



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:10 AM UTC

PDB ID : 1XVF / pdb_00001xvf
Title : soluble methane monooxygenase hydroxylase: chloropropanol soaked structure
Authors : Sazinsky, M.H.; Lippard, S.J.
Deposited on : 2004-10-27
Resolution : 2.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

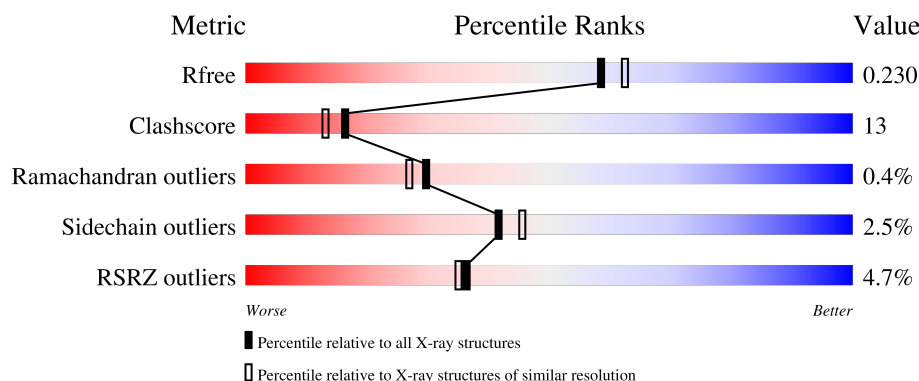
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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% 72% 22% • •
1	B	527	2% 66% 27% • •
2	C	389	0% 78% 20% •
2	D	389	8% 69% 28% •
3	E	170	3% 81% 14% • • •

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Mol	Chain	Length	Quality of chain
3	F	170	21% 66% 28% • •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	3CL	A	1300	-	X	-	-
5	3CL	B	1303	-	X	-	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 18639 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	510	Total	C	N	O	S	0	0	0
			4138	2649	709	762	18			
1	B	510	Total	C	N	O	S	0	0	0
			4137	2646	711	762	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
			3163	2036	545	574	8			
2	D	388	Total	C	N	O	S	0	0	0
			3151	2028	543	572	8			

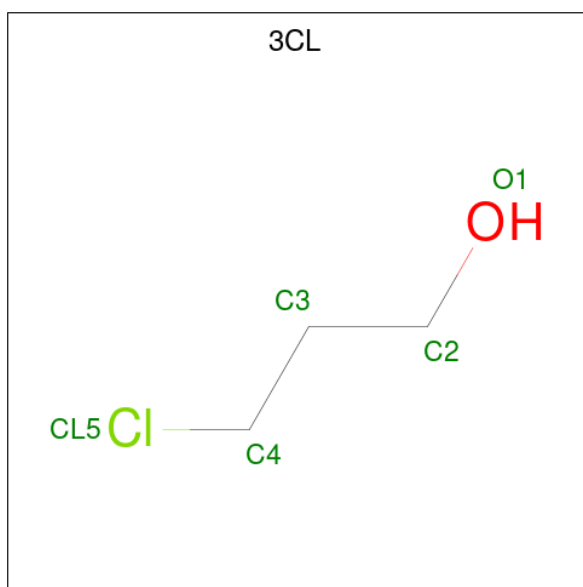
- Molecule 3 is a protein called Methane monooxygenase component A gamma chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	166	Total	C	N	O	S	0	0	0
			1364	864	245	250	5			
3	F	166	Total	C	N	O	S	0	0	0
			1358	860	243	250	5			

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

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

- Molecule 5 is 3-CHLOROPROPANOL (CCD ID: 3CL) (formula: C₃H₇ClO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	Cl	O	0	0
			5	3	1	1		
5	A	1	Total	C	Cl	O	0	0
			5	3	1	1		
5	A	1	Total	C	Cl	O	0	1
			5	3	1	1		
5	A	1	Total	C	Cl	O	0	1
			5	3	1	1		
5	B	1	Total	C	Cl	O	0	0
			5	3	1	1		
5	B	1	Total	C	Cl	O	0	0
			5	3	1	1		
5	B	1	Total	C	Cl	O	0	0
			5	3	1	1		
5	D	1	Total	C	Cl	O	0	0
			5	3	1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	289	Total	O	0	0
			289	289		
6	B	283	Total	O	0	0
			283	283		
6	C	300	Total	O	0	0
			300	300		
6	D	186	Total	O	0	0
			186	186		

