



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:42 PM UTC

PDB ID : 1WYU / pdb_00001wyu
Title : Crystal structure of glycine decarboxylase (P-protein) of the glycine cleavage system, in holo form
Authors : Nakai, T.; Nakagawa, N.; Maoka, N.; Masui, R.; Kuramitsu, S.; Kamiya, N.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2005-02-17
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

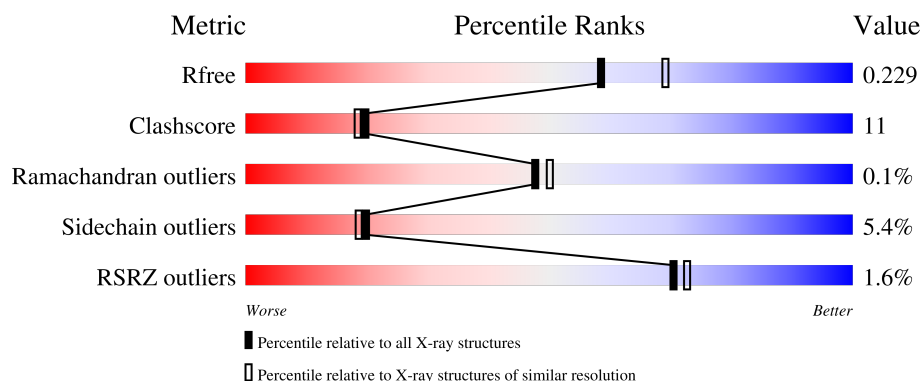
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

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



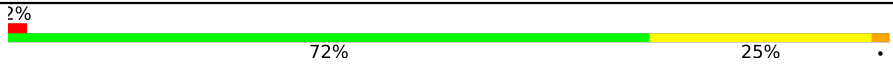
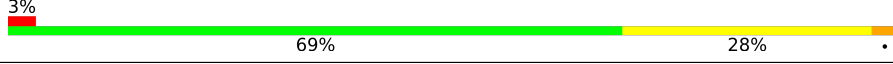
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	438	0% 78% 19% .
1	C	438	0% 76% 21% .
1	E	438	0% 78% 20% .
1	G	438	78% 19% .
2	B	474	2% 71% 25% .

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Mol	Chain	Length	Quality of chain
2	D	474	 2% 72% 25% .
2	F	474	 2% 75% 21% .
2	H	474	 3% 69% 28% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 30337 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 glycine dehydrogenase (decarboxylating) subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	0	0	0
			3320	2129	575	607	9			
1	C	437	Total	C	N	O	S	0	0	0
			3320	2129	575	607	9			
1	E	437	Total	C	N	O	S	0	0	0
			3320	2129	575	607	9			
1	G	437	Total	C	N	O	S	0	0	0
			3320	2129	575	607	9			

- Molecule 2 is a protein called glycine dehydrogenase subunit 2 (P-protein).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	473	Total	C	N	O	S	0	0	0
			3713	2380	655	666	12			
2	D	473	Total	C	N	O	S	0	0	0
			3713	2380	655	666	12			
2	F	473	Total	C	N	O	S	0	0	0
			3713	2380	655	666	12			
2	H	473	Total	C	N	O	S	0	0	0
			3713	2380	655	666	12			

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: $C_8H_{10}NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	F	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	H	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

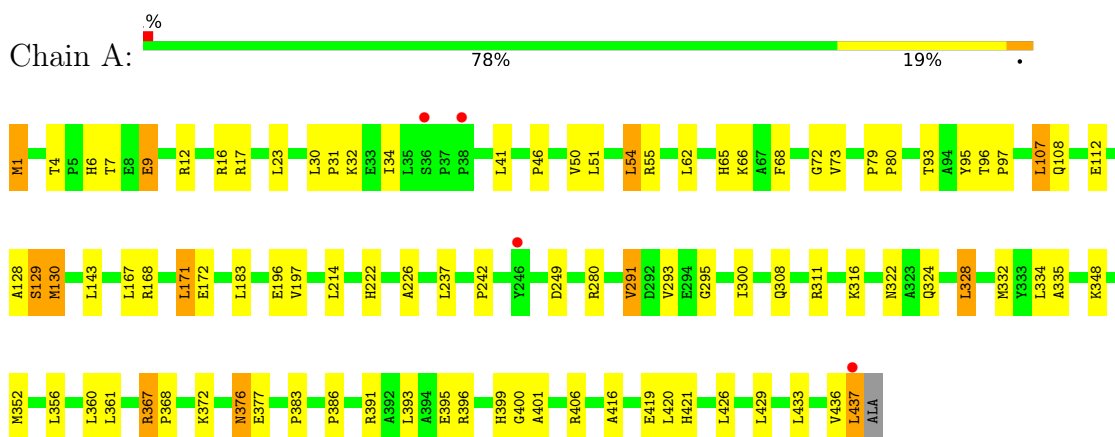
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	281	Total	O	0	0
			281	281		
4	B	286	Total	O	0	0
			286	286		
4	C	277	Total	O	0	0
			277	277		
4	D	233	Total	O	0	0
			233	233		
4	E	283	Total	O	0	0
			283	283		
4	F	272	Total	O	0	0
			272	272		
4	G	286	Total	O	0	0
			286	286		
4	H	227	Total	O	0	0
			227	227		

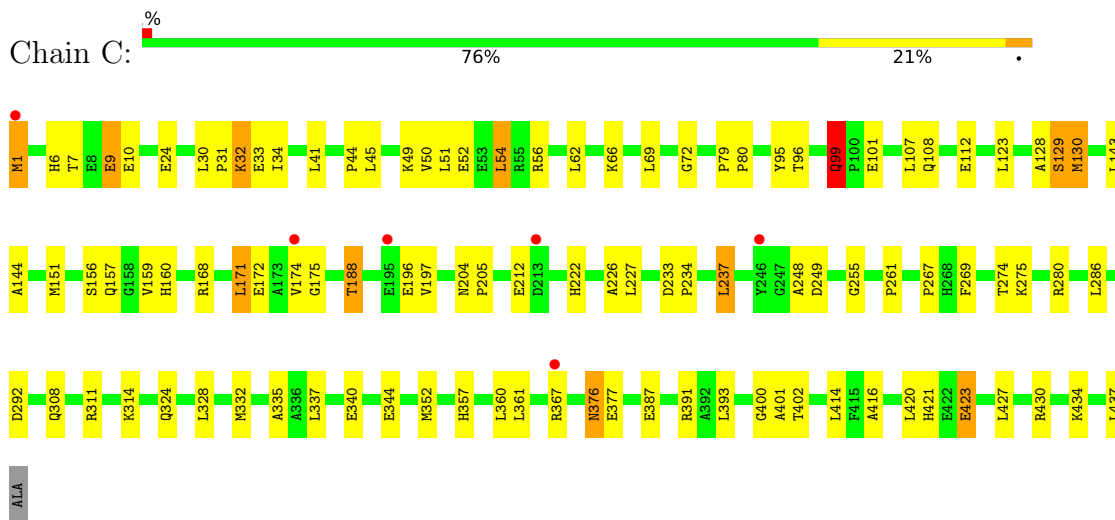
3 Residue-property plots

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

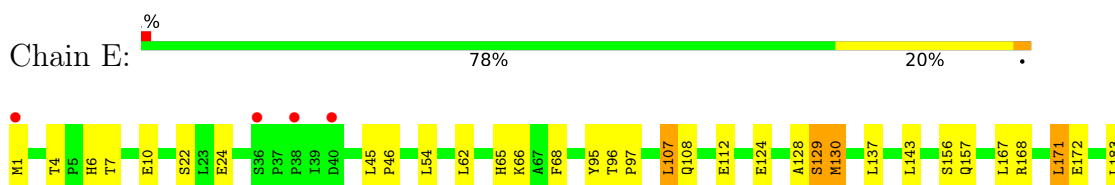
- Molecule 1: glycine dehydrogenase (decarboxylating) subunit 1

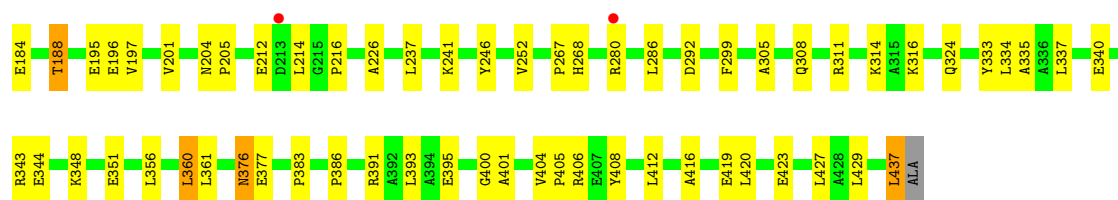


- Molecule 1: glycine dehydrogenase (decarboxylating) subunit 1

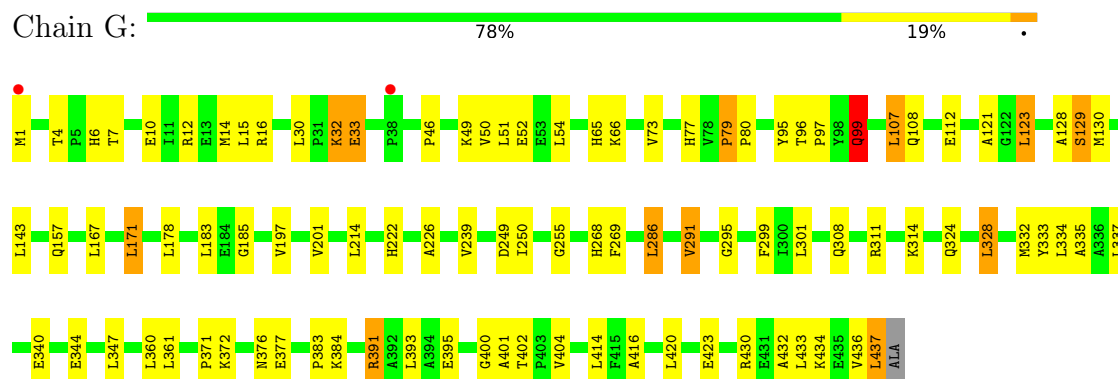


- Molecule 1: glycine dehydrogenase (decarboxylating) subunit 1

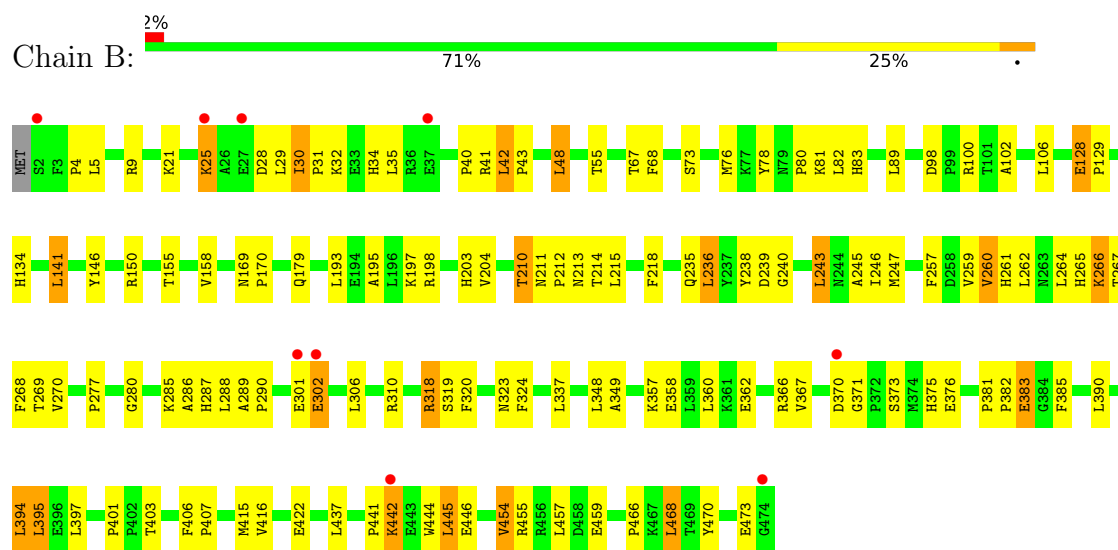




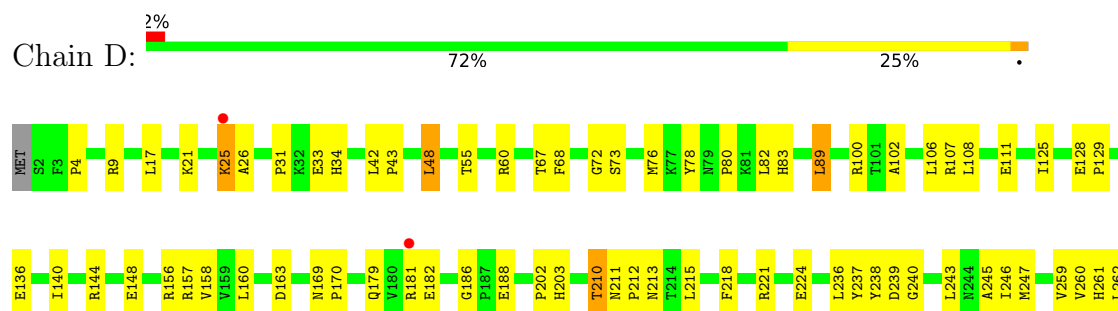
• Molecule 1: glycine dehydrogenase (decarboxylating) subunit 1

