



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:25 PM UTC

PDB ID : 1FYZ / pdb_00001fyz
Title : METHANE MONOOXYGENASE HYDROXYLASE, FORM II REDUCED
BY SOAKING
Authors : Whittington, D.A.; Lippard, S.J.
Deposited on : 2000-10-03
Resolution : 2.15 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

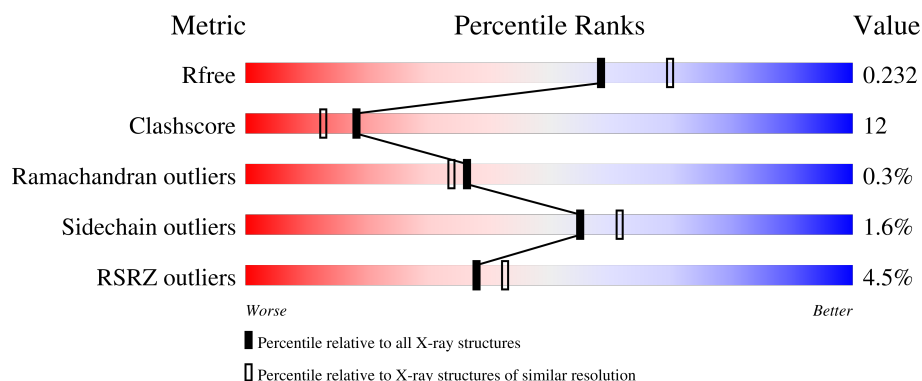
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	3% 72% 24% ..
1	B	527	3% 70% 26% ..
2	C	389	78% 20% .
2	D	389	9% 67% 30% ..
3	E	170	% 81% 15% ..

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Mol	Chain	Length	Quality of chain
3	F	170	16% 66% 31% ..

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 18742 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
			4185	2677	721	769	18			
1	B	511	Total	C	N	O	S	0	0	0
			4185	2677	721	769	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	387	Total	C	N	O	S	0	0	0
			3183	2048	549	578	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	167	Total	C	N	O	S	0	0	0
			1375	872	247	251	5			
3	F	168	Total	C	N	O	S	0	0	0
			1386	878	250	253	5			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total 2	Fe 2	0	0
4	B	2	Total 2	Fe 2	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	Ca 1	0	0
5	C	2	Total 2	Ca 2	0	0

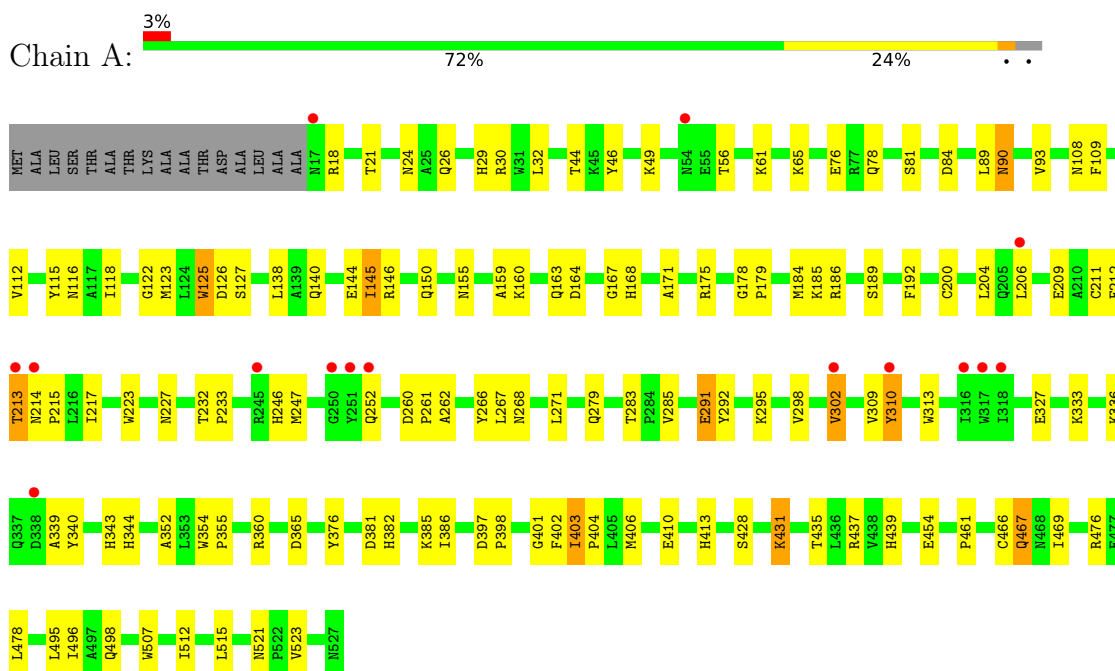
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	281	Total 281	O 281	0	0
6	B	263	Total 263	O 263	0	0
6	C	298	Total 298	O 298	0	0
6	D	171	Total 171	O 171	0	0
6	E	166	Total 166	O 166	0	0
6	F	49	Total 49	O 49	0	0

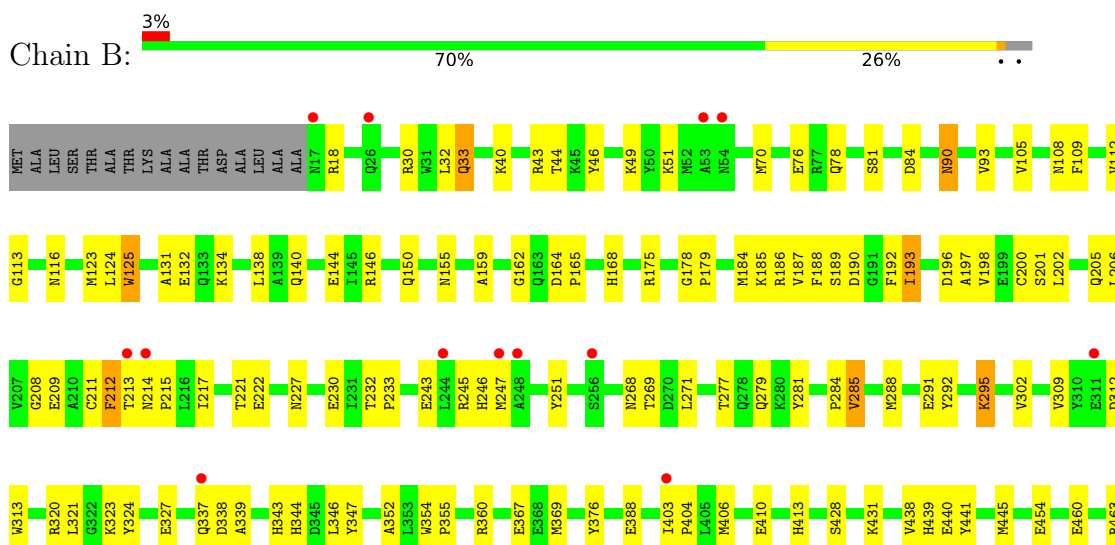
3 Residue-property plots [i](#)

