



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:15 AM UTC

PDB ID : 1FZ2 / pdb_00001fz2
Title : METHANE MONOOXYGENASE HYDROXYLASE, FORM II MIXED-VALENT GENERATED BY CRYSTAL 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

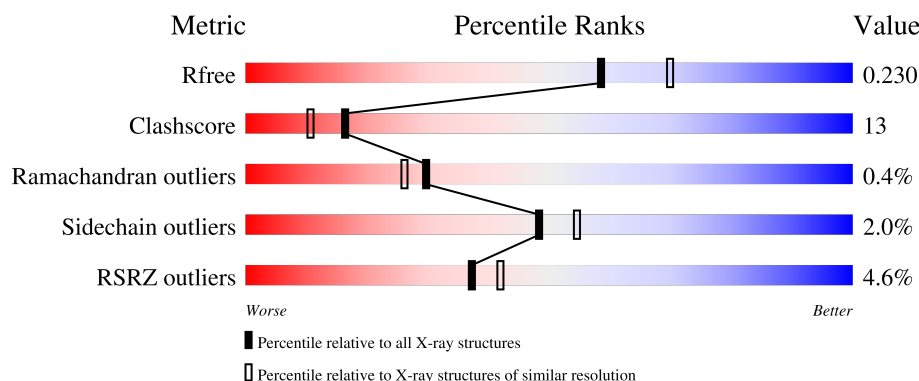
1 Overall quality at a glance

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	2% 69% 26% ..
1	B	527	2% 69% 26% ..
2	C	389	75% 23% .
2	D	389	10% 65% 31% ..
3	E	170	4% 73% 22% ..

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Mol	Chain	Length	Quality of chain
3	F	170	18% 66% 29% ..

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 18664 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	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	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
			1382	875	249	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	3	Total 3	Ca 3	0	0

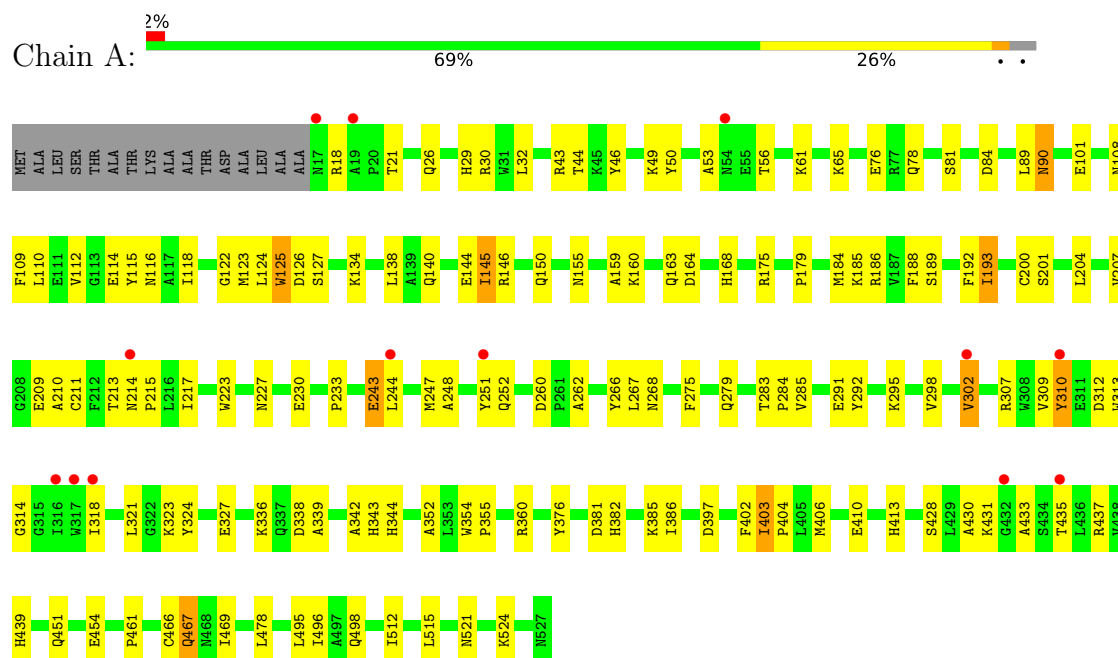
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	272	Total 272	O 272	0	0
6	B	251	Total 251	O 251	0	0
6	C	288	Total 288	O 288	0	0
6	D	133	Total 133	O 133	0	0
6	E	168	Total 168	O 168	0	0
6	F	49	Total 49	O 49	0	0

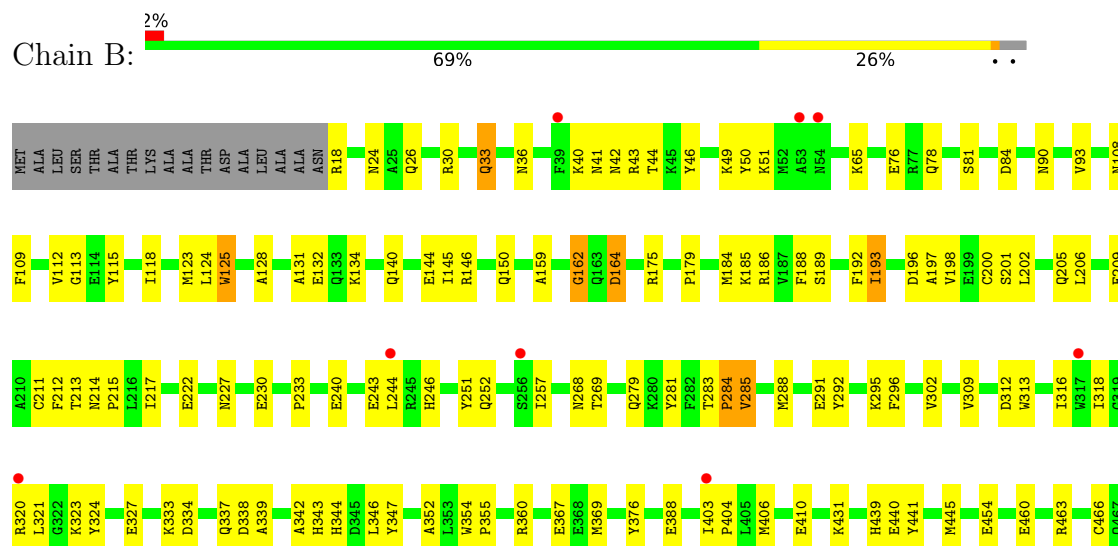
3 Residue-property plots

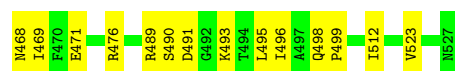
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: METHANE MONOOXYGENASE COMPONENT A, ALPHA CHAIN



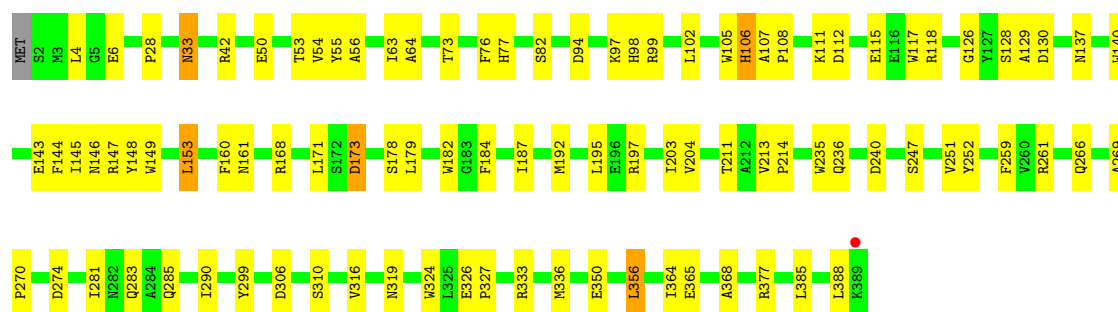
• Molecule 1: METHANE MONOOXYGENASE COMPONENT A, ALPHA CHAIN





