



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:26 PM UTC

PDB ID : 1FZ5 / pdb_00001fz5
Title : METHANE MONOOXYGENASE HYDROXYLASE, FORM II CRYSTALLIZED ANAEROBICALLY FROM REDUCED ENZYME
Authors : Whittington, D.A.; Lippard, S.J.
Deposited on : 2000-10-03
Resolution : 2.40 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)	:	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

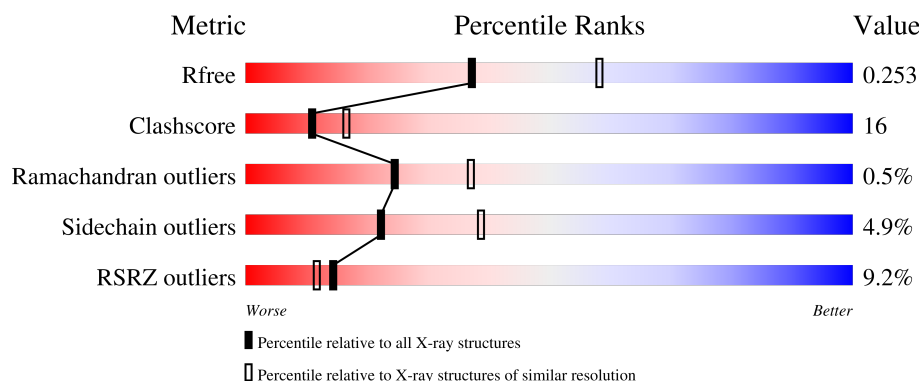
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

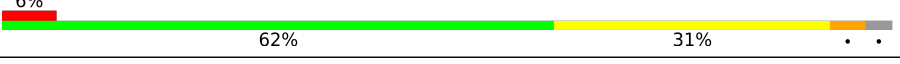
The reported resolution of this entry is 2.40 Å.

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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	527	
1	B	527	
2	C	389	
2	D	389	
3	E	170	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	170	24% 59% 33% 7%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 18004 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 METHANE MONOOXYGENASE COMPONENT A, ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	511	Total	C	N	O	S	0	0	0
			4181	2675	721	767	18			
1	B	510	Total	C	N	O	S	0	0	0
			4177	2673	719	767	18			

- Molecule 2 is a protein called METHANE MONOOXYGENASE COMPONENT A, BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	388	Total	C	N	O	S	0	0	0
			3193	2054	551	580	8			
2	D	386	Total	C	N	O	S	0	0	0
			3175	2042	548	577	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	370	ARG	ALA	conflict	UNP P18798
D	370	ARG	ALA	conflict	UNP P18798

- Molecule 3 is a protein called METHANE MONOOXYGENASE COMPONENT A, GAMMA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	166	Total	C	N	O	S	0	0	0
			1368	867	246	250	5			
3	F	168	Total	C	N	O	S	0	0	0
			1382	875	249	253	5			

- Molecule 4 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Fe 1 1	0	0
4	B	1	Total Fe 1 1	0	0

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Ca 1 1	0	0
5	C	1	Total Ca 1 1	0	0

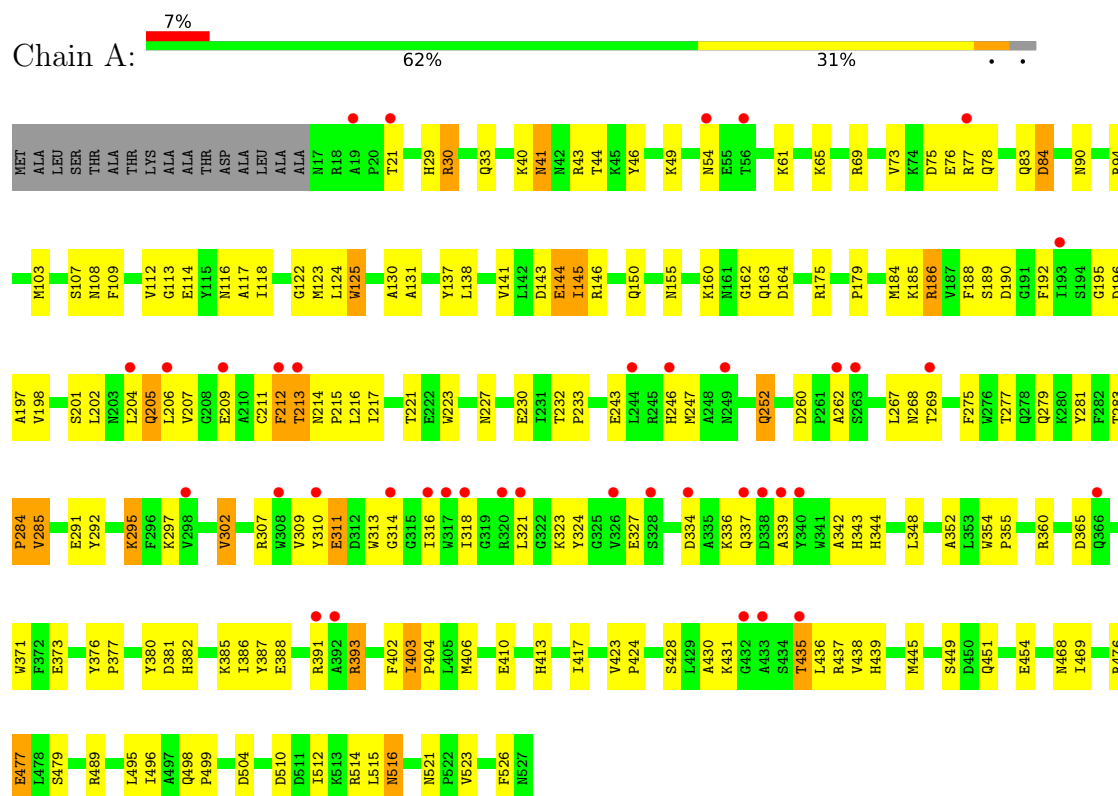
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	133	Total O 133 133	0	0
6	B	89	Total O 89 89	0	0
6	C	178	Total O 178 178	0	0
6	D	42	Total O 42 42	0	0
6	E	70	Total O 70 70	0	0
6	F	12	Total O 12 12	0	0

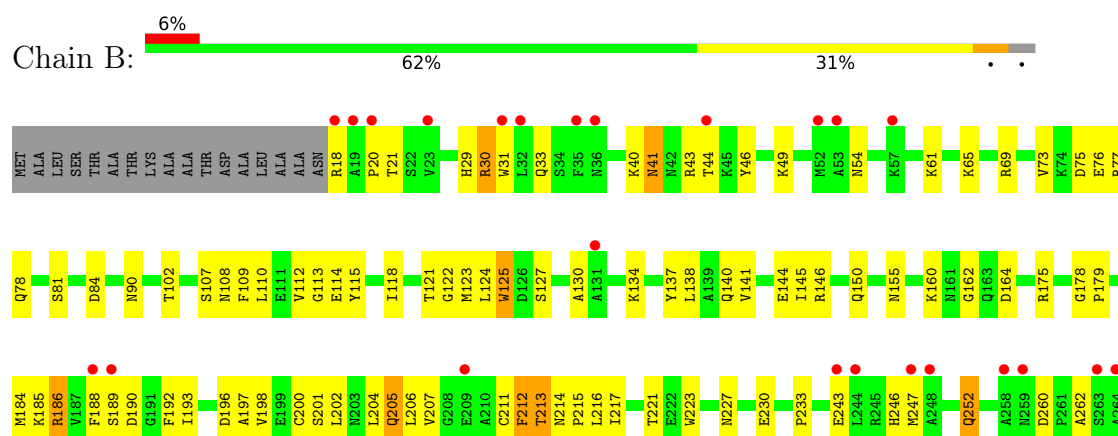
3 Residue-property plots [i](#)

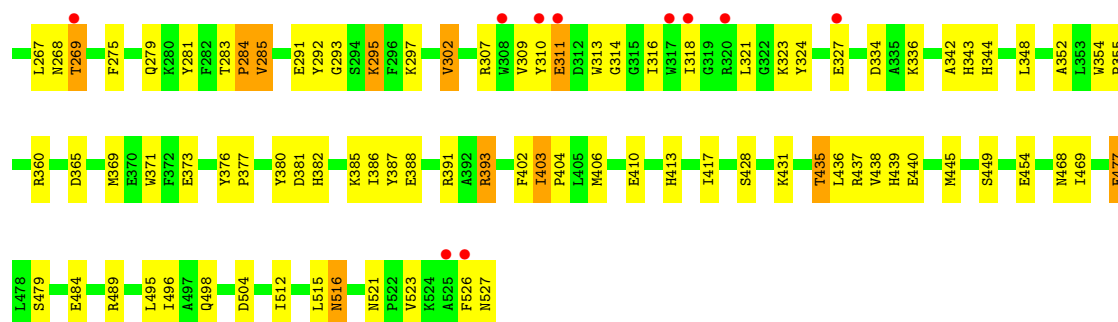
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: METHANE MONOOXYGENASE COMPONENT A, ALPHA CHAIN



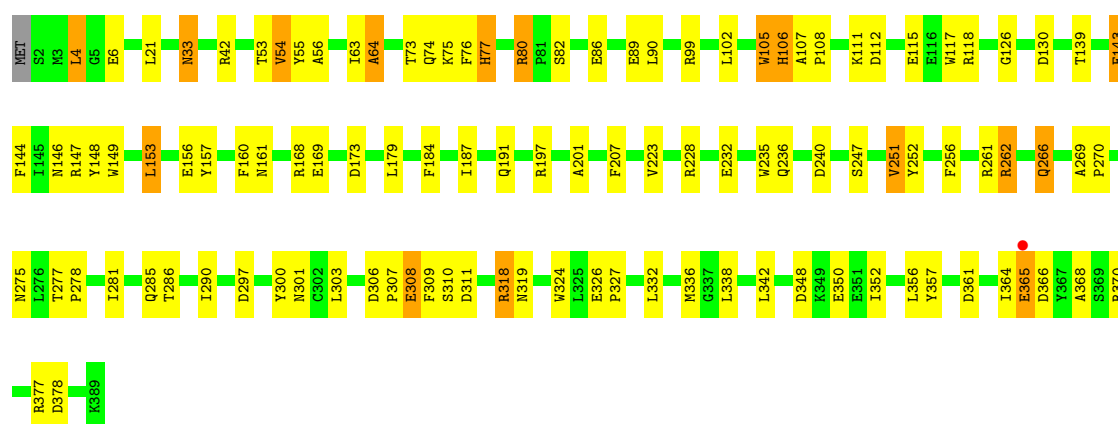
• Molecule 1: METHANE MONOOXYGENASE COMPONENT A, ALPHA CHAIN