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



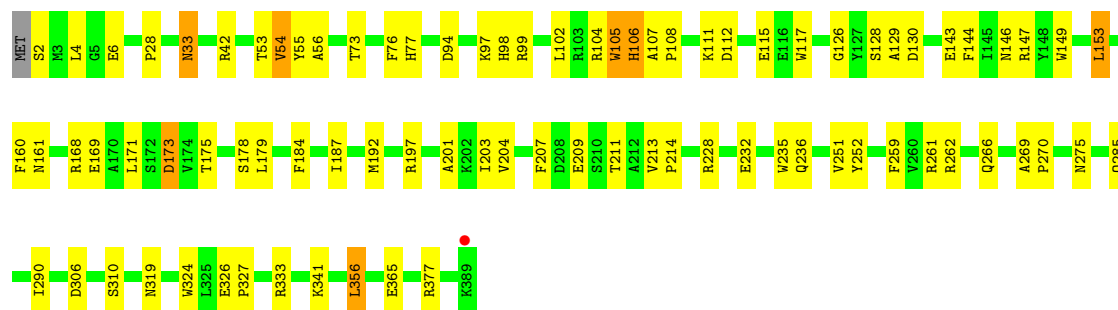
• Molecule 1: METHANE MONOOXYGENASE COMPONENT A, ALPHA CHAIN





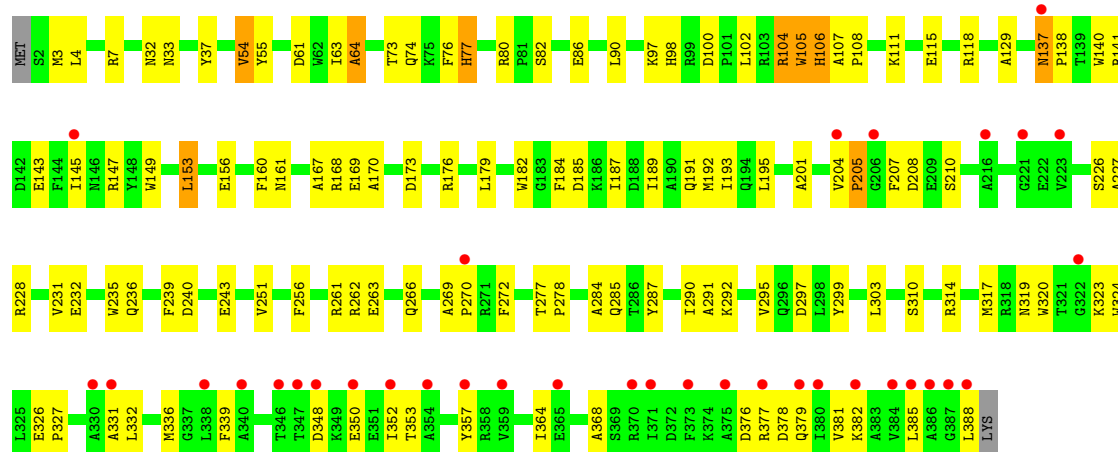
• Molecule 2: METHANE MONOOXYGENASE COMPONENT A, BETA CHAIN

Chain C: 78% 20%



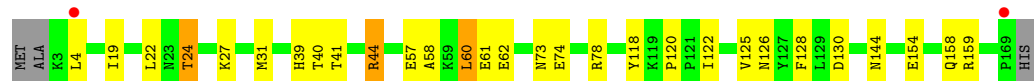
• Molecule 2: METHANE MONOOXYGENASE COMPONENT A, BETA CHAIN

Chain D: 9% 67% 30%



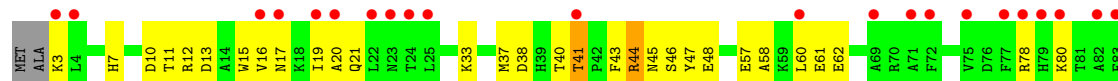
• Molecule 3: METHANE MONOOXYGENASE COMPONENT A, GAMMA CHAIN

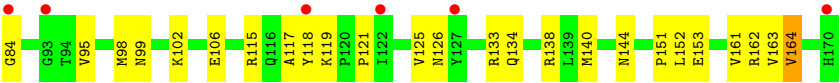
Chain E: 81% 15%



• Molecule 3: METHANE MONOOXYGENASE COMPONENT A, GAMMA CHAIN

Chain F: 16% 66% 31%





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.27Å 171.66Å 221.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.79 – 2.15 29.79 – 2.15	Depositor EDS
% Data completeness (in resolution range)	93.5 (29.79-2.15) 93.5 (29.79-2.15)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.04 (at 2.16Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.189 , 0.230 0.192 , 0.232	Depositor DCC
R_{free} test set	4903 reflections (3.38%)	wwPDB-VP
Wilson B-factor (Å ²)	26.5	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 49.0	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	0.95	EDS
Total number of atoms	18742	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.37% 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: FE2, CA

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	0.36	0/4310	0.90	19/5853 (0.3%)
1	B	0.37	0/4310	0.89	13/5853 (0.2%)
2	C	0.39	0/3289	0.88	15/4464 (0.3%)
2	D	0.34	0/3279	0.84	10/4453 (0.2%)
3	E	0.39	0/1404	0.88	6/1892 (0.3%)
3	F	0.33	0/1416	0.77	1/1907 (0.1%)
All	All	0.36	0/18008	0.87	64/24422 (0.3%)

There are no bond length outliers.

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	339	ALA	N-CA-C	9.52	121.42	111.14
1	A	309	VAL	N-CA-C	8.10	118.14	110.53
1	B	309	VAL	N-CA-C	7.41	117.49	110.53
3	E	122	ILE	N-CA-C	-7.33	104.06	110.74
1	B	93	VAL	N-CA-C	7.05	117.87	111.81
2	C	149	TRP	N-CA-C	-6.88	103.87	111.36
2	D	204	VAL	CA-C-N	6.87	128.43	119.84
2	D	204	VAL	C-N-CA	6.87	128.43	119.84
1	B	496	ILE	N-CA-C	-6.84	104.10	110.53
1	B	431	LYS	N-CA-C	-6.82	104.99	113.38
1	A	339	ALA	N-CA-C	6.67	118.64	111.36
2	D	105	TRP	N-CA-C	-6.67	100.35	109.95
2	C	105	TRP	N-CA-C	-6.64	100.14	110.17
1	B	193	ILE	N-CA-C	6.46	119.85	113.71
2	C	106	HIS	N-CA-C	6.43	118.82	111.11
1	A	164	ASP	CA-C-N	6.41	125.98	119.19
1	A	164	ASP	C-N-CA	6.41	125.98	119.19
1	B	285	VAL	N-CA-C	6.37	116.53	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	295	LYS	N-CA-C	-6.35	103.43	112.13
3	E	118	TYR	N-CA-C	6.31	121.75	113.30
1	A	285	VAL	N-CA-C	6.28	117.06	110.72
2	C	377	ARG	N-CA-C	6.26	118.10	111.28
2	C	236	GLN	N-CA-C	6.23	121.04	113.38
1	A	122	GLY	N-CA-C	-6.12	104.94	112.77
2	C	56	ALA	N-CA-C	-6.10	104.75	111.82
3	E	130	ASP	N-CA-C	-6.09	104.75	111.82
1	A	397	ASP	CA-C-N	5.96	125.84	119.28
1	A	397	ASP	C-N-CA	5.96	125.84	119.28
2	C	252	TYR	N-CA-C	5.95	117.45	110.97
1	A	496	ILE	N-CA-C	-5.94	104.95	110.53
1	B	178	GLY	CA-C-N	5.88	125.42	119.19
1	B	178	GLY	C-N-CA	5.88	125.42	119.19
3	E	73	ASN	N-CA-C	-5.87	102.96	110.53
3	F	118	TYR	N-CA-C	5.64	120.15	112.88
2	C	53	THR	N-CA-C	5.58	120.36	112.93
3	E	39	HIS	N-CA-C	5.56	121.94	113.61
1	A	145	ILE	N-CA-C	-5.52	105.15	110.72
1	A	178	GLY	CA-C-N	5.50	125.02	119.19
1	A	178	GLY	C-N-CA	5.50	125.02	119.19
2	C	171	LEU	N-CA-C	5.47	119.58	113.02
2	C	144	PHE	N-CA-C	5.46	118.40	111.69
1	A	478	LEU	N-CA-C	5.45	117.65	111.11
1	A	291	GLU	N-CA-C	5.44	117.29	111.36
2	D	54	VAL	N-CA-C	5.43	116.26	108.93
1	A	267	LEU	N-CA-C	5.37	117.57	111.02
2	D	104	ARG	N-CA-C	5.34	117.01	108.41
2	C	54	VAL	N-CA-C	5.33	116.57	109.37
3	E	74	GLU	N-CA-C	5.33	117.09	111.28
1	A	266	TYR	N-CA-C	5.33	121.19	114.31
1	A	431	LYS	N-CA-C	-5.32	106.64	113.23
2	D	236	GLN	N-CA-C	5.32	119.92	113.38
2	C	104	ARG	N-CA-C	5.26	116.82	108.67
2	C	169	GLU	N-CA-C	5.25	119.84	113.38
2	C	77	HIS	N-CA-C	-5.21	102.33	110.10
1	B	312	ASP	N-CA-C	5.21	116.64	110.97
2	D	137	ASN	CA-C-N	5.18	124.62	119.24
2	D	137	ASN	C-N-CA	5.18	124.62	119.24
2	D	77	HIS	N-CA-C	-5.17	102.39	110.10
2	C	275	ASN	N-CA-C	-5.16	107.04	113.38
1	B	205	GLN	N-CA-C	5.15	119.44	111.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	212	PHE	N-CA-C	5.14	119.17	112.13
2	D	106	HIS	N-CA-C	5.09	117.22	111.11
1	A	213	THR	N-CA-C	5.06	117.20	111.02
1	B	212	PHE	N-CA-C	5.01	118.63	111.02