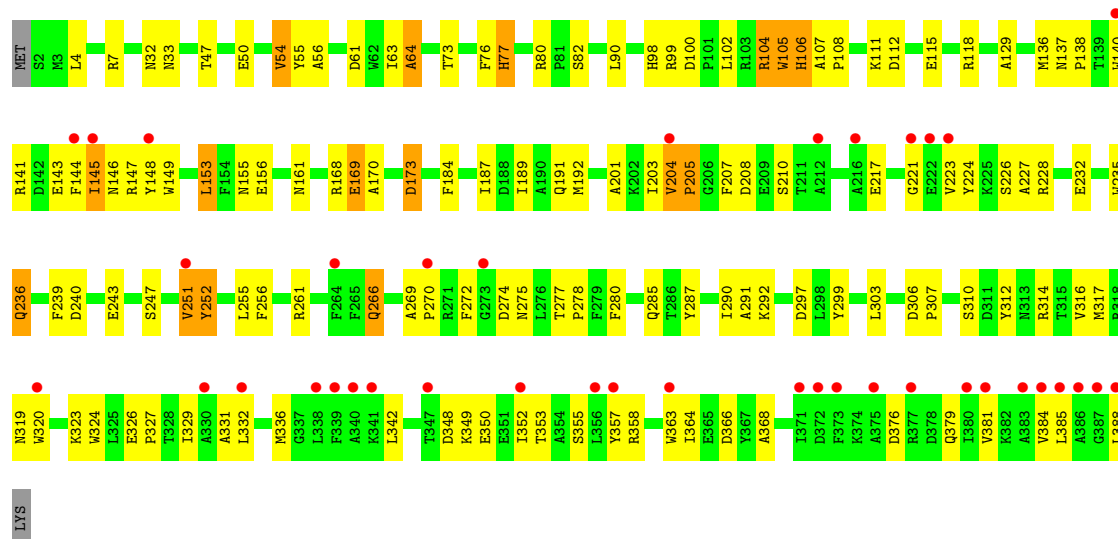
• Molecule 2: METHANE MONOOXYGENASE COMPONENT A, BETA CHAIN

Chain C: 75% 23%



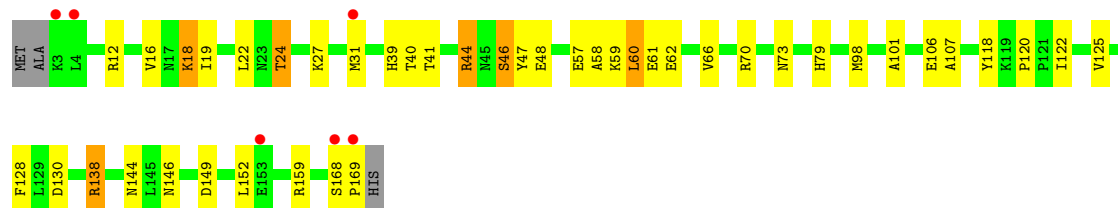
• Molecule 2: METHANE MONOOXYGENASE COMPONENT A, BETA CHAIN

Chain D: 10% 65% 31%

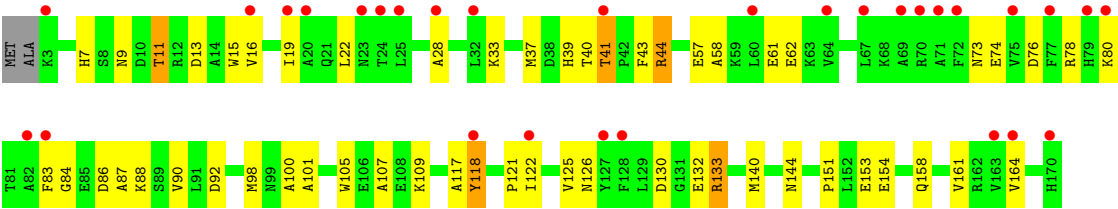


• Molecule 3: METHANE MONOOXYGENASE COMPONENT A, GAMMA CHAIN

Chain E: 4% 73% 22%



• 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	71.37Å 171.89Å 221.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.83 – 2.15 29.83 – 2.15	Depositor EDS
% Data completeness (in resolution range)	94.8 (29.83-2.15) 94.9 (29.83-2.15)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.50 (at 2.16Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.191 , 0.229 0.193 , 0.230	Depositor DCC
R_{free} test set	5021 reflections (3.38%)	wwPDB-VP
Wilson B-factor (Å ²)	27.2	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.8	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	18664	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.49% 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	0.36	0/4310	0.89	18/5853 (0.3%)
1	B	0.36	0/4302	0.89	14/5842 (0.2%)
2	C	0.40	0/3289	0.88	16/4464 (0.4%)
2	D	0.34	0/3279	0.84	10/4453 (0.2%)
3	E	0.41	0/1404	0.89	6/1892 (0.3%)
3	F	0.33	0/1412	0.79	2/1903 (0.1%)
All	All	0.37	0/17996	0.87	66/24407 (0.3%)

There are no bond length outliers.

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	339	ALA	N-CA-C	9.44	121.34	111.14
1	A	309	VAL	N-CA-C	8.82	118.82	110.53
1	B	496	ILE	N-CA-C	-7.82	103.18	110.53
2	C	149	TRP	N-CA-C	-7.69	102.98	111.36
2	D	204	VAL	CA-C-N	7.44	129.14	119.84
2	D	204	VAL	C-N-CA	7.44	129.14	119.84
2	C	105	TRP	N-CA-C	-7.31	99.42	109.95
3	E	130	ASP	N-CA-C	-7.22	103.49	111.36
1	A	496	ILE	N-CA-C	-6.98	103.97	110.53
1	B	431	LYS	N-CA-C	-6.86	104.72	113.23
1	B	285	VAL	N-CA-C	6.85	116.99	110.42
2	C	106	HIS	N-CA-C	6.77	119.23	111.11
1	B	309	VAL	N-CA-C	6.74	117.53	110.72
1	A	164	ASP	CA-C-N	6.66	126.25	119.19
1	A	164	ASP	C-N-CA	6.66	126.25	119.19
2	D	105	TRP	N-CA-C	-6.60	100.20	110.17
1	B	243	GLU	N-CA-C	6.59	119.29	111.71
2	C	236	GLN	N-CA-C	6.46	121.32	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	266	TYR	N-CA-C	6.39	122.15	113.97
1	B	164	ASP	CA-C-N	6.32	126.23	119.28
1	B	164	ASP	C-N-CA	6.32	126.23	119.28
3	E	122	ILE	N-CA-C	-6.23	105.07	110.74
2	D	104	ARG	N-CA-C	6.09	118.22	108.41
1	A	243	GLU	N-CA-C	5.95	119.80	112.54
2	C	377	ARG	N-CA-C	5.92	117.74	111.28
2	C	299	TYR	N-CA-C	5.92	119.69	112.23
1	B	93	VAL	N-CA-C	5.91	117.29	111.67
3	F	39	HIS	N-CA-C	5.90	121.81	113.02
2	C	252	TYR	N-CA-C	5.88	117.37	110.97
1	A	339	ALA	N-CA-C	5.87	117.48	111.14
3	E	118	TYR	N-CA-C	5.86	121.15	113.30
2	C	144	PHE	N-CA-C	5.84	118.88	111.69
1	A	285	VAL	N-CA-C	5.81	115.99	110.53
2	C	56	ALA	N-CA-C	-5.71	105.20	111.82
1	A	145	ILE	N-CA-C	-5.63	105.03	110.72
2	C	77	HIS	N-CA-C	-5.59	101.76	110.10
3	E	73	ASN	N-CA-C	-5.56	103.35	110.53
1	B	193	ILE	N-CA-C	5.55	120.89	109.34
2	D	106	HIS	N-CA-C	5.55	117.77	111.11
3	F	118	TYR	N-CA-C	5.53	120.02	112.88
3	E	39	HIS	N-CA-C	5.50	121.86	113.61
1	B	342	ALA	N-CA-C	5.49	117.70	111.11
1	A	122	GLY	N-CA-C	-5.49	106.02	113.37
2	C	148	TYR	N-CA-C	5.47	118.42	111.69
1	A	478	LEU	N-CA-C	5.44	117.64	111.11
2	C	137	ASN	CA-C-N	5.39	125.04	119.05
2	C	137	ASN	C-N-CA	5.39	125.04	119.05
1	B	205	GLN	N-CA-C	5.38	119.79	111.56
1	B	162	GLY	N-CA-C	5.33	120.75	112.60
1	A	267	LEU	N-CA-C	5.32	117.51	111.02
2	D	77	HIS	N-CA-C	-5.31	102.18	110.10
1	A	50	TYR	N-CA-C	5.24	117.84	110.14
2	C	171	LEU	N-CA-C	5.22	119.28	113.02
2	C	63	ILE	N-CA-C	-5.21	99.00	107.28
1	A	291	GLU	N-CA-C	5.19	117.02	111.36
2	D	236	GLN	N-CA-C	5.14	119.70	113.38
1	A	431	LYS	N-CA-C	-5.11	106.89	113.23
1	B	312	ASP	N-CA-C	5.11	116.70	111.03
1	A	193	ILE	N-CA-C	5.11	119.96	109.34
2	C	53	THR	N-CA-C	5.07	119.67	112.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^o)	Ideal(^o)
2	D	56	ALA	N-CA-C	-5.06	105.95	111.82
1	A	397	ASP	CA-C-N	5.05	124.84	119.28
1	A	397	ASP	C-N-CA	5.05	124.84	119.28
3	E	79	HIS	N-CA-C	5.05	121.14	114.12
2	D	54	VAL	N-CA-C	5.04	115.74	108.93
2	D	169	GLU	N-CA-C	5.03	119.56	113.38