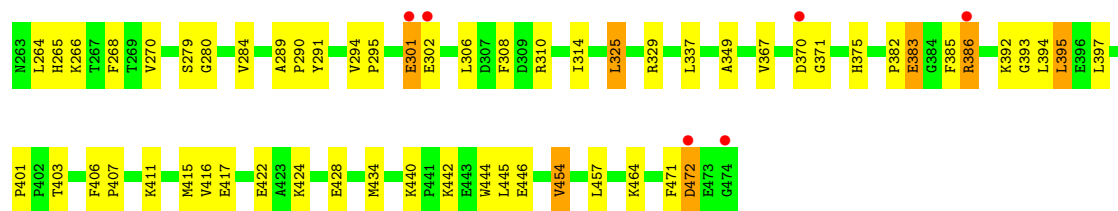


• Molecule 2: glycine dehydrogenase subunit 2 (P-protein)

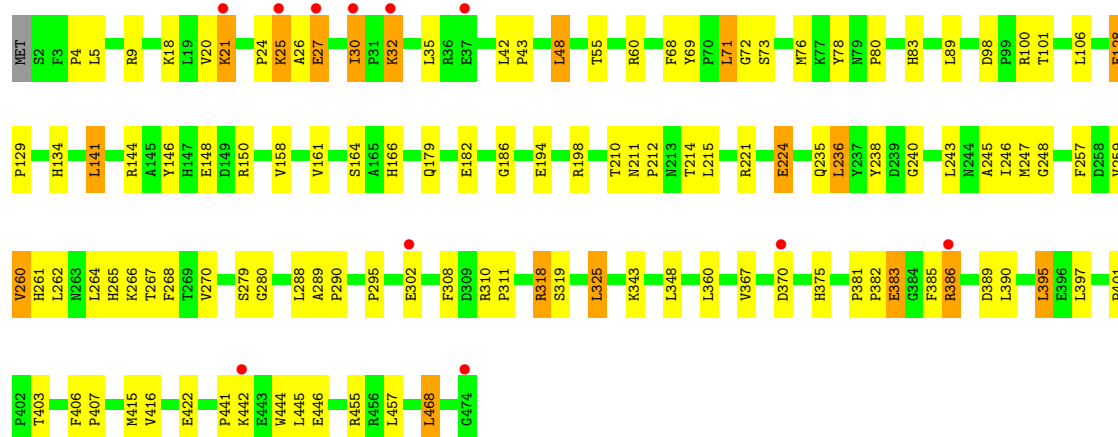
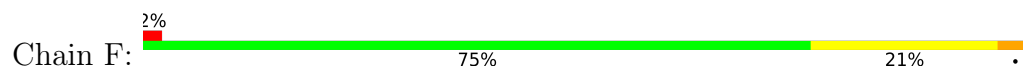


• Molecule 2: glycine dehydrogenase subunit 2 (P-protein)

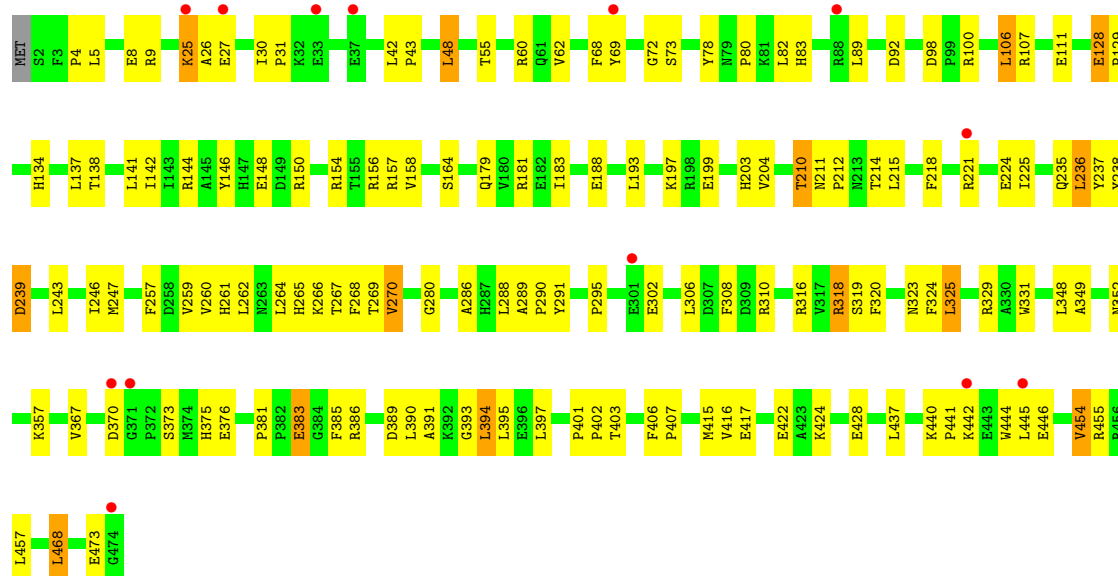




• Molecule 2: glycine dehydrogenase subunit 2 (P-protein)



• Molecule 2: glycine dehydrogenase subunit 2 (P-protein)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	134.87Å 166.67Å 189.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.57 – 2.10 49.57 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.9 (49.57-2.10) 98.9 (49.57-2.10)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 2.08Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.189 , 0.229 0.189 , 0.229	Depositor DCC
R_{free} test set	12319 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	26.5	Xtriage
Anisotropy	0.441	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 44.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	30337	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.85% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.37	0/3395	0.89	7/4617 (0.2%)
1	C	0.36	0/3395	0.87	6/4617 (0.1%)
1	E	0.38	0/3395	0.88	8/4617 (0.2%)
1	G	0.37	0/3395	0.89	10/4617 (0.2%)
2	B	0.39	1/3808 (0.0%)	0.92	19/5162 (0.4%)
2	D	0.38	1/3808 (0.0%)	0.90	16/5162 (0.3%)
2	F	0.39	1/3808 (0.0%)	0.91	13/5162 (0.3%)
2	H	0.38	1/3808 (0.0%)	0.90	19/5162 (0.4%)
All	All	0.38	4/28812 (0.0%)	0.90	98/39116 (0.3%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	266	LYS	CE-NZ	-6.91	1.28	1.49
2	B	266	LYS	CE-NZ	-6.79	1.28	1.49
2	H	266	LYS	CE-NZ	-6.63	1.29	1.49
2	F	266	LYS	CE-NZ	-6.58	1.29	1.49

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	371	GLY	N-CA-C	-9.18	101.12	112.23
1	E	308	GLN	N-CA-C	8.46	120.50	111.28
1	C	308	GLN	N-CA-C	8.29	120.31	111.28
1	A	308	GLN	N-CA-C	7.43	120.32	111.33
2	D	246	ILE	N-CA-C	7.31	119.16	112.43
2	F	268	PHE	N-CA-C	6.94	120.41	112.57
2	F	210	THR	N-CA-C	-6.93	98.94	109.95
2	B	210	THR	N-CA-C	-6.89	99.00	109.95
2	H	268	PHE	N-CA-C	6.88	120.34	112.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	324	GLN	N-CA-C	6.87	119.35	111.11
2	D	268	PHE	N-CA-C	6.83	120.29	112.57
2	B	215	LEU	N-CA-C	-6.81	104.59	113.17
2	H	210	THR	N-CA-C	-6.76	99.66	110.14
1	G	308	GLN	N-CA-C	6.70	119.43	111.33
2	F	416	VAL	N-CA-C	6.63	117.42	107.80
2	B	416	VAL	N-CA-C	6.57	117.59	107.99
1	G	324	GLN	N-CA-C	6.53	118.95	111.11
2	F	246	ILE	N-CA-C	6.48	119.42	113.20
2	B	268	PHE	N-CA-C	6.44	120.76	112.26
2	F	215	LEU	N-CA-C	-6.35	105.57	113.38
2	D	416	VAL	N-CA-C	6.33	116.98	107.80
1	C	324	GLN	N-CA-C	6.32	118.73	111.02
2	D	210	THR	N-CA-C	-6.21	100.08	109.95
2	B	179	GLN	N-CA-C	-6.19	101.36	110.52
2	F	179	GLN	N-CA-C	-6.16	101.40	110.52
1	G	214	LEU	N-CA-C	6.16	118.97	111.82
2	H	269	THR	N-CA-C	6.15	122.11	113.56
2	B	246	ILE	N-CA-C	6.11	119.07	113.20
2	F	310	ARG	CA-C-N	6.10	126.54	119.47
2	F	310	ARG	C-N-CA	6.10	126.54	119.47
2	H	416	VAL	N-CA-C	6.09	116.62	107.80
1	G	99	GLN	CA-C-N	6.07	126.24	119.32
1	G	99	GLN	C-N-CA	6.07	126.24	119.32
2	H	246	ILE	N-CA-C	6.06	118.01	112.43
1	E	201	VAL	N-CA-C	6.04	116.57	107.75
1	E	6	HIS	N-CA-C	6.00	118.90	109.96
1	A	6	HIS	N-CA-C	5.98	119.03	110.24
2	D	179	GLN	N-CA-C	-5.92	101.24	110.42
2	D	337	LEU	N-CA-C	5.92	117.81	111.36
2	B	349	ALA	N-CA-C	-5.89	104.94	111.36
2	D	310	ARG	CA-C-N	5.86	126.27	119.47
2	D	310	ARG	C-N-CA	5.86	126.27	119.47
2	B	55	THR	N-CA-C	-5.82	105.01	111.36
1	A	324	GLN	N-CA-C	5.76	118.04	111.02
2	H	128	GLU	N-CA-C	5.76	120.06	112.35
2	H	310	ARG	CA-C-N	5.75	126.15	119.47
2	H	310	ARG	C-N-CA	5.75	126.15	119.47
2	F	55	THR	N-CA-C	-5.75	105.09	111.36
2	F	158	VAL	N-CA-C	5.74	116.75	108.48
1	E	268	HIS	N-CA-C	-5.70	98.65	110.80
2	H	215	LEU	N-CA-C	-5.70	105.99	113.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	214	LEU	N-CA-C	5.68	118.41	111.82
2	D	67	THR	N-CA-C	5.67	118.02	109.23
1	C	6	HIS	N-CA-C	5.67	118.57	110.24
2	H	239	ASP	N-CA-C	-5.65	99.92	108.67
2	B	269	THR	N-CA-C	5.58	122.21	113.72
1	E	214	LEU	N-CA-C	5.51	118.21	111.82
2	H	179	GLN	N-CA-C	-5.51	102.37	110.52
1	A	93	THR	N-CA-C	5.50	119.69	112.92
2	B	302	GLU	N-CA-C	-5.50	104.93	111.03
2	D	55	THR	N-CA-C	-5.47	105.39	111.36
1	G	268	HIS	N-CA-C	-5.47	99.16	110.80
2	H	270	VAL	N-CA-C	-5.41	103.07	108.96
2	B	267	THR	N-CA-C	5.39	117.16	111.28
2	D	371	GLY	N-CA-C	-5.37	101.38	112.34
2	B	30	ILE	N-CA-C	5.36	113.99	107.61
1	G	6	HIS	N-CA-C	5.31	118.04	110.24
2	F	267	THR	N-CA-C	5.29	117.13	111.36
1	G	157	GLN	N-CA-C	-5.29	106.08	112.54
2	B	67	THR	N-CA-C	5.29	117.42	109.23
2	B	128	GLU	N-CA-C	5.28	119.42	112.35
2	D	215	LEU	N-CA-C	-5.24	106.57	113.17
1	C	99	GLN	CA-C-N	5.22	125.27	119.32
1	C	99	GLN	C-N-CA	5.22	125.27	119.32
2	H	55	THR	N-CA-C	-5.22	105.67	111.36
2	H	324	PHE	N-CA-C	5.21	117.37	111.11
1	E	157	GLN	N-CA-C	-5.21	106.02	112.38
2	H	92	ASP	N-CA-C	5.20	117.91	110.68
1	E	124	GLU	N-CA-C	5.20	119.68	112.45
1	C	157	GLN	N-CA-C	-5.19	106.78	113.01
2	D	128	GLU	N-CA-C	5.17	119.28	112.35
2	D	125	ILE	N-CA-C	5.14	114.97	107.88
2	B	324	PHE	N-CA-C	5.14	117.28	111.11
2	H	60	ARG	N-CA-C	-5.12	105.50	112.26
2	B	285	LYS	N-CA-C	-5.12	103.64	110.55
1	A	7	THR	N-CA-C	-5.10	103.19	110.59
2	H	267	THR	N-CA-C	5.10	116.84	111.28
2	D	60	ARG	N-CA-C	-5.10	105.53	112.26
2	F	60	ARG	N-CA-C	-5.10	105.53	112.26
2	D	349	ALA	N-CA-C	-5.08	105.83	111.36
2	H	286	ALA	N-CA-C	5.05	117.45	111.33
1	G	201	VAL	N-CA-C	5.05	115.18	108.11
1	G	79	PRO	N-CA-C	5.03	116.83	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	242	PRO	N-CA-C	5.02	115.95	110.58
2	H	349	ALA	N-CA-C	-5.01	105.89	111.36
2	F	128	GLU	N-CA-C	5.01	119.07	112.35
2	B	286	ALA	N-CA-C	5.01	117.39	111.33
2	B	337	LEU	N-CA-C	5.00	117.84	111.69

