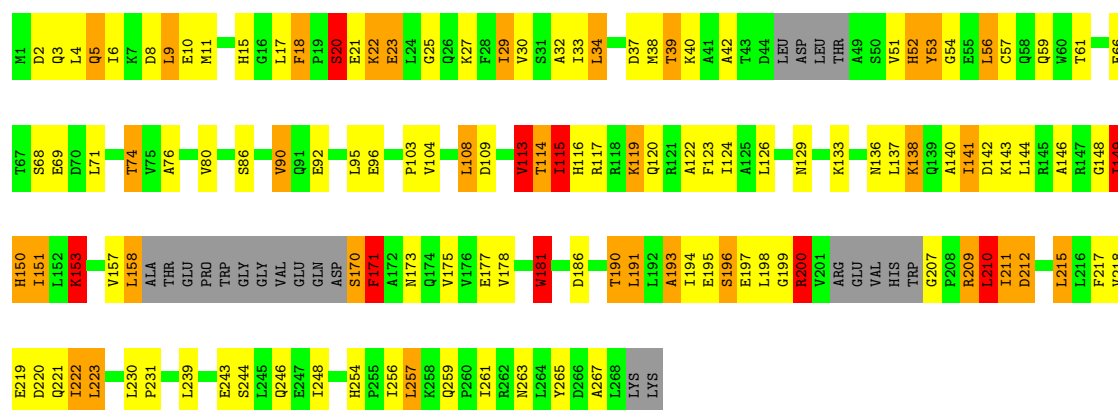
- Molecule 1: DIHYDRONEOPTERIN ALDOLASE 6-HYDROXYMETHYL-7,8-DIHYDROPTERIN SYNTHASE



- Molecule 1: DIHYDRONEOPTERIN ALDOLASE 6-HYDROXYMETHYL-7,8-DIHYDROPTERIN SYNTHASE



Chain D: 45% 31% 12% • 8%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	149.44Å 149.44Å 238.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	127.00 – 2.90	Depositor
% Data completeness (in resolution range)	99.8 (127.00-2.90)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.215 , 0.241	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7968	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	2.08	56/1993 (2.8%)	1.91	60/2700 (2.2%)
1	B	2.16	58/2046 (2.8%)	1.92	63/2772 (2.3%)
1	C	2.00	46/2052 (2.2%)	1.89	59/2783 (2.1%)
1	D	2.01	49/2039 (2.4%)	1.85	52/2763 (1.9%)
All	All	2.06	209/8130 (2.6%)	1.89	234/11018 (2.1%)

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	B	0	1
1	D	0	1
All	All	0	2

All (209) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	194	ILE	CA-CB	-12.76	1.40	1.54
1	C	13	ALA	CA-CB	-10.27	1.40	1.53
1	A	153	LYS	CG-CD	9.80	1.81	1.52
1	C	115	ILE	CA-CB	9.65	1.66	1.54
1	A	154	GLU	C-O	-9.59	1.12	1.23
1	A	108	LEU	C-O	-9.57	1.13	1.23
1	D	115	ILE	CA-CB	9.55	1.65	1.54
1	B	153	LYS	CG-CD	9.24	1.80	1.52
1	B	17	LEU	N-CA	9.06	1.57	1.46
1	C	61	THR	CA-C	8.94	1.64	1.52
1	D	153	LYS	CD-CE	8.76	1.78	1.52
1	A	141	ILE	CG1-CD1	8.72	1.85	1.51
1	B	141	ILE	CG1-CD1	8.68	1.85	1.51
1	B	209	ARG	N-CA	8.33	1.62	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	85	GLU	C-O	-8.25	1.14	1.24
1	A	29	ILE	CG1-CD1	-8.19	1.19	1.51
1	C	153	LYS	CD-CE	8.19	1.77	1.52
1	D	109	ASP	C-O	-8.18	1.14	1.24
1	A	52	HIS	N-CA	8.15	1.55	1.45
1	D	53	TYR	CA-C	-8.01	1.42	1.53
1	A	17	LEU	CG-CD1	7.97	1.78	1.52
1	B	32	ALA	CA-CB	-7.91	1.39	1.54
1	B	267	ALA	CA-C	7.79	1.69	1.52
1	C	32	ALA	CA-CB	-7.76	1.39	1.54
1	D	141	ILE	CG1-CD1	7.72	1.81	1.51
1	A	253	ILE	CG1-CD1	-7.71	1.21	1.51
1	A	61	THR	N-CA	-7.70	1.36	1.46
1	D	68	SER	C-O	7.67	1.32	1.24
1	A	141	ILE	CA-CB	7.60	1.66	1.54
1	C	116	HIS	C-O	-7.60	1.15	1.24
1	B	50	SER	CA-C	7.59	1.61	1.52
1	C	184	ALA	CA-CB	-7.53	1.41	1.53
1	D	52	HIS	N-CA	7.52	1.54	1.45
1	A	40	LYS	C-O	-7.51	1.15	1.24
1	A	68	SER	CA-C	-7.50	1.43	1.53
1	C	68	SER	CA-C	-7.49	1.43	1.52
1	B	149	ILE	CA-C	7.46	1.60	1.52
1	A	17	LEU	N-CA	7.44	1.55	1.46
1	D	181	TRP	CD2-CE2	7.42	1.53	1.41
1	C	151	ILE	C-O	-7.38	1.16	1.24
1	B	154	GLU	C-O	-7.37	1.15	1.23
1	D	248	ILE	CA-CB	-7.36	1.45	1.54
1	B	181	TRP	CD2-CE2	7.31	1.53	1.41
1	B	115	ILE	CB-CG1	-7.28	1.38	1.53
1	A	149	ILE	CA-C	7.21	1.60	1.52
1	C	153	LYS	CG-CD	7.21	1.74	1.52
1	B	51	VAL	CA-C	7.15	1.60	1.53
1	D	222	ILE	C-O	-7.12	1.16	1.24
1	B	236	ALA	C-O	-7.10	1.13	1.24
1	A	229	ILE	CA-CB	-7.09	1.45	1.54
1	B	138	LYS	CE-NZ	7.08	1.70	1.49
1	A	102	ALA	N-CA	-6.99	1.37	1.45
1	B	102	ALA	CA-CB	-6.98	1.44	1.53
1	D	181	TRP	CG-CD2	-6.98	1.31	1.43
1	C	259	GLN	CA-CB	-6.97	1.45	1.53
1	B	159	ALA	CA-CB	-6.95	1.43	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	193	ALA	CA-CB	-6.95	1.42	1.53
1	C	159	ALA	C-O	6.95	1.37	1.23
1	A	235	ILE	CA-CB	-6.93	1.46	1.54
1	B	155	SER	CA-C	-6.93	1.43	1.53
1	D	212	ASP	CA-C	-6.91	1.44	1.52
1	A	153	LYS	CD-CE	6.88	1.73	1.52
1	A	181	TRP	CD2-CE2	6.84	1.52	1.41
1	B	209	ARG	CZ-NH2	6.80	1.42	1.33
1	A	240	PHE	CD1-CE1	6.77	1.58	1.38
1	B	61	THR	CA-C	6.73	1.61	1.52
1	D	66	GLU	C-O	-6.67	1.16	1.24
1	C	109	ASP	N-CA	-6.64	1.37	1.46
1	D	5	GLN	CA-C	-6.58	1.44	1.52
1	A	219	GLU	CD-OE2	6.55	1.37	1.25
1	A	16	GLY	C-O	6.55	1.32	1.23
1	C	26	GLN	N-CA	-6.55	1.38	1.46
1	B	68	SER	CA-C	-6.52	1.44	1.52
1	B	224	TYR	C-O	-6.51	1.16	1.23
1	A	6	ILE	C-O	-6.49	1.17	1.24
1	C	55	GLU	CD-OE2	6.49	1.37	1.25
1	D	153	LYS	CE-NZ	6.43	1.68	1.49
1	D	149	ILE	C-O	-6.42	1.16	1.24
1	A	61	THR	CA-C	6.39	1.61	1.52
1	C	111	CYS	CA-C	-6.37	1.45	1.52
1	D	22	LYS	CD-CE	6.37	1.71	1.52
1	C	181	TRP	CG-CD1	6.36	1.52	1.36
1	B	51	VAL	CA-CB	-6.36	1.45	1.54
1	B	255	PRO	N-CA	6.35	1.55	1.47
1	C	120	GLN	CA-C	6.35	1.60	1.52
1	A	181	TRP	CG-CD1	6.31	1.52	1.36
1	A	247	GLU	C-O	-6.29	1.16	1.24
1	B	115	ILE	CA-CB	6.29	1.61	1.54
1	D	173	ASN	CA-C	-6.26	1.45	1.52
1	B	247	GLU	C-O	-6.25	1.16	1.24
1	D	219	GLU	CD-OE1	6.24	1.37	1.25
1	D	149	ILE	CA-C	6.22	1.59	1.52
1	D	86	SER	C-O	-6.20	1.15	1.24
1	C	57	CYS	CA-C	-6.16	1.44	1.52
1	A	65	GLN	C-O	-6.15	1.15	1.23
1	D	265	TYR	C-O	-6.15	1.16	1.24
1	C	104	VAL	CA-CB	-6.14	1.47	1.54
1	A	183	PRO	CA-C	6.09	1.59	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	109	ASP	N-CA	-6.07	1.39	1.46
1	B	184	ALA	CA-CB	-6.05	1.44	1.53
1	C	223	LEU	CA-C	-6.05	1.45	1.52