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	115	0
1	B	4177	0	3975	135	0
2	C	3193	0	3042	66	0
2	D	3183	0	3029	105	0
3	E	1375	0	1370	31	0
3	F	1382	0	1366	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	3	0	0	0	0
6	A	272	0	0	8	0
6	B	251	0	0	10	0
6	C	288	0	0	6	0
6	D	133	0	0	1	0
6	E	168	0	0	0	0
6	F	49	0	0	2	0
All	All	18664	0	16763	445	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 13.

All (445) 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:B:78:GLN:HE22	1:B:150:GLN:HE21	1.03	1.01
3:F:41:THR:HG23	3:F:43:PHE:H	1.27	1.00
1:B:268:ASN:HD21	1:B:327:GLU:H	1.09	0.98
1:B:123:MET:HE3	1:B:197:ALA:HA	1.49	0.94
1:A:78:GLN:HE22	1:A:150:GLN:HE21	1.13	0.89
1:A:155:ASN:HD22	1:A:168:HIS:HD2	1.21	0.88
1:A:44:THR:HG22	1:A:46:TYR:H	1.37	0.88
1:A:352:ALA:HA	1:A:404:PRO:HB2	1.54	0.87
3:F:40:THR:O	3:F:41:THR:HG22	1.75	0.87
1:B:209:GLU:HA	1:B:213:THR:HB	1.56	0.85
1:A:467:GLN:HG3	6:A:5243:HOH:O	1.79	0.82
2:C:261:ARG:HE	2:C:285:GLN:HE22	1.26	0.82
3:F:80:LYS:HE2	3:F:84:GLY:HA2	1.63	0.80
1:B:352:ALA:HA	1:B:404:PRO:HB2	1.61	0.80
1:B:44:THR:HG22	1:B:46:TYR:H	1.47	0.80
1:B:288:MET:HE1	1:B:346:LEU:CG	2.12	0.79
1:A:209:GLU:HA	1:A:213:THR:HB	1.63	0.79
2:D:90:LEU:HD13	2:D:303:LEU:HD13	1.64	0.79
2:C:146:ASN:HD21	2:C:197:ARG:HH21	1.31	0.79
3:E:19:ILE:HG12	3:E:60:LEU:HD13	1.63	0.79
1:B:214:ASN:HB3	1:B:215:PRO:HD3	1.64	0.79
2:C:102:LEU:HD12	2:C:290:ILE:HG23	1.65	0.79
3:E:41:THR:O	3:E:44:ARG:HD2	1.85	0.76
2:D:319:ASN:OD1	3:F:78:ARG:HD3	1.86	0.76
1:A:268:ASN:HD21	1:A:327:GLU:H	1.30	0.76
1:A:214:ASN:HB3	1:A:215:PRO:HD3	1.66	0.76
1:B:406:MET:O	1:B:410:GLU:HG3	1.85	0.76
3:E:98:MET:HE1	3:E:107:ALA:CB	2.16	0.75
1:A:302:VAL:HG13	1:A:376:TYR:HE2	1.51	0.75
1:B:288:MET:HE1	1:B:346:LEU:CB	2.16	0.74
1:B:439:HIS:HB3	3:F:161:VAL:HG21	1.70	0.73
1:A:406:MET:O	1:A:410:GLU:HG3	1.89	0.73
1:B:78:GLN:NE2	1:B:150:GLN:HE21	1.82	0.73
1:B:108:ASN:HD21	1:B:175:ARG:HH11	1.36	0.73
3:F:133:ARG:HH11	3:F:133:ARG:HB3	1.55	0.72
2:D:102:LEU:HD12	2:D:290:ILE:HG23	1.73	0.71
1:B:288:MET:HE1	1:B:346:LEU:HG	1.71	0.71
3:E:24:THR:HG22	3:E:27:LYS:H	1.56	0.71
1:A:227:ASN:HD21	1:A:295:LYS:H	1.39	0.71
1:B:288:MET:HE1	1:B:346:LEU:HB3	1.73	0.71
2:D:76:PHE:HZ	2:D:168:ARG:HH12	1.37	0.70
1:B:244:LEU:HG	6:B:5195:HOH:O	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:6:GLU:HG3	6:C:5263:HOH:O	1.91	0.69
2:C:102:LEU:CD1	2:C:290:ILE:HG23	2.22	0.69
1:A:76:GLU:HG2	1:B:76:GLU:OE2	1.93	0.69
1:B:24:ASN:OD1	1:B:26:GLN:HG2	1.94	0.68
1:B:302:VAL:HG13	1:B:376:TYR:HE2	1.58	0.68
3:F:153:GLU:H	3:F:153:GLU:CD	2.02	0.68
1:B:227:ASN:HD21	1:B:295:LYS:H	1.40	0.68
1:A:108:ASN:HD21	1:A:175:ARG:HH11	1.40	0.67
1:B:369:MET:HE2	6:B:5159:HOH:O	1.94	0.67
1:A:381:ASP:HA	1:A:385:LYS:HE2	1.75	0.67
2:C:326:GLU:HB3	2:C:327:PRO:HD3	1.76	0.67
1:B:125:TRP:HE1	2:D:161:ASN:ND2	1.93	0.66
1:B:125:TRP:HE1	2:D:161:ASN:HD22	1.43	0.66
2:D:111:LYS:O	2:D:115:GLU:HG3	1.95	0.66
2:C:107:ALA:HB3	2:C:108:PRO:HD3	1.78	0.66
3:F:41:THR:O	3:F:44:ARG:HD2	1.96	0.66
2:C:146:ASN:ND2	2:C:197:ARG:HH21	1.95	0.65
1:B:268:ASN:ND2	1:B:327:GLU:H	1.91	0.65
1:B:288:MET:CE	1:B:346:LEU:HB3	2.26	0.65
2:D:107:ALA:HB3	2:D:108:PRO:HD3	1.79	0.65
2:D:102:LEU:CD1	2:D:290:ILE:HG23	2.27	0.64
3:F:58:ALA:O	3:F:62:GLU:HG3	1.97	0.64
1:B:489:ARG:HD2	1:B:495:LEU:O	1.97	0.64
2:D:145:ILE:O	2:D:149:TRP:HB3	1.98	0.63
3:F:9:ASN:OD1	3:F:11:THR:HG23	1.98	0.63
3:E:98:MET:HE3	3:E:98:MET:O	1.98	0.63
2:D:217:GLU:O	2:D:221:GLY:HA3	1.99	0.63
2:D:326:GLU:HB3	2:D:327:PRO:HD3	1.79	0.63
2:D:100:ASP:OD1	2:D:104:ARG:HD3	1.99	0.63
1:A:244:LEU:HG	6:A:5166:HOH:O	1.98	0.63
1:B:179:PRO:HB3	1:B:469:ILE:HD13	1.80	0.62
3:F:151:PRO:HB2	3:F:153:GLU:OE1	2.00	0.62
1:A:140:GLN:O	1:A:144:GLU:HG2	2.00	0.62
3:F:154:GLU:HG3	3:F:158:GLN:HE21	1.63	0.62
1:A:268:ASN:ND2	1:A:327:GLU:H	1.98	0.62
2:C:42:ARG:HB2	2:C:99:ARG:HH11	1.64	0.62
1:B:240:GLU:HG2	6:B:5194:HOH:O	1.99	0.61
1:B:439:HIS:HB3	3:F:161:VAL:CG2	2.30	0.61
1:A:292:TYR:OH	1:A:344:HIS:HD2	1.82	0.61
3:E:57:GLU:O	3:E:61:GLU:HG3	1.98	0.61
1:A:495:LEU:HD11	1:A:512:ILE:HG13	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:TYR:OH	1:B:344:HIS:HD2	1.84	0.61
1:B:441:TYR:HB2	3:F:161:VAL:HG23	1.82	0.61
2:D:153:LEU:C	2:D:153:LEU:HD12	2.26	0.61
3:E:98:MET:HE1	3:E:107:ALA:HB2	1.83	0.61
1:B:288:MET:HE2	1:B:347:TYR:N	2.15	0.60
3:F:15:TRP:O	3:F:19:ILE:HG23	2.01	0.60
1:A:302:VAL:HG13	1:A:376:TYR:CE2	2.34	0.60
2:C:111:LYS:O	2:C:115:GLU:HG3	2.01	0.60
2:C:112:ASP:OD1	2:D:118:ARG:NH2	2.35	0.60
1:B:33:GLN:HE21	1:B:33:GLN:HA	1.65	0.59
2:C:269:ALA:HB3	2:C:270:PRO:HD3	1.83	0.59
3:E:146:ASN:HB3	3:E:149:ASP:OD2	2.02	0.59
2:C:336:MET:HE3	2:C:388:LEU:HG	1.85	0.59
1:A:279:GLN:HG2	1:A:283:THR:OG1	2.02	0.59
1:A:185:LYS:O	1:A:189:SER:HB2	2.02	0.59
1:B:144:GLU:OE2	1:B:144:GLU:HA	2.03	0.59
2:D:376:ASP:OD2	2:D:379:GLN:HB2	2.03	0.59
1:A:78:GLN:NE2	1:A:150:GLN:HE21	1.94	0.59
2:D:247:SER:HG	2:D:324:TRP:CD1	2.21	0.59
1:B:212:PHE:O	1:B:215:PRO:HD2	2.03	0.58
1:B:333:LYS:HG3	6:B:5108:HOH:O	2.02	0.58
2:C:97:LYS:HD2	6:C:5135:HOH:O	2.03	0.58