There are no chirality outliers.

There are no planarity outliers.

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	3320	0	3363	72	0
1	C	3320	0	3363	78	0
1	E	3320	0	3363	71	0
1	G	3320	0	3363	76	0
2	B	3713	0	3742	106	0
2	D	3713	0	3742	107	0
2	F	3713	0	3742	86	0
2	H	3713	0	3742	112	0
3	B	15	0	7	0	0
3	D	15	0	6	0	0
3	F	15	0	6	0	0
3	H	15	0	7	0	0
4	A	281	0	0	4	0
4	B	286	0	0	2	0
4	C	277	0	0	6	0
4	D	233	0	0	3	0
4	E	283	0	0	6	0
4	F	272	0	0	6	0
4	G	286	0	0	3	0
4	H	227	0	0	4	0
All	All	30337	0	28446	651	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 11.

All (651) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:442:LYS:H	2:D:442:LYS:HD2	1.17	1.09
1:C:32:LYS:H	1:C:32:LYS:HD2	1.19	1.02
2:F:30:ILE:HD11	2:F:35:LEU:HD21	1.41	0.99
2:B:235:GLN:HE22	2:B:287:HIS:HE1	1.10	0.92
1:G:32:LYS:HD3	1:G:32:LYS:H	1.39	0.85
1:C:335:ALA:HA	2:D:43:PRO:HG2	1.58	0.85
1:E:128:ALA:O	1:E:129:SER:HB2	1.76	0.82
2:B:25:LYS:HA	2:B:25:LYS:HE2	1.61	0.81
2:B:442:LYS:H	2:B:442:LYS:HD2	1.46	0.81
2:D:25:LYS:HE3	2:D:26:ALA:H	1.43	0.81
2:D:383:GLU:H	2:D:383:GLU:CD	1.87	0.81
1:E:335:ALA:HA	2:F:43:PRO:HG2	1.64	0.80
1:G:335:ALA:HA	2:H:43:PRO:HG2	1.63	0.80
1:A:436:VAL:HG23	1:A:437:LEU:HD13	1.64	0.79
2:D:442:LYS:HD2	2:D:442:LYS:N	1.97	0.79
2:F:265:HIS:HA	2:F:270:VAL:HB	1.62	0.78
2:H:238:TYR:HB3	2:H:260:VAL:HG22	1.66	0.77
2:B:383:GLU:H	2:B:383:GLU:CD	1.92	0.77
2:H:164:SER:O	2:H:214:THR:HG21	1.84	0.77
2:D:265:HIS:HA	2:D:270:VAL:HB	1.65	0.76
2:H:25:LYS:HE3	2:H:26:ALA:H	1.49	0.76
1:C:66:LYS:HG2	1:C:420:LEU:HD13	1.68	0.76
2:B:80:PRO:HG2	2:B:83:HIS:CE1	2.21	0.76
2:F:383:GLU:CD	2:F:383:GLU:H	1.93	0.75
1:E:156:SER:OG	1:E:188:THR:HG21	1.87	0.75
2:H:25:LYS:HG3	2:H:27:GLU:HG2	1.70	0.74
1:A:32:LYS:H	1:A:32:LYS:HD3	1.53	0.73
2:F:80:PRO:HG2	2:F:83:HIS:CE1	2.24	0.73
2:H:164:SER:HB2	2:H:214:THR:CG2	2.19	0.72
1:A:32:LYS:H	1:A:32:LYS:CD	2.02	0.72
1:G:97:PRO:HG2	1:G:301:LEU:HD21	1.72	0.72
1:C:32:LYS:HD2	1:C:32:LYS:N	2.00	0.72
2:B:310:ARG:HD2	4:B:499:HOH:O	1.88	0.71
2:B:235:GLN:HE22	2:B:287:HIS:CE1	2.02	0.71
2:F:68:PHE:CE1	2:F:422:GLU:HG3	2.26	0.71
1:E:1:MET:HG2	1:E:46:PRO:HA	1.71	0.71
1:E:391:ARG:HG3	1:E:391:ARG:HH11	1.56	0.71
1:A:1:MET:HE2	1:A:1:MET:H1	1.56	0.70
1:C:234:PRO:HA	1:C:237:LEU:HD23	1.73	0.70
2:D:442:LYS:H	2:D:442:LYS:CD	1.94	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:386:ARG:HD3	2:F:386:ARG:N	2.07	0.70
2:H:238:TYR:HD2	2:H:260:VAL:HG13	1.57	0.69
2:F:25:LYS:HE2	2:F:25:LYS:HA	1.72	0.69
2:H:80:PRO:HG2	2:H:83:HIS:CE1	2.28	0.69
2:H:440:LYS:HB2	2:H:445:LEU:HD21	1.75	0.69
2:H:25:LYS:HE3	2:H:26:ALA:N	2.07	0.69
2:F:129:PRO:HG2	2:F:280:GLY:O	1.93	0.68
1:E:188:THR:HG23	1:E:212:GLU:CD	2.18	0.68
2:F:72:GLY:HA3	2:F:415:MET:HG2	1.75	0.68
1:C:1:MET:HE2	1:C:1:MET:H1	1.57	0.68
1:E:391:ARG:NH1	2:F:100:ARG:HD2	2.09	0.68
2:B:358:GLU:O	2:B:362:GLU:HG3	1.94	0.68
1:C:99:GLN:HG3	2:D:395:LEU:HD21	1.75	0.67
2:D:395:LEU:HD13	2:D:401:PRO:HD3	1.77	0.67
1:E:340:GLU:O	1:E:344:GLU:HG3	1.94	0.67
1:C:377:GLU:HG2	1:C:416:ALA:HB2	1.76	0.67
2:B:68:PHE:CE1	2:B:422:GLU:HG3	2.29	0.67
2:D:157:ARG:HA	2:D:157:ARG:HE	1.59	0.67
2:D:367:VAL:CG1	2:D:370:ASP:HB3	2.26	0.66
1:G:32:LYS:H	1:G:32:LYS:CD	2.07	0.66
2:H:158:VAL:HG22	2:H:203:HIS:O	1.96	0.66
1:A:66:LYS:HG2	1:A:420:LEU:HD13	1.78	0.66
1:G:377:GLU:HG2	1:G:416:ALA:HB2	1.78	0.66
2:H:318:ARG:HD3	2:H:319:SER:O	1.95	0.66
2:H:221:ARG:HE	2:H:221:ARG:HA	1.62	0.66
1:A:335:ALA:HA	2:B:43:PRO:HG2	1.76	0.65
2:B:367:VAL:CG1	2:B:370:ASP:HB3	2.26	0.65
1:G:50:VAL:O	1:G:54:LEU:HD23	1.96	0.65
1:G:99:GLN:HG3	2:H:395:LEU:HD21	1.77	0.65
2:B:265:HIS:HA	2:B:270:VAL:HB	1.77	0.65
2:D:294:VAL:CG2	2:D:308:PHE:HA	2.28	0.64
2:H:383:GLU:CD	2:H:383:GLU:H	2.03	0.64
2:B:158:VAL:HG12	2:B:203:HIS:O	1.98	0.64
2:D:83:HIS:HB3	2:D:329:ARG:HD2	1.80	0.64
1:G:77:HIS:HB2	1:G:420:LEU:HD21	1.79	0.64
1:G:107:LEU:HD11	1:G:301:LEU:CD2	2.28	0.64
2:D:33:GLU:CD	2:D:33:GLU:H	2.05	0.64
2:D:221:ARG:NH2	2:D:224:GLU:HG3	2.13	0.64
2:D:442:LYS:O	2:D:446:GLU:HG3	1.98	0.63
2:B:243:LEU:HD13	2:B:247:MET:HB3	1.81	0.63
1:C:391:ARG:HG3	1:C:391:ARG:HH11	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:464:LYS:HE2	2:D:464:LYS:HA	1.79	0.63
2:F:26:ALA:O	2:F:30:ILE:HD13	1.99	0.63
2:B:195:ALA:O	2:B:198:ARG:HG2	1.98	0.63
2:D:144:ARG:O	2:D:148:GLU:HG3	1.98	0.63
1:E:128:ALA:O	1:E:129:SER:CB	2.47	0.63
1:G:1:MET:HG2	1:G:46:PRO:HA	1.81	0.62
2:H:4:PRO:HG2	2:H:9:ARG:NH2	2.14	0.62
2:B:198:ARG:NH1	2:B:198:ARG:HB3	2.13	0.62
2:H:129:PRO:HG2	2:H:280:GLY:O	2.00	0.62
2:D:386:ARG:H	2:D:386:ARG:NE	1.98	0.62
1:A:377:GLU:HG2	1:A:416:ALA:HB2	1.81	0.62
2:F:144:ARG:O	2:F:148:GLU:HG3	2.00	0.62
1:C:430:ARG:O	1:C:434:LYS:HG3	2.00	0.62
2:H:243:LEU:O	2:H:243:LEU:HD13	1.99	0.62
2:D:80:PRO:HG2	2:D:83:HIS:CE1	2.35	0.62
2:D:301:GLU:HG2	2:D:302:GLU:OE2	2.00	0.62
2:D:25:LYS:HE3	2:D:26:ALA:N	2.13	0.62
2:D:129:PRO:HG2	2:D:280:GLY:O	2.00	0.61
2:F:30:ILE:HD11	2:F:35:LEU:CD2	2.26	0.61
2:D:72:GLY:HA2	2:D:417:GLU:HB2	1.82	0.61
2:F:21:LYS:NZ	2:F:21:LYS:HB3	2.15	0.61
2:H:211:ASN:HA	2:H:212:PRO:C	2.25	0.61
1:E:377:GLU:HG2	1:E:416:ALA:HB2	1.80	0.61
1:G:33:GLU:H	1:G:33:GLU:CD	2.07	0.61
1:A:130:MET:HA	1:A:130:MET:HE2	1.83	0.61
2:H:5:LEU:HB2	2:H:8:GLU:HG3	1.83	0.61
1:E:68:PHE:CD2	1:E:429:LEU:HD22	2.36	0.61
1:G:107:LEU:HD11	1:G:301:LEU:HD22	1.82	0.61
1:G:311:ARG:HG3	1:G:314:LYS:HB2	1.82	0.60
2:H:265:HIS:HA	2:H:270:VAL:HB	1.82	0.60
2:H:393:GLY:O	2:H:397:LEU:HD13	2.01	0.60
1:G:433:LEU:O	1:G:436:VAL:HG22	2.00	0.60
1:E:383:PRO:HG2	1:E:437:LEU:HG	1.83	0.60
2:B:48:LEU:HG	2:D:78:TYR:HB2	1.84	0.60
2:B:32:LYS:HD2	2:B:35:LEU:HD12	1.84	0.60
2:D:411:LYS:NZ	2:D:411:LYS:HB3	2.17	0.60
1:G:12:ARG:HG3	1:G:16:ARG:HH12	1.67	0.60
1:A:32:LYS:HD3	1:A:32:LYS:N	2.15	0.60
2:B:129:PRO:HG2	2:B:280:GLY:O	2.02	0.60
1:E:66:LYS:HG2	1:E:420:LEU:HD13	1.83	0.59
1:A:1:MET:HG3	1:A:46:PRO:HA	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:391:ARG:HD3	4:G:591:HOH:O	2.02	0.59
2:H:395:LEU:CD1	2:H:401:PRO:HD3	2.32	0.59
2:D:4:PRO:HG2	2:D:9:ARG:CZ	2.33	0.59
2:H:262:LEU:O	2:H:280:GLY:HA2	2.02	0.59
1:C:1:MET:HE2	1:C:1:MET:N	2.17	0.59
2:B:78:TYR:HB2	2:D:48:LEU:HG	1.84	0.59
2:B:106:LEU:HD11	2:B:306:LEU:HD21	1.85	0.59
2:D:243:LEU:HD13	2:D:243:LEU:O	2.03	0.59
2:F:221:ARG:NH2	2:F:224:GLU:HG3	2.18	0.59
2:H:83:HIS:HB3	2:H:329:ARG:HD2	1.85	0.59
1:C:130:MET:HA	1:C:130:MET:HE2	1.85	0.58
1:C:391:ARG:NH1	2:D:100:ARG:HD2	2.18	0.58
1:A:352:MET:HE2	1:A:421:HIS:O	2.03	0.58
1:E:168:ARG:O	1:E:172:GLU:HG3	2.03	0.58
2:F:78:TYR:HB2	2:H:48:LEU:HG	1.85	0.58
1:G:32:LYS:HG2	1:G:33:GLU:OE2	2.03	0.58
1:A:222:HIS:HE1	1:A:249:ASP:OD2	1.85	0.58
2:B:158:VAL:HG13	2:B:204:VAL:HA	1.85	0.58
1:C:423:GLU:O	1:C:427:LEU:HD23	2.04	0.58
1:G:128:ALA:O	1:G:129:SER:CB	2.52	0.58
1:E:351:GLU:OE1	2:F:24:PRO:HB3	2.03	0.58
2:H:156:ARG:O	2:H:157:ARG:HD2	2.03	0.58
2:H:98:ASP:OD2	2:H:100:ARG:HB2	2.04	0.58
2:B:158:VAL:CG1	2:B:204:VAL:HA	2.34	0.58
1:E:311:ARG:HG3	1:E:314:LYS:HB2	1.85	0.58
2:F:403:THR:HB	2:F:415:MET:HB3	1.85	0.58
2:B:395:LEU:HD13	2:B:401:PRO:HD3	1.85	0.58
1:G:30:LEU:HD22	2:H:218:PHE:CG	2.39	0.58
1:C:340:GLU:O	1:C:344:GLU:HG3	2.03	0.57
2:D:454:VAL:HG11	2:D:457:LEU:HD21	1.85	0.57
1:G:391:ARG:HG3	1:G:391:ARG:HH11	1.69	0.57
1:C:233:ASP:O	1:C:237:LEU:HD22	2.04	0.57
2:B:4:PRO:HG2	2:B:9:ARG:NH2	2.20	0.57
1:C:95:TYR:HB2	2:D:76:MET:CE	2.34	0.57