1	B	256	ILE	CA-C	-6.00	1.44	1.52
1	B	50	SER	C-O	6.00	1.31	1.23
1	D	219	GLU	CD-OE2	5.99	1.36	1.25
1	A	116	HIS	C-O	-5.96	1.17	1.23
1	C	108	LEU	C-O	-5.93	1.17	1.23
1	A	150	HIS	N-CA	5.88	1.53	1.46
1	C	193	ALA	CA-CB	-5.86	1.44	1.53
1	D	80	VAL	CA-CB	-5.85	1.47	1.54
1	C	3	GLN	CA-C	-5.85	1.45	1.52
1	D	122	ALA	CA-CB	-5.84	1.44	1.54
1	B	172	ALA	CA-CB	-5.84	1.44	1.53
1	D	207	GLY	N-CA	5.82	1.54	1.45
1	D	209	ARG	CB-CG	-5.82	1.35	1.52
1	B	223	LEU	CG-CD2	5.81	1.71	1.52
1	D	20	SER	CB-OG	5.81	1.53	1.42
1	A	222	ILE	C-O	-5.81	1.17	1.24
1	B	19	PRO	CA-C	5.80	1.62	1.52
1	A	22	LYS	CA-C	-5.79	1.45	1.52
1	A	212	ASP	N-CA	-5.78	1.39	1.46
1	A	225	THR	CA-C	-5.78	1.45	1.52
1	B	42	ALA	C-O	-5.77	1.16	1.24
1	C	259	GLN	C-O	-5.77	1.19	1.24
1	D	108	LEU	C-O	-5.77	1.16	1.23
1	C	122	ALA	CA-C	5.76	1.59	1.52
1	C	181	TRP	CG-CD2	-5.75	1.33	1.43
1	B	17	LEU	CG-CD1	5.74	1.71	1.52
1	B	94	LYS	CA-CB	-5.74	1.44	1.53
1	C	40	LYS	CE-NZ	5.72	1.66	1.49
1	C	29	ILE	CG1-CD1	-5.72	1.29	1.51
1	B	256	ILE	CG1-CD1	-5.71	1.29	1.51
1	A	237	GLU	C-O	-5.69	1.16	1.24
1	A	88	PRO	C-O	-5.68	1.16	1.24
1	A	54	GLY	C-O	5.68	1.30	1.23
1	A	223	LEU	CG-CD2	5.66	1.71	1.52
1	D	153	LYS	CG-CD	5.64	1.69	1.52
1	B	32	ALA	C-O	-5.64	1.16	1.23
1	B	116	HIS	C-O	-5.62	1.17	1.24
1	C	181	TRP	CD2-CE2	5.61	1.50	1.41
1	D	104	VAL	C-O	5.60	1.31	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	141	ILE	CA-CB	5.59	1.63	1.54
1	A	181	TRP	CG-CD2	-5.59	1.33	1.43
1	C	113	VAL	CA-C	-5.58	1.45	1.52
1	B	89	LEU	CG-CD1	5.57	1.71	1.52
1	C	259	GLN	N-CA	5.57	1.50	1.45
1	C	103	PRO	C-O	-5.57	1.16	1.24
1	B	44	ASP	C-O	5.56	1.34	1.23
1	C	80	VAL	CA-CB	-5.56	1.47	1.54
1	A	4	LEU	CA-C	-5.56	1.46	1.52
1	C	115	ILE	CB-CG1	-5.54	1.42	1.53
1	A	33	ILE	CA-CB	-5.53	1.47	1.54
1	A	131	GLY	C-O	5.53	1.31	1.23
1	C	267	ALA	N-CA	5.52	1.56	1.46
1	A	89	LEU	CG-CD2	5.52	1.70	1.52
1	C	141	ILE	CG1-CD1	5.51	1.73	1.51
1	D	42	ALA	CA-CB	-5.50	1.44	1.53
1	D	259	GLN	CA-CB	-5.50	1.47	1.53
1	D	199	GLY	N-CA	5.50	1.53	1.45
1	D	104	VAL	CA-CB	-5.49	1.47	1.54
1	B	183	PRO	C-O	-5.47	1.17	1.23
1	B	66	GLU	CD-OE1	5.45	1.35	1.25
1	A	37	ASP	CA-C	5.44	1.59	1.52
1	D	263	ASN	CA-C	-5.43	1.45	1.52
1	B	229	ILE	C-O	-5.43	1.18	1.24
1	D	115	ILE	C-O	-5.43	1.17	1.24
1	D	141	ILE	CA-CB	5.42	1.62	1.54
1	B	153	LYS	CD-CE	5.41	1.68	1.52
1	D	210	LEU	CA-C	-5.40	1.45	1.52
1	C	115	ILE	C-O	-5.38	1.18	1.24
1	B	125	ALA	CA-CB	-5.38	1.45	1.53
1	A	58	GLN	CG-CD	5.36	1.65	1.52
1	B	38	MET	C-O	-5.34	1.16	1.24
1	A	257	LEU	C-O	-5.34	1.17	1.24
1	A	51	VAL	N-CA	5.32	1.56	1.46
1	C	16	GLY	N-CA	5.31	1.50	1.45
1	B	29	ILE	CG1-CD1	-5.30	1.31	1.51
1	D	261	ILE	CA-CB	-5.27	1.48	1.54
1	D	181	TRP	CG-CD1	5.26	1.50	1.36
1	A	5	GLN	CA-C	-5.26	1.46	1.52
1	D	90	VAL	CA-CB	-5.25	1.48	1.54
1	B	200	ARG	NE-CZ	5.24	1.38	1.33
1	B	113	VAL	N-CA	-5.22	1.40	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	115	ILE	CB-CG1	-5.22	1.43	1.53
1	B	136	ASN	CA-C	-5.22	1.46	1.52
1	A	240	PHE	CD2-CE2	5.18	1.54	1.38
1	B	235	ILE	C-O	-5.18	1.18	1.24
1	C	29	ILE	N-CA	-5.16	1.40	1.46
1	D	5	GLN	C-O	-5.13	1.17	1.23
1	A	116	HIS	N-CA	5.13	1.52	1.46
1	B	135	ALA	CA-CB	-5.13	1.44	1.53
1	B	194	ILE	CA-C	5.12	1.59	1.52
1	D	103	PRO	CA-CB	-5.12	1.50	1.53
1	C	141	ILE	CA-C	5.10	1.59	1.52
1	B	94	LYS	CB-CG	-5.10	1.37	1.52
1	B	41	ALA	CA-CB	-5.09	1.45	1.53
1	B	10	GLU	C-O	-5.08	1.17	1.23
1	A	104	VAL	C-O	5.08	1.30	1.24
1	B	104	VAL	CA-CB	-5.08	1.47	1.54
1	D	157	VAL	C-O	-5.08	1.18	1.24
1	A	218	VAL	CB-CG1	-5.06	1.35	1.52
1	C	102	ALA	CA-CB	-5.06	1.45	1.53
1	B	6	ILE	C-O	-5.06	1.18	1.24
1	A	19	PRO	CA-C	5.06	1.60	1.52
1	B	138	LYS	CD-CE	5.05	1.67	1.52
1	C	19	PRO	CA-C	5.05	1.60	1.52
1	C	3	GLN	CA-CB	-5.05	1.45	1.53
1	A	85	GLU	CA-C	-5.03	1.46	1.52
1	D	151	ILE	C-O	-5.03	1.18	1.23
1	D	42	ALA	C-O	-5.00	1.17	1.24

All (234) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	143	LYS	N-CA-C	-10.28	100.16	111.36
1	C	53	TYR	CB-CA-C	-10.26	94.77	110.88
1	C	18	PHE	CA-C-N	-9.28	110.19	119.56
1	C	18	PHE	C-N-CA	-9.28	110.19	119.56
1	A	104	VAL	CA-C-N	-9.04	104.27	121.54
1	A	104	VAL	C-N-CA	-9.04	104.27	121.54
1	B	267	ALA	O-C-N	-8.67	109.12	123.00
1	C	211	ILE	CB-CA-C	-8.56	100.06	111.70
1	D	209	ARG	N-CA-C	8.54	124.07	111.34
1	B	220	ASP	N-CA-CB	-8.45	96.63	110.40
1	A	143	LYS	N-CA-C	-8.22	102.40	111.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	11	MET	CA-CB-CG	-8.17	97.76	114.10
1	B	209	ARG	NE-CZ-NH2	8.08	126.47	119.20
1	A	211	ILE	CB-CA-C	-8.02	95.56	111.60
1	C	102	ALA	CA-C-N	-8.01	109.83	119.84
1	C	102	ALA	C-N-CA	-8.01	109.83	119.84
1	D	141	ILE	N-CA-C	-8.00	101.06	111.05
1	A	253	ILE	N-CA-C	7.92	119.99	108.58
1	B	104	VAL	CA-C-N	-7.83	106.59	121.54