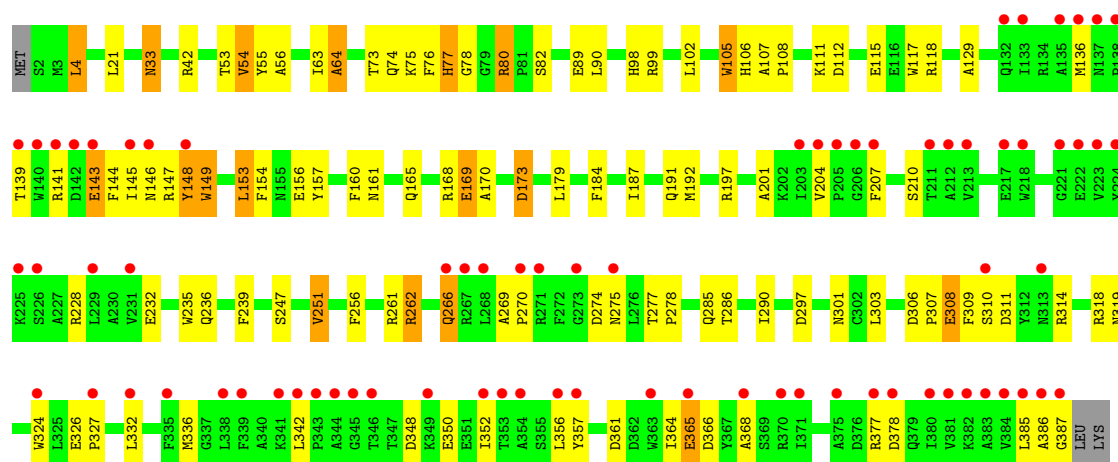
• Molecule 2: METHANE MONOOXYGENASE COMPONENT A, BETA CHAIN

Chain C: 71% 24% .



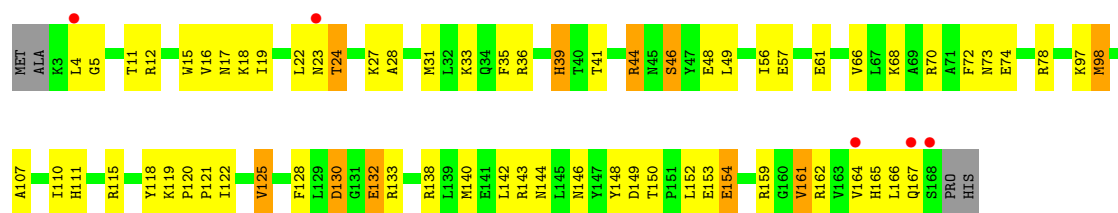
• Molecule 2: METHANE MONOOXYGENASE COMPONENT A, BETA CHAIN

Chain D: 19% 69% 25% 5% .

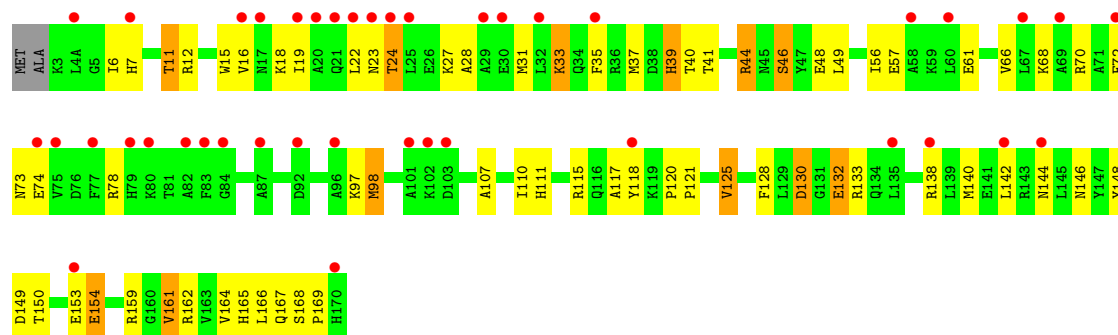


• Molecule 3: METHANE MONOOXYGENASE COMPONENT A, GAMMA CHAIN

Chain E: 3% 57% 35% 6% .



● Molecule 3: METHANE MONOOXYGENASE COMPONENT A, GAMMA CHAIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.24Å 171.57Å 220.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.40 – 2.40 46.40 – 2.40	Depositor EDS
% Data completeness (in resolution range)	89.2 (46.40-2.40) 89.3 (46.40-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.72 (at 2.39Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.218 , 0.253 0.219 , 0.253	Depositor DCC
R_{free} test set	3359 reflections (3.22%)	wwPDB-VP
Wilson B-factor (Å ²)	33.5	Xtriage
Anisotropy	0.169	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 42.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	18004	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% 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: CA, FE2

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	0.43	0/4306	0.95	24/5848 (0.4%)
1	B	0.43	0/4302	0.94	21/5842 (0.4%)
2	C	0.46	0/3289	0.92	17/4464 (0.4%)
2	D	0.40	0/3271	0.90	16/4442 (0.4%)
3	E	0.48	0/1396	0.92	7/1880 (0.4%)
3	F	0.40	0/1412	0.88	4/1903 (0.2%)
All	All	0.43	0/17976	0.93	89/24379 (0.4%)

There are no bond length outliers.

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	318	ARG	NE-CZ-NH1	-8.05	113.45	121.50
2	C	318	ARG	NE-CZ-NH2	7.89	126.30	119.20
1	A	30	ARG	NE-CZ-NH2	7.83	126.25	119.20
1	A	77	ARG	NE-CZ-NH2	7.70	126.13	119.20
1	A	391	ARG	NE-CZ-NH2	7.56	126.00	119.20
3	F	118	TYR	N-CA-C	7.28	122.27	112.88
1	A	77	ARG	NE-CZ-NH1	-7.25	114.25	121.50
1	A	391	ARG	NE-CZ-NH1	-7.25	114.25	121.50
3	F	130	ASP	N-CA-C	-7.18	103.54	111.36
1	A	145	ILE	N-CA-C	-7.17	103.47	110.72
1	A	30	ARG	NE-CZ-NH1	-7.10	114.40	121.50
3	E	118	TYR	N-CA-C	7.00	121.92	112.88
1	A	309	VAL	N-CA-C	6.98	117.77	110.72
1	B	431	LYS	N-CA-C	-6.91	105.00	113.50
3	E	130	ASP	N-CA-C	-6.89	103.85	111.36
1	B	309	VAL	N-CA-C	6.82	117.61	110.72
1	A	431	LYS	N-CA-C	-6.66	105.31	113.50
2	C	106	HIS	N-CA-C	6.58	119.05	111.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	39	HIS	N-CA-C	6.40	123.02	114.12
2	D	236	GLN	N-CA-C	6.37	121.22	113.38
2	D	318	ARG	NE-CZ-NH2	-6.32	113.51	119.20
3	E	122	ILE	N-CA-C	-6.31	105.00	110.74
2	D	106	HIS	N-CA-C	6.27	118.67	111.02
2	C	105	TRP	N-CA-C	-6.24	100.75	110.17
2	D	105	TRP	N-CA-C	-6.23	100.76	110.17
3	F	39	HIS	N-CA-C	6.22	122.94	113.61
1	A	164	ASP	CA-C-N	6.17	125.58	118.85
1	A	164	ASP	C-N-CA	6.17	125.58	118.85
1	B	77	ARG	NE-CZ-NH2	-6.10	113.71	119.20
1	B	164	ASP	CA-C-N	6.04	125.43	118.85
1	B	164	ASP	C-N-CA	6.04	125.43	118.85
2	D	149	TRP	N-CA-C	-5.93	104.73	111.14
1	A	122	GLY	N-CA-C	-5.92	105.44	113.37
2	C	236	GLN	N-CA-C	5.84	120.57	113.38
2	C	149	TRP	N-CA-C	-5.83	104.84	111.14
2	C	262	ARG	N-CA-C	5.79	118.46	111.40
1	B	84	ASP	N-CA-C	5.73	117.94	108.48
2	D	318	ARG	NE-CZ-NH1	5.69	127.19	121.50
1	A	496	ILE	N-CA-C	-5.68	105.19	110.53
1	B	496	ILE	N-CA-C	-5.66	105.21	110.53
2	D	148	TYR	N-CA-C	5.64	117.50	111.36
1	A	30	ARG	CD-NE-CZ	5.61	132.25	124.40
2	D	286	THR	N-CA-C	-5.59	105.10	111.14
1	B	162	GLY	N-CA-C	5.57	121.69	112.66
1	B	122	GLY	N-CA-C	-5.54	105.95	113.37
3	F	73	ASN	N-CA-C	-5.51	102.74	110.35
2	C	169	GLU	N-CA-C	5.46	120.21	113.50
1	B	391	ARG	NE-CZ-NH2	-5.46	114.29	119.20
2	C	53	THR	N-CA-C	5.45	119.59	112.13
1	B	30	ARG	NE-CZ-NH2	-5.43	114.32	119.20
1	A	267	LEU	N-CA-C	5.40	117.61	111.02
1	A	162	GLY	N-CA-C	5.37	121.36	112.66
2	D	77	HIS	N-CA-C	-5.36	102.11	110.10
1	A	84	ASP	N-CA-C	5.36	117.33	108.48
3	E	73	ASN	N-CA-C	-5.36	102.95	110.35
1	A	212	PHE	N-CA-C	5.35	119.46	112.13
2	C	56	ALA	N-CA-C	-5.33	105.64	111.82
1	A	205	GLN	N-CA-C	5.32	119.46	111.96
1	B	205	GLN	N-CA-C	5.32	119.46	111.96
2	D	54	VAL	N-CA-C	5.31	116.25	109.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	366	ASP	N-CA-C	5.30	119.60	113.18
2	C	318	ARG	CD-NE-CZ	5.28	131.80	124.40
3	E	5	GLY	N-CA-C	5.28	120.58	112.51
1	A	391	ARG	CD-NE-CZ	5.27	131.78	124.40
2	C	286	THR	N-CA-C	-5.26	105.63	111.36
1	A	295	LYS	N-CA-C	-5.25	104.94	112.13
1	A	339	ALA	N-CA-C	5.25	117.80	111.40
2	D	366	ASP	N-CA-C	5.25	119.53	113.18
2	D	169	GLU	N-CA-C	5.23	119.94	113.50
2	D	262	ARG	N-CA-C	5.22	117.76	111.40
2	C	148	TYR	N-CA-C	5.20	117.03	111.36
2	D	53	THR	N-CA-C	5.15	119.03	112.12
2	D	318	ARG	CD-NE-CZ	5.15	131.61	124.40
1	B	30	ARG	CD-NE-CZ	5.15	131.61	124.40
1	A	285	VAL	N-CA-C	5.12	115.89	110.72
1	B	178	GLY	CA-C-N	5.11	124.80	119.64
1	B	178	GLY	C-N-CA	5.11	124.80	119.64
1	B	295	LYS	N-CA-C	-5.11	105.13	112.13
2	D	56	ALA	N-CA-C	-5.11	105.79	111.36
1	B	391	ARG	CD-NE-CZ	5.08	131.51	124.40
3	E	143	ARG	N-CA-C	5.05	116.87	111.36
1	B	212	PHE	N-CA-C	5.05	118.89	112.12
1	B	285	VAL	N-CA-C	5.05	115.28	110.53
2	C	252	TYR	N-CA-C	5.05	116.47	110.97
2	C	54	VAL	N-CA-C	5.04	115.91	109.30
1	B	267	LEU	N-CA-C	5.04	117.17	111.02
1	A	77	ARG	CD-NE-CZ	5.02	131.43	124.40
1	B	193	ILE	N-CA-C	5.02	118.54	113.47
2	C	77	HIS	N-CA-C	-5.02	102.62	110.10