1:C:128:ALA:O	1:C:129:SER:CB	2.52	0.57
2:D:245:ALA:HB2	2:D:375:HIS:HB3	1.86	0.57
2:H:144:ARG:O	2:H:148:GLU:HG3	2.04	0.57
1:A:1:MET:HE2	1:A:1:MET:N	2.19	0.57
2:B:442:LYS:HD2	2:B:442:LYS:N	2.17	0.57
1:A:108:GLN:O	1:A:112:GLU:HG3	2.04	0.57
2:B:442:LYS:H	2:B:442:LYS:CD	2.10	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:222:HIS:HE1	1:G:249:ASP:OD2	1.87	0.57
2:H:68:PHE:CE1	2:H:422:GLU:HG3	2.39	0.57
2:B:243:LEU:CD1	2:B:247:MET:HB3	2.34	0.57
2:D:243:LEU:CD1	2:D:247:MET:HG2	2.35	0.57
1:C:72:GLY:HA3	4:C:531:HOH:O	2.04	0.57
1:G:436:VAL:HG23	1:G:437:LEU:HD13	1.86	0.56
2:D:367:VAL:HG12	2:D:370:ASP:HB3	1.87	0.56
2:F:4:PRO:HG2	2:F:9:ARG:CZ	2.35	0.56
1:A:62:LEU:HD22	1:A:399:HIS:NE2	2.20	0.56
2:F:442:LYS:O	2:F:446:GLU:HG3	2.05	0.56
2:H:4:PRO:HG2	2:H:9:ARG:CZ	2.35	0.56
2:F:236:LEU:HD22	2:F:257:PHE:CE1	2.40	0.56
2:F:386:ARG:HD3	2:F:386:ARG:H	1.70	0.56
2:H:403:THR:HB	2:H:415:MET:HB3	1.87	0.56
2:B:235:GLN:NE2	2:B:287:HIS:HE1	1.92	0.56
2:D:264:LEU:HD22	2:D:279:SER:HB3	1.88	0.56
2:F:318:ARG:HD3	2:F:319:SER:O	2.05	0.56
1:G:372:LYS:HB2	1:G:372:LYS:NZ	2.21	0.56
1:A:291:VAL:HG22	1:A:295:GLY:C	2.31	0.56
1:A:168:ARG:O	1:A:172:GLU:HG3	2.06	0.56
1:G:391:ARG:O	1:G:395:GLU:HG3	2.06	0.56
2:F:245:ALA:HB2	2:F:375:HIS:HB3	1.88	0.55
2:H:375:HIS:CE1	2:H:376:GLU:HG2	2.41	0.55
1:G:99:GLN:HG2	2:H:395:LEU:HD11	1.89	0.55
2:H:391:ALA:O	2:H:395:LEU:HD13	2.07	0.55
2:H:146:TYR:O	2:H:150:ARG:HG3	2.06	0.55
2:F:441:PRO:HG2	2:F:444:TRP:HB2	1.88	0.55
2:F:4:PRO:HG2	2:F:9:ARG:NH2	2.22	0.55
2:F:30:ILE:HD13	2:F:30:ILE:H	1.72	0.55
1:G:384:LYS:HD2	1:G:437:LEU:HD12	1.89	0.55
2:H:394:LEU:HD13	2:H:437:LEU:HD11	1.87	0.55
1:C:50:VAL:O	1:C:54:LEU:HD22	2.07	0.55
2:H:188:GLU:HB2	4:H:660:HOH:O	2.06	0.55
2:B:68:PHE:HE1	2:B:422:GLU:HG3	1.71	0.55
2:B:357:LYS:HE2	2:B:373:SER:OG	2.07	0.55
1:G:391:ARG:HG3	1:G:391:ARG:NH1	2.21	0.55
1:C:188:THR:HG23	1:C:212:GLU:CD	2.32	0.54
1:G:128:ALA:O	1:G:129:SER:HB3	2.06	0.54
2:H:406:PHE:HA	2:H:407:PRO:C	2.32	0.54
2:H:442:LYS:O	2:H:446:GLU:HG3	2.07	0.54
2:H:289:ALA:N	2:H:290:PRO:HD2	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:441:PRO:HG2	2:H:444:TRP:HB2	1.88	0.54
2:F:68:PHE:HE1	2:F:422:GLU:HG3	1.71	0.54
2:F:243:LEU:CD1	2:F:247:MET:HB3	2.38	0.54
2:D:102:ALA:O	2:D:106:LEU:HD23	2.07	0.54
1:A:128:ALA:O	1:A:129:SER:CB	2.55	0.54
2:B:25:LYS:HA	2:B:25:LYS:CE	2.36	0.54
2:B:198:ARG:HH11	2:B:198:ARG:CB	2.21	0.54
2:D:158:VAL:HG11	2:D:181:ARG:HG3	1.89	0.54
1:E:167:LEU:HG	1:E:171:LEU:HD22	1.88	0.54
1:E:348:LYS:HE3	2:F:20:VAL:HG13	1.90	0.54
1:A:128:ALA:O	1:A:129:SER:HB3	2.07	0.53
1:A:406:ARG:HG2	1:A:406:ARG:HH11	1.72	0.53
1:A:367:ARG:HG3	1:A:368:PRO:HD2	1.91	0.53
1:C:144:ALA:HA	1:C:227:LEU:HD12	1.90	0.53
2:D:411:LYS:HB3	2:D:411:LYS:HZ3	1.73	0.53
1:G:12:ARG:HG3	1:G:16:ARG:NH1	2.23	0.53
1:C:128:ALA:O	1:C:129:SER:HB3	2.09	0.53
1:E:196:GLU:H	1:E:196:GLU:CD	2.17	0.53
2:D:289:ALA:N	2:D:290:PRO:HD2	2.23	0.53
2:D:31:PRO:HG2	2:D:34:HIS:HD2	1.74	0.53
2:D:464:LYS:HE2	2:D:464:LYS:CA	2.38	0.53
1:E:65:HIS:O	1:E:66:LYS:HB2	2.09	0.53
1:G:432:ALA:O	1:G:436:VAL:HG13	2.09	0.53
2:H:164:SER:HB2	2:H:214:THR:HG21	1.90	0.53
2:B:4:PRO:HG2	2:B:9:ARG:CZ	2.40	0.52
2:F:318:ARG:CD	2:F:319:SER:O	2.57	0.52
2:B:375:HIS:CE1	2:B:376:GLU:HG2	2.44	0.52
2:D:160:LEU:HD23	2:D:181:ARG:HB2	1.90	0.52
2:F:146:TYR:O	2:F:150:ARG:HG3	2.09	0.52
1:A:391:ARG:O	1:A:395:GLU:HG3	2.10	0.52
2:D:294:VAL:HG23	2:D:308:PHE:HA	1.91	0.52
1:G:291:VAL:HG22	1:G:295:GLY:C	2.34	0.52
1:A:1:MET:H1	1:A:1:MET:CE	2.23	0.52
1:A:376:ASN:H	1:A:376:ASN:HD22	1.57	0.52
1:A:391:ARG:HG3	1:A:391:ARG:HH11	1.75	0.52
1:C:108:GLN:O	1:C:112:GLU:HG3	2.09	0.52
1:E:65:HIS:CE1	1:E:66:LYS:HG3	2.45	0.52
2:F:265:HIS:CA	2:F:270:VAL:HB	2.37	0.52
2:D:31:PRO:HB2	2:D:33:GLU:OE2	2.09	0.52
2:F:367:VAL:CG1	2:F:370:ASP:HB3	2.40	0.52
2:B:30:ILE:HB	2:B:35:LEU:HD21	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:72:GLY:HA3	2:D:415:MET:HG2	1.92	0.52
1:C:7:THR:OG1	1:C:10:GLU:HG3	2.10	0.52
1:C:32:LYS:H	1:C:32:LYS:CD	1.94	0.52
1:E:391:ARG:O	1:E:395:GLU:HG3	2.10	0.52
2:H:62:VAL:HG23	2:H:69:TYR:OH	2.10	0.52
1:G:340:GLU:O	1:G:344:GLU:HG3	2.10	0.52
2:H:367:VAL:CG1	2:H:370:ASP:HB3	2.40	0.52
1:C:1:MET:H1	1:C:1:MET:CE	2.23	0.51
2:D:106:LEU:HD11	2:D:306:LEU:HD21	1.92	0.51
1:A:167:LEU:HG	1:A:171:LEU:HD22	1.91	0.51
1:A:17:ARG:NH2	2:B:362:GLU:OE1	2.43	0.51
2:F:238:TYR:CE2	2:F:240:GLY:HA2	2.45	0.51
2:F:318:ARG:HD3	2:F:319:SER:N	2.25	0.51
1:G:12:ARG:HD3	4:G:721:HOH:O	2.10	0.51
2:H:236:LEU:HD22	2:H:257:PHE:CE1	2.45	0.51
1:E:280:ARG:O	1:E:280:ARG:HD3	2.10	0.51
2:B:394:LEU:HD13	2:B:437:LEU:CD1	2.41	0.51
1:C:222:HIS:HE1	1:C:249:ASP:OD2	1.93	0.51
2:D:238:TYR:HB3	2:D:260:VAL:HG12	1.92	0.51
1:A:32:LYS:H	1:A:32:LYS:CE	2.24	0.51
2:B:211:ASN:HA	2:B:212:PRO:C	2.35	0.51
1:E:4:THR:HG21	2:F:348:LEU:HD12	1.93	0.51
2:H:237:TYR:OH	2:H:261:HIS:HB3	2.11	0.51
2:B:442:LYS:O	2:B:446:GLU:HG3	2.11	0.51
2:B:81:LYS:HE3	4:B:526:HOH:O	2.09	0.51
2:H:243:LEU:CD1	2:H:247:MET:HG2	2.41	0.51
2:B:318:ARG:HD3	2:B:319:SER:O	2.10	0.50
1:C:314:LYS:NZ	1:C:314:LYS:HB3	2.25	0.50
2:B:301:GLU:HA	2:B:301:GLU:OE1	2.10	0.50
2:D:31:PRO:HG2	2:D:34:HIS:CD2	2.46	0.50
2:D:471:PHE:O	2:D:472:ASP:C	2.55	0.50
1:E:280:ARG:NH1	1:E:316:LYS:NZ	2.59	0.50
1:C:9:GLU:H	1:C:9:GLU:CD	2.18	0.50
2:D:302:GLU:CD	2:D:302:GLU:H	2.18	0.50
1:E:65:HIS:HD2	4:F:732:HOH:O	1.94	0.50
1:A:376:ASN:H	1:A:376:ASN:ND2	2.10	0.50
2:H:394:LEU:HD13	2:H:437:LEU:CD1	2.41	0.50
1:C:143:LEU:HD23	1:C:143:LEU:C	2.37	0.50
1:C:311:ARG:HG3	1:C:314:LYS:HB2	1.93	0.50
2:F:243:LEU:HD13	2:F:247:MET:HB3	1.93	0.50
1:A:300:ILE:HD13	2:B:459:GLU:HG2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:394:LEU:HD13	2:B:437:LEU:HD11	1.93	0.50
2:H:72:GLY:HA2	2:H:417:GLU:HB3	1.92	0.50
2:D:386:ARG:H	2:D:386:ARG:HE	1.60	0.50
2:H:72:GLY:HA3	2:H:415:MET:HG2	1.92	0.50
2:F:211:ASN:HA	2:F:212:PRO:C	2.37	0.49
2:D:4:PRO:HG2	2:D:9:ARG:NH2	2.26	0.49
2:B:289:ALA:N	2:B:290:PRO:HD2	2.27	0.49
1:C:30:LEU:HD22	2:D:218:PHE:CG	2.47	0.49
1:E:241:LYS:HD3	1:E:246:TYR:CZ	2.46	0.49
1:A:433:LEU:HA	1:A:436:VAL:HG22	1.93	0.49
1:C:212:GLU:HG3	4:C:696:HOH:O	2.12	0.49
2:H:381:PRO:HB3	2:H:390:LEU:CD1	2.43	0.49
1:A:9:GLU:CD	1:A:9:GLU:H	2.20	0.49
2:F:48:LEU:HG	2:H:78:TYR:HB2	1.94	0.49
1:A:372:LYS:N	1:A:372:LYS:HD2	2.27	0.49
2:B:28:ASP:C	2:B:29:LEU:HD22	2.38	0.49
2:H:395:LEU:HD12	2:H:401:PRO:HD3	1.94	0.49
2:D:294:VAL:CG2	2:D:295:PRO:HA	2.42	0.49
2:H:260:VAL:HG12	2:H:261:HIS:N	2.26	0.49
2:B:31:PRO:HG2	2:B:34:HIS:HD2	1.77	0.49
2:D:188:GLU:HB2	4:D:616:HOH:O	2.13	0.49
2:D:301:GLU:N	2:D:301:GLU:OE1	2.45	0.49
1:A:356:LEU:HB2	1:A:426:LEU:HD22	1.95	0.48
1:A:376:ASN:HD22	1:A:376:ASN:N	2.11	0.48
2:B:146:TYR:O	2:B:150:ARG:HG3	2.12	0.48
2:D:261:HIS:CD2	2:D:261:HIS:C	2.91	0.48
1:A:300:ILE:CD1	2:B:459:GLU:HG2	2.42	0.48
1:E:1:MET:HE3	1:E:45:LEU:C	2.38	0.48
1:G:108:GLN:O	1:G:112:GLU:HG3	2.13	0.48
2:H:107:ARG:O	2:H:111:GLU:HG3	2.12	0.48
2:F:161:VAL:O	2:F:182:GLU:HA	2.13	0.48
2:F:21:LYS:HB3	2:F:21:LYS:HZ3	1.77	0.48
1:E:130:MET:HE2	1:E:130:MET:HA	1.94	0.48
2:H:158:VAL:CG2	2:H:204:VAL:HA	2.43	0.48
1:E:22:SER:OG	1:E:24:GLU:HG2	2.14	0.48
1:E:108:GLN:O	1:E:112:GLU:HG3	2.14	0.48
1:E:391:ARG:HG3	1:E:391:ARG:NH1	2.27	0.48
2:D:454:VAL:CG1	2:D:457:LEU:HD21	2.43	0.48
1:E:7:THR:OG1	1:E:10:GLU:HG3	2.14	0.48