1	B	104	VAL	C-N-CA	-7.83	106.59	121.54
1	C	115	ILE	CA-CB-CG2	7.74	123.65	110.50
1	C	104	VAL	CA-C-N	-7.68	106.88	121.54
1	C	104	VAL	C-N-CA	-7.68	106.88	121.54
1	A	141	ILE	CB-CG1-CD1	7.38	129.31	113.80
1	B	104	VAL	CB-CA-C	-7.37	103.48	111.59
1	B	256	ILE	CA-CB-CG1	-7.36	97.89	110.40
1	C	219	GLU	CA-C-N	7.33	132.32	120.60
1	C	219	GLU	C-N-CA	7.33	132.32	120.60
1	D	219	GLU	CA-C-N	7.32	132.95	120.72
1	D	219	GLU	C-N-CA	7.32	132.95	120.72
1	A	252	PHE	CA-C-N	-7.17	113.12	122.37
1	A	252	PHE	C-N-CA	-7.17	113.12	122.37
1	D	23	GLU	N-CA-C	-7.17	102.88	111.69
1	B	51	VAL	CA-C-O	-7.11	113.38	121.98
1	A	78	LYS	N-CA-C	-7.07	103.50	111.14
1	D	113	VAL	CA-C-N	-7.01	112.91	122.86
1	D	113	VAL	C-N-CA	-7.01	112.91	122.86
1	B	115	ILE	CA-CB-CG2	6.96	122.34	110.50
1	D	200	ARG	CA-C-N	6.95	130.10	116.20
1	B	17	LEU	N-CA-CB	6.94	120.60	110.26
1	D	141	ILE	CB-CG1-CD1	6.90	128.30	113.80
1	B	170	SER	N-CA-C	6.87	125.43	110.80
1	C	153	LYS	CA-C-N	-6.87	112.64	122.94
1	C	153	LYS	C-N-CA	-6.87	112.64	122.94
1	A	68	SER	CB-CA-C	-6.85	99.44	111.22
1	B	29	ILE	CG1-CB-CG2	-6.84	90.17	110.70
1	C	11	MET	CA-C-N	-6.82	112.50	122.65
1	C	11	MET	C-N-CA	-6.82	112.50	122.65
1	D	142	ASP	CA-C-N	6.79	129.38	120.28
1	D	142	ASP	C-N-CA	6.79	129.38	120.28
1	A	8	ASP	N-CA-C	6.79	121.03	111.52
1	A	263	ASN	N-CA-C	6.76	118.73	111.36
1	A	113	VAL	CA-C-N	-6.71	113.31	122.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	113	VAL	C-N-CA	-6.71	113.31	122.77
1	A	267	ALA	O-C-N	-6.71	112.27	123.00
1	B	68	SER	CB-CA-C	-6.67	99.25	110.19
1	D	119	LYS	CG-CD-CE	-6.66	95.99	111.30
1	A	266	ASP	N-CA-C	6.64	120.97	112.34
1	A	255	PRO	CA-C-N	-6.61	114.55	122.35
1	A	255	PRO	C-N-CA	-6.61	114.55	122.35
1	A	17	LEU	N-CA-CB	6.57	119.86	110.13
1	A	115	ILE	CA-CB-CG2	6.56	121.66	110.50
1	C	190	THR	N-CA-C	-6.56	104.75	112.89
1	C	74	THR	N-CA-CB	6.53	119.48	110.01
1	C	226	ASP	N-CA-C	6.52	120.10	111.75
1	A	222	ILE	CA-C-O	-6.49	114.45	120.22
1	C	153	LYS	CG-CD-CE	6.49	126.22	111.30
1	D	153	LYS	CA-C-N	-6.48	113.85	122.99
1	D	153	LYS	C-N-CA	-6.48	113.85	122.99
1	A	59	GLN	N-CA-C	-6.45	104.17	111.14
1	C	266	ASP	CA-C-O	-6.41	111.35	120.51
1	D	248	ILE	CA-C-N	-6.40	116.42	122.37
1	D	248	ILE	C-N-CA	-6.40	116.42	122.37
1	B	18	PHE	CA-C-N	-6.39	113.04	119.56
1	B	18	PHE	C-N-CA	-6.39	113.04	119.56
1	B	249	ALA	CA-C-N	-6.39	113.22	119.87
1	B	249	ALA	C-N-CA	-6.39	113.22	119.87
1	B	266	ASP	CA-C-O	-6.39	111.37	120.51
1	C	99	LYS	CA-C-N	-6.38	113.24	119.87
1	C	99	LYS	C-N-CA	-6.38	113.24	119.87
1	B	252	PHE	CA-C-N	-6.37	114.90	122.93
1	B	252	PHE	C-N-CA	-6.37	114.90	122.93
1	C	100	PRO	CA-C-N	-6.36	112.47	122.65
1	C	100	PRO	C-N-CA	-6.36	112.47	122.65
1	C	68	SER	CB-CA-C	-6.35	100.43	110.79
1	D	115	ILE	CA-CB-CG2	6.26	121.14	110.50
1	C	141	ILE	CB-CG1-CD1	6.25	126.93	113.80
1	D	259	GLN	N-CA-C	6.21	118.23	108.55
1	A	219	GLU	CA-C-N	6.17	131.02	120.72
1	A	219	GLU	C-N-CA	6.17	131.02	120.72
1	A	266	ASP	CA-C-N	-6.14	110.64	121.70
1	A	266	ASP	C-N-CA	-6.14	110.64	121.70
1	A	24	LEU	CB-CA-C	-6.13	98.51	109.24
1	B	217	PHE	CA-C-N	-6.11	115.35	123.17
1	B	217	PHE	C-N-CA	-6.11	115.35	123.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	23	GLU	CA-C-O	-6.10	113.95	120.42
1	A	74	THR	N-CA-CB	6.09	119.07	110.12
1	C	108	LEU	CA-C-N	-6.08	111.17	122.60
1	C	108	LEU	C-N-CA	-6.08	111.17	122.60
1	B	209	ARG	NE-CZ-NH1	-6.06	115.44	121.50
1	D	29	ILE	CG1-CB-CG2	-6.03	92.62	110.70
1	D	200	ARG	CA-C-O	-6.01	110.58	120.80
1	D	66	GLU	CB-CA-C	-6.00	100.47	110.68
1	D	17	LEU	CD1-CG-CD2	-5.99	97.62	110.80
1	C	94	LYS	CD-CE-NZ	-5.93	92.91	111.90
1	B	99	LYS	CA-C-N	-5.93	113.64	120.04
1	B	99	LYS	C-N-CA	-5.93	113.64	120.04
1	D	68	SER	CB-CA-C	-5.93	101.20	110.74
1	B	219	GLU	CB-CA-C	-5.92	109.73	116.54
1	D	25	GLY	N-CA-C	-5.92	104.05	112.81
1	C	43	THR	CA-CB-OG1	-5.92	100.72	109.60
1	A	5	GLN	N-CA-C	5.91	118.84	109.50
1	D	149	ILE	CA-CB-CG2	5.90	120.53	110.50
1	C	221	GLN	CA-C-N	-5.90	113.67	122.70
1	C	221	GLN	C-N-CA	-5.90	113.67	122.70
1	A	181	TRP	N-CA-C	-5.88	105.76	113.17
1	A	108	LEU	O-C-N	-5.88	116.70	122.99
1	A	244	SER	N-CA-C	-5.87	105.95	113.23
1	C	59	GLN	CB-CA-C	-5.85	101.66	110.90
1	C	5	GLN	N-CA-C	5.84	119.00	109.24
1	A	8	ASP	CB-CA-C	-5.84	104.04	111.86
1	C	25	GLY	N-CA-C	-5.83	101.71	112.62
1	C	115	ILE	CB-CG1-CD1	-5.83	101.56	113.80
1	B	266	ASP	N-CA-C	5.80	123.17	110.80
1	C	22	LYS	CD-CE-NZ	-5.80	93.35	111.90
1	B	100	PRO	CA-C-N	-5.79	113.40	122.73
1	B	100	PRO	C-N-CA	-5.79	113.40	122.73
1	D	104	VAL	CB-CA-C	-5.79	103.64	111.63
1	A	211	ILE	N-CA-CB	5.79	121.33	111.50
1	B	176	VAL	CG1-CB-CG2	-5.78	98.08	110.80
1	B	187	LEU	N-CA-C	-5.77	104.89	111.07