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	4181	0	3977	160	0
1	B	4177	0	3975	162	0
2	C	3193	0	3042	93	0
2	D	3175	0	3018	97	0
3	E	1368	0	1363	60	0
3	F	1382	0	1366	64	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
6	A	133	0	0	3	0
6	B	89	0	0	3	0
6	C	178	0	0	8	0
6	D	42	0	0	0	0
6	E	70	0	0	1	0
6	F	12	0	0	0	0
All	All	18004	0	16741	563	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 16.

All (563) 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:A:352:ALA:HA	1:A:404:PRO:HB2	1.36	1.06
1:B:352:ALA:HA	1:B:404:PRO:HB2	1.38	1.02
1:A:355:PRO:HG2	1:A:403:ILE:HD11	1.43	0.99
1:B:355:PRO:HG2	1:B:403:ILE:HD11	1.42	0.99
2:C:270:PRO:HB3	2:D:270:PRO:HB3	1.45	0.98
2:D:146:ASN:HD21	2:D:197:ARG:HH21	1.12	0.98
2:C:146:ASN:HD21	2:C:197:ARG:HH21	1.12	0.95
2:C:319:ASN:HA	3:E:74:GLU:OE1	1.68	0.94
3:F:15:TRP:O	3:F:19:ILE:HG13	1.69	0.92
1:A:252:GLN:HA	1:A:252:GLN:NE2	1.85	0.92
2:D:261:ARG:HE	2:D:285:GLN:HE22	1.17	0.91
1:B:78:GLN:HE22	1:B:150:GLN:HE21	1.03	0.90
3:F:132:GLU:OE2	3:F:132:GLU:HA	1.67	0.90
1:A:78:GLN:HE22	1:A:150:GLN:HE21	0.92	0.89
3:E:132:GLU:HA	3:E:132:GLU:OE2	1.71	0.89
1:A:123:MET:HE2	1:A:197:ALA:HA	1.54	0.89
3:E:15:TRP:O	3:E:19:ILE:HG13	1.73	0.89
2:C:261:ARG:HE	2:C:285:GLN:HE22	1.16	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:GLN:HA	1:B:252:GLN:NE2	1.88	0.85
1:A:252:GLN:HA	1:A:252:GLN:HE21	1.39	0.85
2:D:319:ASN:HA	3:F:74:GLU:OE1	1.77	0.84
1:A:78:GLN:NE2	1:A:150:GLN:HE21	1.75	0.83
1:A:44:THR:HG22	1:A:46:TYR:H	1.44	0.82
1:B:44:THR:HG22	1:B:46:TYR:H	1.43	0.80
1:B:227:ASN:HD21	1:B:295:LYS:H	1.28	0.80
1:B:269:THR:HG22	3:F:148:TYR:CE1	2.18	0.79
1:A:78:GLN:HE22	1:A:150:GLN:NE2	1.76	0.78
1:B:123:MET:HE2	1:B:197:ALA:HA	1.66	0.78
1:B:252:GLN:HA	1:B:252:GLN:HE21	1.48	0.77
3:E:98:MET:HE2	3:E:98:MET:HA	1.65	0.76
3:F:98:MET:HE2	3:F:98:MET:HA	1.68	0.76
1:B:41:ASN:HD22	1:B:41:ASN:N	1.84	0.76
1:A:118:ILE:HG12	1:A:144:GLU:HB3	1.68	0.75
1:A:41:ASN:N	1:A:41:ASN:HD22	1.83	0.75
1:A:381:ASP:HA	1:A:385:LYS:HE2	1.68	0.75
3:E:138:ARG:HH21	3:E:142:LEU:HD21	1.51	0.74
2:D:146:ASN:ND2	2:D:197:ARG:HH21	1.83	0.74
1:A:355:PRO:HG2	1:A:403:ILE:CD1	2.18	0.74
1:B:381:ASP:HA	1:B:385:LYS:HE2	1.70	0.74
2:C:146:ASN:ND2	2:C:197:ARG:HH21	1.83	0.74
3:F:12:ARG:O	3:F:16:VAL:HG23	1.88	0.73
1:B:307:ARG:HA	1:B:311:GLU:HG3	1.71	0.73
2:D:76:PHE:HZ	2:D:168:ARG:HH12	1.37	0.73
1:A:292:TYR:OH	1:A:344:HIS:HD2	1.71	0.72
1:B:292:TYR:OH	1:B:344:HIS:HD2	1.73	0.72
1:A:355:PRO:CG	1:A:403:ILE:HD11	2.18	0.72
1:A:307:ARG:HA	1:A:311:GLU:HG3	1.72	0.72
2:C:102:LEU:CD1	2:C:290:ILE:HG23	2.20	0.72
2:C:365:GLU:HA	2:C:365:GLU:OE1	1.90	0.72
3:F:138:ARG:HH21	3:F:142:LEU:HD21	1.53	0.72
1:B:495:LEU:HD11	1:B:512:ILE:HG13	1.72	0.71
2:D:385:LEU:C	2:D:387:GLY:H	1.98	0.71
1:A:117:ALA:HB3	1:A:144:GLU:CG	2.20	0.71
2:C:326:GLU:HB3	2:C:327:PRO:HD3	1.71	0.71
1:A:117:ALA:HB3	1:A:144:GLU:HG2	1.72	0.71
2:C:76:PHE:HZ	2:C:168:ARG:HH12	1.38	0.71
2:C:261:ARG:HE	2:C:285:GLN:NE2	1.89	0.71
2:D:261:ARG:HE	2:D:285:GLN:NE2	1.89	0.70
1:B:213:THR:O	1:B:217:ILE:HG12	1.91	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:24:THR:HG22	3:E:27:LYS:H	1.55	0.70
2:C:223:VAL:HG13	6:C:5175:HOH:O	1.92	0.70
1:B:78:GLN:NE2	1:B:150:GLN:HE21	1.85	0.70
2:C:361:ASP:O	2:C:365:GLU:HB2	1.92	0.70
1:B:436:LEU:HB3	3:F:167:GLN:HE21	1.57	0.70
1:A:213:THR:O	1:A:217:ILE:HG12	1.91	0.69
1:A:495:LEU:HD11	1:A:512:ILE:HG13	1.73	0.69
1:A:108:ASN:HD21	1:A:175:ARG:HH11	1.40	0.69
3:E:12:ARG:O	3:E:16:VAL:HG23	1.92	0.69
1:B:160:LYS:HA	2:D:33:ASN:HB2	1.74	0.69
2:D:102:LEU:CD1	2:D:290:ILE:HG23	2.21	0.69
1:B:355:PRO:HG2	1:B:403:ILE:CD1	2.19	0.68
1:B:134:LYS:HD3	2:D:161:ASN:HD21	1.57	0.68
1:A:160:LYS:HA	2:C:33:ASN:HB2	1.74	0.68
1:B:355:PRO:CG	1:B:403:ILE:HD11	2.20	0.68
1:B:206:LEU:HB2	6:B:5079:HOH:O	1.93	0.67
2:C:111:LYS:O	2:C:115:GLU:HG3	1.94	0.67
1:A:107:SER:HB3	1:A:155:ASN:HD21	1.59	0.67
2:D:111:LYS:O	2:D:115:GLU:HG3	1.94	0.67
1:A:269:THR:HG22	3:E:148:TYR:CE1	2.30	0.67
2:D:228:ARG:O	2:D:232:GLU:HG3	1.94	0.66
3:E:17:ASN:HB3	6:E:214:HOH:O	1.94	0.66
1:A:76:GLU:HG2	1:B:76:GLU:HG2	1.78	0.66
1:A:124:LEU:HD21	1:A:201:SER:HB2	1.77	0.66
2:D:326:GLU:HB3	2:D:327:PRO:HD3	1.76	0.66
3:F:39:HIS:CD2	3:F:49:LEU:HD12	2.30	0.66
1:B:78:GLN:HE22	1:B:150:GLN:NE2	1.87	0.66
1:B:526:PHE:O	1:B:527:ASN:ND2	2.29	0.66
1:A:214:ASN:HB3	1:A:215:PRO:HD3	1.77	0.66
2:D:365:GLU:OE1	2:D:365:GLU:HA	1.95	0.66
1:B:123:MET:HB2	2:D:168:ARG:HD3	1.77	0.65
1:A:117:ALA:CB	1:A:144:GLU:HG2	2.26	0.65
3:F:41:THR:O	3:F:44:ARG:HD2	1.97	0.65
1:B:138:LEU:HD22	2:D:160:PHE:CZ	2.32	0.65
1:B:214:ASN:HB3	1:B:215:PRO:HD3	1.79	0.65
2:D:90:LEU:HD13	2:D:303:LEU:HD13	1.80	0.64
3:E:150:THR:HG23	3:E:154:GLU:HG2	1.79	0.64
2:C:102:LEU:HD12	2:C:290:ILE:HG23	1.79	0.64
2:D:146:ASN:HD21	2:D:197:ARG:NH2	1.90	0.64
1:A:438:VAL:HB	3:E:164:VAL:HG23	1.77	0.64
1:A:227:ASN:HD21	1:A:295:LYS:H	1.45	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:ASN:HD21	1:B:175:ARG:HH11	1.44	0.64
2:C:228:ARG:O	2:C:232:GLU:HG3	1.98	0.64
1:B:184:MET:CE	1:B:188:PHE:HB2	2.27	0.64
1:B:526:PHE:HE2	3:F:165:HIS:HD2	1.46	0.64
3:F:24:THR:HG22	3:F:27:LYS:H	1.61	0.64
2:C:90:LEU:HD13	2:C:303:LEU:HD13	1.80	0.63
2:C:146:ASN:HD21	2:C:197:ARG:NH2	1.91	0.63
2:D:385:LEU:O	2:D:387:GLY:N	2.31	0.63
2:C:308:GLU:HG2	2:C:309:PHE:CE1	2.34	0.63
2:D:153:LEU:C	2:D:153:LEU:HD12	2.24	0.63
1:A:184:MET:CE	1:A:188:PHE:HB2	2.28	0.63
2:D:361:ASP:O	2:D:365:GLU:HB2	1.99	0.63
3:F:150:THR:HG23	3:F:154:GLU:HG2	1.81	0.62
2:D:336:MET:CE	2:D:356:LEU:HD11	2.29	0.62
1:A:123:MET:HE2	1:A:197:ALA:CA	2.25	0.62
3:E:41:THR:O	3:E:44:ARG:HD2	1.98	0.62
2:C:348:ASP:O	2:C:352:ILE:HG13	1.99	0.62
3:E:39:HIS:CD2	3:E:49:LEU:HD12	2.34	0.62
1:B:184:MET:HE3	1:B:188:PHE:HB2	1.81	0.62
1:B:108:ASN:HD21	1:B:175:ARG:HD3	1.65	0.61
1:B:179:PRO:HB3	1:B:469:ILE:HD13	1.82	0.61
1:B:49:LYS:CE	3:F:144:ASN:HD22	2.13	0.61
1:A:190:ASP:HB3	2:C:74:GLN:O	2.00	0.61
2:D:33:ASN:C	2:D:33:ASN:HD22	2.07	0.61
2:D:348:ASP:O	2:D:352:ILE:HG13	2.00	0.61
1:A:445:MET:HE3	1:A:523:VAL:HG22	1.82	0.61
1:B:314:GLY:HA2	1:B:318:ILE:HD12	1.83	0.61
1:A:310:TYR:CZ	1:A:336:LYS:HD2	2.35	0.61
2:D:89:GLU:CD	3:F:125:VAL:HG13	2.26	0.60
2:D:385:LEU:C	2:D:387:GLY:N	2.59	0.60
2:C:89:GLU:CD	3:E:125:VAL:HG13	2.26	0.60
1:A:108:ASN:HD21	1:A:175:ARG:HD3	1.66	0.60
1:B:107:SER:HB3	1:B:155:ASN:HD21	1.65	0.60
1:B:269:THR:HG22	3:F:148:TYR:HE1	1.62	0.60