1:B:123:MET:HE1	1:B:200:CYS:SG	2.44	0.58
1:B:269:THR:HG23	6:B:5224:HOH:O	2.02	0.58
3:F:13:ASP:O	3:F:16:VAL:HG22	2.03	0.58
1:B:227:ASN:ND2	1:B:295:LYS:H	2.01	0.58
2:C:247:SER:HG	2:C:324:TRP:CD1	2.21	0.58
1:A:109:PHE:O	1:A:112:VAL:HG12	2.04	0.58
1:A:184:MET:HE3	1:A:188:PHE:HB2	1.85	0.58
2:D:357:TYR:CE1	2:D:381:VAL:HG11	2.38	0.58
1:A:155:ASN:HD22	1:A:168:HIS:CD2	2.13	0.57
1:B:495:LEU:HD11	1:B:512:ILE:HG13	1.86	0.57
2:D:228:ARG:O	2:D:232:GLU:HG3	2.04	0.57
1:B:49:LYS:HD3	3:F:144:ASN:HD22	1.70	0.57
3:F:61:GLU:HB3	3:F:121:PRO:HD3	1.85	0.57
2:D:261:ARG:HE	2:D:285:GLN:HE22	1.50	0.57
3:E:98:MET:HE1	3:E:107:ALA:HB1	1.87	0.57
1:B:192:PHE:O	1:B:200:CYS:HB3	2.05	0.57
1:B:18:ARG:O	2:D:129:ALA:HA	2.04	0.57
1:B:51:LYS:HG3	6:B:5199:HOH:O	2.04	0.57
1:A:313:TRP:CZ3	1:A:318:ILE:HD11	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:GLN:HE22	1:B:132:GLU:H	1.50	0.56
2:D:98:HIS:HD2	2:D:297:ASP:OD1	1.88	0.56
1:B:360:ARG:HG2	1:B:498:GLN:HB2	1.88	0.56
2:C:179:LEU:HD12	2:C:182:TRP:CE3	2.41	0.56
1:A:108:ASN:HD21	1:A:175:ARG:HD3	1.71	0.56
3:E:58:ALA:O	3:E:62:GLU:HG3	2.06	0.56
3:F:41:THR:HG23	3:F:43:PHE:N	2.10	0.56
1:A:227:ASN:ND2	1:A:295:LYS:H	2.04	0.55
2:C:259:PHE:CE1	2:C:356:LEU:HD13	2.41	0.55
1:A:179:PRO:HB3	1:A:469:ILE:HD13	1.87	0.55
1:B:268:ASN:HD21	1:B:327:GLU:N	1.92	0.55
3:F:130:ASP:OD1	3:F:133:ARG:NH1	2.40	0.55
3:E:101:ALA:HA	3:E:106:GLU:OE2	2.07	0.55
2:D:61:ASP:OD1	3:F:7:HIS:HD2	1.89	0.55
1:B:495:LEU:HD11	1:B:512:ILE:CG1	2.37	0.55
1:A:213:THR:O	1:A:217:ILE:HG12	2.06	0.55
1:A:439:HIS:HE1	1:A:454:GLU:OE1	1.89	0.54
1:B:337:GLN:HG3	1:B:338:ASP:N	2.23	0.54
2:D:348:ASP:OD2	2:D:350:GLU:HB2	2.07	0.54
1:B:369:MET:HE1	1:B:388:GLU:OE2	2.07	0.54
2:D:148:TYR:HE2	2:D:223:VAL:HG21	1.72	0.54
1:A:495:LEU:HD11	1:A:512:ILE:CG1	2.36	0.54
1:B:108:ASN:HD21	1:B:175:ARG:HD3	1.72	0.54
2:C:211:THR:O	2:C:214:PRO:HD2	2.07	0.54
1:B:211:CYS:HB2	1:B:313:TRP:CD1	2.42	0.54
1:A:314:GLY:HA2	1:A:318:ILE:HD12	1.89	0.54
1:B:33:GLN:NE2	1:B:132:GLU:H	2.05	0.54
2:C:94:ASP:HB3	2:C:97:LYS:HG3	1.90	0.54
3:E:98:MET:HE2	3:E:138:ARG:CG	2.38	0.54
6:C:5103:HOH:O	3:E:125:VAL:HG22	2.07	0.54
3:E:18:LYS:HB2	3:E:18:LYS:NZ	2.23	0.54
2:D:324:TRP:C	2:D:327:PRO:HD2	2.33	0.54
3:F:19:ILE:HD12	3:F:19:ILE:C	2.33	0.54
2:C:42:ARG:HB2	2:C:99:ARG:NH1	2.23	0.53
1:B:206:LEU:HD11	1:B:321:LEU:HD11	1.89	0.53
2:C:350:GLU:HB3	6:C:5197:HOH:O	2.08	0.53
2:D:156:GLU:HA	2:D:156:GLU:OE2	2.08	0.53
1:A:268:ASN:HD21	1:A:327:GLU:N	2.05	0.53
1:B:115:TYR:OH	2:D:173:ASP:HA	2.08	0.53
2:D:77:HIS:CD2	3:F:140:MET:HG2	2.43	0.53
3:F:61:GLU:O	3:F:121:PRO:HG2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:ASP:CG	1:B:489:ARG:HH22	2.16	0.53
1:B:198:VAL:O	1:B:202:LEU:HG	2.08	0.53
2:D:47:THR:OG1	2:D:50:GLU:HG3	2.09	0.53
2:C:211:THR:C	2:C:214:PRO:HD2	2.34	0.53
1:A:360:ARG:HG2	1:A:498:GLN:HB2	1.91	0.53
2:C:270:PRO:HB3	2:D:270:PRO:HB3	1.90	0.53
2:D:143:GLU:O	2:D:147:ARG:HB3	2.09	0.53
1:B:244:LEU:HB2	6:B:5234:HOH:O	2.09	0.53
1:A:53:ALA:HB1	6:A:5184:HOH:O	2.09	0.52
1:B:222:GLU:OE1	2:D:7:ARG:HD3	2.09	0.52
1:B:186:ARG:HD3	1:B:186:ARG:C	2.34	0.52
1:B:439:HIS:HE1	1:B:454:GLU:OE1	1.92	0.52
1:B:460:GLU:OE1	1:B:463:ARG:HD3	2.10	0.52
2:C:333:ARG:HD2	6:C:5230:HOH:O	2.08	0.52
1:A:313:TRP:CH2	1:A:318:ILE:HD11	2.44	0.52
1:B:108:ASN:ND2	1:B:175:ARG:HH11	2.05	0.52
1:A:110:LEU:O	1:A:114:GLU:HG2	2.09	0.52
1:B:43:ARG:HD2	1:B:43:ARG:C	2.34	0.52
2:C:336:MET:CE	2:C:385:LEU:HD23	2.40	0.52
1:B:269:THR:HG21	6:F:369:HOH:O	2.08	0.52
2:D:201:ALA:HA	2:D:207:PHE:HB3	1.91	0.52
2:D:269:ALA:HB3	2:D:270:PRO:HD3	1.91	0.52
1:B:50:TYR:CD2	1:B:257:ILE:HD12	2.44	0.52
1:B:281:TYR:CZ	1:B:285:VAL:HG21	2.44	0.52
2:D:187:ILE:O	2:D:191:GLN:HG3	2.10	0.52
1:B:30:ARG:HG2	1:B:30:ARG:HH11	1.75	0.51
1:A:260:ASP:OD2	1:A:262:ALA:HB3	2.10	0.51
2:D:137:ASN:HB3	2:D:272:PHE:HB3	1.92	0.51
1:A:403:ILE:HD13	1:A:515:LEU:HD11	1.93	0.51
3:F:125:VAL:HG23	3:F:126:ASN:N	2.25	0.51
1:A:344:HIS:HE1	1:A:376:TYR:CD2	2.28	0.51
1:B:78:GLN:HE22	1:B:150:GLN:NE2	1.88	0.51
1:B:124:LEU:HD21	1:B:201:SER:HB2	1.92	0.51
2:D:240:ASP:HB2	3:F:125:VAL:HG21	1.92	0.51
3:E:66:VAL:HG12	3:E:70:ARG:HH21	1.76	0.51
3:F:57:GLU:O	3:F:61:GLU:HG3	2.11	0.51
2:D:323:LYS:HB2	3:F:78:ARG:NH1	2.25	0.51
3:E:41:THR:O	3:E:44:ARG:CD	2.56	0.51
2:C:365:GLU:HG3	6:C:5210:HOH:O	2.09	0.51
1:B:193:ILE:HD11	2:D:82:SER:HB3	1.93	0.51
1:A:204:LEU:O	1:A:209:GLU:HG3	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:490:SER:OG	2:D:32:ASN:HB2	2.10	0.50
1:A:144:GLU:HA	1:A:144:GLU:OE2	2.11	0.50
1:B:186:ARG:HA	2:D:73:THR:OG1	2.10	0.50
1:A:65:LYS:HB3	2:C:117:TRP:CG	2.47	0.50
2:C:50:GLU:OE1	2:C:99:ARG:NH1	2.45	0.50
2:D:138:PRO:HA	2:D:141:ARG:NH1	2.26	0.50
3:E:44:ARG:HD3	3:E:47:TYR:CZ	2.47	0.50
1:A:108:ASN:ND2	1:A:175:ARG:HH11	2.09	0.50
1:A:160:LYS:HE3	6:A:5061:HOH:O	2.10	0.50
1:A:252:GLN:HB3	6:A:5045:HOH:O	2.11	0.50
1:A:307:ARG:HG2	1:A:312:ASP:OD2	2.12	0.50
1:A:413:HIS:HD2	1:A:428:SER:OG	1.95	0.50
1:A:435:THR:HG22	3:E:168:SER:HA	1.93	0.50
1:B:320:ARG:HH11	1:B:320:ARG:HB3	1.76	0.50
2:C:161:ASN:HB3	2:C:235:TRP:CE2	2.46	0.50