1	D	257	LEU	N-CA-C	-5.75	106.27	113.28
1	B	113	VAL	N-CA-C	-5.74	99.86	108.12
1	D	59	GLN	CB-CA-C	-5.74	101.83	110.90
1	D	104	VAL	N-CA-C	-5.73	101.64	109.55
1	D	150	HIS	N-CA-C	5.70	118.83	109.76
1	B	6	ILE	CG1-CB-CG2	-5.69	93.64	110.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	209	ARG	N-CA-C	5.68	126.92	111.00
1	A	147	ARG	NE-CZ-NH1	-5.68	115.82	121.50
1	C	109	ASP	N-CA-C	-5.67	105.14	112.68
1	D	8	ASP	CB-CA-C	-5.65	103.87	111.89
1	B	107	SER	N-CA-C	5.63	117.86	109.59
1	A	9	LEU	CB-CA-C	-5.62	101.83	110.26
1	A	74	THR	CA-CB-CG2	5.62	120.05	110.50
1	B	250	PRO	CA-C-N	-5.61	113.68	122.65
1	B	250	PRO	C-N-CA	-5.61	113.68	122.65
1	A	61	THR	OG1-CB-CG2	-5.60	98.10	109.30
1	B	74	THR	N-CA-CB	5.60	118.45	110.16
1	B	5	GLN	N-CA-C	5.56	118.28	109.50
1	A	235	ILE	N-CA-C	5.55	116.18	110.36
1	B	232	HIS	N-CA-C	-5.52	103.08	109.93
1	A	98	LYS	CD-CE-NZ	-5.52	94.23	111.90
1	A	266	ASP	CA-C-O	-5.51	113.10	119.61
1	B	115	ILE	CB-CG1-CD1	-5.51	102.23	113.80
1	B	133	LYS	CG-CD-CE	5.51	123.98	111.30
1	D	207	GLY	CA-C-N	5.49	125.25	119.76
1	D	207	GLY	C-N-CA	5.49	125.25	119.76
1	A	52	HIS	CB-CA-C	-5.46	100.27	109.50
1	D	71	LEU	CB-CG-CD2	-5.46	94.33	110.70
1	A	176	VAL	CG1-CB-CG2	-5.44	98.83	110.80
1	A	246	GLN	CB-CG-CD	-5.44	103.35	112.60
1	D	76	ALA	N-CA-C	-5.44	105.44	111.36
1	D	104	VAL	CA-C-N	-5.43	111.16	121.54
1	D	104	VAL	C-N-CA	-5.43	111.16	121.54
1	B	210	LEU	N-CA-C	5.43	117.64	111.02
1	A	222	ILE	CB-CG1-CD1	-5.43	102.40	113.80
1	C	141	ILE	N-CA-CB	5.40	119.02	110.54
1	D	220	ASP	N-CA-CB	-5.40	101.42	110.39
1	A	141	ILE	N-CA-CB	5.40	119.01	110.54
1	B	219	GLU	CA-C-N	5.39	130.57	121.14
1	B	219	GLU	C-N-CA	5.39	130.57	121.14
1	C	90	VAL	N-CA-C	5.39	116.20	108.93
1	C	43	THR	CA-CB-CG2	5.38	119.65	110.50
1	B	253	ILE	N-CA-C	5.38	116.05	108.36
1	B	61	THR	CB-CA-C	5.37	120.98	110.67
1	C	222	ILE	CB-CA-C	5.37	117.42	110.12
1	B	20	SER	N-CA-C	-5.35	105.49	112.23
1	B	11	MET	CA-CB-CG	-5.34	103.41	114.10
1	C	84	PHE	N-CA-C	-5.34	105.46	111.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	209	ARG	CB-CA-C	-5.34	104.14	112.31
1	D	4	LEU	CA-C-N	-5.34	113.18	122.37
1	D	4	LEU	C-N-CA	-5.34	113.18	122.37
1	A	66	GLU	CB-CA-C	-5.29	100.19	110.46
1	D	22	LYS	N-CA-CB	5.29	118.37	110.22
1	A	104	VAL	N-CA-C	-5.28	100.78	109.12
1	C	210	LEU	CB-CA-C	-5.27	100.08	110.10
1	D	51	VAL	CA-C-O	-5.26	114.74	120.84
1	B	218	VAL	CB-CA-C	5.25	116.92	111.09
1	A	158	LEU	N-CA-C	5.25	117.08	108.52
1	B	53	TYR	N-CA-C	5.24	116.69	110.97
1	D	30	VAL	N-CA-C	5.24	115.51	108.17
1	C	110	THR	N-CA-C	5.23	116.24	108.60
1	D	90	VAL	N-CA-C	5.23	116.15	109.30
1	A	230	LEU	CB-CA-C	-5.23	101.04	108.88
1	C	196	SER	CB-CA-C	-5.22	102.65	110.90
1	D	18	PHE	CA-C-N	-5.22	114.24	119.56
1	D	18	PHE	C-N-CA	-5.22	114.24	119.56
1	C	63	TRP	N-CA-C	-5.22	105.77	111.82
1	B	32	ALA	N-CA-C	5.19	117.08	109.24
1	B	238	ARG	NE-CZ-NH1	-5.18	116.32	121.50
1	B	266	ASP	CA-C-N	-5.18	112.38	121.70
1	B	266	ASP	C-N-CA	-5.18	112.38	121.70
1	B	137	LEU	N-CA-C	-5.18	105.55	111.14
1	B	211	ILE	CB-CA-C	-5.18	101.55	110.30
1	A	149	ILE	CB-CA-C	5.17	117.87	111.15
1	C	218	VAL	CB-CA-C	5.17	116.83	111.09
1	B	156	SER	CA-C-N	-5.16	116.29	122.90
1	B	156	SER	C-N-CA	-5.16	116.29	122.90
1	A	220	ASP	N-CA-CB	-5.16	101.83	110.39
1	C	126	LEU	CA-C-N	-5.14	117.66	121.61
1	C	126	LEU	C-N-CA	-5.14	117.66	121.61
1	C	256	ILE	N-CA-C	5.13	117.02	111.58
1	C	48	THR	N-CA-C	-5.13	106.28	112.54
1	B	221	GLN	CA-C-N	-5.12	116.05	123.11
1	B	221	GLN	C-N-CA	-5.12	116.05	123.11
1	D	5	GLN	CA-C-O	-5.12	114.46	120.60
1	C	266	ASP	N-CA-C	5.12	121.70	110.80
1	C	87	TYR	CA-C-N	-5.11	114.35	119.56
1	C	87	TYR	C-N-CA	-5.11	114.35	119.56
1	C	17	LEU	N-CA-CB	5.08	118.07	110.19
1	A	243	GLU	CB-CA-C	-5.08	102.84	110.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	250	PRO	N-CA-C	-5.07	107.52	113.86
1	A	104	VAL	CB-CA-C	-5.07	104.13	111.68
1	D	171	PHE	CA-C-O	-5.05	115.33	120.99
1	A	257	LEU	N-CA-C	-5.05	107.12	113.28
1	D	141	ILE	N-CA-CB	5.04	119.27	110.65
1	D	140	ALA	CA-C-O	-5.04	115.51	120.90
1	A	100	PRO	CB-CA-C	-5.03	104.70	111.85
1	B	196	SER	CA-C-N	-5.03	113.90	122.56
1	B	196	SER	C-N-CA	-5.03	113.90	122.56
1	A	118	ARG	NE-CZ-NH2	5.03	123.72	119.20
1	C	22	LYS	N-CA-C	-5.01	106.99	113.01
1	C	17	LEU	N-CA-C	-5.01	104.83	112.04
1	D	196	SER	CA-CB-OG	-5.01	101.08	111.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	266	ASP	Peptide
1	D	223	LEU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1953	0	1967	102	0
1	B	2006	0	2016	89	0
1	C	2011	0	2026	117	0
1	D	1998	0	2010	92	0
All	All	7968	0	8019	379	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 24.