1:A:476:ARG:HD3	3:E:4:LEU:HG	1.84	0.60
2:C:338:LEU:HB2	6:C:5175:HOH:O	2.00	0.60
2:D:102:LEU:HD12	2:D:290:ILE:HG23	1.82	0.60
2:D:308:GLU:HG2	2:D:309:PHE:CE1	2.37	0.60
1:A:118:ILE:HD13	1:A:145:ILE:HG12	1.84	0.60
2:C:336:MET:CE	2:C:356:LEU:HD11	2.32	0.60
1:B:445:MET:HE3	1:B:523:VAL:HG22	1.83	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:247:SER:HG	2:C:324:TRP:CD1	2.20	0.59
2:D:357:TYR:CD2	2:D:377:ARG:NH1	2.70	0.59
3:F:57:GLU:O	3:F:61:GLU:HG3	2.01	0.59
1:B:230:GLU:C	1:B:233:PRO:HD2	2.27	0.59
1:A:230:GLU:C	1:A:233:PRO:HD2	2.28	0.59
1:A:314:GLY:HA2	1:A:318:ILE:HD12	1.84	0.59
2:C:105:TRP:O	2:C:108:PRO:HD2	2.02	0.59
3:F:111:HIS:HE1	3:F:132:GLU:OE2	1.86	0.59
3:F:22:LEU:HD11	3:F:31:MET:SD	2.43	0.58
1:A:243:GLU:O	1:A:247:MET:HG2	2.03	0.58
1:B:323:LYS:HE2	1:B:324:TYR:CE1	2.38	0.58
2:C:139:THR:O	2:C:143:GLU:HB3	2.03	0.58
1:A:207:VAL:HG22	1:A:313:TRP:CZ2	2.39	0.58
3:E:111:HIS:HE1	3:E:132:GLU:OE2	1.87	0.58
1:A:65:LYS:HD2	2:C:117:TRP:HB2	1.86	0.57
2:C:364:ILE:HA	2:C:368:ALA:HB3	1.85	0.57
2:D:139:THR:O	2:D:143:GLU:HB3	2.04	0.57
2:C:6:GLU:HG3	6:C:5095:HOH:O	2.04	0.57
3:F:165:HIS:ND1	3:F:166:LEU:N	2.53	0.57
2:D:105:TRP:O	2:D:108:PRO:HD2	2.05	0.57
3:F:153:GLU:H	3:F:153:GLU:CD	2.12	0.57
1:A:29:HIS:CD2	1:A:61:LYS:HA	2.40	0.57
1:A:185:LYS:O	1:A:189:SER:HB2	2.05	0.57
2:D:336:MET:HE2	2:D:356:LEU:HD11	1.86	0.57
1:A:206:LEU:HD11	1:A:321:LEU:HD11	1.87	0.57
1:B:30:ARG:O	1:B:30:ARG:HD3	2.05	0.57
1:B:124:LEU:HD21	1:B:201:SER:HB2	1.85	0.56
1:B:207:VAL:HG22	1:B:313:TRP:CZ2	2.40	0.56
2:C:153:LEU:C	2:C:153:LEU:HD12	2.30	0.56
2:C:357:TYR:CD2	2:C:377:ARG:NH1	2.73	0.56
1:B:30:ARG:HD3	1:B:30:ARG:C	2.29	0.56
2:C:33:ASN:C	2:C:33:ASN:HD22	2.13	0.56
1:A:323:LYS:HE2	1:A:324:TYR:CE1	2.40	0.56
2:D:187:ILE:O	2:D:191:GLN:HG3	2.04	0.56
1:B:403:ILE:HG22	1:B:406:MET:HG3	1.88	0.56
1:A:393:ARG:CG	1:A:393:ARG:HH11	2.19	0.56
1:A:436:LEU:HB3	3:E:167:GLN:HE21	1.71	0.56
1:B:227:ASN:ND2	1:B:295:LYS:H	1.99	0.56
2:C:187:ILE:O	2:C:191:GLN:HG3	2.06	0.56
1:B:190:ASP:HB3	2:D:74:GLN:O	2.06	0.56
3:E:111:HIS:CE1	3:E:132:GLU:OE2	2.59	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:98:MET:CE	3:F:110:ILE:HB	2.36	0.56
1:A:438:VAL:HG12	3:E:164:VAL:HG21	1.86	0.55
2:C:86:GLU:HG2	6:C:5132:HOH:O	2.06	0.55
2:C:107:ALA:HB3	2:C:108:PRO:HD3	1.87	0.55
1:B:243:GLU:O	1:B:247:MET:HG2	2.05	0.55
1:B:477:GLU:OE2	1:B:479:SER:N	2.38	0.55
2:D:364:ILE:HA	2:D:368:ALA:HB3	1.86	0.55
3:E:22:LEU:HD11	3:E:31:MET:SD	2.46	0.55
1:A:41:ASN:N	1:A:41:ASN:ND2	2.53	0.55
1:A:314:GLY:HA2	1:A:318:ILE:CD1	2.37	0.55
1:B:516:ASN:C	1:B:516:ASN:HD22	2.15	0.55
2:C:336:MET:HE2	2:C:356:LEU:HD11	1.88	0.55
1:A:184:MET:HE3	1:A:188:PHE:HB2	1.87	0.55
1:B:33:GLN:HE22	1:B:130:ALA:HB1	1.72	0.55
3:E:15:TRP:CD1	3:E:56:ILE:HD13	2.41	0.55
1:A:76:GLU:OE2	1:B:76:GLU:HG2	2.06	0.55
1:B:310:TYR:CZ	1:B:336:LYS:HD2	2.41	0.55
3:F:111:HIS:CE1	3:F:132:GLU:OE2	2.59	0.55
1:A:186:ARG:HA	2:C:73:THR:OG1	2.06	0.55
1:B:185:LYS:O	1:B:189:SER:HB2	2.06	0.55
1:B:140:GLN:O	1:B:144:GLU:HG2	2.07	0.55
1:B:314:GLY:HA2	1:B:318:ILE:CD1	2.37	0.55
3:E:57:GLU:O	3:E:61:GLU:HG3	2.06	0.55
1:B:206:LEU:HD11	1:B:321:LEU:HD11	1.90	0.54
2:D:146:ASN:HD22	2:D:197:ARG:HE	1.56	0.54
1:A:209:GLU:OE2	1:A:246:HIS:ND1	2.39	0.54
1:B:369:MET:HE2	6:B:5084:HOH:O	2.07	0.54
3:E:153:GLU:CD	3:E:153:GLU:H	2.15	0.54
3:F:61:GLU:HB3	3:F:121:PRO:HD3	1.89	0.54
1:A:211:CYS:HB2	1:A:313:TRP:CD1	2.43	0.54
3:E:35:PHE:CE1	3:E:39:HIS:HD2	2.26	0.54
1:B:436:LEU:HB3	3:F:167:GLN:NE2	2.22	0.54
2:C:306:ASP:O	2:C:310:SER:HB2	2.08	0.54
1:B:438:VAL:HG12	3:F:164:VAL:HG21	1.90	0.54
2:D:156:GLU:HA	2:D:156:GLU:OE2	2.09	0.53
1:A:108:ASN:ND2	1:A:175:ARG:HH11	2.05	0.53
3:E:165:HIS:ND1	3:E:166:LEU:N	2.57	0.53
1:A:252:GLN:NE2	1:A:252:GLN:CA	2.68	0.53
2:D:33:ASN:C	2:D:33:ASN:ND2	2.66	0.53
3:E:98:MET:CE	3:E:110:ILE:HB	2.38	0.53
2:C:235:TRP:CD1	2:C:235:TRP:C	2.84	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:438:VAL:HG12	3:F:164:VAL:CG2	2.38	0.53
2:C:261:ARG:NE	2:C:285:GLN:HE22	1.98	0.53
2:D:319:ASN:OD1	3:F:78:ARG:HD3	2.08	0.53
3:F:68:LYS:HG3	3:F:72:PHE:CD2	2.43	0.53
1:A:438:VAL:HG12	3:E:164:VAL:CG2	2.39	0.53
2:D:235:TRP:CD1	2:D:235:TRP:C	2.87	0.53
3:E:132:GLU:OE2	3:E:132:GLU:CA	2.50	0.53
3:F:146:ASN:HB3	3:F:149:ASP:OD2	2.09	0.53
1:A:114:GLU:O	1:A:144:GLU:HG3	2.09	0.53
2:C:146:ASN:HD22	2:C:197:ARG:HE	1.57	0.53
1:A:269:THR:HG22	3:E:148:TYR:HE1	1.72	0.52
3:F:46:SER:OG	3:F:48:GLU:HG2	2.09	0.52
1:A:146:ARG:HB2	2:C:106:HIS:CE1	2.44	0.52
1:A:403:ILE:HG22	1:A:406:MET:HG3	1.91	0.52
1:A:83:GLN:HG2	6:A:5091:HOH:O	2.09	0.52
1:B:29:HIS:CD2	1:B:61:LYS:HA	2.44	0.52
3:E:46:SER:OG	3:E:48:GLU:HG2	2.10	0.52
1:B:313:TRP:CZ3	1:B:318:ILE:HD11	2.45	0.52
1:B:354:TRP:CG	1:B:355:PRO:HD3	2.45	0.52
2:D:107:ALA:HB3	2:D:108:PRO:HD3	1.90	0.52
1:B:393:ARG:NH1	6:B:5051:HOH:O	2.39	0.52
3:F:98:MET:HE1	3:F:107:ALA:HA	1.92	0.52
1:B:198:VAL:O	1:B:202:LEU:HG	2.09	0.52
3:E:61:GLU:HB3	3:E:121:PRO:HD3	1.92	0.52
1:A:107:SER:HB3	1:A:155:ASN:ND2	2.24	0.52
1:B:118:ILE:HD13	1:B:145:ILE:HG12	1.92	0.52
2:C:75:LYS:HB3	2:C:80:ARG:O	2.09	0.52
1:A:33:GLN:HA	1:A:131:ALA:HB3	1.92	0.52
1:B:110:LEU:O	1:B:114:GLU:HG2	2.10	0.52
3:E:146:ASN:HB3	3:E:149:ASP:OD2	2.10	0.52
1:A:179:PRO:HB3	1:A:469:ILE:HD13	1.91	0.51
1:B:196:ASP:HB2	3:F:140:MET:SD	2.51	0.51
1:A:192:PHE:CE2	1:A:204:LEU:HA	2.45	0.51
1:A:33:GLN:HE22	1:A:130:ALA:HB1	1.74	0.51
1:B:526:PHE:HE2	3:F:165:HIS:CD2	2.27	0.51
1:A:138:LEU:HD22	2:C:160:PHE:CZ	2.45	0.51
1:A:313:TRP:CZ3	1:A:318:ILE:HD11	2.46	0.51
1:A:76:GLU:HG2	1:B:76:GLU:OE2	2.10	0.51
1:A:221:THR:HG22	1:A:233:PRO:HA	1.92	0.51
1:B:108:ASN:ND2	1:B:175:ARG:HH11	2.09	0.51
2:C:21:LEU:HD22	2:D:4:LEU:HD21	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:SER:HB3	1:B:155:ASN:ND2	2.26	0.51
1:A:380:TYR:CE2	1:A:388:GLU:OE1	2.64	0.51
3:E:98:MET:HE1	3:E:107:ALA:HA	1.93	0.51
3:F:130:ASP:OD1	3:F:133:ARG:NH1	2.44	0.51
2:D:269:ALA:HB3	2:D:270:PRO:HD3	1.93	0.51
1:A:109:PHE:O	1:A:112:VAL:HG12	2.11	0.50
1:A:206:LEU:HD11	1:A:321:LEU:CD1	2.41	0.50
2:D:143:GLU:HG2	2:D:144:PHE:CE1	2.46	0.50
1:A:118:ILE:CG1	1:A:144:GLU:HB3	2.39	0.50
1:A:477:GLU:OE2	1:A:479:SER:N	2.40	0.50
2:C:269:ALA:HB3	2:C:270:PRO:HD3	1.92	0.50
1:A:439:HIS:HE1	1:A:454:GLU:OE1	1.95	0.50
1:A:516:ASN:C	1:A:516:ASN:HD22	2.18	0.50
1:B:221:THR:HG22	1:B:233:PRO:HA	1.92	0.50
1:A:186:ARG:HD3	1:A:186:ARG:C	2.36	0.50