2:C:261:ARG:HE	2:C:285:GLN:NE2	2.04	0.50
1:A:44:THR:HG23	1:A:126:ASP:OD1	2.12	0.50
1:A:186:ARG:HA	2:C:73:THR:OG1	2.12	0.50
1:B:291:GLU:OE1	1:B:343:HIS:HE1	1.94	0.50
2:D:54:VAL:O	2:D:55:TYR:HB2	2.11	0.50
3:F:33:LYS:O	3:F:37:MET:HG2	2.11	0.50
2:C:54:VAL:O	2:C:55:TYR:HB2	2.12	0.50
1:A:338:ASP:OD1	1:A:433:ALA:HB2	2.11	0.49
2:C:235:TRP:CD1	2:C:235:TRP:C	2.90	0.49
2:D:82:SER:O	2:D:168:ARG:NH2	2.45	0.49
2:D:336:MET:HE3	2:D:388:LEU:HD21	1.94	0.49
1:B:344:HIS:HE1	1:B:376:TYR:CD2	2.30	0.49
2:C:98:HIS:HE1	2:C:178:SER:OG	1.94	0.49
1:B:140:GLN:HG3	1:B:246:HIS:CD2	2.47	0.49
1:A:26:GLN:HG2	6:A:5178:HOH:O	2.10	0.49
1:B:230:GLU:C	1:B:233:PRO:HD2	2.37	0.49
1:B:367:GLU:HG3	6:B:5018:HOH:O	2.12	0.49
2:D:243:GLU:HB2	2:D:320:TRP:CZ2	2.48	0.49
1:A:243:GLU:O	1:A:247:MET:HG2	2.13	0.49
1:B:125:TRP:CD1	1:B:125:TRP:C	2.90	0.49
2:D:247:SER:O	2:D:251:VAL:HB	2.13	0.49
3:E:98:MET:HE2	3:E:138:ARG:HG2	1.93	0.49
3:F:98:MET:HE1	3:F:107:ALA:O	2.13	0.49
1:B:49:LYS:CE	3:F:144:ASN:HD22	2.27	0.48
1:B:185:LYS:O	1:B:189:SER:HB2	2.13	0.48
1:B:206:LEU:HD11	1:B:321:LEU:CD1	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:324:TRP:HA	2:D:327:PRO:HD2	1.96	0.48
2:D:364:ILE:HA	2:D:368:ALA:HB3	1.95	0.48
3:E:22:LEU:HD11	3:E:31:MET:SD	2.53	0.48
1:A:49:LYS:HD3	3:E:144:ASN:HD22	1.78	0.48
1:B:302:VAL:HG13	1:B:376:TYR:CE2	2.44	0.48
2:D:189:ILE:HD11	2:D:287:TYR:CD1	2.49	0.48
1:A:134:LYS:HD3	2:C:161:ASN:HD21	1.77	0.48
3:E:46:SER:OG	3:E:48:GLU:HG2	2.14	0.48
2:D:323:LYS:HB2	3:F:78:ARG:HH11	1.77	0.48
1:B:313:TRP:CZ2	1:B:318:ILE:HD11	2.48	0.48
2:D:140:TRP:HB2	2:D:272:PHE:CD2	2.49	0.48
1:A:402:PHE:O	1:A:403:ILE:HD12	2.14	0.48
1:A:192:PHE:O	1:A:200:CYS:HB3	2.14	0.48
1:B:184:MET:HE2	1:B:188:PHE:HB2	1.95	0.48
1:A:159:ALA:O	2:C:33:ASN:HB2	2.14	0.47
2:D:136:MET:HE2	2:D:274:ASP:OD1	2.14	0.47
1:A:451:GLN:HB2	3:E:152:LEU:HD11	1.95	0.47
1:A:466:CYS:HB2	2:C:73:THR:HA	1.95	0.47
1:B:196:ASP:HB2	3:F:140:MET:SD	2.55	0.47
1:B:128:ALA:O	1:B:134:LYS:HE2	2.14	0.47
2:D:184:PHE:O	2:D:187:ILE:HG22	2.15	0.47
1:A:125:TRP:HE1	2:C:161:ASN:ND2	2.12	0.47
1:B:251:TYR:HE2	1:B:320:ARG:HH12	1.62	0.47
1:B:354:TRP:CG	1:B:355:PRO:HD3	2.50	0.47
2:C:336:MET:HE2	2:C:385:LEU:HD23	1.97	0.47
2:D:299:TYR:O	2:D:317:MET:HE1	2.15	0.47
1:A:118:ILE:HD13	1:A:145:ILE:HG12	1.97	0.47
1:B:323:LYS:HE2	1:B:324:TYR:CZ	2.50	0.47
2:C:118:ARG:NH2	2:D:111:LYS:HD3	2.29	0.47
2:D:148:TYR:CE2	2:D:223:VAL:HG21	2.49	0.47
1:B:146:ARG:HB2	2:D:106:HIS:CE1	2.50	0.46
2:D:161:ASN:HB3	2:D:235:TRP:CE2	2.50	0.46
3:F:90:VAL:HG11	3:F:118:TYR:CE2	2.50	0.46
3:F:105:TRP:O	3:F:109:LYS:HG3	2.15	0.46
1:B:468:ASN:CG	1:B:471:GLU:HG3	2.40	0.46
2:C:213:VAL:HB	2:C:214:PRO:HD3	1.97	0.46
2:C:364:ILE:HA	2:C:368:ALA:HB3	1.97	0.46
3:F:22:LEU:HD13	3:F:28:ALA:HA	1.97	0.46
1:A:81:SER:OG	1:B:84:ASP:HB3	2.15	0.46
1:B:140:GLN:HG3	1:B:246:HIS:CE1	2.50	0.46
1:B:186:ARG:HD3	1:B:186:ARG:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:THR:O	1:B:217:ILE:HG12	2.14	0.46
1:A:186:ARG:HD3	1:A:186:ARG:C	2.40	0.46
2:D:192:MET:HE3	2:D:280:PHE:CD2	2.51	0.46
2:D:277:THR:HB	2:D:278:PRO:HD3	1.98	0.46
1:A:310:TYR:CE1	1:A:336:LYS:HD2	2.51	0.46
1:A:248:ALA:O	1:A:252:GLN:HB2	2.16	0.46
1:A:439:HIS:CE1	1:A:454:GLU:OE1	2.69	0.46
1:B:49:LYS:CD	3:F:144:ASN:HD22	2.29	0.45
1:B:334:ASP:HA	1:B:337:GLN:HG2	1.99	0.45
1:A:403:ILE:HD13	1:A:515:LEU:CD1	2.46	0.45
1:A:163:GLN:O	2:C:28:PRO:HA	2.16	0.45
1:A:230:GLU:C	1:A:233:PRO:HD2	2.42	0.45
2:C:192:MET:HE2	2:C:283:GLN:OE1	2.16	0.45
1:A:163:GLN:HG2	6:A:5119:HOH:O	2.15	0.45
1:B:41:ASN:O	2:D:236:GLN:HB3	2.17	0.45
2:D:349:LYS:HA	2:D:352:ILE:HG12	1.98	0.45
1:A:343:HIS:CD2	1:A:343:HIS:H	2.35	0.45
1:A:382:HIS:O	1:A:386:ILE:HG13	2.17	0.45
1:B:164:ASP:OD1	1:B:489:ARG:NH2	2.50	0.45
1:B:466:CYS:HB2	2:D:73:THR:HA	1.99	0.45
2:C:140:TRP:NE1	2:C:145:ILE:HD11	2.32	0.45
2:C:153:LEU:C	2:C:153:LEU:HD12	2.42	0.45
1:A:46:TYR:CD2	1:A:123:MET:HE3	2.52	0.45
1:A:101:GLU:CD	1:A:360:ARG:HD3	2.41	0.45
1:A:116:ASN:CG	1:A:189:SER:HA	2.42	0.45
3:F:132:GLU:HG3	6:F:352:HOH:O	2.16	0.45
1:A:310:TYR:CZ	1:A:336:LYS:HD2	2.52	0.44
1:A:115:TYR:OH	2:C:173:ASP:HA	2.17	0.44
2:D:98:HIS:CD2	2:D:99:ARG:N	2.84	0.44
2:D:329:ILE:HG23	2:D:384:VAL:HG22	1.98	0.44
2:D:144:PHE:CE2	2:D:342:LEU:HD23	2.52	0.44
1:A:435:THR:HG22	3:E:169:PRO:HD3	2.00	0.44
1:B:302:VAL:CG1	1:B:376:TYR:HE2	2.29	0.44
2:D:275:ASN:C	2:D:278:PRO:HD2	2.42	0.44
1:B:30:ARG:HG2	1:B:30:ARG:NH1	2.32	0.44
1:B:403:ILE:HG22	1:B:406:MET:SD	2.58	0.44
2:D:105:TRP:O	2:D:108:PRO:HD2	2.16	0.44
1:A:521:ASN:HB3	1:A:524:LYS:HG2	2.00	0.44
1:B:65:LYS:HE2	2:D:192:MET:HE2	1.99	0.44
2:D:292:LYS:HE3	2:D:366:ASP:OD2	2.18	0.44
1:A:32:LEU:C	1:A:32:LEU:HD23	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:GLN:HG3	6:B:5206:HOH:O	2.18	0.44
2:C:143:GLU:O	2:C:147:ARG:HB3	2.18	0.44
2:D:235:TRP:CD1	2:D:235:TRP:C	2.94	0.44
2:D:255:LEU:HD21	2:D:363:TRP:CG	2.52	0.44
1:A:138:LEU:HD22	2:C:160:PHE:CZ	2.53	0.44
1:A:461:PRO:HG2	3:E:159:ARG:CZ	2.47	0.44
2:D:240:ASP:HB2	3:F:125:VAL:CG2	2.47	0.44
2:D:324:TRP:O	2:D:327:PRO:HD2	2.18	0.44