All (379) 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:C:153:LYS:CE	1:C:153:LYS:CD	1.77	1.62
1:A:153:LYS:CD	1:A:153:LYS:CG	1.81	1.58
1:A:17:LEU:CG	1:A:17:LEU:CD1	1.78	1.58
1:D:141:ILE:CD1	1:D:141:ILE:CG1	1.81	1.56
1:D:153:LYS:CD	1:D:153:LYS:CE	1.78	1.56
1:D:153:LYS:CE	1:D:153:LYS:NZ	1.68	1.55
1:B:153:LYS:CD	1:B:153:LYS:CG	1.80	1.54
1:B:141:ILE:CD1	1:B:141:ILE:CG1	1.85	1.52
1:B:138:LYS:CE	1:B:138:LYS:NZ	1.70	1.51
1:A:141:ILE:CD1	1:A:141:ILE:CG1	1.85	1.49
1:D:149:ILE:C	1:D:149:ILE:HD12	1.56	1.24
1:D:37:ASP:OD1	1:D:39:THR:HG22	1.38	1.21
1:D:211:ILE:HD12	1:D:211:ILE:H	1.12	1.11
1:A:37:ASP:OD1	1:A:39:THR:HG22	1.48	1.11
1:D:211:ILE:HD12	1:D:211:ILE:N	1.65	1.04
1:B:149:ILE:C	1:B:149:ILE:HD12	1.87	0.99
1:B:9:LEU:HD13	1:B:11:MET:HE2	1.44	0.99
1:D:115:ILE:C	1:D:115:ILE:HD12	1.88	0.98
1:D:15:HIS:HD2	1:D:69:GLU:H	1.08	0.97
1:D:129:ASN:HA	1:D:133:LYS:HD3	1.46	0.97
1:C:123:PHE:CE1	1:C:177:GLU:HG3	1.99	0.96
1:A:149:ILE:C	1:A:149:ILE:HD12	1.92	0.95
1:B:108:LEU:HD11	1:B:111:CYS:SG	2.07	0.94
1:C:37:ASP:OD1	1:C:39:THR:HG22	1.68	0.94
1:C:115:ILE:HD12	1:C:115:ILE:C	1.93	0.93
1:D:149:ILE:C	1:D:149:ILE:CD1	2.41	0.93
1:B:4:LEU:HD11	1:B:53:TYR:HE2	1.34	0.92
1:D:120:GLN:HE21	1:D:221:GLN:HE22	1.10	0.91
1:A:120:GLN:HE21	1:A:221:GLN:HE22	1.10	0.91
1:D:149:ILE:HD12	1:D:150:HIS:N	1.87	0.90
1:B:15:HIS:HD2	1:B:69:GLU:H	1.19	0.90
1:D:37:ASP:OD1	1:D:39:THR:CG2	2.19	0.89
1:C:15:HIS:HD2	1:C:69:GLU:H	1.20	0.88
1:D:18:PHE:HB2	1:D:21:GLU:HG3	1.53	0.88
1:A:171:PHE:CD1	1:A:173:ASN:ND2	2.43	0.87
1:B:138:LYS:NZ	1:B:138:LYS:HB3	1.89	0.86
1:C:9:LEU:HD13	1:C:11:MET:HE2	1.55	0.86
1:B:222:ILE:HD12	1:B:256:ILE:HD11	1.56	0.86
1:B:149:ILE:HD12	1:B:150:HIS:N	1.92	0.84
1:C:39:THR:HG21	1:D:186:ASP:OD2	1.78	0.84
1:D:15:HIS:CD2	1:D:69:GLU:H	1.96	0.83
1:A:37:ASP:OD1	1:A:39:THR:CG2	2.27	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:HIS:HD2	1:A:69:GLU:H	1.27	0.82
1:B:37:ASP:OD1	1:B:39:THR:HG22	1.79	0.82
1:B:138:LYS:HB3	1:B:138:LYS:HZ3	1.44	0.82
1:C:253:ILE:HD13	1:D:256:ILE:HD13	1.60	0.81
1:A:42:ALA:O	1:B:74:THR:HB	1.80	0.81
1:C:42:ALA:O	1:D:74:THR:HB	1.80	0.81
1:C:9:LEU:HD13	1:C:11:MET:CE	2.10	0.81
1:C:120:GLN:HE21	1:C:221:GLN:HE22	1.28	0.81
1:A:9:LEU:HD13	1:A:11:MET:CE	2.11	0.80
1:B:9:LEU:HD13	1:B:11:MET:CE	2.11	0.79
1:B:15:HIS:CD2	1:B:69:GLU:H	2.01	0.79
1:C:57:CYS:O	1:C:61:THR:HG22	1.83	0.79
1:D:9:LEU:HD13	1:D:11:MET:HE2	1.62	0.79
1:C:198:LEU:HD12	1:C:211:ILE:HG12	1.64	0.78
1:D:108:LEU:N	1:D:108:LEU:HD23	2.01	0.76
1:B:108:LEU:CD1	1:B:111:CYS:SG	2.72	0.76
1:A:171:PHE:CE1	1:A:173:ASN:ND2	2.53	0.76
1:A:254:HIS:HD2	1:A:256:ILE:H	1.32	0.76
1:D:223:LEU:HG	1:D:230:LEU:HD12	1.66	0.76
1:A:15:HIS:CD2	1:A:69:GLU:H	2.06	0.74
1:B:120:GLN:HE21	1:B:221:GLN:HE22	1.35	0.74
1:A:222:ILE:HD12	1:A:256:ILE:HD11	1.70	0.73
1:D:92:GLU:OE1	1:D:116:HIS:HE1	1.71	0.73
1:D:108:LEU:HD23	1:D:108:LEU:H	1.55	0.72
1:D:138:LYS:NZ	1:D:138:LYS:HB3	2.04	0.71
1:A:126:LEU:N	1:A:126:LEU:HD12	2.05	0.71
1:D:209:ARG:O	1:D:210:LEU:HB2	1.88	0.71
1:D:34:LEU:N	1:D:34:LEU:HD23	2.05	0.71
1:D:9:LEU:HD13	1:D:11:MET:CE	2.21	0.70
1:B:186:ASP:O	1:B:190:THR:HG23	1.91	0.70
1:C:18:PHE:HB2	1:C:21:GLU:HG3	1.74	0.70
1:D:198:LEU:O	1:D:210:LEU:HD13	1.92	0.69
1:A:39:THR:HG21	1:B:186:ASP:OD2	1.92	0.69
1:C:39:THR:HG21	1:D:186:ASP:CG	2.18	0.69
1:C:15:HIS:CD2	1:C:69:GLU:H	2.08	0.69
1:A:17:LEU:CD1	1:A:17:LEU:CD2	2.69	0.68
1:A:9:LEU:HD13	1:A:11:MET:HE2	1.74	0.68
1:B:4:LEU:HD11	1:B:53:TYR:CE2	2.24	0.68
1:A:120:GLN:NE2	1:A:221:GLN:HE22	1.88	0.68
1:C:198:LEU:CD1	1:C:211:ILE:HG12	2.24	0.68
1:D:211:ILE:N	1:D:211:ILE:CD1	2.47	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:196:SER:C	1:C:198:LEU:H	2.02	0.68
1:D:120:GLN:NE2	1:D:221:GLN:HE22	1.90	0.67
1:C:38:MET:HE1	1:D:113:VAL:HG22	1.76	0.67
1:C:254:HIS:HD2	1:C:257:LEU:H	1.43	0.67
1:C:149:ILE:CD1	1:C:178:VAL:HB	2.24	0.67
1:D:129:ASN:HB3	1:D:171:PHE:CD2	2.29	0.66
1:B:126:LEU:HD12	1:B:126:LEU:N	2.10	0.66
1:C:128:SER:HB2	1:C:210:LEU:O	1.95	0.66
1:A:15:HIS:HD2	1:A:69:GLU:N	1.94	0.66
1:A:38:MET:HE1	1:B:113:VAL:HG22	1.77	0.66
1:C:92:GLU:OE1	1:C:116:HIS:HE1	1.79	0.65
1:C:15:HIS:HD2	1:C:69:GLU:N	1.94	0.65
1:B:16:GLY:O	1:B:22:LYS:HE2	1.97	0.65
1:C:39:THR:HB	1:D:117:ARG:NH2	2.13	0.64
1:C:108:LEU:N	1:C:108:LEU:HD23	2.12	0.64
1:C:231:PRO:HD2	1:C:256:ILE:HD12	1.80	0.64
1:B:15:HIS:HD2	1:B:69:GLU:N	1.94	0.64
1:D:129:ASN:HB2	1:D:170:SER:O	1.97	0.64
1:C:253:ILE:HD13	1:D:256:ILE:CD1	2.28	0.63
1:C:37:ASP:OD1	1:C:39:THR:CG2	2.46	0.63
1:C:57:CYS:O	1:C:61:THR:CG2	2.48	0.62
1:D:209:ARG:O	1:D:210:LEU:CB	2.47	0.62
1:D:115:ILE:HD12	1:D:116:HIS:N	2.14	0.61
1:C:128:SER:CB	1:C:210:LEU:O	2.48	0.61
1:D:15:HIS:HD2	1:D:69:GLU:N	1.90	0.61
1:A:129:ASN:O	1:A:130:MET:HG2	2.00	0.61
1:C:115:ILE:HD12	1:C:116:HIS:N	2.14	0.61
1:C:254:HIS:CD2	1:C:257:LEU:H	2.19	0.61
1:A:222:ILE:HG12	1:A:222:ILE:O	2.00	0.60