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	4185	0	3981	107	0
1	B	4185	0	3981	137	0
2	C	3193	0	3042	65	0
2	D	3183	0	3029	94	0
3	E	1375	0	1370	18	0
3	F	1386	0	1377	50	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	1	0	0	0	0
5	C	2	0	0	0	0
6	A	281	0	0	5	0
6	B	263	0	0	7	0
6	C	298	0	0	9	0
6	D	171	0	0	3	0
6	E	166	0	0	0	0
6	F	49	0	0	1	0
All	All	18742	0	16780	416	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 12.

All (416) 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)
3:F:41:THR:HG23	3:F:43:PHE:H	1.27	0.99
1:A:44:THR:HG22	1:A:46:TYR:H	1.32	0.95
1:B:78:GLN:HE22	1:B:150:GLN:HE21	1.02	0.94
1:A:352:ALA:HA	1:A:404:PRO:HB2	1.50	0.93
1:A:78:GLN:HE22	1:A:150:GLN:HE21	1.01	0.91
1:A:435:THR:HG21	1:A:437:ARG:HE	1.36	0.91
1:B:268:ASN:HD21	1:B:327:GLU:H	1.20	0.90
3:F:80:LYS:HE2	3:F:84:GLY:HA2	1.51	0.90
1:A:467:GLN:HG3	6:A:5252:HOH:O	1.69	0.90
1:A:435:THR:CG2	1:A:437:ARG:HE	1.88	0.86
2:C:261:ARG:HE	2:C:285:GLN:HE22	1.21	0.85
1:A:209:GLU:HA	1:A:213:THR:HB	1.59	0.84
3:E:19:ILE:HG12	3:E:60:LEU:HD13	1.59	0.84
1:A:109:PHE:HB3	1:A:184:MET:HE3	1.61	0.82
1:B:288:MET:HE1	1:B:346:LEU:HG	1.59	0.82
3:F:41:THR:O	3:F:44:ARG:HD2	1.80	0.82
1:B:352:ALA:HA	1:B:404:PRO:HB2	1.59	0.81
1:B:123:MET:HE3	1:B:197:ALA:HA	1.63	0.80
1:B:406:MET:O	1:B:410:GLU:HG3	1.81	0.80
1:A:268:ASN:HD21	1:A:327:GLU:H	1.31	0.79
1:B:44:THR:HG22	1:B:46:TYR:H	1.47	0.79
1:B:188:PHE:HZ	1:B:213:THR:HG22	1.48	0.79
1:A:108:ASN:HD21	1:A:175:ARG:HH11	1.29	0.78
1:B:288:MET:HE1	1:B:346:LEU:CG	2.14	0.77
1:A:155:ASN:HD22	1:A:168:HIS:HD2	1.33	0.77
1:B:208:GLY:O	1:B:213:THR:HG23	1.85	0.76
1:A:406:MET:O	1:A:410:GLU:HG3	1.86	0.76
1:A:78:GLN:NE2	1:A:150:GLN:HE21	1.81	0.75
1:B:209:GLU:HA	1:B:213:THR:OG1	1.87	0.75
3:F:40:THR:O	3:F:41:THR:HG22	1.89	0.72
2:D:319:ASN:OD1	3:F:78:ARG:HD3	1.88	0.72
1:B:78:GLN:NE2	1:B:150:GLN:HE21	1.83	0.72
3:F:13:ASP:O	3:F:16:VAL:HG22	1.90	0.72
2:D:102:LEU:CD1	2:D:290:ILE:HG23	2.20	0.72
2:D:167:ALA:O	2:D:176:ARG:NH1	2.23	0.72
1:A:302:VAL:HG13	1:A:376:TYR:HE2	1.56	0.71
2:C:146:ASN:HD21	2:C:197:ARG:HH21	1.36	0.71
1:B:108:ASN:HD21	1:B:175:ARG:HH11	1.37	0.71
1:A:78:GLN:HE22	1:A:150:GLN:NE2	1.82	0.71
1:B:33:GLN:HE22	1:B:132:GLU:H	1.40	0.70
2:D:352:ILE:HD11	2:D:388:LEU:HD11	1.74	0.70
3:F:3:LYS:HG3	3:F:10:ASP:OD2	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:ARG:O	2:D:129:ALA:HA	1.92	0.69
1:B:33:GLN:HE21	1:B:33:GLN:HA	1.56	0.69
2:D:102:LEU:HD13	2:D:290:ILE:HG23	1.75	0.69
3:E:41:THR:O	3:E:44:ARG:HD2	1.92	0.68
1:B:489:ARG:HD2	1:B:495:LEU:O	1.93	0.68
2:D:228:ARG:O	2:D:232:GLU:HG3	1.93	0.68
2:D:326:GLU:HB3	2:D:327:PRO:HD3	1.76	0.67
2:C:42:ARG:HB2	2:C:99:ARG:HH11	1.59	0.67
1:B:30:ARG:O	1:B:30:ARG:HD3	1.95	0.67
3:F:58:ALA:O	3:F:62:GLU:HG3	1.95	0.67
1:B:288:MET:HE2	1:B:347:TYR:N	2.09	0.66
3:F:57:GLU:O	3:F:61:GLU:HG3	1.95	0.66
1:B:179:PRO:HB3	1:B:469:ILE:HD13	1.77	0.66
2:C:326:GLU:HB3	2:C:327:PRO:HD3	1.76	0.66
2:C:102:LEU:CD1	2:C:290:ILE:HG23	2.26	0.66
2:C:76:PHE:HZ	2:C:168:ARG:HH12	1.42	0.65
2:D:261:ARG:HE	2:D:285:GLN:HE22	1.44	0.65
2:D:201:ALA:HA	2:D:207:PHE:HB3	1.77	0.65
1:B:184:MET:HE2	1:B:188:PHE:HB2	1.78	0.65
1:B:369:MET:HE1	1:B:388:GLU:OE2	1.96	0.65
2:C:97:LYS:HD2	6:C:5058:HOH:O	1.97	0.65
2:D:153:LEU:C	2:D:153:LEU:HD12	2.22	0.65
2:D:111:LYS:O	2:D:115:GLU:HG3	1.96	0.64
3:E:24:THR:HG22	3:E:27:LYS:H	1.63	0.64
1:A:268:ASN:ND2	1:A:327:GLU:H	1.95	0.64
3:F:15:TRP:O	3:F:19:ILE:HG23	1.97	0.64
1:A:476:ARG:HD3	3:E:4:LEU:HG	1.79	0.64
1:B:227:ASN:HD21	1:B:295:LYS:H	1.44	0.64
3:F:153:GLU:H	3:F:153:GLU:CD	2.05	0.63
1:A:381:ASP:HA	1:A:385:LYS:HE2	1.80	0.63
2:D:100:ASP:OD1	2:D:104:ARG:HD3	1.99	0.63
2:D:187:ILE:O	2:D:191:GLN:HG3	1.98	0.63
2:C:333:ARG:HD3	6:C:5162:HOH:O	1.98	0.62
1:B:439:HIS:HD2	3:F:163:VAL:HA	1.64	0.62
2:D:76:PHE:HZ	2:D:168:ARG:HH12	1.48	0.62
1:A:302:VAL:HG13	1:A:376:TYR:CE2	2.34	0.62
1:B:268:ASN:ND2	1:B:327:GLU:H	1.95	0.62
1:B:70:MET:HE1	1:B:245:ARG:NH1	2.14	0.62
2:D:357:TYR:CE1	2:D:381:VAL:HG11	2.35	0.62
1:B:367:GLU:HG3	6:B:5014:HOH:O	2.00	0.62
1:B:247:MET:HE2	1:B:247:MET:HA	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:TYR:OH	1:B:344:HIS:HD2	1.83	0.62
2:C:270:PRO:HB3	2:D:270:PRO:HB3	1.81	0.62
1:B:44:THR:HG21	6:B:5215:HOH:O	2.00	0.62
2:C:365:GLU:HG3	6:C:5182:HOH:O	2.00	0.61
1:B:214:ASN:HD21	1:B:247:MET:HE3	1.64	0.61
2:C:333:ARG:HD2	6:C:5161:HOH:O	2.00	0.61
1:A:108:ASN:ND2	1:A:175:ARG:HH11	1.98	0.61
1:B:302:VAL:HG13	1:B:376:TYR:HE2	1.66	0.61
2:C:107:ALA:HB3	2:C:108:PRO:HD3	1.83	0.60
1:A:292:TYR:OH	1:A:344:HIS:HD2	1.82	0.60
2:D:90:LEU:HD13	2:D:303:LEU:HD13	1.83	0.60
1:B:369:MET:HE2	6:B:5158:HOH:O	2.02	0.60
1:B:526:PHE:O	1:B:527:ASN:HB2	2.02	0.60
2:C:6:GLU:HG3	6:C:5133:HOH:O	2.02	0.59