2:C:76:PHE:HZ	2:C:168:ARG:HH12	1.66	0.43
3:E:120:PRO:HD3	3:E:128:PHE:CG	2.53	0.43
1:B:140:GLN:HG3	1:B:246:HIS:NE2	2.33	0.43
2:D:239:PHE:HB2	3:F:126:ASN:HA	2.00	0.43
3:F:74:GLU:O	3:F:78:ARG:HG3	2.17	0.43
1:A:184:MET:HE3	1:A:188:PHE:CB	2.48	0.43
1:A:323:LYS:HE2	1:A:324:TYR:CZ	2.53	0.43
1:B:288:MET:CE	1:B:347:TYR:N	2.82	0.43
3:E:40:THR:C	3:E:41:THR:HG23	2.42	0.43
1:B:468:ASN:OD1	1:B:471:GLU:HG3	2.18	0.43
2:D:208:ASP:OD2	2:D:210:SER:HB3	2.19	0.43
2:D:352:ILE:HD11	2:D:388:LEU:HD11	2.01	0.43
1:A:56:THR:CG2	1:A:252:GLN:HE21	2.32	0.43
1:A:89:LEU:HD21	1:B:230:GLU:HG3	2.00	0.43
2:D:63:ILE:O	2:D:64:ALA:C	2.61	0.43
2:D:138:PRO:HA	2:D:141:ARG:HH12	1.82	0.43
1:B:109:PHE:O	1:B:112:VAL:HG12	2.19	0.43
1:B:476:ARG:HG3	1:B:476:ARG:HH11	1.83	0.43
2:C:126:GLY:O	2:C:130:ASP:HB2	2.19	0.43
3:F:41:THR:O	3:F:44:ARG:CD	2.65	0.43
2:C:118:ARG:NH2	2:D:112:ASP:OD1	2.52	0.42
2:D:192:MET:HE3	2:D:280:PHE:CE2	2.53	0.42
1:A:44:THR:OG1	1:A:127:SER:HA	2.19	0.42
1:B:159:ALA:O	2:D:33:ASN:HB2	2.19	0.42
2:D:228:ARG:HG2	2:D:228:ARG:HH11	1.83	0.42
1:A:146:ARG:HB2	2:C:106:HIS:CE1	2.54	0.42
1:B:36:ASN:HD21	1:B:42:ASN:HD21	1.66	0.42
1:B:227:ASN:HD21	1:B:296:PHE:H	1.67	0.42
2:C:33:ASN:N	2:C:33:ASN:HD22	2.16	0.42
2:D:226:SER:HB2	2:D:331:ALA:HA	2.01	0.42
1:A:43:ARG:C	1:A:43:ARG:HD2	2.44	0.42
1:B:140:GLN:O	1:B:144:GLU:HG2	2.19	0.42
2:D:312:TYR:O	2:D:316:VAL:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:12:ARG:O	3:E:16:VAL:HG23	2.19	0.42
3:E:66:VAL:CG1	3:E:70:ARG:HH21	2.31	0.42
3:F:33:LYS:HE3	3:F:117:ALA:HB2	2.02	0.42
1:A:84:ASP:HB3	1:B:81:SER:OG	2.20	0.42
2:D:352:ILE:HG13	2:D:353:THR:N	2.34	0.42
3:F:40:THR:O	3:F:41:THR:CG2	2.58	0.42
2:D:169:GLU:O	2:D:170:ALA:C	2.61	0.42
2:D:266:GLN:HA	2:D:266:GLN:HE21	1.84	0.42
2:D:357:TYR:CE1	2:D:381:VAL:HG21	2.55	0.42
3:F:100:ALA:O	3:F:101:ALA:C	2.62	0.42
1:A:251:TYR:CD2	1:A:321:LEU:HD21	2.54	0.42
1:B:316:ILE:O	1:B:320:ARG:HG3	2.20	0.42
2:D:291:ALA:HB2	6:D:431:HOH:O	2.20	0.42
1:A:21:THR:HG22	2:C:128:SER:CB	2.50	0.42
1:A:352:ALA:CA	1:A:404:PRO:HB2	2.37	0.42
1:B:209:GLU:HA	1:B:213:THR:CB	2.40	0.42
1:B:460:GLU:HB3	1:B:463:ARG:HG3	2.02	0.42
1:A:211:CYS:HB2	1:A:313:TRP:CD1	2.55	0.42
1:A:430:ALA:HA	6:A:5265:HOH:O	2.19	0.42
1:B:283:THR:HB	1:B:284:PRO:HD3	2.02	0.42
2:D:98:HIS:CD2	2:D:99:ARG:H	2.38	0.42
1:B:491:ASP:O	1:B:493:LYS:HG3	2.20	0.41
2:D:261:ARG:HE	2:D:285:GLN:NE2	2.17	0.41
2:D:336:MET:HE2	2:D:385:LEU:HA	2.01	0.41
1:B:162:GLY:HA3	6:B:5040:HOH:O	2.19	0.41
1:B:288:MET:HB2	1:B:288:MET:HE3	1.70	0.41
2:D:203:ILE:HG13	2:D:204:VAL:HG23	2.01	0.41
1:A:18:ARG:O	2:C:129:ALA:HA	2.20	0.41
1:A:354:TRP:CG	1:A:355:PRO:HD3	2.56	0.41
1:A:284:PRO:HB3	1:A:342:ALA:HB1	2.02	0.41
3:F:33:LYS:HE3	3:F:117:ALA:CB	2.50	0.41
1:A:207:VAL:HG11	1:A:275:PHE:HA	2.02	0.41
1:B:50:TYR:CD1	1:B:50:TYR:N	2.89	0.41
1:B:445:MET:HE3	1:B:523:VAL:HG22	2.02	0.41
2:D:310:SER:O	2:D:314:ARG:HG3	2.21	0.41
1:A:56:THR:HG23	1:A:252:GLN:HE21	1.86	0.41
1:A:90:ASN:HD22	1:A:90:ASN:HA	1.61	0.41
1:A:193:ILE:HD11	2:C:82:SER:HB3	2.02	0.41
1:A:283:THR:HB	1:A:284:PRO:HD3	2.03	0.41
1:B:118:ILE:HD13	1:B:145:ILE:HG12	2.01	0.41
1:B:403:ILE:HG23	1:B:406:MET:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:184:PHE:O	2:C:187:ILE:HG22	2.20	0.41
3:F:88:LYS:O	3:F:92:ASP:OD1	2.38	0.41
1:A:124:LEU:HD21	1:A:201:SER:HB2	2.02	0.41
2:C:306:ASP:O	2:C:310:SER:HB2	2.19	0.41
2:D:256:PHE:HA	2:D:332:LEU:HD21	2.03	0.41
1:A:123:MET:SD	2:C:168:ARG:NH1	2.94	0.41
1:A:354:TRP:N	1:A:355:PRO:CD	2.84	0.41
1:B:246:HIS:CD2	1:B:246:HIS:N	2.88	0.41
2:C:316:VAL:O	2:C:319:ASN:HB3	2.21	0.41
2:D:226:SER:CB	2:D:331:ALA:HA	2.50	0.41
2:D:355:SER:O	2:D:358:ARG:HB2	2.21	0.41
3:F:73:ASN:ND2	3:F:76:ASP:OD2	2.54	0.41
1:A:29:HIS:CD2	1:A:61:LYS:HA	2.56	0.41
2:C:203:ILE:HG13	2:C:204:VAL:HG23	2.02	0.41
2:D:102:LEU:HB2	2:D:104:ARG:HD2	2.04	0.41
3:E:59:LYS:HA	3:E:59:LYS:HD3	1.93	0.41
1:A:437:ARG:NH1	1:A:454:GLU:OE2	2.49	0.40
1:B:33:GLN:HA	1:B:131:ALA:HB3	2.03	0.40
1:B:113:GLY:HA3	1:B:188:PHE:CD2	2.56	0.40
2:D:145:ILE:HG22	2:D:146:ASN:N	2.36	0.40
3:F:33:LYS:HB2	3:F:83:PHE:HZ	1.86	0.40
3:F:86:ASP:O	3:F:87:ALA:C	2.64	0.40
1:B:320:ARG:HB3	1:B:320:ARG:NH1	2.35	0.40
2:C:266:GLN:HB2	2:C:281:ILE:HG21	2.04	0.40
2:D:306:ASP:HA	2:D:307:PRO:HD3	1.90	0.40
1:B:403:ILE:CG2	1:B:406:MET:HG3	2.52	0.40
2:D:224:TYR:O	2:D:227:ALA:HB3	2.21	0.40
1:A:125:TRP:HE1	2:C:161:ASN:HD22	1.70	0.40
1:A:223:TRP:CE2	1:A:298:VAL:HB	2.56	0.40
1:B:354:TRP:CH2	1:B:499:PRO:HD3	2.56	0.40
1:A:210:ALA:HA	1:A:247:MET:HE1	2.02	0.40
2:C:240:ASP:HB2	3:E:125:VAL:CG2	2.51	0.40
2:C:274:ASP:OD1	2:C:274:ASP:C	2.64	0.40
2:D:155:ASN:ND2	2:D:252:TYR:OH	2.54	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	509/527 (97%)	486 (96%)	23 (4%)	0	100	100
1	B	508/527 (96%)	480 (94%)	26 (5%)	2 (0%)	30	26
2	C	386/389 (99%)	376 (97%)	8 (2%)	2 (0%)	24	20
2	D	385/389 (99%)	362 (94%)	19 (5%)	4 (1%)	12	8
3	E	165/170 (97%)	162 (98%)	3 (2%)	0	100	100
3	F	166/170 (98%)	160 (96%)	5 (3%)	1 (1%)	21	15
All	All	2119/2172 (98%)	2026 (96%)	84 (4%)	9 (0%)	30	26