1:B:17:LEU:N	1:B:17:LEU:HD12	2.16	0.60
1:D:108:LEU:N	1:D:108:LEU:CD2	2.65	0.60
1:A:218:VAL:HG13	1:A:218:VAL:O	2.01	0.60
1:B:115:ILE:C	1:B:115:ILE:HD12	2.27	0.60
1:A:200:ARG:HH11	1:A:200:ARG:HB2	1.66	0.60
1:B:149:ILE:CD1	1:B:178:VAL:HB	2.31	0.60
1:A:37:ASP:CG	1:A:39:THR:HG22	2.26	0.60
1:A:254:HIS:CD2	1:A:256:ILE:H	2.17	0.60
1:A:4:LEU:HD11	1:A:53:TYR:CE2	2.37	0.59
1:A:149:ILE:CD1	1:A:178:VAL:HB	2.32	0.59
1:C:217:PHE:CD2	1:C:231:PRO:HB3	2.38	0.59
1:C:120:GLN:NE2	1:C:221:GLN:HE22	2.01	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:ASP:OD1	1:B:39:THR:CG2	2.50	0.59
1:C:151:ILE:N	1:C:151:ILE:HD12	2.17	0.59
1:A:24:LEU:HG	1:D:20:SER:HB2	1.84	0.58
1:C:39:THR:HB	1:D:117:ARG:HH21	1.68	0.58
1:D:138:LYS:HB3	1:D:138:LYS:HZ3	1.65	0.58
1:D:217:PHE:CD2	1:D:231:PRO:HB3	2.38	0.58
1:B:149:ILE:HD11	1:B:178:VAL:HB	1.85	0.58
1:A:171:PHE:HD1	1:A:173:ASN:ND2	2.01	0.57
1:C:240:PHE:H	1:C:240:PHE:HD2	1.50	0.57
1:C:195:GLU:HA	1:C:211:ILE:HD13	1.87	0.57
1:A:175:VAL:HG23	1:A:176:VAL:N	2.19	0.57
1:A:175:VAL:CG2	1:A:176:VAL:N	2.68	0.57
1:B:209:ARG:HD3	1:B:212:ASP:OD1	2.05	0.57
1:D:52:HIS:O	1:D:56:LEU:HB2	2.05	0.56
1:C:45:LEU:N	1:C:45:LEU:HD23	2.20	0.56
1:C:129:ASN:HA	1:C:133:LYS:HG2	1.85	0.56
1:A:149:ILE:HD12	1:A:150:HIS:N	2.20	0.56
1:D:53:TYR:O	1:D:54:GLY:C	2.49	0.56
1:A:186:ASP:O	1:A:190:THR:HG23	2.05	0.56
1:C:5:GLN:HG3	1:C:7:LYS:HE3	1.88	0.56
1:C:2:ASP:HB2	1:C:38:MET:HG3	1.87	0.56
1:B:254:HIS:HD2	1:B:256:ILE:H	1.53	0.56
1:A:200:ARG:HB2	1:A:200:ARG:NH1	2.20	0.56
1:A:138:LYS:HZ2	1:A:138:LYS:HB3	1.71	0.56
1:A:5:GLN:HG3	1:A:7:LYS:HE3	1.88	0.55
1:A:9:LEU:HD13	1:A:11:MET:HE3	1.88	0.55
1:A:253:ILE:HD12	1:B:256:ILE:HD13	1.89	0.55
1:A:96:GLU:HA	1:A:114:THR:HB	1.87	0.55
1:B:57:CYS:O	1:B:61:THR:HG22	2.05	0.55
1:C:95:LEU:C	1:C:95:LEU:HD13	2.31	0.55
1:D:57:CYS:O	1:D:61:THR:HG22	2.05	0.55
1:A:115:ILE:HD12	1:A:115:ILE:C	2.31	0.55
1:A:218:VAL:O	1:A:221:GLN:HB2	2.06	0.55
1:D:200:ARG:NH1	1:D:212:ASP:OD1	2.39	0.55
1:A:17:LEU:HD12	1:A:17:LEU:N	2.23	0.54
1:A:149:ILE:HD13	1:A:178:VAL:HB	1.89	0.54
1:C:199:GLY:O	1:C:210:LEU:HD13	2.07	0.54
1:A:123:PHE:CE1	1:A:177:GLU:HG3	2.42	0.54
1:B:151:ILE:HD12	1:B:151:ILE:N	2.22	0.54
1:D:193:ALA:O	1:D:197:GLU:HG2	2.08	0.54
1:C:265:TYR:O	1:C:266:ASP:C	2.44	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:PRO:HD2	1:A:256:ILE:HD12	1.91	0.53
1:B:254:HIS:CD2	1:B:256:ILE:H	2.27	0.53
1:C:126:LEU:HD12	1:C:126:LEU:N	2.24	0.53
1:C:138:LYS:NZ	1:C:138:LYS:HB3	2.24	0.53
1:C:194:ILE:O	1:C:195:GLU:C	2.51	0.52
1:A:193:ALA:O	1:A:197:GLU:HG2	2.10	0.52
1:A:16:GLY:O	1:A:22:LYS:HE2	2.10	0.52
1:B:149:ILE:C	1:B:149:ILE:CD1	2.62	0.52
1:C:2:ASP:C	1:C:3:GLN:HG2	2.34	0.52
1:C:53:TYR:N	1:C:53:TYR:CD2	2.72	0.52
1:A:222:ILE:O	1:A:222:ILE:CG1	2.58	0.51
1:C:134:GLN:OE1	1:C:134:GLN:HA	2.10	0.51
1:C:133:LYS:HE2	1:C:170:SER:O	2.09	0.51
1:D:186:ASP:O	1:D:190:THR:HG23	2.11	0.51
1:C:158:LEU:N	1:C:158:LEU:HD12	2.25	0.51
1:A:129:ASN:C	1:A:130:MET:CG	2.84	0.51
1:A:57:CYS:O	1:A:61:THR:HG22	2.11	0.51
1:B:92:GLU:OE1	1:B:116:HIS:HE1	1.94	0.51
1:A:39:THR:HG21	1:B:186:ASP:CG	2.36	0.50
1:B:29:ILE:HB	1:B:98:LYS:HB2	1.92	0.50
1:C:211:ILE:HD12	1:C:211:ILE:H	1.76	0.50
1:C:240:PHE:HA	1:C:243:GLU:HB2	1.92	0.50
1:D:96:GLU:HG3	1:D:114:THR:HB	1.93	0.50
1:B:254:HIS:CD2	1:B:257:LEU:H	2.30	0.50
1:D:230:LEU:HA	1:D:231:PRO:C	2.36	0.50
1:A:2:ASP:OD1	1:B:115:ILE:HA	2.11	0.50
1:D:2:ASP:HB2	1:D:38:MET:HG3	1.93	0.50
1:A:39:THR:HB	1:B:117:ARG:HH21	1.75	0.50
1:B:175:VAL:CG1	1:B:244:SER:HB2	2.42	0.50
1:C:27:LYS:HD3	1:C:29:ILE:HD11	1.93	0.50
1:A:120:GLN:HE21	1:A:221:GLN:NE2	1.93	0.50
1:A:151:ILE:N	1:A:151:ILE:HD12	2.27	0.49
1:A:175:VAL:HG23	1:A:176:VAL:H	1.77	0.49
1:D:126:LEU:N	1:D:126:LEU:HD12	2.26	0.49
1:D:200:ARG:HD2	1:D:211:ILE:O	2.13	0.49
1:B:188:LEU:HD22	1:B:228:LEU:HB2	1.95	0.49
1:C:140:ALA:O	1:C:141:ILE:C	2.54	0.49
1:A:58:GLN:HA	1:A:61:THR:HG22	1.95	0.49
1:B:49:ALA:C	1:B:89:LEU:HD11	2.37	0.49
1:B:261:ILE:O	1:B:262:ARG:C	2.55	0.49
1:C:30:VAL:HG12	1:C:31:SER:N	2.27	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:240:PHE:N	1:C:240:PHE:CD2	2.79	0.49
1:C:46:ASP:OD1	1:C:46:ASP:C	2.56	0.49
1:A:92:GLU:HB2	1:A:118:ARG:HG3	1.93	0.48
1:B:211:ILE:O	1:B:211:ILE:HD12	2.13	0.48
1:D:37:ASP:CG	1:D:39:THR:HG22	2.29	0.48
1:B:66:GLU:HB3	1:B:67:THR:HG23	1.95	0.48
1:A:218:VAL:HG12	1:A:230:LEU:HD13	1.95	0.48
1:B:124:ILE:HD13	1:B:191:LEU:HD11	1.93	0.48
1:A:72:ILE:HB	1:A:97:LEU:HD22	1.94	0.48
1:C:72:ILE:HB	1:C:97:LEU:HD13	1.95	0.48
1:B:2:ASP:C	1:B:3:GLN:HG2	2.39	0.48
1:D:23:GLU:HA	1:D:23:GLU:OE1	2.13	0.48
1:A:186:ASP:O	1:A:190:THR:CG2	2.62	0.48
1:A:155:SER:OG	1:A:244:SER:HB2	2.14	0.48
1:B:230:LEU:HA	1:B:231:PRO:C	2.38	0.48
1:C:66:GLU:CB	1:C:67:THR:HG23	2.44	0.48
1:C:97:LEU:HD23	1:C:97:LEU:C	2.39	0.48
1:C:158:LEU:N	1:C:158:LEU:CD1	2.77	0.48
1:C:8:ASP:O	1:D:108:LEU:HA	2.14	0.47