2:H:210:THR:HG22	2:H:239:ASP:HB3	1.95	0.48
2:D:136:GLU:O	2:D:140:ILE:HG12	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:430:ARG:O	1:G:434:LYS:HG3	2.14	0.48
2:B:134:HIS:HE1	2:B:318:ARG:HB3	1.79	0.48
2:F:32:LYS:HE3	2:F:35:LEU:HB2	1.96	0.48
1:G:49:LYS:HE3	1:G:52:GLU:OE1	2.14	0.48
2:B:238:TYR:HB3	2:B:260:VAL:HG12	1.95	0.47
2:F:128:GLU:N	2:F:129:PRO:HD2	2.29	0.47
2:F:381:PRO:HB3	2:F:390:LEU:CD1	2.44	0.47
2:B:367:VAL:HG12	2:B:370:ASP:HB3	1.96	0.47
1:C:45:LEU:HD22	1:C:49:LYS:HG2	1.97	0.47
2:D:370:ASP:HA	4:D:594:HOH:O	2.13	0.47
1:G:197:VAL:O	1:G:226:ALA:HB2	2.14	0.47
2:B:245:ALA:HB2	2:B:375:HIS:HB3	1.94	0.47
2:B:454:VAL:HG11	2:B:457:LEU:HD21	1.97	0.47
2:D:264:LEU:HD22	2:D:279:SER:CB	2.43	0.47
2:D:393:GLY:O	2:D:397:LEU:HD13	2.14	0.47
2:F:455:ARG:HB3	4:F:579:HOH:O	2.14	0.47
1:C:69:LEU:HA	4:C:592:HOH:O	2.14	0.47
1:C:168:ARG:O	1:C:172:GLU:HG3	2.14	0.47
1:E:216:PRO:HG2	4:E:592:HOH:O	2.14	0.47
2:F:238:TYR:HB3	2:F:260:VAL:HG12	1.97	0.47
2:D:169:ASN:HB2	2:D:170:PRO:CD	2.45	0.47
2:D:291:TYR:O	2:D:314:ILE:HG23	2.15	0.47
1:E:333:TYR:CE1	1:E:337:LEU:HD12	2.48	0.47
1:G:402:THR:HB	1:G:414:LEU:HB2	1.96	0.47
1:A:73:VAL:HG23	2:B:320:PHE:CZ	2.50	0.47
1:A:386:PRO:HG2	4:A:671:HOH:O	2.15	0.47
2:B:98:ASP:OD2	2:B:100:ARG:HB2	2.14	0.47
1:E:137:LEU:HA	1:E:252:VAL:HG21	1.97	0.47
1:G:239:VAL:HG21	1:G:347:LEU:HD21	1.96	0.47
2:B:406:PHE:HA	2:B:407:PRO:C	2.40	0.47
1:E:212:GLU:HG3	4:E:648:HOH:O	2.14	0.47
1:E:343:ARG:HH22	2:F:25:LYS:NZ	2.13	0.47
1:G:65:HIS:O	1:G:66:LYS:HB2	2.15	0.47
2:H:454:VAL:HG11	2:H:457:LEU:HD21	1.96	0.47
1:A:293:VAL:HG12	2:B:455:ARG:HB2	1.97	0.47
2:B:29:LEU:HD22	2:B:29:LEU:N	2.29	0.47
2:B:381:PRO:HB3	2:B:390:LEU:CD1	2.45	0.47
2:H:158:VAL:HG23	2:H:204:VAL:HA	1.96	0.47
2:F:318:ARG:NE	4:F:626:HOH:O	2.25	0.47
2:H:137:LEU:O	2:H:141:LEU:HD13	2.15	0.47
1:A:12:ARG:HG2	1:A:12:ARG:HH11	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:325:LEU:O	2:D:329:ARG:HG2	2.15	0.46
1:E:65:HIS:ND1	1:E:66:LYS:HG3	2.30	0.46
1:E:95:TYR:CG	1:E:96:THR:N	2.83	0.46
1:A:46:PRO:HD3	2:D:21:LYS:HG2	1.97	0.46
1:A:348:LYS:HG3	1:A:419:GLU:HA	1.98	0.46
2:B:403:THR:HB	2:B:415:MET:HB3	1.96	0.46
1:C:352:MET:HE2	1:C:421:HIS:O	2.15	0.46
1:E:97:PRO:HG3	1:E:107:LEU:HD13	1.97	0.46
1:E:376:ASN:HD22	1:E:376:ASN:H	1.64	0.46
2:F:386:ARG:HG2	2:F:389:ASP:OD2	2.15	0.46
2:H:221:ARG:HA	2:H:221:ARG:NE	2.29	0.46
2:D:262:LEU:O	2:D:280:GLY:HA2	2.15	0.46
1:E:299:PHE:CZ	2:F:5:LEU:HD21	2.50	0.46
1:G:7:THR:OG1	1:G:10:GLU:HG3	2.15	0.46
1:A:95:TYR:HB2	2:B:76:MET:CE	2.46	0.46
2:D:211:ASN:HA	2:D:212:PRO:C	2.40	0.46
2:D:406:PHE:HA	2:D:407:PRO:C	2.41	0.46
2:H:80:PRO:CG	2:H:83:HIS:CE1	2.98	0.46
2:D:265:HIS:CA	2:D:270:VAL:HB	2.40	0.46
1:E:188:THR:HG23	1:E:212:GLU:OE1	2.15	0.46
1:C:101:GLU:CD	2:D:392:LYS:HZ2	2.24	0.46
2:B:40:PRO:HG2	2:B:42:LEU:HD22	1.98	0.46
1:E:195:GLU:HG2	4:E:704:HOH:O	2.16	0.46
2:H:142:ILE:HG23	2:H:291:TYR:HB2	1.98	0.46
2:H:193:LEU:O	2:H:197:LYS:HG3	2.16	0.46
2:B:31:PRO:HG2	2:B:34:HIS:CD2	2.50	0.46
2:B:394:LEU:HD23	2:B:401:PRO:HA	1.97	0.46
1:C:156:SER:OG	1:C:188:THR:HG21	2.16	0.46
1:E:391:ARG:HH11	1:E:391:ARG:CG	2.27	0.46
2:F:235:GLN:HE21	2:F:288:LEU:HD11	1.79	0.46
2:H:30:ILE:HG23	2:H:31:PRO:HD2	1.97	0.46
2:B:444:TRP:CE3	2:B:445:LEU:HD12	2.51	0.46
2:D:294:VAL:HG23	2:D:295:PRO:HA	1.98	0.46
2:F:262:LEU:O	2:F:280:GLY:HA2	2.16	0.46
1:C:357:HIS:O	1:C:361:LEU:HD13	2.16	0.45
1:E:95:TYR:HB2	2:F:76:MET:CE	2.46	0.45
1:E:400:GLY:O	1:E:401:ALA:HB3	2.15	0.45
1:C:51:LEU:HG	2:D:82:LEU:HD11	1.98	0.45
1:G:50:VAL:O	1:G:54:LEU:CD2	2.63	0.45
2:H:138:THR:O	2:H:142:ILE:HG13	2.16	0.45
2:H:386:ARG:HG2	2:H:389:ASP:OD2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:306:LEU:N	2:H:306:LEU:HD22	2.31	0.45
2:H:325:LEU:O	2:H:329:ARG:HG2	2.16	0.45
2:D:210:THR:CG2	2:D:239:ASP:HB3	2.47	0.45
1:G:249:ASP:C	1:G:250:ILE:HG13	2.40	0.45
1:G:299:PHE:CZ	2:H:5:LEU:HD21	2.51	0.45
1:A:280:ARG:NH2	1:A:311:ARG:HH22	2.13	0.45
1:A:322:ASN:O	2:B:277:PRO:HA	2.16	0.45
1:A:376:ASN:ND2	4:A:526:HOH:O	2.50	0.45
2:F:395:LEU:HD13	2:F:401:PRO:HD3	1.98	0.45
1:A:433:LEU:O	1:A:436:VAL:HG22	2.16	0.45
2:B:382:PRO:HG2	2:B:385:PHE:CD1	2.52	0.45
1:G:14:MET:HE1	2:H:352:ASN:OD1	2.17	0.45
1:G:301:LEU:HD23	4:G:504:HOH:O	2.16	0.45
1:A:4:THR:HG21	2:B:348:LEU:HD12	1.98	0.45
2:B:262:LEU:O	2:B:280:GLY:HA2	2.16	0.45
2:D:294:VAL:HG21	2:D:308:PHE:HA	1.98	0.45
1:E:305:ALA:HB3	4:E:678:HOH:O	2.16	0.45
2:F:26:ALA:HB1	2:F:35:LEU:HD21	1.98	0.45
2:F:382:PRO:HG2	2:F:385:PHE:CD1	2.52	0.45
1:G:95:TYR:CG	1:G:96:THR:N	2.85	0.45
1:A:51:LEU:HG	2:B:82:LEU:HD11	1.97	0.45
1:G:121:ALA:HB1	1:G:123:LEU:HD23	1.98	0.45
1:A:143:LEU:C	1:A:143:LEU:HD23	2.42	0.45
2:H:455:ARG:HB3	4:H:548:HOH:O	2.16	0.45
1:A:31:PRO:HG2	1:A:34:ILE:HG12	1.99	0.45
1:A:383:PRO:HG2	1:A:437:LEU:HG	1.99	0.45
2:B:210:THR:HG22	2:B:239:ASP:HB3	1.98	0.45
1:C:197:VAL:O	1:C:226:ALA:HB2	2.17	0.45
1:C:261:PRO:HG2	4:C:502:HOH:O	2.17	0.45
1:G:12:ARG:NE	1:G:16:ARG:HH12	2.15	0.45
2:B:236:LEU:HD22	2:B:257:PHE:CE1	2.52	0.44
2:F:25:LYS:HD3	2:F:27:GLU:HG3	1.99	0.44
1:A:400:GLY:O	1:A:401:ALA:HB3	2.17	0.44
2:D:25:LYS:HE3	2:D:25:LYS:HA	1.98	0.44
2:F:248:GLY:HA3	2:F:343:LYS:HG2	1.99	0.44
2:B:444:TRP:HE3	2:B:445:LEU:HD12	1.83	0.44
2:F:134:HIS:HE1	2:F:318:ARG:HB3	1.81	0.44
1:A:66:LYS:HD2	4:C:657:HOH:O	2.17	0.44
1:A:95:TYR:CG	1:A:96:THR:N	2.85	0.44
2:B:318:ARG:NH2	2:B:323:ASN:OD1	2.50	0.44
1:E:197:VAL:O	1:E:226:ALA:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:245:ALA:HB2	2:B:375:HIS:CG	2.53	0.44
1:E:348:LYS:HG3	1:E:419:GLU:HA	1.98	0.44
1:A:396:ARG:HH11	1:A:396:ARG:HG3	1.83	0.44
2:B:210:THR:OG1	2:B:213:ASN:HA	2.17	0.44
1:C:95:TYR:HB2	2:D:76:MET:HE1	1.99	0.44
1:C:95:TYR:CG	1:C:96:THR:N	2.86	0.44
1:C:255:GLY:HA3	1:C:269:PHE:CE1	2.52	0.44
1:E:204:ASN:HA	1:E:205:PRO:C	2.42	0.44
1:E:292:ASP:OD1	1:E:292:ASP:C	2.61	0.44
2:H:402:PRO:HB2	2:H:415:MET:O	2.18	0.44
2:B:102:ALA:O	2:B:106:LEU:HD23	2.18	0.44
2:B:381:PRO:HB2	2:B:385:PHE:HB2	1.99	0.44
1:C:376:ASN:HD22	1:C:376:ASN:H	1.66	0.44
1:C:174:VAL:HG22	1:C:174:VAL:O	2.18	0.44
1:G:97:PRO:HB2	1:G:107:LEU:HD22	1.99	0.44
1:C:400:GLY:O	1:C:401:ALA:HB3	2.18	0.43
2:F:129:PRO:CG	2:F:280:GLY:O	2.62	0.43
2:H:80:PRO:HG2	2:H:83:HIS:ND1	2.34	0.43
1:A:30:LEU:HD22	2:B:218:PHE:CG	2.53	0.43
2:B:198:ARG:NH1	2:B:198:ARG:CB	2.78	0.43
2:B:466:PRO:HB2	2:B:468:LEU:CD1	2.48	0.43
1:C:248:ALA:O	1:C:275:LYS:HE3	2.19	0.43
1:C:391:ARG:HG3	1:C:391:ARG:NH1	2.31	0.43
1:E:376:ASN:H	1:E:376:ASN:ND2	2.16	0.43
1:G:391:ARG:NH1	2:H:100:ARG:CZ	2.81	0.43
1:E:143:LEU:HD23	1:E:143:LEU:C	2.42	0.43
1:G:167:LEU:HG	1:G:171:LEU:HD22	2.00	0.43
2:H:394:LEU:HD12	2:H:394:LEU:HA	1.90	0.43
1:C:79:PRO:HA	1:C:80:PRO:HD2	1.84	0.43
1:C:204:ASN:HA	1:C:205:PRO:C	2.43	0.43
1:G:328:LEU:O	1:G:332:MET:HG3	2.19	0.43
2:H:316:ARG:NH1	2:H:316:ARG:HG2	2.34	0.43
2:F:30:ILE:HD13	2:F:30:ILE:N	2.34	0.43
1:C:267:PRO:HD2	2:D:325:LEU:HB2	2.00	0.43
2:F:30:ILE:HG12	2:F:35:LEU:HG	1.99	0.43
2:H:381:PRO:HB2	2:H:385:PHE:HB2	2.00	0.43
1:A:65:HIS:O	1:A:66:LYS:HB2	2.19	0.43
1:E:406:ARG:HD2	4:E:554:HOH:O	2.17	0.43
2:H:134:HIS:HE1	2:H:318:ARG:HB3	1.84	0.43
2:H:318:ARG:NH2	2:H:323:ASN:OD1	2.51	0.43
1:G:185:GLY:O	1:G:371:PRO:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:72:GLY:HA2	2:H:417:GLU:CB	2.49	0.43
2:H:210:THR:CG2	2:H:239:ASP:HB3	2.49	0.43