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	64	ALA
3	F	122	ILE
1	B	40	LYS
2	D	252	TYR
2	C	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	432/442 (98%)	427 (99%)	5 (1%)	63	70
2	C	322/323 (100%)	316 (98%)	6 (2%)	50	56
2	D	321/323 (99%)	314 (98%)	7 (2%)	45	51
3	E	145/147 (99%)	139 (96%)	6 (4%)	27	26
3	F	145/147 (99%)	140 (97%)	5 (3%)	32	33
All	All	1798/1824 (99%)	1762 (98%)	36 (2%)	48	54

All (36) 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
1	B	440	GLU
2	C	4	LEU
2	C	33	ASN
2	C	153	LEU
2	C	173	ASP
2	C	195	LEU
2	C	356	LEU
2	D	4	LEU
2	D	80	ARG
2	D	145	ILE
2	D	153	LEU
2	D	173	ASP
2	D	205	PRO
2	D	266	GLN
3	E	18	LYS
3	E	24	THR
3	E	44	ARG
3	E	46	SER
3	E	60	LEU

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Mol	Chain	Res	Type
3	E	138	ARG
3	F	11	THR
3	F	41	THR
3	F	44	ARG
3	F	133	ARG
3	F	164	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	78	GLN
1	A	83	GLN
1	A	90	ASN
1	A	100	ASN
1	A	108	ASN
1	A	155	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	412	ASN
1	A	413	HIS
1	A	439	HIS
1	A	442	ASN
1	A	486	HIS
1	B	26	GLN
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	205	GLN
1	B	214	ASN