1:B:123:MET:HE1	1:B:200:CYS:SG	2.42	0.59
2:D:145:ILE:O	2:D:149:TRP:HB3	2.02	0.59
3:E:22:LEU:HD11	3:E:31:MET:SD	2.42	0.59
3:F:41:THR:HG23	3:F:43:PHE:N	2.10	0.59
1:B:439:HIS:HE1	1:B:454:GLU:OE1	1.85	0.59
2:D:208:ASP:OD2	2:D:210:SER:HB3	2.02	0.59
2:C:261:ARG:HE	2:C:285:GLN:NE2	1.96	0.59
1:A:125:TRP:HE1	2:C:161:ASN:ND2	2.01	0.59
2:C:269:ALA:HB3	2:C:270:PRO:HD3	1.84	0.59
1:A:185:LYS:O	1:A:189:SER:HB2	2.02	0.58
1:B:288:MET:HE1	1:B:346:LEU:CB	2.33	0.58
1:A:279:GLN:HG2	1:A:283:THR:OG1	2.03	0.58
2:C:146:ASN:ND2	2:C:197:ARG:HH21	2.01	0.58
1:A:44:THR:OG1	1:A:127:SER:HA	2.04	0.58
1:A:204:LEU:O	1:A:209:GLU:HG3	2.03	0.57
2:C:211:THR:O	2:C:214:PRO:HD2	2.04	0.57
1:B:214:ASN:HB2	1:B:215:PRO:HD3	1.85	0.57
1:A:56:THR:HG23	1:A:252:GLN:HE21	1.70	0.57
1:A:227:ASN:HD21	1:A:295:LYS:H	1.52	0.57
2:D:61:ASP:OD1	3:F:7:HIS:HD2	1.87	0.57
1:A:140:GLN:O	1:A:144:GLU:HG2	2.04	0.57
1:A:333:LYS:HG2	6:A:5248:HOH:O	2.05	0.57
2:D:378:ASP:O	2:D:382:LYS:HG3	2.04	0.57
1:B:33:GLN:NE2	1:B:132:GLU:H	2.02	0.56
2:D:352:ILE:CD1	2:D:388:LEU:HD11	2.33	0.56
1:A:521:ASN:OD1	1:A:523:VAL:HG12	2.06	0.56
1:B:439:HIS:HB3	3:F:161:VAL:HG21	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:ILE:HD13	1:A:515:LEU:HD11	1.87	0.56
1:B:245:ARG:HG3	1:B:245:ARG:HH11	1.71	0.56
2:D:256:PHE:HA	2:D:332:LEU:HD21	1.87	0.56
2:C:94:ASP:HB3	2:C:97:LYS:HG3	1.88	0.56
1:A:403:ILE:HD13	1:A:515:LEU:CD1	2.36	0.56
3:F:19:ILE:HD12	3:F:19:ILE:C	2.31	0.55
1:B:188:PHE:CZ	1:B:213:THR:HG22	2.36	0.55
1:A:125:TRP:HE1	2:C:161:ASN:HD22	1.54	0.55
1:B:186:ARG:HD3	1:B:186:ARG:C	2.32	0.55
2:C:211:THR:C	2:C:214:PRO:HD2	2.32	0.55
1:A:495:LEU:HD11	1:A:512:ILE:HG13	1.88	0.54
1:B:108:ASN:HD21	1:B:175:ARG:HD3	1.72	0.54
1:A:108:ASN:HD21	1:A:175:ARG:HD3	1.72	0.54
1:A:109:PHE:O	1:A:112:VAL:HG12	2.07	0.54
1:B:193:ILE:HD11	2:D:82:SER:HB3	1.90	0.54
1:B:439:HIS:HB3	3:F:161:VAL:CG2	2.37	0.54
2:C:112:ASP:OD1	2:D:118:ARG:NH2	2.41	0.54
2:D:105:TRP:O	2:D:108:PRO:HD2	2.07	0.54
3:F:80:LYS:CE	3:F:84:GLY:HA2	2.31	0.54
1:B:213:THR:O	1:B:217:ILE:HG12	2.07	0.54
2:D:107:ALA:HB3	2:D:108:PRO:HD3	1.89	0.54
1:A:495:LEU:HD11	1:A:512:ILE:CG1	2.38	0.54
1:B:32:LEU:C	1:B:32:LEU:HD23	2.33	0.54
1:A:76:GLU:HG2	1:B:76:GLU:OE2	2.08	0.54
1:A:439:HIS:HE1	1:A:454:GLU:OE1	1.90	0.54
3:F:44:ARG:HD3	3:F:47:TYR:CZ	2.43	0.54
2:D:82:SER:O	2:D:168:ARG:NH2	2.40	0.54
1:A:214:ASN:HB2	1:A:215:PRO:HD3	1.90	0.54
1:A:344:HIS:HE1	1:A:376:TYR:CD2	2.26	0.53
1:A:213:THR:O	1:A:217:ILE:HG12	2.08	0.53
1:A:360:ARG:HG2	1:A:498:GLN:HB2	1.90	0.53
2:D:324:TRP:O	2:D:327:PRO:HD2	2.09	0.53
3:E:4:LEU:HG	3:E:4:LEU:O	2.09	0.53
1:A:160:LYS:HD2	6:A:5238:HOH:O	2.08	0.53
1:B:144:GLU:OE2	1:B:144:GLU:HA	2.09	0.53
1:B:291:GLU:OE1	1:B:343:HIS:HE1	1.90	0.53
3:F:151:PRO:HB2	3:F:153:GLU:OE1	2.08	0.53
6:C:5117:HOH:O	3:E:125:VAL:HG22	2.08	0.53
2:D:323:LYS:HB2	3:F:78:ARG:HH11	1.74	0.53
1:B:403:ILE:HG22	1:B:406:MET:SD	2.49	0.53
2:D:324:TRP:C	2:D:327:PRO:HD2	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:381:VAL:O	2:D:385:LEU:HB2	2.08	0.53
1:B:140:GLN:HG3	1:B:246:HIS:CE1	2.44	0.52
1:B:186:ARG:HD3	1:B:186:ARG:O	2.09	0.52
2:C:42:ARG:HB2	2:C:99:ARG:NH1	2.24	0.52
1:B:269:THR:HG23	6:B:5097:HOH:O	2.09	0.52
1:B:302:VAL:HG13	1:B:376:TYR:CE2	2.45	0.52
1:A:179:PRO:HB3	1:A:469:ILE:HD13	1.91	0.52
2:C:98:HIS:HE1	2:C:178:SER:OG	1.92	0.52
1:B:78:GLN:HE22	1:B:150:GLN:NE2	1.86	0.52
1:B:281:TYR:CZ	1:B:285:VAL:HG21	2.44	0.52
2:C:175:THR:O	2:C:179:LEU:HD13	2.10	0.52
2:D:310:SER:O	2:D:314:ARG:HG3	2.09	0.52
2:D:352:ILE:HG13	2:D:353:THR:N	2.24	0.52
2:C:2:SER:HB2	6:C:5232:HOH:O	2.09	0.52
2:D:277:THR:HB	2:D:278:PRO:HD3	1.92	0.52
1:B:108:ASN:ND2	1:B:175:ARG:HH11	2.04	0.51
1:B:288:MET:CE	1:B:346:LEU:HB3	2.40	0.51
2:D:161:ASN:HB3	2:D:235:TRP:CE2	2.45	0.51
3:E:41:THR:O	3:E:44:ARG:CD	2.56	0.51
3:E:57:GLU:O	3:E:61:GLU:HG3	2.10	0.51
1:B:212:PHE:O	1:B:215:PRO:HD2	2.11	0.51
1:B:51:LYS:HG3	6:B:5190:HOH:O	2.10	0.51
1:B:344:HIS:HE1	1:B:376:TYR:CD2	2.29	0.51
1:A:21:THR:HG22	2:C:128:SER:CB	2.41	0.51
1:B:495:LEU:HD11	1:B:512:ILE:CG1	2.41	0.51
2:C:201:ALA:HA	2:C:207:PHE:HB3	1.92	0.51
2:C:235:TRP:CD1	2:C:235:TRP:C	2.89	0.51
1:B:490:SER:OG	2:D:32:ASN:HB2	2.11	0.50
1:B:211:CYS:HB2	1:B:313:TRP:CD1	2.46	0.50
1:A:18:ARG:O	2:C:129:ALA:HA	2.12	0.50
1:B:164:ASP:CG	1:B:489:ARG:HH22	2.19	0.50
1:B:466:CYS:HB2	2:D:73:THR:HA	1.94	0.50
1:B:222:GLU:OE1	2:D:7:ARG:HD3	2.12	0.50
3:F:61:GLU:HB3	3:F:121:PRO:HD3	1.94	0.50
1:A:81:SER:OG	1:B:84:ASP:HB3	2.11	0.50
1:A:84:ASP:HB3	1:B:81:SER:OG	2.11	0.50
1:B:192:PHE:O	1:B:200:CYS:HB3	2.11	0.50
1:A:109:PHE:HD2	1:A:184:MET:CE	2.25	0.50
1:A:206:LEU:HD23	1:A:271:LEU:HD13	1.93	0.50
2:D:54:VAL:O	2:D:55:TYR:HB2	2.12	0.50
2:D:102:LEU:HB2	2:D:104:ARG:HD2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:454:GLU:OE2	3:F:152:LEU:HD13	2.12	0.50