1:B:218:VAL:O	1:B:221:GLN:HB2	2.14	0.47
1:C:66:GLU:HB3	1:C:67:THR:HG23	1.94	0.47
1:A:92:GLU:OE1	1:A:116:HIS:HE1	1.97	0.47
1:C:96:GLU:HB2	1:C:114:THR:HB	1.95	0.47
1:B:17:LEU:HD12	1:B:17:LEU:H	1.80	0.47
1:D:146:ALA:C	1:D:148:GLY:H	2.22	0.47
1:A:17:LEU:CD1	1:A:17:LEU:N	2.78	0.47
1:A:181:TRP:CD1	1:A:181:TRP:C	2.93	0.47
1:B:238:ARG:O	1:B:239:LEU:C	2.57	0.47
1:C:2:ASP:OD1	1:D:117:ARG:NH1	2.47	0.47
1:C:242:LEU:O	1:C:243:GLU:C	2.58	0.47
1:B:71:LEU:HB2	1:B:74:THR:HG23	1.97	0.47
1:B:135:ALA:O	1:B:139:GLN:HG3	2.15	0.47
1:C:17:LEU:HD12	1:C:17:LEU:N	2.29	0.47
1:C:183:PRO:HG2	1:C:186:ASP:OD2	2.15	0.47
1:C:265:TYR:O	1:C:267:ALA:N	2.48	0.47
1:A:183:PRO:O	1:A:184:ALA:C	2.58	0.47
1:C:53:TYR:O	1:C:54:GLY:C	2.56	0.47
1:C:108:LEU:HD23	1:C:108:LEU:H	1.78	0.46
1:D:90:VAL:O	1:D:119:LYS:HE3	2.15	0.46
1:D:254:HIS:CD2	1:D:257:LEU:H	2.33	0.46
1:B:95:LEU:HD13	1:B:95:LEU:C	2.41	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:LEU:HD11	1:B:111:CYS:HG	1.76	0.46
1:A:108:LEU:N	1:A:108:LEU:HD23	2.31	0.46
1:A:253:ILE:CD1	1:B:256:ILE:HD13	2.46	0.46
1:B:175:VAL:HG12	1:B:244:SER:HB2	1.98	0.46
1:B:200:ARG:HB2	1:B:200:ARG:CZ	2.45	0.46
1:B:222:ILE:HG12	1:B:222:ILE:O	2.15	0.46
1:B:254:HIS:HD2	1:B:257:LEU:H	1.62	0.46
1:A:138:LYS:HB3	1:A:138:LYS:NZ	2.31	0.45
1:B:5:GLN:OE1	1:B:7:LYS:HE2	2.16	0.45
1:C:217:PHE:CE2	1:C:231:PRO:HB3	2.52	0.45
1:C:92:GLU:OE1	1:C:116:HIS:CE1	2.67	0.45
1:C:95:LEU:C	1:C:95:LEU:CD1	2.89	0.45
1:B:37:ASP:CG	1:B:39:THR:HG22	2.41	0.45
1:C:144:LEU:HD12	1:C:144:LEU:HA	1.57	0.45
1:A:261:ILE:O	1:A:262:ARG:C	2.59	0.45
1:C:196:SER:C	1:C:198:LEU:N	2.67	0.45
1:D:92:GLU:OE1	1:D:116:HIS:CE1	2.61	0.45
1:A:144:LEU:HD12	1:A:144:LEU:HA	1.68	0.45
1:B:132:ASP:O	1:B:133:LYS:C	2.59	0.45
1:C:5:GLN:HB2	1:C:32:ALA:O	2.16	0.45
1:C:37:ASP:CG	1:C:39:THR:HG22	2.40	0.45
1:C:222:ILE:HD13	1:C:222:ILE:HG21	1.50	0.45
1:D:200:ARG:NH1	1:D:209:ARG:HG2	2.32	0.45
1:A:254:HIS:CD2	1:A:257:LEU:H	2.35	0.45
1:D:53:TYR:N	1:D:53:TYR:CD2	2.84	0.45
1:C:123:PHE:CE1	1:C:177:GLU:CG	2.86	0.45
1:D:215:LEU:HD23	1:D:215:LEU:HA	1.62	0.45
1:D:6:ILE:N	1:D:6:ILE:HD12	2.32	0.45
1:D:124:ILE:HD13	1:D:191:LEU:HD11	1.98	0.45
1:D:198:LEU:O	1:D:210:LEU:CD1	2.64	0.45
1:B:152:LEU:HD23	1:B:152:LEU:HA	1.50	0.44
1:D:181:TRP:CD1	1:D:181:TRP:C	2.95	0.44
1:B:17:LEU:N	1:B:17:LEU:CD1	2.80	0.44
1:C:58:GLN:C	1:C:61:THR:HG22	2.42	0.44
1:C:52:HIS:HD2	1:C:55:GLU:HG3	1.82	0.44
1:C:243:GLU:HA	1:C:265:TYR:CE1	2.52	0.44
1:A:140:ALA:O	1:A:141:ILE:C	2.60	0.44
1:A:200:ARG:HH11	1:A:200:ARG:CB	2.30	0.44
1:B:153:LYS:CD	1:B:153:LYS:CB	2.82	0.44
1:A:129:ASN:C	1:A:130:MET:HG2	2.43	0.44
1:C:231:PRO:HG3	1:C:255:PRO:HG2	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:ILE:HD12	1:A:116:HIS:N	2.33	0.44
1:D:5:GLN:HB2	1:D:32:ALA:O	2.17	0.44
1:A:95:LEU:HD13	1:A:95:LEU:C	2.43	0.44
1:B:222:ILE:HD13	1:B:222:ILE:HG21	1.62	0.44
1:C:149:ILE:HD12	1:C:149:ILE:C	2.42	0.44
1:A:4:LEU:HD11	1:A:53:TYR:HE2	1.83	0.43
1:B:4:LEU:CD1	1:B:53:TYR:HE2	2.19	0.43
1:C:102:ALA:O	1:C:104:VAL:N	2.51	0.43
1:A:14:TYR:CD1	1:A:14:TYR:N	2.86	0.43
1:A:58:GLN:CA	1:A:61:THR:HG22	2.49	0.43
1:A:132:ASP:O	1:A:133:LYS:C	2.61	0.43
1:A:217:PHE:CD2	1:A:231:PRO:HB3	2.53	0.43
1:C:53:TYR:HB2	1:C:54:GLY:H	1.56	0.43
1:D:194:ILE:O	1:D:195:GLU:C	2.61	0.43
1:D:210:LEU:HD23	1:D:210:LEU:HA	1.86	0.43
1:A:10:GLU:C	1:A:11:MET:HG3	2.44	0.43
1:B:209:ARG:HD3	1:B:209:ARG:HH11	1.58	0.43
1:C:149:ILE:HD11	1:C:178:VAL:HB	1.99	0.43
1:A:95:LEU:C	1:A:95:LEU:CD1	2.92	0.43
1:B:181:TRP:CD1	1:B:181:TRP:C	2.97	0.43
1:D:133:LYS:O	1:D:136:ASN:HB2	2.18	0.43
1:D:149:ILE:CD1	1:D:178:VAL:HB	2.49	0.43
1:A:230:LEU:HA	1:A:230:LEU:HD23	1.83	0.43
1:B:144:LEU:HA	1:B:144:LEU:HD12	1.72	0.43
1:B:248:ILE:HD13	1:B:248:ILE:HG21	1.71	0.43
1:C:66:GLU:C	1:C:67:THR:CG2	2.90	0.43
1:C:66:GLU:C	1:C:67:THR:HG23	2.43	0.43
1:C:61:THR:O	1:C:65:GLN:HG3	2.18	0.43
1:C:157:VAL:C	1:C:158:LEU:HD12	2.44	0.43
1:D:33:ILE:C	1:D:34:LEU:HD23	2.44	0.43
1:C:58:GLN:O	1:C:61:THR:CG2	2.67	0.43
1:D:256:ILE:HD13	1:D:256:ILE:HG21	1.87	0.43
1:B:106:LEU:HA	1:B:106:LEU:HD23	1.85	0.42
1:C:132:ASP:O	1:C:133:LYS:C	2.62	0.42
1:D:123:PHE:CE1	1:D:177:GLU:HG3	2.54	0.42
1:A:38:MET:CE	1:B:113:VAL:HG22	2.47	0.42
1:C:123:PHE:CZ	1:C:177:GLU:HG3	2.51	0.42
1:C:149:ILE:HD12	1:C:150:HIS:N	2.35	0.42
1:D:2:ASP:C	1:D:3:GLN:CG	2.91	0.42
1:A:222:ILE:HG21	1:A:222:ILE:HD13	1.49	0.42
1:C:136:ASN:ND2	1:C:136:ASN:H	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:GLU:HB3	1:A:220:ASP:H	1.17	0.42
1:B:241:VAL:O	1:B:245:LEU:HB2	2.20	0.42
1:C:215:LEU:HA	1:C:215:LEU:HD23	1.73	0.42
1:B:60:TRP:O	1:B:64:PHE:HB2	2.19	0.42
1:B:176:VAL:HG12	1:B:177:GLU:N	2.33	0.42
1:C:218:VAL:HG12	1:C:230:LEU:HD11	2.01	0.42
1:B:56:LEU:HD23	1:B:56:LEU:HA	1.81	0.42
1:C:43:THR:HG22	1:C:44:ASP:OD1	2.20	0.42
1:D:254:HIS:HD2	1:D:257:LEU:H	1.67	0.42
1:B:53:TYR:O	1:B:54:GLY:C	2.63	0.41
1:B:175:VAL:CG2	1:B:176:VAL:N	2.83	0.41