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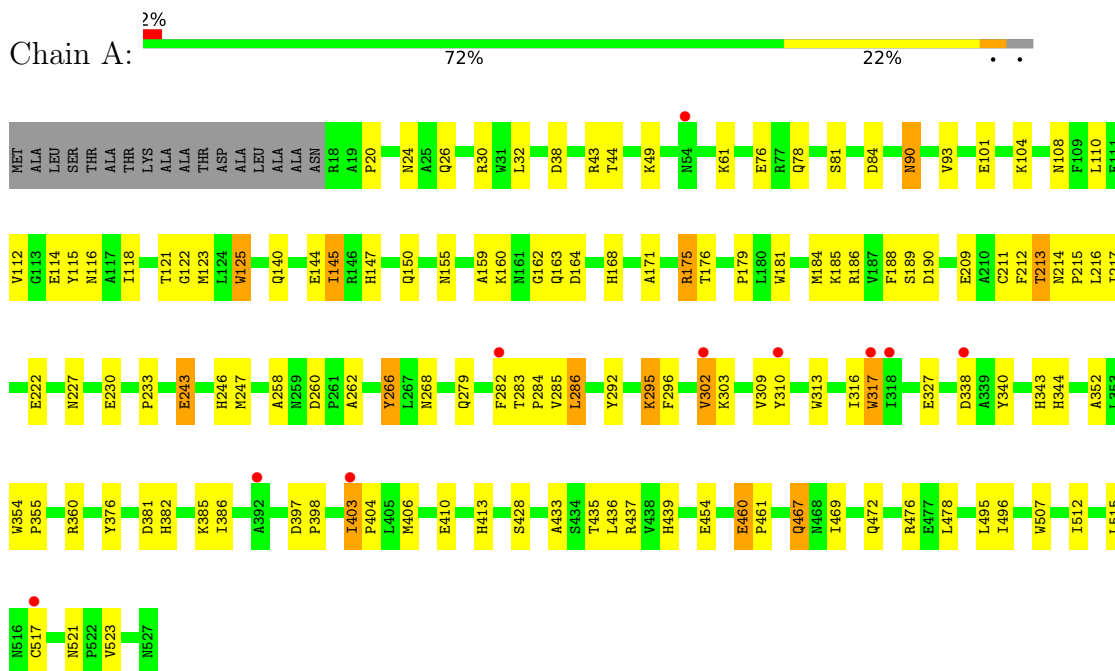
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	160	Total 160	O 160	0	0
6	F	66	Total 66	O 66	0	0

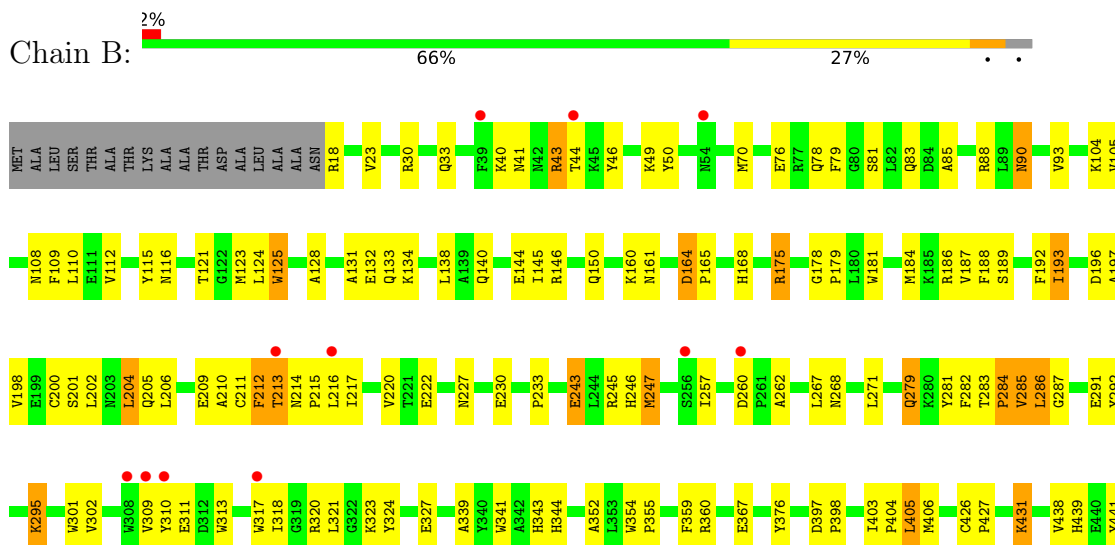
3 Residue-property plots [i](#)