2:D:377:ARG:O	2:D:381:VAL:HG23	2.11	0.50
1:A:160:LYS:HA	2:C:33:ASN:HB2	1.94	0.50
2:C:111:LYS:O	2:C:115:GLU:HG3	2.11	0.49
1:B:164:ASP:OD1	1:B:489:ARG:NH2	2.45	0.49
2:C:153:LEU:C	2:C:153:LEU:HD12	2.37	0.49
2:C:102:LEU:HD12	2:C:290:ILE:HG23	1.94	0.49
2:C:192:MET:HE2	2:C:192:MET:HA	1.94	0.49
2:C:203:ILE:HG13	2:C:204:VAL:HG23	1.94	0.49
1:B:43:ARG:HD2	1:B:43:ARG:C	2.37	0.49
2:D:364:ILE:HA	2:D:368:ALA:HB3	1.95	0.49
1:B:438:VAL:HB	3:F:164:VAL:HG22	1.93	0.49
2:C:54:VAL:O	2:C:55:TYR:HB2	2.13	0.49
2:D:261:ARG:HE	2:D:285:GLN:NE2	2.09	0.49
1:A:186:ARG:HA	2:C:73:THR:OG1	2.13	0.49
1:B:251:TYR:HE2	1:B:320:ARG:HH12	1.61	0.49
2:C:213:VAL:HB	2:C:214:PRO:HD3	1.95	0.49
1:A:401:GLY:HA2	1:A:515:LEU:CD2	2.43	0.49
1:B:320:ARG:HH11	1:B:320:ARG:HB3	1.78	0.49
1:B:162:GLY:HA3	6:B:5119:HOH:O	2.13	0.48
1:B:49:LYS:CE	3:F:144:ASN:HD22	2.26	0.48
1:B:413:HIS:HD2	1:B:428:SER:OG	1.96	0.48
2:D:156:GLU:HA	2:D:156:GLU:OE2	2.12	0.48
2:D:226:SER:HB2	2:D:331:ALA:HA	1.95	0.48
1:A:109:PHE:CB	1:A:184:MET:HE3	2.39	0.48
1:A:163:GLN:O	2:C:28:PRO:HA	2.14	0.48
1:B:138:LEU:HD22	2:D:160:PHE:CZ	2.48	0.48
1:A:123:MET:HB2	2:C:168:ARG:HD3	1.94	0.48
1:B:526:PHE:O	1:B:527:ASN:CB	2.61	0.48
2:C:126:GLY:O	2:C:130:ASP:HB2	2.13	0.48
1:A:56:THR:CG2	1:A:252:GLN:HE21	2.26	0.48
1:A:138:LEU:HD22	2:C:160:PHE:CZ	2.48	0.48
1:A:115:TYR:OH	2:C:173:ASP:HA	2.14	0.48
1:B:185:LYS:O	1:B:189:SER:HB2	2.14	0.48
1:A:227:ASN:ND2	1:A:295:LYS:H	2.12	0.48
1:A:146:ARG:HB2	2:C:106:HIS:CE1	2.49	0.47
2:C:319:ASN:OD1	3:E:78:ARG:HD3	2.14	0.47
2:D:269:ALA:HB3	2:D:270:PRO:HD3	1.96	0.47
2:D:169:GLU:O	2:D:170:ALA:C	2.56	0.47
3:E:154:GLU:O	3:E:158:GLN:HG3	2.12	0.47
3:F:38:ASP:HA	3:F:45:ASN:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:LYS:HD3	3:E:144:ASN:HD22	1.80	0.47
3:F:19:ILE:HD12	3:F:20:ALA:N	2.29	0.47
1:B:232:THR:HB	1:B:233:PRO:HD3	1.96	0.47
2:C:143:GLU:O	2:C:147:ARG:HB3	2.14	0.47
2:C:161:ASN:HB3	2:C:235:TRP:CE2	2.49	0.47
2:D:192:MET:HA	2:D:192:MET:HE2	1.97	0.47
1:B:30:ARG:HD3	1:B:30:ARG:C	2.40	0.47
1:B:146:ARG:HB2	2:D:106:HIS:CE1	2.50	0.47
1:B:198:VAL:O	1:B:202:LEU:HG	2.14	0.47
1:B:440:GLU:OE1	3:F:162:ARG:HD3	2.15	0.47
2:C:228:ARG:O	2:C:232:GLU:HG3	2.15	0.47
2:D:143:GLU:O	2:D:147:ARG:HB3	2.15	0.47
2:D:184:PHE:O	2:D:187:ILE:HG22	2.15	0.47
3:F:33:LYS:O	3:F:37:MET:HG2	2.13	0.47
1:A:26:GLN:HG2	6:A:5123:HOH:O	2.15	0.47
1:A:232:THR:HB	1:A:233:PRO:HD3	1.96	0.47
1:B:32:LEU:HD23	1:B:32:LEU:O	2.15	0.47
1:B:460:GLU:OE1	1:B:463:ARG:HD3	2.15	0.47
2:C:341:LYS:HE3	6:C:5159:HOH:O	2.14	0.47
2:D:77:HIS:CD2	3:F:140:MET:HG2	2.50	0.47
2:D:348:ASP:OD2	2:D:350:GLU:HB2	2.14	0.46
3:E:58:ALA:O	3:E:62:GLU:HG3	2.15	0.46
3:F:133:ARG:NH1	3:F:134:GLN:HG3	2.30	0.46
1:B:159:ALA:O	2:D:33:ASN:HB2	2.15	0.46
1:B:206:LEU:HD23	1:B:271:LEU:HD13	1.97	0.46
1:B:208:GLY:C	1:B:213:THR:HG23	2.39	0.46
2:C:261:ARG:NE	2:C:285:GLN:HE22	2.02	0.46
2:D:140:TRP:HB2	2:D:272:PHE:CD2	2.51	0.46
1:A:354:TRP:CG	1:A:355:PRO:HD3	2.51	0.46
1:B:186:ARG:HA	2:D:73:THR:OG1	2.15	0.46
2:C:105:TRP:O	2:C:108:PRO:HD2	2.15	0.46
2:D:235:TRP:CD1	2:D:235:TRP:C	2.93	0.46
3:E:120:PRO:HD3	3:E:128:PHE:CG	2.51	0.46
1:B:360:ARG:HG2	1:B:498:GLN:HB2	1.98	0.46
2:D:137:ASN:HB3	2:D:272:PHE:HB3	1.98	0.46
1:B:196:ASP:HB2	3:F:140:MET:SD	2.56	0.46
2:D:353:THR:O	2:D:357:TYR:HD1	1.99	0.46
3:F:16:VAL:O	3:F:19:ILE:HG13	2.16	0.46
3:E:4:LEU:O	3:E:4:LEU:CG	2.63	0.46
1:A:186:ARG:HD3	1:A:186:ARG:C	2.40	0.45
3:F:12:ARG:O	3:F:16:VAL:HG13	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:ASP:OD2	1:A:365:ASP:C	2.59	0.45
1:B:337:GLN:HG3	1:B:338:ASP:N	2.32	0.45
1:A:352:ALA:CA	1:A:404:PRO:HB2	2.33	0.45
1:A:402:PHE:O	1:A:403:ILE:HD12	2.16	0.45
2:C:209:GLU:HG2	6:C:5044:HOH:O	2.15	0.45
1:A:439:HIS:CE1	1:A:454:GLU:OE1	2.70	0.45
1:B:354:TRP:CG	1:B:355:PRO:HD3	2.52	0.45
1:B:288:MET:HE1	1:B:346:LEU:HB3	1.98	0.45
1:B:495:LEU:HD11	1:B:512:ILE:HG13	1.97	0.45
2:D:77:HIS:CG	3:F:140:MET:HG2	2.52	0.45
2:D:97:LYS:NZ	6:D:534:HOH:O	2.48	0.45
1:A:89:LEU:HD21	1:B:230:GLU:HG3	1.99	0.45
1:A:382:HIS:O	1:A:386:ILE:HG13	2.17	0.45
1:B:445:MET:HE3	1:B:523:VAL:HG22	1.98	0.45
1:B:320:ARG:NH1	1:B:320:ARG:CB	2.80	0.44
1:B:441:TYR:HB2	3:F:161:VAL:HG23	1.99	0.44
2:D:189:ILE:HD12	2:D:284:ALA:HB2	1.98	0.44
3:F:98:MET:HG3	3:F:138:ARG:HG2	1.98	0.44
2:C:259:PHE:CE1	2:C:356:LEU:HD13	2.52	0.44
2:D:243:GLU:HB2	2:D:320:TRP:CZ2	2.52	0.44
2:D:299:TYR:O	2:D:317:MET:HE1	2.18	0.44
1:A:223:TRP:CE2	1:A:298:VAL:HB	2.52	0.44
1:B:344:HIS:HE1	1:B:376:TYR:CE2	2.35	0.44
1:B:125:TRP:CD1	1:B:125:TRP:C	2.95	0.44
1:A:413:HIS:HD2	1:A:428:SER:OG	2.00	0.44
1:A:461:PRO:HG2	3:E:159:ARG:CZ	2.47	0.44
3:E:40:THR:C	3:E:41:THR:HG23	2.42	0.44
1:B:125:TRP:HE1	2:D:161:ASN:ND2	2.15	0.44