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Mol	Chain	Res	Type
1	B	227	ASN
1	B	249	ASN
1	B	268	ASN
1	B	273	ASN
1	B	278	GLN
1	B	279	GLN
1	B	343	HIS
1	B	344	HIS
1	B	413	HIS
1	B	439	HIS
1	B	451	GLN
1	B	486	HIS
1	B	516	ASN
1	B	527	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	98	HIS
2	D	125	GLN
2	D	161	ASN
2	D	266	GLN
2	D	285	GLN
2	D	293	GLN
2	D	296	GLN
2	D	301	ASN
2	D	379	GLN
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	111	HIS
3	F	144	ASN

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Mol	Chain	Res	Type
3	F	158	GLN
3	F	167	GLN

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 8 ligands modelled in this entry, 8 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%)	-0.02	13 (2%) 58 62	18, 30, 51, 74	0
1	B	510/527 (96%)	0.03	8 (1%) 70 74	19, 32, 52, 66	0
2	C	388/389 (99%)	-0.50	1 (0%) 90 91	15, 23, 39, 58	0
2	D	387/389 (99%)	0.68	39 (10%) 12 14	20, 40, 64, 73	0
3	E	167/170 (98%)	-0.28	6 (3%) 46 50	17, 26, 41, 74	0
3	F	168/170 (98%)	1.22	30 (17%) 3 4	32, 50, 68, 76	0
All	All	2131/2172 (98%)	0.11	97 (4%) 37 42	15, 32, 58, 76	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	83	PHE	5.3
2	D	352	ILE	4.2
3	F	118	TYR	3.7
2	D	384	VAL	3.5
3	F	28	ALA	3.5
3	F	82	ALA	3.5
2	D	380	ILE	3.4
2	D	332	LEU	3.4
3	E	4	LEU	3.4
1	B	53	ALA	3.3
2	D	388	LEU	3.2
3	E	169	PRO	3.2
3	F	122	ILE	3.2
1	B	403	ILE	3.2
3	F	41	THR	3.1
1	A	317	TRP	3.1
2	D	385	LEU	3.1
1	B	244	LEU	3.0
2	D	223	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
2	D	339	PHE	3.0
3	F	25	LEU	2.9
2	D	145	ILE	2.9
3	F	72	PHE	2.9
3	F	20	ALA	2.9
3	F	69	ALA	2.9
1	A	17	ASN	2.8
2	D	375	ALA	2.8
2	D	387	GLY	2.8
1	A	244	LEU	2.8
3	F	70	ARG	2.8
1	A	318	ILE	2.8
3	E	168	SER	2.8
1	A	251	TYR	2.8
3	F	71	ALA	2.7
3	F	67	LEU	2.7
2	D	371	ILE	2.7
3	F	19	ILE	2.7
3	F	24	THR	2.6
2	D	357	TYR	2.6
2	D	270	PRO	2.6
2	D	381	VAL	2.6
2	D	320	TRP	2.6
2	D	330	ALA	2.5
3	F	77	PHE	2.5
2	C	389	LYS	2.5
2	D	144	PHE	2.5
3	F	75	VAL	2.5
1	B	54	ASN	2.5
2	D	221	GLY	2.5
3	F	164	VAL	2.4
1	A	310	TYR	2.4
3	F	60	LEU	2.4
1	A	316	ILE	2.4
3	F	170	HIS	2.4
1	A	54	ASN	2.4
1	B	256	SER	2.4
2	D	222	GLU	2.4
2	D	372	ASP	2.4
2	D	373	PHE	2.4
3	F	163	VAL	2.4
3	F	127	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	19	ALA	2.3
2	D	383	ALA	2.3
2	D	386	ALA	2.3
1	A	214	ASN	2.3
2	D	338	LEU	2.3
3	F	23	ASN	2.3
3	F	3	LYS	2.3
3	F	16	VAL	2.3
2	D	148	TYR	2.3
3	F	79	HIS	2.3
2	D	204	VAL	2.3
2	D	363	TRP	2.3
1	A	435	THR	2.3
1	A	432	GLY	2.3
2	D	273	GLY	2.3
3	F	32	LEU	2.3
1	B	317	TRP	2.3
2	D	347	THR	2.2
1	B	320	ARG	2.2
1	A	302	VAL	2.2
2	D	341	LYS	2.2
3	E	3	LYS	2.2
2	D	340	ALA	2.2
2	D	356	LEU	2.2
3	F	128	PHE	2.2
2	D	216	ALA	2.2
2	D	140	TRP	2.2
3	E	153	GLU	2.1
2	D	264	PHE	2.1
3	F	64	VAL	2.1
2	D	212	ALA	2.1
3	F	80	LYS	2.1
1	B	39	PHE	2.1
2	D	251	VAL	2.0
3	E	31	MET	2.0
2	D	377	ARG	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
4	FE2	A	5002	1/1	0.90	0.10	63,63,63,63	0
5	CA	C	5006	1/1	0.92	0.07	53,53,53,53	0
4	FE2	B	5004	1/1	0.93	0.08	66,66,66,66	0
5	CA	C	5008	1/1	0.93	0.07	55,55,55,55	0
4	FE2	A	5001	1/1	0.97	0.07	37,37,37,37	0
4	FE2	B	5003	1/1	0.98	0.04	34,34,34,34	0
5	CA	C	5007	1/1	0.98	0.06	39,39,39,39	0
5	CA	A	5005	1/1	0.98	0.06	37,37,37,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.