2:D:163:ASP:HA	2:D:182:GLU:CD	2.43	0.43
1:G:49:LYS:HA	1:G:49:LYS:HD2	1.83	0.43
1:G:255:GLY:HA3	1:G:269:PHE:CE1	2.54	0.43
2:H:154:ARG:HG3	2:H:154:ARG:HH11	1.84	0.43
1:A:406:ARG:HG2	1:A:406:ARG:NH1	2.32	0.43
1:G:383:PRO:HG2	1:G:437:LEU:HG	2.01	0.43
1:C:196:GLU:CD	1:C:196:GLU:H	2.27	0.42
1:C:376:ASN:H	1:C:376:ASN:ND2	2.16	0.42
1:G:400:GLY:O	1:G:401:ALA:HB3	2.18	0.42
2:H:357:LYS:HD2	2:H:373:SER:OG	2.18	0.42
4:A:718:HOH:O	2:B:266:LYS:HE2	2.19	0.42
1:C:54:LEU:HB3	2:D:89:LEU:HD23	2.00	0.42
1:E:391:ARG:NH1	2:F:98:ASP:OD2	2.52	0.42
2:D:107:ARG:O	2:D:111:GLU:HG3	2.20	0.42
2:D:238:TYR:CE2	2:D:240:GLY:HA2	2.54	0.42
2:D:440:LYS:HG2	2:D:444:TRP:CE3	2.54	0.42
1:E:376:ASN:HD22	1:E:376:ASN:N	2.18	0.42
2:F:69:TYR:HD1	2:F:71:LEU:HD22	1.84	0.42
1:G:30:LEU:HD22	2:H:218:PHE:CD2	2.54	0.42
1:G:291:VAL:CG2	1:G:295:GLY:C	2.92	0.42
2:D:302:GLU:CD	2:D:302:GLU:N	2.78	0.42
1:E:299:PHE:HZ	2:F:5:LEU:HD21	1.85	0.42
2:F:166:HIS:HA	2:F:406:PHE:CZ	2.54	0.42
1:G:4:THR:HG21	2:H:348:LEU:HD12	2.00	0.42
1:A:97:PRO:HG3	1:A:107:LEU:HD13	2.01	0.42
2:B:210:THR:CG2	2:B:239:ASP:HB3	2.50	0.42
1:C:24:GLU:OE1	1:C:24:GLU:N	2.42	0.42
1:C:328:LEU:O	1:C:332:MET:HG3	2.19	0.42
2:D:72:GLY:HA2	2:D:417:GLU:CB	2.49	0.42
2:F:68:PHE:CD1	2:F:422:GLU:HG3	2.54	0.42
2:H:238:TYR:CB	2:H:260:VAL:HG22	2.44	0.42
1:A:79:PRO:HA	1:A:80:PRO:HD2	1.85	0.42
1:A:196:GLU:OE2	1:A:197:VAL:HG23	2.19	0.42
1:E:383:PRO:CG	1:E:437:LEU:HG	2.47	0.42
2:F:261:HIS:CD2	2:F:261:HIS:C	2.98	0.42
2:H:295:PRO:HB3	2:H:308:PHE:CE1	2.54	0.42
1:C:52:GLU:O	1:C:56:ARG:HG3	2.20	0.42
1:C:387:GLU:HG3	4:C:517:HOH:O	2.20	0.42
2:B:238:TYR:CE2	2:B:240:GLY:HA2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:441:PRO:HG2	2:B:444:TRP:HB2	2.02	0.42
2:D:68:PHE:CE1	2:D:422:GLU:HG3	2.55	0.42
2:D:382:PRO:HG2	2:D:385:PHE:CD1	2.54	0.42
1:G:12:ARG:CD	1:G:16:ARG:HH12	2.33	0.42
2:H:106:LEU:HD11	2:H:306:LEU:HD21	2.01	0.42
2:H:128:GLU:N	2:H:129:PRO:HD2	2.35	0.42
2:H:181:ARG:HD2	2:H:199:GLU:OE1	2.20	0.42
2:B:169:ASN:HB2	2:B:170:PRO:CD	2.50	0.42
1:C:151:MET:HE3	1:C:175:GLY:C	2.45	0.42
1:C:314:LYS:HB3	1:C:314:LYS:HZ2	1.84	0.42
2:D:403:THR:HB	2:D:415:MET:HB3	2.02	0.42
1:G:143:LEU:C	1:G:143:LEU:HD23	2.44	0.42
1:A:95:TYR:O	1:A:96:THR:C	2.61	0.42
2:B:235:GLN:HE21	2:B:288:LEU:HD11	1.85	0.42
2:B:261:HIS:CD2	2:B:261:HIS:C	2.98	0.42
2:F:146:TYR:O	2:F:150:ARG:CG	2.68	0.42
2:H:211:ASN:CA	2:H:212:PRO:C	2.93	0.42
1:C:402:THR:HB	1:C:414:LEU:HB2	2.02	0.41
1:G:171:LEU:HD23	1:G:178:LEU:HB2	2.02	0.41
2:B:238:TYR:HB2	2:B:257:PHE:CD1	2.55	0.41
2:D:243:LEU:HD12	2:D:247:MET:HG2	2.00	0.41
2:D:259:VAL:HG23	2:D:284:VAL:HG12	2.02	0.41
1:G:311:ARG:HG3	1:G:314:LYS:CB	2.50	0.41
1:G:372:LYS:HB2	1:G:372:LYS:HZ3	1.83	0.41
2:B:21:LYS:HE2	1:C:44:PRO:O	2.20	0.41
2:D:186:GLY:HA3	4:D:628:HOH:O	2.20	0.41
2:D:210:THR:OG1	2:D:213:ASN:HA	2.20	0.41
1:G:54:LEU:CD2	2:H:331:TRP:HZ3	2.33	0.41
1:G:97:PRO:HG3	1:G:107:LEU:HD13	2.02	0.41
1:G:404:VAL:CG2	1:G:414:LEU:HG	2.50	0.41
2:H:221:ARG:NH1	2:H:224:GLU:HG2	2.35	0.41
2:H:238:TYR:HB2	2:H:257:PHE:CD1	2.54	0.41
2:H:445:LEU:N	2:H:445:LEU:HD22	2.34	0.41
1:A:280:ARG:NH1	1:A:316:LYS:NZ	2.68	0.41
2:B:366:ARG:NH1	2:B:381:PRO:O	2.54	0.41
1:C:143:LEU:HD23	1:C:143:LEU:O	2.20	0.41
1:C:159:VAL:O	1:C:160:HIS:C	2.62	0.41
1:C:280:ARG:HG3	1:C:280:ARG:HH11	1.86	0.41
2:F:194:GLU:O	2:F:198:ARG:HD3	2.20	0.41
2:H:156:ARG:C	2:H:157:ARG:HD2	2.45	0.41
2:D:108:LEU:C	2:D:108:LEU:HD23	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:395:LEU:CD1	2:D:401:PRO:HD3	2.49	0.41
1:E:405:PRO:HG2	1:E:408:TYR:CD2	2.56	0.41
2:F:289:ALA:N	2:F:290:PRO:HD2	2.35	0.41
2:H:389:ASP:HB3	2:H:445:LEU:HB3	2.03	0.41
1:A:50:VAL:O	1:A:54:LEU:HD22	2.19	0.41
1:E:356:LEU:HG	1:E:360:LEU:HD22	2.02	0.41
1:E:404:VAL:HB	1:E:412:LEU:HB2	2.02	0.41
2:F:311:PRO:HG2	4:F:573:HOH:O	2.19	0.41
2:H:4:PRO:HB3	4:H:635:HOH:O	2.19	0.41
2:H:221:ARG:O	2:H:225:ILE:HG13	2.21	0.41
2:H:316:ARG:HG2	2:H:316:ARG:HH11	1.86	0.41
1:A:291:VAL:CG2	1:A:295:GLY:C	2.94	0.41
1:A:328:LEU:O	1:A:332:MET:HG3	2.21	0.41
2:B:357:LYS:HZ3	2:B:370:ASP:HB2	1.86	0.41
1:C:337:LEU:HD13	2:D:17:LEU:HB2	2.02	0.41
2:D:78:TYR:CZ	2:D:80:PRO:HA	2.56	0.41
2:D:424:LYS:O	2:D:428:GLU:HG3	2.21	0.41
2:F:141:LEU:HD12	2:F:141:LEU:HA	1.85	0.41
2:F:264:LEU:HD22	2:F:279:SER:OG	2.21	0.41
2:F:468:LEU:HB3	4:F:497:HOH:O	2.19	0.41
1:G:286:LEU:CD2	2:H:468:LEU:HG	2.50	0.41
2:H:235:GLN:HE21	2:H:288:LEU:HD11	1.85	0.41
1:A:72:GLY:HA3	4:A:647:HOH:O	2.20	0.41
2:B:141:LEU:HD12	2:B:141:LEU:HA	1.94	0.41
2:B:383:GLU:CD	2:B:383:GLU:N	2.71	0.41
1:C:101:GLU:CD	1:C:101:GLU:H	2.29	0.41
1:E:267:PRO:HD2	2:F:325:LEU:HB2	2.01	0.41
2:B:41:ARG:HH22	2:B:473:GLU:CD	2.29	0.41
2:B:80:PRO:HG2	2:B:83:HIS:ND1	2.36	0.41
2:B:155:THR:O	2:B:203:HIS:HA	2.20	0.41
1:C:123:LEU:HD13	1:C:274:THR:HA	2.03	0.41
1:C:151:MET:HE1	1:C:174:VAL:O	2.21	0.41
1:C:292:ASP:OD1	1:C:292:ASP:C	2.64	0.41
2:D:136:GLU:HA	2:D:237:TYR:OH	2.21	0.41
2:D:156:ARG:HD3	2:D:202:PRO:O	2.21	0.41
1:E:1:MET:HE3	1:E:46:PRO:N	2.36	0.41
1:E:386:PRO:HG2	4:E:687:HOH:O	2.21	0.41
1:G:333:TYR:CE2	1:G:337:LEU:HD12	2.56	0.41
2:H:288:LEU:C	2:H:290:PRO:HD2	2.45	0.41
2:H:370:ASP:HA	4:H:675:HOH:O	2.20	0.41
2:H:424:LYS:O	2:H:428:GLU:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:PHE:CD2	1:A:429:LEU:HD22	2.56	0.41
1:A:197:VAL:O	1:A:226:ALA:HB2	2.21	0.41
2:D:237:TYR:CD1	2:D:259:VAL:HG13	2.56	0.41
2:D:245:ALA:HB2	2:D:375:HIS:CG	2.56	0.41
1:E:280:ARG:NH1	1:E:316:LYS:HZ1	2.18	0.41
1:E:391:ARG:HA	2:F:98:ASP:OD2	2.21	0.41
2:F:295:PRO:HB3	2:F:308:PHE:CE1	2.56	0.41
2:F:406:PHE:HA	2:F:407:PRO:C	2.45	0.41
2:B:193:LEU:O	2:B:197:LYS:HG3	2.21	0.40
1:C:335:ALA:HA	2:D:43:PRO:CG	2.41	0.40
2:D:102:ALA:O	2:D:106:LEU:CD2	2.69	0.40
1:G:73:VAL:HG23	2:H:320:PHE:CZ	2.56	0.40
2:B:214:THR:O	2:B:415:MET:HE3	2.21	0.40
2:B:357:LYS:NZ	2:B:370:ASP:HB2	2.35	0.40
2:D:370:ASP:O	2:D:370:ASP:CG	2.64	0.40
2:H:260:VAL:CG1	2:H:261:HIS:N	2.83	0.40
1:A:280:ARG:O	1:A:280:ARG:HD3	2.21	0.40
2:B:5:LEU:HD13	2:B:470:TYR:HD1	1.86	0.40
2:B:25:LYS:HE2	2:B:25:LYS:CA	2.42	0.40
2:B:128:GLU:N	2:B:129:PRO:HD2	2.36	0.40
1:C:95:TYR:O	1:C:96:THR:C	2.65	0.40
2:D:203:HIS:CD2	2:D:203:HIS:H	2.37	0.40
1:E:62:LEU:HB3	2:F:101:THR:HB	2.04	0.40
1:E:377:GLU:HG2	1:E:416:ALA:CB	2.50	0.40
2:F:18:LYS:HB2	1:G:1:MET:HG3	2.03	0.40
2:F:164:SER:HB2	2:F:214:THR:OG1	2.22	0.40
2:F:186:GLY:HA3	4:F:638:HOH:O	2.21	0.40
1:G:12:ARG:CG	1:G:16:ARG:HH12	2.31	0.40
1:G:51:LEU:HG	2:H:82:LEU:HD11	2.02	0.40
1:G:79:PRO:HA	1:G:80:PRO:HD2	1.88	0.40
2:H:183:ILE:HG22	2:H:199:GLU:HG3	2.03	0.40
1:A:436:VAL:HG23	1:A:437:LEU:CD1	2.44	0.40
2:B:466:PRO:HB2	2:B:468:LEU:HD11	2.03	0.40
1:C:31:PRO:O	1:C:34:ILE:HG12	2.21	0.40
1:C:171:LEU:HA	1:C:171:LEU:HD12	1.89	0.40
2:D:394:LEU:HD11	2:D:434:MET:SD	2.62	0.40
1:E:292:ASP:HA	2:F:457:LEU:HA	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	435/438 (99%)	418 (96%)	16 (4%)	1 (0%)	43	44
1	C	435/438 (99%)	421 (97%)	13 (3%)	1 (0%)	43	44
1	E	435/438 (99%)	421 (97%)	13 (3%)	1 (0%)	43	44
1	G	435/438 (99%)	416 (96%)	18 (4%)	1 (0%)	43	44
2	B	471/474 (99%)	458 (97%)	13 (3%)	0	100	100
2	D	471/474 (99%)	455 (97%)	15 (3%)	1 (0%)	43	44
2	F	471/474 (99%)	453 (96%)	18 (4%)	0	100	100
2	H	471/474 (99%)	456 (97%)	15 (3%)	0	100	100
All	All	3624/3648 (99%)	3498 (96%)	121 (3%)	5 (0%)	48	50