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

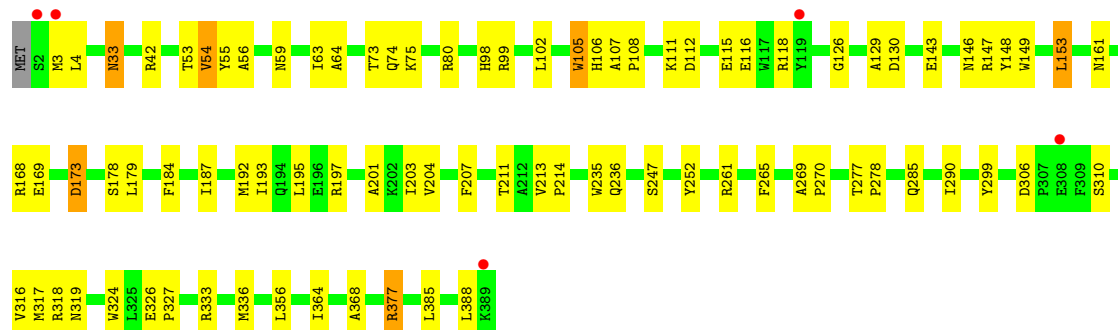
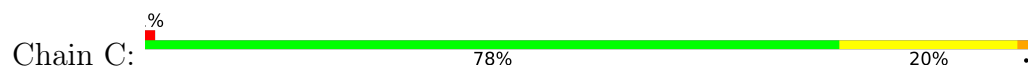


- Molecule 1: Methane monooxygenase component A alpha chain

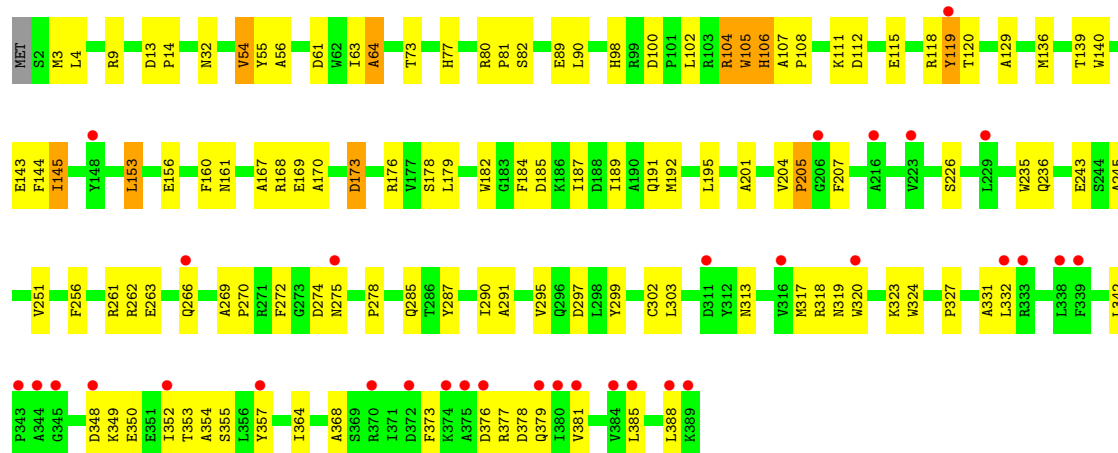




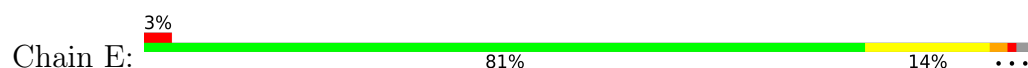
• Molecule 2: Methane monooxygenase component A beta chain



• Molecule 2: Methane monooxygenase component A beta chain



• Molecule 3: Methane monooxygenase component A gamma chain



• 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	70.83Å 171.47Å 221.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 2.00 19.98 – 2.00	Depositor EDS
% Data completeness (in resolution range)	93.8 (19.98-2.00) 93.8 (19.98-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.03 (at 2.01Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.202 , 0.230 0.201 , 0.230	Depositor DCC
R_{free} test set	16940 reflections (9.37%)	wwPDB-VP
Wilson B-factor (Å ²)	24.2	Xtriage
Anisotropy	0.218	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 51.0	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	18639	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.31% 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: FE, 3CL

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	0.39	0/4263	0.94	21/5797 (0.4%)
1	B	0.39	0/4262	0.95	22/5796 (0.4%)
2	C	0.42	0/3259	0.90	13/4430 (0.3%)
2	D	0.39	0/3247	0.93	14/4417 (0.3%)
3	E	0.46	0/1392	1.84	9/1876 (0.5%)
3	F	0.33	0/1387	0.83	3/1873 (0.2%)
All	All	0.40	0/17810	1.02	82/24189 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	3

There are no bond length outliers.