1:B:344:HIS:HE1	1:B:376:TYR:CD2	2.29	0.50
1:B:439:HIS:HE1	1:B:454:GLU:OE1	1.94	0.50
1:B:186:ARG:HD3	1:B:186:ARG:C	2.36	0.50
2:C:365:GLU:OE1	2:C:365:GLU:CA	2.59	0.50
3:F:41:THR:O	3:F:44:ARG:CD	2.60	0.50
3:F:15:TRP:CD1	3:F:56:ILE:HD13	2.47	0.50
3:E:41:THR:O	3:E:44:ARG:CD	2.60	0.50
3:E:162:ARG:CZ	3:E:164:VAL:HG12	2.41	0.50
1:B:260:ASP:OD2	1:B:262:ALA:HB3	2.12	0.50
1:A:196:ASP:HB2	3:E:140:MET:SD	2.51	0.50
1:A:260:ASP:OD2	1:A:262:ALA:HB3	2.12	0.49
1:B:65:LYS:HE2	2:D:192:MET:HE2	1.94	0.49
2:C:33:ASN:C	2:C:33:ASN:ND2	2.69	0.49
2:C:143:GLU:HG2	2:C:144:PHE:CE1	2.47	0.49
1:B:43:ARG:HD2	1:B:43:ARG:C	2.37	0.49
1:B:206:LEU:HD11	1:B:321:LEU:CD1	2.43	0.49
1:B:352:ALA:CA	1:B:404:PRO:HB2	2.27	0.49
1:A:313:TRP:O	1:A:318:ILE:HG13	2.13	0.49
2:D:365:GLU:OE1	2:D:365:GLU:CA	2.60	0.49
3:F:162:ARG:CZ	3:F:164:VAL:HG12	2.43	0.49
2:C:4:LEU:HD21	2:D:21:LEU:HD22	1.93	0.49
1:A:284:PRO:HB3	1:A:342:ALA:HB1	1.94	0.49
3:E:4:LEU:HG	3:E:4:LEU:O	2.12	0.49
1:B:207:VAL:HG11	1:B:275:PHE:HA	1.94	0.49
2:D:54:VAL:O	2:D:55:TYR:HB2	2.12	0.49
1:A:354:TRP:CG	1:A:355:PRO:HD3	2.48	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:PHE:CE2	1:B:204:LEU:HA	2.48	0.49
2:C:143:GLU:HG2	2:C:144:PHE:CD1	2.48	0.49
1:A:360:ARG:HG2	1:A:498:GLN:HB2	1.93	0.49
1:B:284:PRO:HB3	1:B:342:ALA:HB1	1.95	0.49
1:B:526:PHE:CE2	3:F:165:HIS:HD2	2.30	0.49
1:B:302:VAL:HG12	1:B:376:TYR:OH	2.13	0.49
1:B:360:ARG:HG2	1:B:498:GLN:HB2	1.94	0.49
2:D:143:GLU:HG2	2:D:144:PHE:CD1	2.47	0.49
1:A:65:LYS:HB3	2:C:117:TRP:CG	2.48	0.49
1:A:207:VAL:HG22	1:A:313:TRP:HZ2	1.78	0.49
1:A:302:VAL:HG12	1:A:376:TYR:OH	2.13	0.48
1:B:268:ASN:HD21	1:B:327:GLU:H	1.59	0.48
1:B:313:TRP:O	1:B:318:ILE:HG13	2.13	0.48
1:A:292:TYR:OH	1:A:344:HIS:CD2	2.60	0.48
1:B:186:ARG:HA	2:D:73:THR:OG1	2.13	0.48
1:B:438:VAL:HB	3:F:164:VAL:HG23	1.96	0.48
2:C:156:GLU:OE2	2:C:156:GLU:HA	2.14	0.48
2:C:277:THR:HB	2:C:278:PRO:HD3	1.94	0.48
1:A:113:GLY:HA3	1:A:188:PHE:CD2	2.49	0.48
1:A:344:HIS:HE1	1:A:376:TYR:CD2	2.32	0.48
1:B:382:HIS:O	1:B:386:ILE:HG13	2.14	0.48
2:C:112:ASP:OD1	2:D:118:ARG:NH2	2.47	0.48
2:D:324:TRP:O	2:D:327:PRO:HD2	2.13	0.48
3:F:40:THR:O	3:F:41:THR:OG1	2.31	0.48
1:A:521:ASN:OD1	1:A:523:VAL:HG12	2.14	0.48
1:B:41:ASN:N	1:B:41:ASN:ND2	2.54	0.48
1:B:380:TYR:CE2	1:B:388:GLU:OE1	2.67	0.48
2:C:54:VAL:O	2:C:55:TYR:HB2	2.13	0.48
2:D:146:ASN:ND2	2:D:197:ARG:NH2	2.57	0.48
1:B:252:GLN:HE21	1:B:252:GLN:CA	2.24	0.48
1:B:144:GLU:OE2	1:B:144:GLU:HA	2.14	0.47
1:A:204:LEU:HG	1:A:205:GLN:HG3	1.96	0.47
1:A:252:GLN:HE21	1:A:252:GLN:CA	2.18	0.47
1:B:413:HIS:HD2	1:B:428:SER:OG	1.98	0.47
1:A:43:ARG:C	1:A:43:ARG:HD2	2.38	0.47
1:A:123:MET:HB2	2:C:168:ARG:HD3	1.96	0.47
2:D:324:TRP:C	2:D:327:PRO:HD2	2.39	0.47
1:B:204:LEU:HG	1:B:205:GLN:HG3	1.96	0.47
1:B:406:MET:O	1:B:410:GLU:HG3	2.14	0.47
2:C:319:ASN:OD1	3:E:78:ARG:HD3	2.14	0.47
3:E:66:VAL:HG12	3:E:70:ARG:HH21	1.79	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:130:ASP:OD1	3:E:133:ARG:NH1	2.47	0.47
3:F:35:PHE:CE1	3:F:39:HIS:HD2	2.32	0.47
1:A:49:LYS:CE	3:E:144:ASN:HD22	2.28	0.47
1:A:382:HIS:O	1:A:386:ILE:HG13	2.14	0.47
1:A:413:HIS:HD2	1:A:428:SER:OG	1.97	0.47
1:A:198:VAL:O	1:A:202:LEU:HG	2.14	0.47
1:A:373:GLU:OE2	1:A:377:PRO:HA	2.15	0.47
1:A:406:MET:O	1:A:410:GLU:HG3	2.13	0.47
1:B:393:ARG:HH11	1:B:393:ARG:CG	2.27	0.47
2:D:82:SER:O	2:D:168:ARG:NH2	2.48	0.47
2:D:306:ASP:O	2:D:310:SER:HB2	2.14	0.47
3:E:159:ARG:HG3	3:E:161:VAL:HG12	1.97	0.47
1:B:417:ILE:HG13	1:B:468:ASN:HB2	1.97	0.47
1:B:440:GLU:OE1	3:F:162:ARG:NH1	2.39	0.47
2:D:75:LYS:HB3	2:D:80:ARG:O	2.15	0.47
2:D:256:PHE:HA	2:D:332:LEU:HD21	1.97	0.47
3:E:98:MET:HE1	3:E:110:ILE:HB	1.97	0.47
3:E:150:THR:CG2	3:E:154:GLU:HG2	2.45	0.47
1:A:116:ASN:CG	1:A:189:SER:HA	2.41	0.47
1:A:439:HIS:CG	3:E:161:VAL:HG21	2.50	0.47
1:B:365:ASP:OD2	1:B:365:ASP:C	2.58	0.46
2:C:42:ARG:HB2	2:C:99:ARG:HG3	1.97	0.46
2:D:157:TYR:O	2:D:160:PHE:HB3	2.15	0.46
1:B:65:LYS:HD2	2:D:117:TRP:HB2	1.96	0.46
1:B:211:CYS:HB2	1:B:313:TRP:CD1	2.50	0.46
2:D:275:ASN:C	2:D:278:PRO:HD2	2.39	0.46
1:A:430:ALA:HA	6:A:5054:HOH:O	2.15	0.46
2:C:146:ASN:ND2	2:C:197:ARG:NH2	2.58	0.46
2:D:336:MET:HE1	2:D:356:LEU:HD11	1.97	0.46
1:A:108:ASN:HD21	1:A:175:ARG:CD	2.28	0.46
1:A:195:GLY:HA2	6:C:5060:HOH:O	2.14	0.46
1:B:49:LYS:HE3	3:F:144:ASN:HD22	1.79	0.46
1:B:302:VAL:HG12	1:B:376:TYR:CZ	2.50	0.46
2:D:161:ASN:HB3	2:D:235:TRP:CE2	2.51	0.46
1:A:268:ASN:HD21	1:A:327:GLU:H	1.62	0.46
1:B:75:ASP:OD2	1:B:146:ARG:NH1	2.48	0.46
1:B:313:TRP:CE3	1:B:318:ILE:HD11	2.51	0.46
2:C:80:ARG:HB2	6:C:5062:HOH:O	2.15	0.46
1:B:125:TRP:CD1	1:B:125:TRP:C	2.94	0.46
2:C:318:ARG:NH2	6:C:5034:HOH:O	2.48	0.46
1:A:211:CYS:HB2	1:A:313:TRP:CG	2.49	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:VAL:HG12	1:A:376:TYR:CZ	2.51	0.46
1:A:437:ARG:NH1	1:A:454:GLU:OE2	2.48	0.46
1:B:65:LYS:HB3	2:D:117:TRP:CG	2.50	0.46
1:B:291:GLU:OE1	1:B:343:HIS:HE1	1.98	0.46
1:B:521:ASN:OD1	1:B:523:VAL:HG12	2.16	0.46
1:B:207:VAL:O	1:B:211:CYS:HB3	2.16	0.46
3:F:98:MET:HE1	3:F:110:ILE:HB	1.97	0.46
1:A:65:LYS:HB3	2:C:117:TRP:CD2	2.51	0.45
1:B:484:GLU:OE1	3:F:6:ILE:N	2.46	0.45
2:D:348:ASP:OD2	2:D:350:GLU:HB3	2.15	0.45
1:A:186:ARG:HA	2:C:73:THR:HG1	1.80	0.45
1:A:186:ARG:HD2	1:A:277:THR:HG23	1.99	0.45
1:B:393:ARG:HB3	1:B:402:PHE:CD2	2.51	0.45
1:B:109:PHE:O	1:B:112:VAL:HG12	2.16	0.45
1:B:202:LEU:HD22	1:B:206:LEU:HD23	1.99	0.45
2:C:80:ARG:HG3	3:E:132:GLU:OE1	2.16	0.45
3:F:66:VAL:HG12	3:F:70:ARG:HH21	1.80	0.45
1:A:202:LEU:HD22	1:A:206:LEU:HD23	1.98	0.45
1:A:417:ILE:HG13	1:A:468:ASN:HB2	1.98	0.45
1:B:108:ASN:HD21	1:B:175:ARG:CD	2.29	0.45
1:B:281:TYR:CZ	1:B:285:VAL:HG21	2.52	0.45
1:B:292:TYR:OH	1:B:344:HIS:CD2	2.62	0.45
2:C:77:HIS:CD2	3:E:140:MET:HG2	2.51	0.45
2:D:184:PHE:O	2:D:187:ILE:HG22	2.17	0.45
1:A:75:ASP:OD2	1:A:146:ARG:NH1	2.49	0.45
1:A:212:PHE:O	1:A:216:LEU:HB3	2.16	0.45
1:B:373:GLU:OE2	1:B:377:PRO:HA	2.17	0.45
1:A:113:GLY:HA2	1:A:188:PHE:HB3	1.99	0.45
1:A:125:TRP:CD1	1:A:125:TRP:C	2.95	0.45
1:A:125:TRP:HE1	2:C:161:ASN:ND2	2.14	0.45
1:B:123:MET:HE2	1:B:197:ALA:CA	2.42	0.45
2:D:143:GLU:O	2:D:147:ARG:HB3	2.17	0.45
3:F:98:MET:HE2	3:F:110:ILE:HD12	1.98	0.45
3:F:159:ARG:HG3	3:F:161:VAL:HG12	1.98	0.44
1:A:283:THR:HB	1:A:284:PRO:HD3	1.99	0.44
1:B:283:THR:HB	1:B:284:PRO:HD3	1.98	0.44
2:D:262:ARG:HA	2:D:266:GLN:HB3	1.99	0.44
3:E:115:ARG:NH1	3:E:132:GLU:OE1	2.48	0.44
3:F:33:LYS:O	3:F:37:MET:HG2	2.18	0.44