1:B:186:ARG:CZ	1:B:277:THR:HG23	2.48	0.44
1:B:354:TRP:CH2	1:B:499:PRO:HD3	2.52	0.44
2:C:4:LEU:HD23	6:D:454:HOH:O	2.17	0.44
2:D:239:PHE:HB2	3:F:126:ASN:HA	1.99	0.44
1:A:44:THR:HG23	1:A:126:ASP:OD1	2.18	0.44
1:A:24:ASN:OD1	1:A:26:GLN:HG2	2.18	0.44
1:B:155:ASN:OD1	1:B:168:HIS:HD2	2.01	0.44
3:F:46:SER:OG	3:F:48:GLU:HG2	2.18	0.44
1:A:398:PRO:HG3	1:A:507:TRP:CD1	2.53	0.44
1:A:466:CYS:HB2	2:C:73:THR:HA	1.98	0.44
1:B:323:LYS:HE2	1:B:324:TYR:CZ	2.52	0.44
1:A:144:GLU:HA	1:A:144:GLU:OE2	2.18	0.43
1:B:140:GLN:O	1:B:144:GLU:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:VAL:O	1:B:109:PHE:HB2	2.18	0.43
1:B:184:MET:CE	1:B:188:PHE:HB2	2.47	0.43
1:B:288:MET:HE2	1:B:347:TYR:CA	2.48	0.43
2:D:138:PRO:HA	2:D:141:ARG:NH1	2.33	0.43
2:D:263:GLU:OE2	2:D:263:GLU:HA	2.19	0.43
3:F:61:GLU:O	3:F:121:PRO:HG2	2.17	0.43
1:A:260:ASP:OD2	1:A:262:ALA:HB3	2.18	0.43
2:C:306:ASP:O	2:C:310:SER:HB2	2.17	0.43
1:B:33:GLN:HA	1:B:131:ALA:HB3	2.00	0.43
1:A:146:ARG:HG2	1:A:150:GLN:OE1	2.19	0.43
1:B:33:GLN:HA	1:B:33:GLN:NE2	2.27	0.43
2:D:377:ARG:HG3	2:D:377:ARG:HH11	1.82	0.43
3:F:17:ASN:O	3:F:21:GLN:HG2	2.19	0.43
1:A:211:CYS:HB2	1:A:313:TRP:CD1	2.54	0.43
1:A:302:VAL:HG11	1:A:340:TYR:CE1	2.54	0.43
1:A:76:GLU:HG2	1:B:76:GLU:HG2	2.01	0.43
1:B:165:PRO:HG3	6:B:5118:HOH:O	2.19	0.43
2:C:262:ARG:HA	2:C:266:GLN:HB3	2.01	0.43
2:D:227:ALA:O	2:D:231:VAL:HG23	2.18	0.43
3:F:33:LYS:HE3	3:F:117:ALA:HA	2.00	0.43
1:B:109:PHE:O	1:B:112:VAL:HG12	2.19	0.43
1:B:243:GLU:C	1:B:245:ARG:H	2.26	0.43
1:B:230:GLU:C	1:B:233:PRO:HD2	2.44	0.43
2:C:269:ALA:N	2:C:270:PRO:CD	2.82	0.43
1:A:65:LYS:HB3	2:C:117:TRP:CG	2.54	0.42
1:B:320:ARG:HH11	1:B:320:ARG:CB	2.32	0.42
3:F:41:THR:O	3:F:44:ARG:CD	2.60	0.42
1:B:116:ASN:CG	1:B:189:SER:HA	2.44	0.42
1:B:184:MET:HE3	1:B:187:VAL:HG23	2.02	0.42
1:B:323:LYS:HE2	1:B:324:TYR:CE1	2.54	0.42
2:D:357:TYR:CZ	2:D:381:VAL:HG21	2.54	0.42
3:E:125:VAL:HG23	3:E:126:ASN:N	2.34	0.42
1:A:32:LEU:C	1:A:32:LEU:HD23	2.44	0.42
2:C:102:LEU:HD13	2:C:290:ILE:HG23	2.02	0.42
3:F:125:VAL:HG22	6:F:1064:HOH:O	2.19	0.42
1:B:217:ILE:O	1:B:221:THR:HG23	2.19	0.42
2:D:240:ASP:HB2	3:F:125:VAL:CG2	2.49	0.42
1:A:159:ALA:O	2:C:33:ASN:HB2	2.19	0.42
1:B:190:ASP:HB3	2:D:74:GLN:O	2.20	0.42
2:C:33:ASN:N	2:C:33:ASN:HD22	2.16	0.42
2:D:323:LYS:HB2	3:F:78:ARG:NH1	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:63:ILE:O	2:D:64:ALA:C	2.61	0.42
1:A:118:ILE:HD13	1:A:145:ILE:HG12	2.01	0.42
1:A:214:ASN:ND2	1:A:247:MET:SD	2.93	0.42
1:B:206:LEU:HD11	1:B:321:LEU:CD1	2.50	0.42
2:D:195:LEU:C	2:D:195:LEU:HD23	2.45	0.42
1:A:382:HIS:CD2	1:A:431:LYS:HG3	2.55	0.41
3:F:19:ILE:HG22	3:F:60:LEU:HD13	2.02	0.41
1:A:116:ASN:CG	1:A:189:SER:HA	2.46	0.41
2:D:98:HIS:HD2	2:D:297:ASP:OD1	2.03	0.41
1:B:113:GLY:HA3	1:B:188:PHE:CD2	2.55	0.41
1:A:192:PHE:O	1:A:200:CYS:HB3	2.20	0.41
2:C:324:TRP:C	2:C:327:PRO:HD2	2.45	0.41
2:D:291:ALA:O	2:D:295:VAL:HG23	2.21	0.41
1:A:291:GLU:OE1	1:A:343:HIS:HE1	2.03	0.41
1:B:134:LYS:HD3	2:D:161:ASN:HD21	1.85	0.41
1:B:288:MET:CE	1:B:347:TYR:N	2.82	0.41
2:C:184:PHE:O	2:C:187:ILE:HG22	2.21	0.41
1:A:125:TRP:CD1	1:A:125:TRP:C	2.99	0.41
1:A:140:GLN:HG3	1:A:246:HIS:CE1	2.55	0.41
1:B:90:ASN:HD22	1:B:90:ASN:HA	1.64	0.41
1:B:124:LEU:HD21	1:B:201:SER:HB2	2.03	0.41
1:B:243:GLU:C	1:B:245:ARG:N	2.78	0.41
2:D:37:TYR:CD1	2:D:37:TYR:C	2.99	0.41
2:D:176:ARG:HH11	2:D:176:ARG:HG3	1.86	0.41
2:D:336:MET:O	2:D:339:PHE:HD1	2.04	0.41
2:D:376:ASP:OD2	2:D:379:GLN:HG2	2.21	0.41
1:A:90:ASN:HD22	1:A:90:ASN:HA	1.60	0.41
1:A:109:PHE:HD2	1:A:184:MET:HE2	1.85	0.41
1:A:382:HIS:CB	1:A:431:LYS:HD2	2.51	0.41
2:D:179:LEU:HD23	2:D:182:TRP:CE3	2.56	0.41
2:D:185:ASP:O	2:D:189:ILE:HG12	2.21	0.40
3:F:95:VAL:HG12	3:F:99:ASN:ND2	2.35	0.40
3:F:102:LYS:HG2	3:F:106:GLU:OE1	2.20	0.40
1:A:44:THR:HG21	6:A:5166:HOH:O	2.21	0.40
1:A:167:GLY:O	1:A:171:ALA:HB2	2.21	0.40
1:B:184:MET:HE2	1:B:188:PHE:CB	2.48	0.40
2:D:262:ARG:O	2:D:266:GLN:HB3	2.21	0.40
1:A:29:HIS:CD2	1:A:61:LYS:HA	2.56	0.40
1:A:260:ASP:OD1	1:A:261:PRO:HD2	2.21	0.40
1:A:310:TYR:CE1	1:A:336:LYS:HD2	2.56	0.40
2:D:189:ILE:HD11	2:D:287:TYR:CD1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:VAL:HG11	2:D:3:MET:HG2	2.03	0.40
2:D:86:GLU:HG2	6:D:449:HOH:O	2.21	0.40
2:D:153:LEU:HA	2:D:193:ILE:HD12	2.04	0.40
2:D:189:ILE:HD11	2:D:284:ALA:HA	2.03	0.40
3:F:115:ARG:O	3:F:119:LYS:HB2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	509/527 (97%)	487 (96%)	22 (4%)	0	100	100
1	B	509/527 (97%)	483 (95%)	24 (5%)	2 (0%)	30	26
2	C	386/389 (99%)	377 (98%)	8 (2%)	1 (0%)	36	34
2	D	385/389 (99%)	368 (96%)	14 (4%)	3 (1%)	16	10
3	E	165/170 (97%)	163 (99%)	2 (1%)	0	100	100
3	F	166/170 (98%)	161 (97%)	5 (3%)	0	100	100
All	All	2120/2172 (98%)	2039 (96%)	75 (4%)	6 (0%)	36	34