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	120	PRO	CA-C-N	47.77	179.55	119.84
3	E	120	PRO	C-N-CA	47.77	179.55	119.84
2	D	119	TYR	O-C-N	12.61	135.20	122.09
3	E	120	PRO	C-N-CD	-11.62	77.35	125.00
1	B	339	ALA	N-CA-C	8.87	120.72	111.14
1	B	496	ILE	N-CA-C	-7.87	103.13	110.53
3	E	167	GLN	N-CA-C	-7.87	97.32	109.52
1	A	164	ASP	CA-C-N	7.76	127.39	119.56
1	A	164	ASP	C-N-CA	7.76	127.39	119.56
1	B	285	VAL	N-CA-C	7.75	117.86	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	204	VAL	CA-C-N	7.53	129.25	119.84
2	D	204	VAL	C-N-CA	7.53	129.25	119.84
2	D	373	PHE	N-CA-C	-7.50	97.83	109.76
3	E	130	ASP	N-CA-C	-7.42	103.27	111.36
1	B	309	VAL	N-CA-C	7.38	117.36	110.42
2	C	105	TRP	N-CA-C	-7.35	99.36	109.95
1	B	431	LYS	N-CA-C	-7.30	104.52	113.50
2	C	149	TRP	N-CA-C	-6.95	103.79	111.36
3	E	121	PRO	CA-N-CD	-6.86	102.40	112.00
1	B	164	ASP	CA-C-N	6.86	126.82	119.28
1	B	164	ASP	C-N-CA	6.86	126.82	119.28
3	F	39	HIS	N-CA-C	6.85	122.60	112.94
1	B	426	CYS	CA-C-N	6.83	127.10	119.32
1	B	426	CYS	C-N-CA	6.83	127.10	119.32
2	D	119	TYR	CB-CG-CD1	-6.65	110.83	120.80
2	D	119	TYR	CB-CG-CD2	6.65	130.77	120.80
1	A	309	VAL	N-CA-C	6.64	116.80	110.42
2	D	105	TRP	N-CA-C	-6.59	100.21	110.17
1	B	93	VAL	N-CA-C	6.56	117.90	111.67
2	C	106	HIS	N-CA-C	6.48	118.89	111.11
1	A	285	VAL	N-CA-C	6.36	116.99	110.82
1	A	397	ASP	CA-C-N	6.29	125.97	119.56
1	A	397	ASP	C-N-CA	6.29	125.97	119.56
1	A	212	PHE	N-CA-C	6.17	120.89	112.68
2	C	236	GLN	N-CA-C	6.08	120.86	113.38
2	D	106	HIS	N-CA-C	6.03	118.35	111.11
2	D	120	THR	N-CA-C	-6.03	104.61	111.07
1	A	213	THR	N-CA-C	6.02	117.51	111.07
2	C	169	GLU	N-CA-C	6.00	120.77	113.38
1	A	496	ILE	N-CA-C	-6.00	104.89	110.53
1	A	145	ILE	N-CA-C	-5.83	104.83	110.72
2	C	252	TYR	N-CA-C	5.83	117.33	110.97
2	C	148	TYR	N-CA-C	5.81	118.83	111.69
3	E	39	HIS	N-CA-C	5.80	122.31	113.61
1	A	258	ALA	N-CA-C	5.68	117.47	111.28
2	D	54	VAL	N-CA-C	5.67	116.58	108.93
1	B	478	LEU	N-CA-C	5.66	117.92	111.02
1	A	243	GLU	N-CA-C	5.65	118.20	111.71
1	B	295	LYS	N-CA-C	-5.64	104.00	111.96
1	A	266	TYR	N-CA-C	5.63	121.57	114.31
1	A	122	GLY	N-CA-C	-5.62	105.58	112.77
1	B	145	ILE	N-CA-C	-5.59	105.07	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	118	TYR	N-CA-C	5.51	120.69	113.30
2	D	56	ALA	N-CA-C	-5.51	105.43	111.82
1	B	267	LEU	N-CA-C	5.50	117.73	111.02
3	F	6	ILE	N-CA-C	5.49	120.77	109.34
2	C	63	ILE	N-CA-C	-5.44	98.63	107.28
1	A	295	LYS	N-CA-C	-5.43	104.30	111.96
1	A	317	TRP	N-CA-C	5.41	117.60	111.11
1	B	212	PHE	N-CA-C	5.40	119.53	112.13
3	F	118	TYR	N-CA-C	5.38	119.83	112.88
2	D	104	ARG	N-CA-C	5.33	117.00	108.41
1	B	490	SER	N-CA-C	5.33	118.57	111.75
2	C	377	ARG	N-CA-C	5.33	117.09	111.28
1	B	204	LEU	N-CA-C	5.32	116.94	111.03
2	C	53	THR	N-CA-C	5.31	119.99	112.93
2	D	119	TYR	CA-C-O	-5.29	115.24	120.90
2	C	54	VAL	N-CA-C	5.27	116.48	109.37
1	A	460	GLU	CA-C-N	5.26	125.31	119.32
1	A	460	GLU	C-N-CA	5.26	125.31	119.32
1	B	247	MET	N-CA-C	-5.25	105.45	111.07
1	B	193	ILE	N-CA-C	5.24	120.24	109.34
1	B	243	GLU	N-CA-C	5.24	117.74	111.71
1	A	162	GLY	N-CA-C	5.20	120.56	112.60
2	C	265	PHE	N-CA-C	5.20	117.02	111.36
1	B	178	GLY	CA-C-N	5.18	124.68	119.19
1	B	178	GLY	C-N-CA	5.18	124.68	119.19
2	D	318	ARG	N-CA-C	-5.16	105.65	111.28
1	A	104	LYS	N-CA-C	-5.15	105.56	111.07
2	C	56	ALA	N-CA-C	-5.14	105.80	111.71
1	A	478	LEU	N-CA-C	5.09	117.22	111.11
3	E	79	HIS	N-CA-C	5.08	121.22	113.61