1:B:344:HIS:HE1	1:B:376:TYR:CE2	2.35	0.44
2:C:306:ASP:HA	2:C:307:PRO:HD3	1.86	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:136:MET:HE2	2:D:274:ASP:OD1	2.17	0.44
1:A:124:LEU:HB3	1:A:137:TYR:CE1	2.53	0.44
1:A:163:GLN:HG2	6:A:5012:HOH:O	2.16	0.44
1:B:44:THR:HG23	1:B:127:SER:HA	2.00	0.44
1:B:65:LYS:HB3	2:D:117:TRP:CD2	2.53	0.44
2:C:256:PHE:HA	2:C:332:LEU:HD21	1.99	0.44
2:D:144:PHE:CZ	2:D:342:LEU:HD23	2.53	0.44
1:A:207:VAL:HG11	1:A:275:PHE:HA	1.99	0.44
1:A:313:TRP:CE3	1:A:318:ILE:HD11	2.52	0.44
1:B:54:ASN:C	1:B:54:ASN:OD1	2.61	0.44
1:B:207:VAL:HG22	1:B:313:TRP:HZ2	1.79	0.44
2:C:157:TYR:O	2:C:160:PHE:HB3	2.18	0.44
2:C:247:SER:O	2:C:251:VAL:HB	2.18	0.44
2:C:324:TRP:C	2:C:327:PRO:HD2	2.42	0.44
1:A:223:TRP:CZ3	1:A:297:LYS:HA	2.53	0.43
1:A:291:GLU:OE1	1:A:343:HIS:HE1	2.01	0.43
1:B:212:PHE:O	1:B:216:LEU:HB3	2.18	0.43
2:C:275:ASN:C	2:C:278:PRO:HD2	2.43	0.43
2:D:169:GLU:O	2:D:170:ALA:C	2.60	0.43
1:B:348:LEU:HD23	1:B:387:TYR:CE2	2.53	0.43
2:C:143:GLU:O	2:C:147:ARG:HB3	2.17	0.43
2:C:144:PHE:CZ	2:C:342:LEU:HD23	2.54	0.43
2:C:161:ASN:HB3	2:C:235:TRP:CE2	2.52	0.43
3:E:98:MET:HE2	3:E:110:ILE:HD12	2.00	0.43
1:A:348:LEU:HD23	1:A:387:TYR:CE2	2.54	0.43
1:A:451:GLN:HB2	3:E:152:LEU:HD11	2.00	0.43
1:B:403:ILE:HD12	1:B:515:LEU:CD1	2.49	0.43
2:C:184:PHE:O	2:C:187:ILE:HG22	2.18	0.43
2:C:336:MET:HE1	2:C:356:LEU:HD11	2.01	0.43
3:E:161:VAL:HG23	3:E:162:ARG:N	2.33	0.43
3:F:6:ILE:HG22	3:F:7:HIS:ND1	2.33	0.43
3:F:161:VAL:HG23	3:F:162:ARG:N	2.34	0.43
1:A:403:ILE:HD12	1:A:515:LEU:CD1	2.48	0.43
3:E:98:MET:HE3	3:E:110:ILE:CG2	2.49	0.43
3:F:150:THR:CG2	3:F:154:GLU:HG2	2.48	0.43
1:A:352:ALA:CA	1:A:404:PRO:HB2	2.25	0.43
1:A:393:ARG:HB3	1:A:402:PHE:CD2	2.54	0.43
1:A:445:MET:HE1	1:A:526:PHE:HB2	2.01	0.43
2:D:80:ARG:HG3	3:F:132:GLU:OE1	2.19	0.43
2:D:98:HIS:HD2	2:D:297:ASP:OD1	2.02	0.43
3:F:22:LEU:HD13	3:F:28:ALA:HA	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:ASP:OD2	1:A:365:ASP:C	2.61	0.43
1:A:435:THR:HG22	1:A:449:SER:O	2.18	0.43
1:B:297:LYS:HG2	1:B:371:TRP:CE2	2.53	0.43
1:A:281:TYR:CZ	1:A:285:VAL:HG21	2.54	0.43
1:B:102:THR:OG1	1:B:293:GLY:HA3	2.19	0.43
1:B:243:GLU:OE1	1:B:246:HIS:ND1	2.52	0.43
2:D:78:GLY:O	3:F:115:ARG:HD3	2.18	0.42
3:E:68:LYS:HG3	3:E:72:PHE:CD2	2.54	0.42
2:C:82:SER:O	2:C:168:ARG:NH2	2.52	0.42
2:D:63:ILE:O	2:D:64:ALA:C	2.61	0.42
2:D:306:ASP:HA	2:D:307:PRO:HD3	1.88	0.42
2:D:77:HIS:CD2	3:F:140:MET:HG2	2.54	0.42
2:D:141:ARG:HD2	2:D:204:VAL:HG21	2.02	0.42
2:D:277:THR:HB	2:D:278:PRO:HD3	2.00	0.42
3:E:153:GLU:CD	3:E:153:GLU:N	2.78	0.42
1:A:393:ARG:CG	1:A:393:ARG:NH1	2.80	0.42
1:B:69:ARG:O	1:B:73:VAL:HG23	2.20	0.42
2:D:310:SER:O	2:D:314:ARG:HG3	2.20	0.42
3:E:15:TRP:CZ3	3:E:18:LYS:HD3	2.55	0.42
3:F:168:SER:HA	3:F:169:PRO:HD2	1.91	0.42
1:B:516:ASN:O	1:B:516:ASN:ND2	2.48	0.42
2:C:201:ALA:HA	2:C:207:PHE:HB3	2.02	0.42
2:C:338:LEU:CB	6:C:5175:HOH:O	2.64	0.42
2:D:153:LEU:HD12	2:D:154:PHE:N	2.34	0.42
3:F:120:PRO:HD3	3:F:128:PHE:CG	2.55	0.42
1:A:54:ASN:OD1	1:A:54:ASN:C	2.61	0.42
1:A:184:MET:HE2	1:A:188:PHE:HB2	1.98	0.42
2:C:126:GLY:O	2:C:130:ASP:HB2	2.20	0.42
2:D:145:ILE:O	2:D:149:TRP:HB3	2.19	0.42
1:B:137:TYR:O	1:B:141:VAL:HG23	2.19	0.42
1:B:393:ARG:HH11	1:B:393:ARG:HG3	1.84	0.42
1:B:435:THR:HG22	1:B:449:SER:O	2.20	0.42
2:C:54:VAL:HG12	2:C:55:TYR:CD2	2.54	0.42
1:A:84:ASP:HB3	1:B:81:SER:OG	2.20	0.42
1:A:186:ARG:CZ	1:A:277:THR:HG23	2.50	0.42
1:A:360:ARG:HD2	1:A:489:ARG:NH2	2.35	0.42
2:C:118:ARG:NH2	2:D:112:ASP:OD1	2.53	0.42
2:D:297:ASP:O	2:D:301:ASN:HB3	2.20	0.42
3:F:11:THR:HG22	3:F:12:ARG:N	2.34	0.42
3:F:33:LYS:HD2	3:F:117:ALA:HA	2.02	0.42
3:F:153:GLU:CD	3:F:153:GLU:N	2.76	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:HIS:HE1	1:A:376:TYR:CE2	2.38	0.42
2:C:262:ARG:HA	2:C:266:GLN:HB3	2.02	0.42
3:F:15:TRP:CZ3	3:F:18:LYS:HD3	2.55	0.42
1:B:44:THR:CG2	1:B:127:SER:HA	2.50	0.41
1:B:437:ARG:NH1	1:B:454:GLU:OE2	2.49	0.41
1:A:143:ASP:O	1:A:146:ARG:HB3	2.20	0.41
1:B:113:GLY:HA3	1:B:188:PHE:CD2	2.55	0.41
2:C:240:ASP:HB2	3:E:125:VAL:CG2	2.50	0.41
1:A:516:ASN:O	1:A:516:ASN:ND2	2.49	0.41
1:B:75:ASP:O	1:B:76:GLU:C	2.63	0.41
1:B:115:TYR:OH	2:D:173:ASP:HA	2.20	0.41
1:B:445:MET:HE1	1:B:526:PHE:HB2	2.02	0.41
2:C:348:ASP:OD2	2:C:350:GLU:HB3	2.20	0.41
1:B:121:THR:HG21	1:B:140:GLN:CG	2.50	0.41
2:C:300:TYR:CD1	2:C:370:ARG:HG3	2.56	0.41
1:A:297:LYS:HG2	1:A:371:TRP:CE2	2.56	0.41
1:A:445:MET:CE	1:A:526:PHE:HB2	2.51	0.41
1:B:18:ARG:O	2:D:129:ALA:HA	2.20	0.41
1:B:192:PHE:O	1:B:200:CYS:HB3	2.21	0.41
2:C:63:ILE:O	2:C:64:ALA:C	2.64	0.41
2:D:42:ARG:HB2	2:D:99:ARG:HG3	2.01	0.41
1:A:423:VAL:HA	1:A:424:PRO:HD3	1.91	0.41
1:B:31:TRP:CZ2	2:D:210:SER:HA	2.55	0.41
1:B:110:LEU:HD23	1:B:110:LEU:HA	1.89	0.41
1:B:206:LEU:HD12	1:B:206:LEU:HA	1.90	0.41
1:A:103:MET:HE2	1:A:232:THR:OG1	2.20	0.41
1:A:393:ARG:NH1	1:A:393:ARG:HG3	2.35	0.41
2:C:297:ASP:O	2:C:301:ASN:HB3	2.20	0.41
1:A:137:TYR:O	1:A:141:VAL:HG23	2.21	0.41
1:B:18:ARG:HG3	1:B:18:ARG:HH11	1.85	0.41
1:B:121:THR:HG21	1:B:140:GLN:HG2	2.03	0.41
2:C:266:GLN:NE2	2:C:281:ILE:HG22	2.36	0.41
2:D:153:LEU:C	2:D:153:LEU:CD1	2.94	0.41
2:D:165:GLN:OE1	2:D:239:PHE:HA	2.21	0.41
2:D:201:ALA:HA	2:D:207:PHE:HB3	2.02	0.41
2:D:247:SER:O	2:D:251:VAL:HB	2.21	0.41
3:E:36:ARG:NH2	3:E:119:LYS:HD2	2.36	0.41
1:B:223:TRP:CZ3	1:B:297:LYS:HA	2.56	0.41
1:B:360:ARG:HD2	1:B:489:ARG:NH2	2.35	0.41
1:A:146:ARG:HB2	2:C:106:HIS:NE2	2.34	0.40
1:A:209:GLU:HA	1:A:213:THR:HB	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:PRO:HG3	2:D:129:ALA:HB2	2.03	0.40
3:E:4:LEU:O	3:E:4:LEU:CG	2.69	0.40
3:E:22:LEU:HD13	3:E:28:ALA:HA	2.03	0.40
1:A:510:ASP:O	1:A:514:ARG:HG3	2.21	0.40
1:B:124:LEU:HB3	1:B:137:TYR:CE1	2.55	0.40
1:A:69:ARG:O	1:A:73:VAL:HG23	2.21	0.40
2:D:147:ARG:HD2	2:D:148:TYR:CE1	2.56	0.40
2:D:308:GLU:O	2:D:308:GLU:HG3	2.22	0.40
1:A:354:TRP:CH2	1:A:499:PRO:HD3	2.57	0.40
1:B:252:GLN:NE2	1:B:252:GLN:CA	2.70	0.40
3:E:120:PRO:HD3	3:E:128:PHE:CG	2.56	0.40
3:F:74:GLU:O	3:F:78:ARG:HG3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	509/527 (97%)	481 (94%)	25 (5%)	3 (1%)	21	32
1	B	508/527 (96%)	479 (94%)	27 (5%)	2 (0%)	30	43
2	C	386/389 (99%)	368 (95%)	16 (4%)	2 (0%)	24	37
2	D	384/389 (99%)	363 (94%)	18 (5%)	3 (1%)	16	25
3	E	164/170 (96%)	161 (98%)	3 (2%)	0	100	100
3	F	166/170 (98%)	162 (98%)	4 (2%)	0	100	100
All	All	2117/2172 (98%)	2014 (95%)	93 (4%)	10 (0%)	24	37