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	40	LYS
2	D	64	ALA
2	D	205	PRO
2	D	251	VAL
1	B	284	PRO
2	C	251	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	433/442 (98%)	426 (98%)	7 (2%)	55	61
1	B	433/442 (98%)	429 (99%)	4 (1%)	70	77
2	C	322/323 (100%)	318 (99%)	4 (1%)	63	70
2	D	321/323 (99%)	315 (98%)	6 (2%)	50	56
3	E	145/147 (99%)	142 (98%)	3 (2%)	47	52
3	F	146/147 (99%)	142 (97%)	4 (3%)	39	41
All	All	1800/1824 (99%)	1772 (98%)	28 (2%)	55	61

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ARG
1	A	90	ASN
1	A	125	TRP
1	A	302	VAL
1	A	310	TYR
1	A	403	ILE
1	A	467	GLN
1	B	33	GLN
1	B	90	ASN
1	B	125	TRP
1	B	279	GLN
2	C	33	ASN
2	C	153	LEU
2	C	173	ASP
2	C	356	LEU
2	D	4	LEU
2	D	80	ARG
2	D	153	LEU
2	D	173	ASP
2	D	205	PRO
2	D	292	LYS
3	E	24	THR

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Mol	Chain	Res	Type
3	E	44	ARG
3	E	60	LEU
3	F	11	THR
3	F	41	THR
3	F	44	ARG
3	F	164	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	78	GLN
1	A	90	ASN
1	A	100	ASN
1	A	108	ASN
1	A	133	GLN
1	A	155	ASN
1	A	161	ASN
1	A	168	HIS
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	413	HIS
1	A	439	HIS
1	A	442	ASN
1	A	472	GLN
1	A	486	HIS
1	B	33	GLN
1	B	42	ASN
1	B	78	GLN
1	B	90	ASN
1	B	100	ASN
1	B	108	ASN
1	B	168	HIS
1	B	203	ASN
1	B	205	GLN