1:C:230:LEU:HA	1:C:231:PRO:C	2.45	0.41
1:D:158:LEU:HD12	1:D:158:LEU:HA	1.82	0.41
1:A:101:TRP:O	1:A:102:ALA:C	2.63	0.41
1:D:27:LYS:HD3	1:D:29:ILE:HD11	2.02	0.41
1:A:187:LEU:HA	1:A:187:LEU:HD12	1.83	0.41
1:C:6:ILE:O	1:C:31:SER:HA	2.19	0.41
1:C:24:LEU:HA	1:C:24:LEU:HD23	1.79	0.41
1:C:195:GLU:HA	1:C:211:ILE:CD1	2.49	0.41
1:D:10:GLU:O	1:D:11:MET:HG3	2.20	0.41
1:D:151:ILE:N	1:D:151:ILE:HD12	2.35	0.41
1:A:89:LEU:HD23	1:A:89:LEU:HA	1.92	0.41
1:A:101:TRP:N	1:A:101:TRP:CD1	2.88	0.41
1:A:191:LEU:HG	1:A:213:LEU:HB3	2.03	0.41
1:C:47:LEU:HD23	1:C:47:LEU:HA	1.62	0.41
1:A:223:LEU:H	1:A:230:LEU:HB2	1.85	0.41
1:B:17:LEU:H	1:B:17:LEU:CD1	2.32	0.41
1:D:196:SER:C	1:D:198:LEU:N	2.77	0.41
1:A:129:ASN:OD1	1:A:130:MET:HG3	2.21	0.41
1:B:104:VAL:HG12	1:B:105:HIS:N	2.35	0.41
1:B:153:LYS:HD2	1:B:153:LYS:HA	2.03	0.41
1:C:3:GLN:O	1:D:114:THR:HG23	2.21	0.41
1:C:191:LEU:HD12	1:C:191:LEU:HA	1.79	0.41
1:D:153:LYS:HA	1:D:153:LYS:HD2	1.20	0.41
1:D:200:ARG:HE	1:D:200:ARG:HB3	1.81	0.41
1:A:234:TYR:O	1:A:235:ILE:C	2.62	0.41
1:A:254:HIS:HD2	1:A:256:ILE:N	2.09	0.41
1:C:260:PRO:O	1:C:261:ILE:C	2.63	0.41
1:C:136:ASN:ND2	1:C:136:ASN:N	2.69	0.41
1:C:196:SER:O	1:C:198:LEU:N	2.54	0.41
1:B:175:VAL:HG12	1:B:244:SER:CB	2.51	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:254:HIS:HD2	1:D:256:ILE:H	1.69	0.40
1:B:265:TYR:O	1:B:266:ASP:C	2.62	0.40
1:C:153:LYS:HA	1:C:153:LYS:HD2	1.21	0.40
1:D:146:ALA:C	1:D:148:GLY:N	2.79	0.40
1:A:198:LEU:HB2	1:A:211:ILE:HD11	2.04	0.40
1:A:147:ARG:HG3	1:A:147:ARG:HH11	1.86	0.40
1:C:140:ALA:C	1:C:142:ASP:N	2.79	0.40
1:C:218:VAL:HG12	1:C:230:LEU:CD1	2.52	0.40
1:D:254:HIS:CD2	1:D:256:ILE:H	2.40	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	233/270 (86%)	223 (96%)	10 (4%)	0	100	100
1	B	240/270 (89%)	229 (95%)	10 (4%)	1 (0%)	30	59
1	C	243/270 (90%)	223 (92%)	16 (7%)	4 (2%)	7	27
1	D	240/270 (89%)	220 (92%)	18 (8%)	2 (1%)	16	44
All	All	956/1080 (88%)	895 (94%)	54 (6%)	7 (1%)	18	48

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	170	SER
1	C	266	ASP
1	D	210	LEU
1	D	267	ALA
1	C	134	GLN
1	C	147	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	197	GLU

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	215/241 (89%)	186 (86%)	29 (14%)	4	12
1	B	221/241 (92%)	185 (84%)	36 (16%)	2	8
1	C	222/241 (92%)	187 (84%)	35 (16%)	2	8
1	D	220/241 (91%)	186 (84%)	34 (16%)	2	9
All	All	878/964 (91%)	744 (85%)	134 (15%)	3	9

All (134) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	9	LEU
1	A	17	LEU
1	A	20	SER
1	A	40	LYS
1	A	56	LEU
1	A	74	THR
1	A	95	LEU
1	A	113	VAL
1	A	114	THR
1	A	115	ILE
1	A	126	LEU
1	A	138	LYS
1	A	141	ILE
1	A	143	LYS
1	A	149	ILE
1	A	153	LYS
1	A	157	VAL
1	A	175	VAL
1	A	190	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	191	LEU
1	A	200	ARG
1	A	211	ILE
1	A	215	LEU
1	A	222	ILE
1	A	239	LEU
1	A	246	GLN
1	A	256	ILE
1	A	262	ARG
1	B	3	GLN
1	B	9	LEU
1	B	17	LEU
1	B	29	ILE
1	B	40	LYS
1	B	43	THR
1	B	44	ASP
1	B	52	HIS
1	B	56	LEU
1	B	74	THR
1	B	95	LEU
1	B	113	VAL
1	B	114	THR
1	B	115	ILE
1	B	130	MET
1	B	138	LYS
1	B	141	ILE
1	B	143	LYS
1	B	144	LEU
1	B	149	ILE
1	B	153	LYS
1	B	157	VAL
1	B	158	LEU
1	B	175	VAL
1	B	190	THR
1	B	191	LEU
1	B	200	ARG
1	B	211	ILE
1	B	212	ASP
1	B	215	LEU
1	B	218	VAL
1	B	222	ILE
1	B	239	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	244	SER
1	B	253	ILE
1	B	262	ARG
1	C	6	ILE
1	C	9	LEU
1	C	17	LEU
1	C	20	SER
1	C	34	LEU
1	C	40	LYS
1	C	43	THR
1	C	45	LEU
1	C	56	LEU
1	C	74	THR
1	C	93	MET
1	C	95	LEU
1	C	109	ASP
1	C	113	VAL
1	C	114	THR
1	C	115	ILE
1	C	137	LEU
1	C	138	LYS
1	C	141	ILE
1	C	143	LYS
1	C	144	LEU
1	C	149	ILE
1	C	153	LYS
1	C	157	VAL
1	C	170	SER
1	C	175	VAL
1	C	191	LEU
1	C	200	ARG
1	C	211	ILE
1	C	215	LEU
1	C	218	VAL
1	C	222	ILE
1	C	243	GLU
1	C	253	ILE
1	C	258	LYS
1	D	9	LEU
1	D	20	SER
1	D	22	LYS
1	D	34	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	39	THR
1	D	40	LYS
1	D	56	LEU
1	D	74	THR
1	D	95	LEU
1	D	113	VAL
1	D	114	THR
1	D	115	ILE
1	D	137	LEU
1	D	138	LYS
1	D	143	LYS
1	D	144	LEU
1	D	149	ILE
1	D	153	LYS
1	D	158	LEU
1	D	170	SER
1	D	171	PHE
1	D	175	VAL
1	D	181	TRP
1	D	190	THR
1	D	191	LEU
1	D	200	ARG
1	D	211	ILE
1	D	215	LEU
1	D	218	VAL
1	D	222	ILE
1	D	239	LEU
1	D	243	GLU
1	D	244	SER
1	D	246	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	HIS
1	A	59	GLN
1	A	91	GLN
1	A	105	HIS
1	A	116	HIS
1	A	174	GLN
1	A	221	GLN
1	A	246	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	254	HIS
1	B	15	HIS
1	B	26	GLN
1	B	59	GLN
1	B	105	HIS
1	B	116	HIS
1	B	134	GLN
1	B	136	ASN
1	B	139	GLN
1	B	173	ASN
1	B	174	GLN
1	B	221	GLN
1	B	254	HIS
1	C	15	HIS
1	C	59	GLN
1	C	91	GLN
1	C	105	HIS
1	C	116	HIS
1	C	120	GLN
1	C	136	ASN
1	C	174	GLN
1	C	254	HIS
1	D	15	HIS
1	D	91	GLN
1	D	105	HIS
1	D	116	HIS
1	D	120	GLN
1	D	136	ASN
1	D	139	GLN
1	D	254	HIS

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.