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	386	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	64	ALA
2	D	64	ALA
1	A	40	LYS
1	B	40	LYS
2	D	251	VAL
1	A	94	ARG
1	B	284	PRO
2	C	251	VAL
1	A	284	PRO

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	432/442 (98%)	411 (95%)	21 (5%)	22	39
1	B	432/442 (98%)	413 (96%)	19 (4%)	25	43
2	C	322/323 (100%)	310 (96%)	12 (4%)	30	51
2	D	320/323 (99%)	308 (96%)	12 (4%)	29	49
3	E	144/147 (98%)	132 (92%)	12 (8%)	10	17
3	F	145/147 (99%)	133 (92%)	12 (8%)	10	17
All	All	1795/1824 (98%)	1707 (95%)	88 (5%)	22	39

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	THR
1	A	30	ARG
1	A	41	ASN
1	A	90	ASN
1	A	125	TRP
1	A	144	GLU
1	A	186	ARG
1	A	213	THR
1	A	252	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	279	GLN
1	A	302	VAL
1	A	311	GLU
1	A	316	ILE
1	A	334	ASP
1	A	337	GLN
1	A	393	ARG
1	A	403	ILE
1	A	435	THR
1	A	477	GLU
1	A	504	ASP
1	A	516	ASN
1	B	21	THR
1	B	41	ASN
1	B	90	ASN
1	B	125	TRP
1	B	186	ARG
1	B	213	THR
1	B	252	GLN
1	B	269	THR
1	B	279	GLN
1	B	302	VAL
1	B	311	GLU
1	B	316	ILE
1	B	334	ASP
1	B	393	ARG
1	B	403	ILE
1	B	435	THR
1	B	477	GLU
1	B	504	ASP
1	B	516	ASN
2	C	4	LEU
2	C	33	ASN
2	C	80	ARG
2	C	143	GLU
2	C	153	LEU
2	C	173	ASP
2	C	179	LEU
2	C	266	GLN
2	C	308	GLU
2	C	311	ASP
2	C	365	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	378	ASP
2	D	4	LEU
2	D	33	ASN
2	D	80	ARG
2	D	143	GLU
2	D	153	LEU
2	D	173	ASP
2	D	179	LEU
2	D	266	GLN
2	D	308	GLU
2	D	311	ASP
2	D	365	GLU
2	D	378	ASP
3	E	11	THR
3	E	23	ASN
3	E	24	THR
3	E	33	LYS
3	E	44	ARG
3	E	46	SER
3	E	97	LYS
3	E	98	MET
3	E	125	VAL
3	E	132	GLU
3	E	154	GLU
3	E	161	VAL
3	F	11	THR
3	F	23	ASN
3	F	24	THR
3	F	33	LYS
3	F	44	ARG
3	F	46	SER
3	F	97	LYS
3	F	98	MET
3	F	125	VAL
3	F	132	GLU
3	F	154	GLU
3	F	161	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (82) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	41	ASN
1	A	59	GLN
1	A	78	GLN
1	A	90	ASN
1	A	108	ASN
1	A	133	GLN
1	A	155	ASN
1	A	203	ASN
1	A	227	ASN
1	A	249	ASN
1	A	252	GLN
1	A	268	ASN
1	A	273	ASN
1	A	279	GLN
1	A	343	HIS
1	A	344	HIS
1	A	382	HIS
1	A	412	ASN
1	A	413	HIS
1	A	422	GLN
1	A	439	HIS
1	A	442	ASN
1	A	486	HIS
1	B	41	ASN
1	B	59	GLN
1	B	78	GLN
1	B	90	ASN
1	B	108	ASN
1	B	155	ASN
1	B	168	HIS
1	B	203	ASN
1	B	205	GLN
1	B	214	ASN
1	B	227	ASN
1	B	249	ASN
1	B	252	GLN
1	B	268	ASN
1	B	273	ASN
1	B	279	GLN
1	B	343	HIS
1	B	344	HIS
1	B	382	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	412	ASN
1	B	413	HIS
1	B	439	HIS
1	B	442	ASN
1	B	472	GLN
1	B	486	HIS
1	B	527	ASN
2	C	98	HIS
2	C	125	GLN
2	C	146	ASN
2	C	161	ASN
2	C	266	GLN
2	C	275	ASN
2	C	285	GLN
2	C	301	ASN
2	D	33	ASN
2	D	98	HIS
2	D	125	GLN
2	D	132	GLN
2	D	146	ASN
2	D	161	ASN
2	D	266	GLN
2	D	285	GLN
2	D	301	ASN
3	E	39	HIS
3	E	45	ASN
3	E	111	HIS
3	E	134	GLN
3	E	144	ASN
3	E	158	GLN
3	E	167	GLN
3	F	39	HIS
3	F	45	ASN
3	F	111	HIS
3	F	134	GLN
3	F	144	ASN
3	F	158	GLN
3	F	167	GLN
3	F	170	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	511/527 (96%)	0.47	39 (7%)	20 16	22, 42, 71, 88	0
1	B	510/527 (96%)	0.47	34 (6%)	24 20	25, 41, 74, 87	0
2	C	388/389 (99%)	-0.27	1 (0%)	90 88	19, 28, 47, 65	0
2	D	386/389 (99%)	1.08	75 (19%)	3 2	27, 53, 84, 89	0
3	E	166/170 (97%)	-0.03	5 (3%)	52 48	18, 32, 51, 68	0
3	F	168/170 (98%)	1.53	41 (24%)	2 1	42, 62, 83, 92	0
All	All	2129/2172 (98%)	0.49	195 (9%)	14 12	18, 41, 77, 92	0