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	175	ARG	Sidechain
1	B	359	PHE	Mainchain
1	B	88	ARG	Sidechain

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	4138	0	3897	110	0
1	B	4137	0	3888	145	0
2	C	3163	0	2986	71	0
2	D	3151	0	2960	90	0
3	E	1364	0	1352	25	0
3	F	1358	0	1335	51	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	20	0	18	6	0
5	B	15	0	14	2	0
5	D	5	0	5	0	0
6	A	289	0	0	10	0
6	B	283	0	0	5	0
6	C	300	0	0	5	0
6	D	186	0	0	3	0
6	E	160	0	0	1	0
6	F	66	0	0	7	0
All	All	18639	0	16455	439	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 (439) 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:403:ILE:HD11	1:B:515:LEU:CD1	1.57	1.32
1:B:403:ILE:CD1	1:B:515:LEU:CD1	2.20	1.19
1:B:403:ILE:HD11	1:B:515:LEU:HD11	1.21	1.10
2:C:318:ARG:NH2	6:C:614:HOH:O	1.89	1.05
1:B:352:ALA:HA	1:B:404:PRO:HB2	1.45	0.98
3:F:80:LYS:HE2	3:F:84:GLY:HA2	1.48	0.96
1:B:213:THR:OG1	5:B:1303:3CL:CL5	2.23	0.94
1:B:78:GLN:HE22	1:B:150:GLN:HE21	1.16	0.94
1:B:216:LEU:HD13	1:B:286:LEU:HD11	1.50	0.92
3:F:39:HIS:HD2	6:F:848:HOH:O	1.51	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:GLU:OE2	6:A:2212:HOH:O	1.87	0.91
1:B:403:ILE:CD1	1:B:515:LEU:HD13	2.00	0.88
1:A:517:CYS:SG	6:A:2223:HOH:O	2.30	0.88
1:A:78:GLN:HE22	1:A:150:GLN:HE21	1.19	0.86
1:A:467:GLN:HG3	6:A:2125:HOH:O	1.77	0.85
1:B:44:THR:HG22	1:B:46:TYR:H	1.39	0.85
3:F:41:THR:O	3:F:44:ARG:HD2	1.77	0.85
3:E:41:THR:O	3:E:44:ARG:HD2	1.78	0.84
2:C:261:ARG:HE	2:C:285:GLN:HE22	1.26	0.83
1:A:352:ALA:HA	1:A:404:PRO:HB2	1.60	0.82
2:D:167:ALA:O	2:D:176:ARG:NH1	2.13	0.82
2:C:102:LEU:HD12	2:C:290:ILE:HG23	1.61	0.80
1:A:435:THR:HG21	1:A:437:ARG:HE	1.47	0.80
1:B:108:ASN:HD21	1:B:175:ARG:HH11	1.30	0.79
3:F:146:ASN:OD1	6:F:863:HOH:O	2.02	0.77
1:B:179:PRO:HB3	1:B:469:ILE:HD13	1.66	0.77
2:D:319:ASN:OD1	3:F:78:ARG:HD3	1.84	0.77
2:D:261:ARG:HE	2:D:285:GLN:HE22	1.29	0.77