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Mol	Chain	Res	Type
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	411	ASN
1	B	413	HIS
1	B	439	HIS
1	B	451	GLN
1	B	486	HIS
1	B	516	ASN
2	C	33	ASN
2	C	98	HIS
2	C	125	GLN
2	C	146	ASN
2	C	161	ASN
2	C	220	ASN
2	C	285	GLN
2	C	293	GLN
2	C	301	ASN
2	D	57	GLN
2	D	98	HIS
2	D	125	GLN
2	D	161	ASN
2	D	285	GLN
2	D	289	GLN
2	D	293	GLN
2	D	296	GLN
2	D	301	ASN
3	E	23	ASN
3	E	45	ASN
3	E	144	ASN
3	E	158	GLN
3	E	165	HIS
3	F	7	HIS
3	F	45	ASN
3	F	99	ASN
3	F	144	ASN

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 7 ligands modelled in this entry, 7 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%)	-0.04	15 (2%) 53 57	18, 28, 49, 67	0
1	B	511/527 (96%)	-0.00	14 (2%) 56 60	19, 29, 50, 70	0
2	C	388/389 (99%)	-0.50	1 (0%) 90 91	15, 22, 39, 57	0
2	D	387/389 (99%)	0.63	35 (9%) 15 16	21, 38, 61, 70	0
3	E	167/170 (98%)	-0.25	2 (1%) 76 79	17, 24, 40, 68	0
3	F	168/170 (98%)	1.14	28 (16%) 4 5	31, 48, 66, 74	0
All	All	2132/2172 (98%)	0.08	95 (4%) 38 43	15, 30, 56, 74	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	4	LEU	6.5
3	F	83	PHE	4.8
3	F	71	ALA	4.2
2	D	352	ILE	4.1
2	D	380	ILE	4.1
2	D	385	LEU	3.9
3	F	19	ILE	3.8
1	A	17	ASN	3.8
1	B	213	THR	3.4
1	A	214	ASN	3.3
2	D	388	LEU	3.3
2	D	347	THR	3.2
1	A	206	LEU	3.2
1	B	403	ILE	3.2
3	F	72	PHE	3.1
3	F	170	HIS	3.0
1	B	54	ASN	2.9
3	F	20	ALA	2.9
1	A	318	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
2	D	384	VAL	2.8
1	A	251	TYR	2.8
3	F	118	TYR	2.8
2	D	371	ILE	2.8
2	D	382	LYS	2.8
1	B	17	ASN	2.8
3	F	41	THR	2.8
2	D	206	GLY	2.7
2	D	331	ALA	2.7
3	F	24	THR	2.7
3	E	169	PRO	2.7
1	A	317	TRP	2.7
2	D	370	ARG	2.7
2	D	137	ASN	2.6
3	F	122	ILE	2.6
3	F	23	ASN	2.6
1	A	252	GLN	2.6
3	F	84	GLY	2.6
3	F	75	VAL	2.6
1	B	311	GLU	2.6
2	D	221	GLY	2.6
1	A	316	ILE	2.5
2	D	348	ASP	2.5
2	D	223	VAL	2.5
2	D	270	PRO	2.5
2	D	338	LEU	2.5
1	B	214	ASN	2.5
2	D	359	VAL	2.4
3	F	17	ASN	2.4
2	D	346	THR	2.4
2	D	340	ALA	2.4
2	D	375	ALA	2.4
2	D	386	ALA	2.4
1	A	302	VAL	2.4
3	F	93	GLY	2.4
2	D	350	GLU	2.3
2	D	373	PHE	2.3
3	F	16	VAL	2.3
1	A	213	THR	2.3
1	B	517	CYS	2.3
1	A	338	ASP	2.3
1	B	256	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	337	GLN	2.3
2	D	330	ALA	2.3
1	A	250	GLY	2.2
3	F	69	ALA	2.2
3	F	79	HIS	2.2
2	D	145	ILE	2.2
2	D	387	GLY	2.2
3	F	80	LYS	2.2
2	D	204	VAL	2.2
1	B	53	ALA	2.2
2	D	357	TYR	2.2
1	A	245	ARG	2.1
3	F	22	LEU	2.1
1	A	310	TYR	2.1
2	D	216	ALA	2.1
3	F	82	ALA	2.1
3	F	3	LYS	2.1
3	F	60	LEU	2.1
2	D	365	GLU	2.1
2	D	379	GLN	2.1
1	B	247	MET	2.1
3	F	127	TYR	2.1
2	D	322	GLY	2.1
1	B	248	ALA	2.1
2	D	354	ALA	2.1
3	F	25	LEU	2.0
1	B	26	GLN	2.0
2	D	377	ARG	2.0
3	F	78	ARG	2.0
2	C	389	LYS	2.0
3	F	77	PHE	2.0
1	A	54	ASN	2.0
1	B	244	LEU	2.0
3	F	4	LEU	2.0

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

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
5	CA	C	5006	1/1	0.96	0.05	55,55,55,55	0
5	CA	C	5007	1/1	0.97	0.08	38,38,38,38	0
5	CA	A	5005	1/1	0.98	0.04	34,34,34,34	0
4	FE2	A	5002	1/1	0.98	0.04	39,39,39,39	0
4	FE2	B	5004	1/1	0.98	0.03	43,43,43,43	0
4	FE2	A	5001	1/1	0.99	0.02	30,30,30,30	0
4	FE2	B	5003	1/1	1.00	0.01	29,29,29,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.