All (195) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	387	GLY	5.7
1	A	433	ALA	5.2
2	D	353	THR	5.2
2	D	386	ALA	4.8
1	A	338	ASP	4.5
1	B	264	ALA	4.3
3	F	22	LEU	4.1
2	D	224	TYR	4.1
1	B	53	ALA	4.1
3	F	72	PHE	3.9
3	F	4(A)	LEU	3.9
2	D	352	ILE	3.8
1	A	244	LEU	3.8
2	D	354	ALA	3.8
2	D	380	ILE	3.7
3	F	82	ALA	3.7
1	A	54	ASN	3.7
2	D	205	PRO	3.7
1	B	35	PHE	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	270	PRO	3.7
3	E	4	LEU	3.6
3	F	84	GLY	3.6
3	F	77	PHE	3.6
1	B	188	PHE	3.5
2	D	146	ASN	3.5
2	D	206	GLY	3.5
3	F	75	VAL	3.4
2	D	275	ASN	3.4
1	A	310	TYR	3.4
3	E	168	SER	3.4
3	F	20	ALA	3.3
3	F	87	ALA	3.3
1	A	213	THR	3.3
1	B	131	ALA	3.3
3	F	32	LEU	3.2
2	D	136	MET	3.2
1	A	432	GLY	3.1
2	D	385	LEU	3.1
2	D	381	VAL	3.1
2	D	135	ALA	3.1
2	D	223	VAL	3.1
2	D	384	VAL	3.1
1	A	56	THR	3.1
3	E	167	GLN	3.0
1	B	258	ALA	3.0
3	F	25	LEU	3.0
1	A	316	ILE	3.0
2	D	356	LEU	3.0
2	D	141	ARG	3.0
3	F	23	ASN	3.0
1	A	314	GLY	3.0
2	D	137	ASN	3.0
1	A	209	GLU	3.0
2	D	382	LYS	3.0
2	D	383	ALA	2.9
2	D	368	ALA	2.9
3	F	118	TYR	2.9
2	D	225	LYS	2.9
3	F	101	ALA	2.9
2	D	273	GLY	2.9
1	A	326	VAL	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	525	ALA	2.8
2	D	143	GLU	2.8
2	D	133	ILE	2.8
2	D	204	VAL	2.8
3	F	83	PHE	2.8
1	A	318	ILE	2.8
1	A	263	SER	2.8
1	A	337	GLN	2.8
2	D	140	TRP	2.8
3	F	74	GLU	2.8
1	B	526	PHE	2.8
2	D	145	ILE	2.7
1	B	36	ASN	2.7
1	B	244	LEU	2.7
1	B	248	ALA	2.6
2	D	338	LEU	2.6
1	A	339	ALA	2.6
1	B	243	GLU	2.6
2	D	231	VAL	2.6
1	A	328	SER	2.6
2	D	344	ALA	2.6
3	F	80	LYS	2.6
2	D	132	GLN	2.5
2	D	266	GLN	2.5
2	D	212	ALA	2.5
1	A	269	THR	2.5
1	A	308	TRP	2.5
3	F	60	LEU	2.5
3	F	17	ASN	2.5
2	D	226	SER	2.5
2	D	370	ARG	2.5
2	D	377	ARG	2.5
2	D	345	GLY	2.5
2	D	363	TRP	2.5
3	F	102	LYS	2.5
1	B	44	THR	2.5
3	F	30	GLU	2.5
1	B	57	LYS	2.5
2	D	341	LYS	2.5
1	A	391	ARG	2.5
1	A	262	ALA	2.5
1	A	435	THR	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	138	PRO	2.4
2	D	148	TYR	2.4
2	D	357	TYR	2.4
3	E	23	ASN	2.4
2	D	365	GLU	2.4
2	D	142	ASP	2.4
1	A	206	LEU	2.4
2	D	332	LEU	2.4
1	A	317	TRP	2.4
3	F	24	THR	2.4
1	B	311	GLU	2.4
2	D	268	LEU	2.4
2	D	207	PHE	2.4
1	B	247	MET	2.4
2	D	313	ASN	2.4
1	B	318	ILE	2.4
1	B	18	ARG	2.4
2	D	271	ARG	2.4
1	B	310	TYR	2.4
2	D	349	LYS	2.4
1	B	31	TRP	2.4
2	D	217	GLU	2.4
2	D	218	TRP	2.4
3	F	79	HIS	2.3
3	F	103	ASP	2.3
2	D	335	PHE	2.3
1	B	23	VAL	2.3
1	A	392	ALA	2.3
1	B	320	ARG	2.3
2	D	203	ILE	2.3
2	D	343	PRO	2.3
3	F	153	GLU	2.3
1	B	19	ALA	2.2
1	B	269	THR	2.2
2	D	139	THR	2.2
1	A	366	GLN	2.2
1	B	52	MET	2.2
1	B	308	TRP	2.2
3	F	35	PHE	2.2
1	A	320	ARG	2.2
1	A	340	TYR	2.2
1	A	204	LEU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	321	LEU	2.2
3	F	67	LEU	2.2
1	B	263	SER	2.2
2	D	371	ILE	2.2
3	F	7	HIS	2.2
3	F	21	GLN	2.2
1	A	193	ILE	2.2
1	B	317	TRP	2.2
2	D	339	PHE	2.2
1	A	246	HIS	2.2
1	B	259	ASN	2.2
3	F	19	ILE	2.2
1	B	189	SER	2.2
1	A	334	ASP	2.2
3	F	92	ASP	2.2
1	B	20	PRO	2.2
2	D	213	VAL	2.1
3	F	16	VAL	2.1
3	F	142	LEU	2.1
1	B	209	GLU	2.1
3	F	170	HIS	2.1
1	A	19	ALA	2.1
3	F	69	ALA	2.1
3	F	96	ALA	2.1
2	D	221	GLY	2.1
2	C	365	GLU	2.1
3	F	138	ARG	2.1
2	D	378	ASP	2.1
2	D	324	TRP	2.1
3	F	29	ALA	2.1
2	D	229	LEU	2.1
2	D	342	LEU	2.1
3	F	135	LEU	2.1
1	A	21	THR	2.1
1	A	77	ARG	2.1
2	D	375	ALA	2.1
2	D	267	ARG	2.1
2	D	211	THR	2.1
2	D	346	THR	2.1
2	D	310	SER	2.1
3	F	58	ALA	2.0
1	A	212	PHE	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	298	VAL	2.0
3	E	164	VAL	2.0
1	B	32	LEU	2.0
1	B	327	GLU	2.0
2	D	222	GLU	2.0
1	A	249	ASN	2.0
3	F	144	ASN	2.0
2	D	327	PRO	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(Å ²)	Q<0.9
4	FE2	B	5003	1/1	0.90	0.08	58,58,58,58	0
4	FE2	A	5001	1/1	0.93	0.06	56,56,56,56	0
5	CA	C	5006	1/1	0.93	0.08	64,64,64,64	0
5	CA	A	5005	1/1	0.97	0.07	53,53,53,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.