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	129	SER
1	C	129	SER
1	E	129	SER
1	G	129	SER
2	D	472	ASP

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	336/336 (100%)	315 (94%)	21 (6%)	16	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	336/336 (100%)	316 (94%)	20 (6%)	17	15
1	E	336/336 (100%)	319 (95%)	17 (5%)	21	21
1	G	336/336 (100%)	316 (94%)	20 (6%)	17	15
2	B	384/385 (100%)	362 (94%)	22 (6%)	18	17
2	D	384/385 (100%)	371 (97%)	13 (3%)	32	35
2	F	384/385 (100%)	358 (93%)	26 (7%)	14	12
2	H	384/385 (100%)	367 (96%)	17 (4%)	25	26
All	All	2880/2884 (100%)	2724 (95%)	156 (5%)	20	18

All (156) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	9	GLU
1	A	16	ARG
1	A	23	LEU
1	A	41	LEU
1	A	54	LEU
1	A	55	ARG
1	A	107	LEU
1	A	130	MET
1	A	171	LEU
1	A	183	LEU
1	A	237	LEU
1	A	291	VAL
1	A	328	LEU
1	A	334	LEU
1	A	360	LEU
1	A	361	LEU
1	A	367	ARG
1	A	376	ASN
1	A	393	LEU
1	A	437	LEU
2	B	25	LYS
2	B	42	LEU
2	B	48	LEU
2	B	73	SER
2	B	89	LEU
2	B	141	LEU
2	B	236	LEU

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Mol	Chain	Res	Type
2	B	243	LEU
2	B	259	VAL
2	B	260	VAL
2	B	264	LEU
2	B	302	GLU
2	B	318	ARG
2	B	360	LEU
2	B	383	GLU
2	B	394	LEU
2	B	395	LEU
2	B	397	LEU
2	B	442	LYS
2	B	445	LEU
2	B	454	VAL
2	B	468	LEU
1	C	1	MET
1	C	9	GLU
1	C	32	LYS
1	C	33	GLU
1	C	41	LEU
1	C	54	LEU
1	C	62	LEU
1	C	99	GLN
1	C	107	LEU
1	C	130	MET
1	C	171	LEU
1	C	188	THR
1	C	237	LEU
1	C	286	LEU
1	C	360	LEU
1	C	367	ARG
1	C	376	ASN
1	C	393	LEU
1	C	423	GLU
1	C	437	LEU
2	D	25	LYS
2	D	42	LEU
2	D	48	LEU
2	D	73	SER
2	D	89	LEU
2	D	236	LEU
2	D	301	GLU

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Mol	Chain	Res	Type
2	D	325	LEU
2	D	383	GLU
2	D	386	ARG
2	D	395	LEU
2	D	445	LEU
2	D	454	VAL
1	E	54	LEU
1	E	107	LEU
1	E	130	MET
1	E	171	LEU
1	E	183	LEU
1	E	184	GLU
1	E	188	THR
1	E	237	LEU
1	E	286	LEU
1	E	334	LEU
1	E	360	LEU
1	E	361	LEU
1	E	376	ASN
1	E	393	LEU
1	E	423	GLU
1	E	427	LEU
1	E	437	LEU
2	F	21	LYS
2	F	25	LYS
2	F	27	GLU
2	F	30	ILE
2	F	32	LYS
2	F	42	LEU
2	F	48	LEU
2	F	71	LEU
2	F	73	SER
2	F	89	LEU
2	F	106	LEU
2	F	141	LEU
2	F	224	GLU
2	F	236	LEU
2	F	259	VAL
2	F	260	VAL
2	F	302	GLU
2	F	318	ARG
2	F	325	LEU

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Mol	Chain	Res	Type
2	F	360	LEU
2	F	383	GLU
2	F	386	ARG
2	F	395	LEU
2	F	397	LEU
2	F	445	LEU
2	F	468	LEU
1	G	15	LEU
1	G	32	LYS
1	G	33	GLU
1	G	99	GLN
1	G	107	LEU
1	G	123	LEU
1	G	130	MET
1	G	171	LEU
1	G	183	LEU
1	G	286	LEU
1	G	291	VAL
1	G	328	LEU
1	G	334	LEU
1	G	360	LEU
1	G	361	LEU
1	G	376	ASN
1	G	391	ARG
1	G	393	LEU
1	G	423	GLU
1	G	437	LEU
2	H	25	LYS
2	H	42	LEU
2	H	48	LEU
2	H	73	SER
2	H	89	LEU
2	H	106	LEU
2	H	236	LEU
2	H	259	VAL
2	H	264	LEU
2	H	302	GLU
2	H	318	ARG
2	H	325	LEU
2	H	383	GLU
2	H	394	LEU
2	H	454	VAL

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Mol	Chain	Res	Type
2	H	468	LEU
2	H	473	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	GLN
1	A	222	HIS
1	A	354	HIS
1	A	376	ASN
2	B	34	HIS
2	B	169	ASN
2	B	235	GLN
2	B	287	HIS
1	C	222	HIS
1	C	376	ASN
2	D	34	HIS
2	D	179	GLN
2	D	235	GLN
1	E	354	HIS
1	E	376	ASN
2	F	179	GLN
2	F	235	GLN
2	F	465	HIS
1	G	60	GLN
1	G	83	GLN
1	G	222	HIS
1	G	376	ASN
2	H	169	ASN
2	H	179	GLN
2	H	235	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	$\# Z > 2$
3	PLP	B	475	2	15,15,16	1.65	4 (26%)	21,22,23	1.92	4 (19%)
3	PLP	D	475	2	15,15,16	1.60	4 (26%)	21,22,23	1.94	3 (14%)
3	PLP	F	475	2	15,15,16	1.61	4 (26%)	21,22,23	1.89	3 (14%)
3	PLP	H	475	2	15,15,16	1.63	4 (26%)	21,22,23	1.86	3 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PLP	B	475	2	-	0/6/6/8	0/1/1/1
3	PLP	D	475	2	-	0/6/6/8	0/1/1/1
3	PLP	F	475	2	-	0/6/6/8	0/1/1/1
3	PLP	H	475	2	-	0/6/6/8	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	475	PLP	C5-C4	3.11	1.44	1.40
3	H	475	PLP	C5-C4	3.09	1.44	1.40
3	F	475	PLP	C5-C4	3.08	1.44	1.40
3	B	475	PLP	C2-N1	2.93	1.39	1.33
3	D	475	PLP	C5-C4	2.90	1.43	1.40
3	H	475	PLP	C2-N1	2.90	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	475	PLP	C2-N1	2.82	1.38	1.33
3	F	475	PLP	C2-N1	2.74	1.38	1.33
3	D	475	PLP	C3-C2	-2.72	1.38	1.41
3	B	475	PLP	C2A-C2	2.48	1.54	1.50
3	H	475	PLP	C3-C2	-2.39	1.38	1.41
3	B	475	PLP	C3-C2	-2.26	1.38	1.41
3	F	475	PLP	C2A-C2	2.23	1.53	1.50
3	H	475	PLP	C2A-C2	2.15	1.53	1.50
3	D	475	PLP	C2A-C2	2.13	1.53	1.50
3	F	475	PLP	C3-C2	-2.04	1.38	1.41

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	475	PLP	O4P-C5A-C5	6.49	121.52	109.36
3	B	475	PLP	O4P-C5A-C5	6.44	121.42	109.36
3	F	475	PLP	O4P-C5A-C5	6.25	121.07	109.36
3	H	475	PLP	O4P-C5A-C5	5.98	120.57	109.36
3	B	475	PLP	C5-C6-N1	-2.42	119.90	123.83
3	H	475	PLP	C5-C6-N1	-2.40	119.93	123.83
3	D	475	PLP	C5-C6-N1	-2.39	119.94	123.83
3	F	475	PLP	C5-C6-N1	-2.25	120.17	123.83
3	F	475	PLP	C5A-C5-C6	-2.23	115.72	119.36
3	H	475	PLP	C5A-C5-C6	-2.23	115.72	119.36
3	D	475	PLP	C5A-C5-C6	-2.15	115.85	119.36
3	B	475	PLP	C4A-C4-C3	-2.11	117.00	120.52
3	B	475	PLP	C5A-C5-C6	-2.04	116.03	119.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	437/438 (99%)	-0.07	4 (0%) 81 83	19, 26, 40, 48	0
1	C	437/438 (99%)	-0.01	6 (1%) 73 75	19, 27, 40, 47	0
1	E	437/438 (99%)	-0.13	6 (1%) 73 75	18, 25, 38, 49	0
1	G	437/438 (99%)	-0.12	2 (0%) 87 88	19, 26, 40, 48	0
2	B	473/474 (99%)	-0.14	9 (1%) 66 69	16, 24, 42, 57	0
2	D	473/474 (99%)	0.09	8 (1%) 69 71	18, 29, 48, 63	0
2	F	473/474 (99%)	-0.09	11 (2%) 61 64	16, 25, 42, 52	0
2	H	473/474 (99%)	0.15	13 (2%) 56 59	19, 30, 48, 61	0
All	All	3640/3648 (99%)	-0.04	59 (1%) 70 73	16, 27, 43, 63	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	370	ASP	4.0
1	G	1	MET	3.9
2	B	301	GLU	3.9
2	D	472	ASP	3.6
2	F	386	ARG	3.4
2	B	474	GLY	3.3
1	A	38	PRO	3.2
2	F	30	ILE	3.2
2	H	370	ASP	3.1
2	F	302	GLU	3.1
2	H	27	GLU	3.1
2	H	474	GLY	3.0
1	C	367	ARG	3.0
2	H	37	GLU	2.9
2	B	370	ASP	2.9
2	D	302	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	437	LEU	2.8
2	B	37	GLU	2.8
1	C	246	TYR	2.8
1	E	36	SER	2.7
2	D	181	ARG	2.7
1	E	1	MET	2.6
1	E	280	ARG	2.6
2	H	445	LEU	2.6
2	B	2	SER	2.6
2	D	474	GLY	2.5
1	E	38	PRO	2.5
2	H	371	GLY	2.5
2	H	221	ARG	2.5
2	D	301	GLU	2.5
1	A	36	SER	2.4
2	D	370	ASP	2.4
1	C	213	ASP	2.4
2	D	386	ARG	2.4
1	C	1	MET	2.3
2	F	27	GLU	2.3
2	F	474	GLY	2.3
1	A	246	TYR	2.3
2	H	69	TYR	2.3
1	G	38	PRO	2.2
2	H	88	ARG	2.2
2	H	301	GLU	2.2
1	E	40	ASP	2.2
2	H	33	GLU	2.1
2	B	302	GLU	2.1
2	F	37	GLU	2.1
1	C	174	VAL	2.1
2	B	25	LYS	2.1
2	H	25	LYS	2.1
1	C	195	GLU	2.1
2	B	27	GLU	2.1
2	D	25	LYS	2.1
2	H	442	LYS	2.1
2	B	442	LYS	2.0
2	F	32	LYS	2.0
1	E	213	ASP	2.0
2	F	21	LYS	2.0
2	F	25	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
2	F	442	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PLP	D	475	15/16	0.94	0.10	29,36,39,39	0
3	PLP	H	475	15/16	0.96	0.08	24,36,39,39	0
3	PLP	B	475	15/16	0.97	0.07	21,31,34,35	0
3	PLP	F	475	15/16	0.98	0.07	18,26,31,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.