1:B:403:ILE:HD11	1:B:515:LEU:HD12	1.63	0.77
2:C:102:LEU:CD1	2:C:290:ILE:HG23	2.15	0.76
2:C:333:ARG:HD3	6:C:536:HOH:O	1.86	0.75
1:B:33:GLN:HE22	1:B:132:GLU:H	1.31	0.75
2:C:3:MET:HG3	2:C:4:LEU:H	1.52	0.75
3:E:22:LEU:HD11	3:E:31:MET:SD	2.27	0.75
1:A:435:THR:CG2	1:A:437:ARG:HE	1.99	0.74
3:E:98:MET:HE1	3:E:107:ALA:CB	2.17	0.74
3:F:13:ASP:O	3:F:16:VAL:HG22	1.86	0.74
1:B:210:ALA:HA	1:B:247:MET:HE1	1.70	0.74
1:B:123:MET:HE3	1:B:197:ALA:HA	1.68	0.74
2:D:100:ASP:OD1	2:D:104:ARG:HD3	1.89	0.73
3:F:153:GLU:H	3:F:153:GLU:CD	1.95	0.73
1:B:214:ASN:HB3	1:B:215:PRO:HD3	1.70	0.72
1:A:227:ASN:HD21	1:A:295:LYS:H	1.37	0.72
2:C:336:MET:HE3	2:C:388:LEU:HG	1.70	0.72
2:D:256:PHE:HA	2:D:332:LEU:HD21	1.72	0.71
3:E:165:HIS:HE1	3:E:167:GLN:HE21	1.38	0.71
2:D:364:ILE:HA	2:D:368:ALA:HB3	1.70	0.71
3:F:4:LEU:HD21	3:F:10:ASP:H	1.53	0.71
1:B:108:ASN:ND2	1:B:175:ARG:HH11	1.88	0.71
1:B:268:ASN:HD21	1:B:327:GLU:H	1.39	0.71
1:B:403:ILE:HD12	1:B:515:LEU:CD1	2.20	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:19:ILE:HG12	3:E:60:LEU:HD13	1.73	0.70
3:E:24:THR:HG22	3:E:27:LYS:H	1.56	0.70
1:A:476:ARG:HD3	3:E:4:LEU:HG	1.73	0.70
3:F:58:ALA:O	3:F:62:GLU:HG3	1.91	0.70
1:B:70:MET:HE1	1:B:245:ARG:NH1	2.06	0.70
2:C:270:PRO:HB3	2:D:270:PRO:HB3	1.75	0.69
1:B:281:TYR:O	1:B:284:PRO:HD2	1.92	0.69
2:D:192:MET:HA	2:D:192:MET:HE2	1.75	0.69
1:B:439:HIS:HB3	3:F:161:VAL:HG21	1.73	0.68
2:D:323:LYS:HB2	3:F:78:ARG:NH1	2.08	0.68
1:B:33:GLN:NE2	1:B:132:GLU:H	1.90	0.68
1:A:268:ASN:HD21	1:A:327:GLU:H	1.43	0.67
2:C:146:ASN:HD21	2:C:197:ARG:HH21	1.42	0.67
1:A:338:ASP:OD2	1:A:433:ALA:HB2	1.94	0.67
3:E:165:HIS:HE1	3:E:167:GLN:NE2	1.92	0.67
1:A:209:GLU:HA	1:A:213:THR:HB	1.77	0.67
2:D:378:ASP:OD2	6:D:1443:HOH:O	2.12	0.66
2:D:102:LEU:CD1	2:D:290:ILE:HG23	2.26	0.65
1:A:292:TYR:OH	1:A:344:HIS:HD2	1.80	0.65
1:B:206:LEU:HD11	1:B:321:LEU:HD11	1.79	0.65
2:D:354:ALA:O	6:D:1441:HOH:O	2.14	0.65
1:B:213:THR:O	1:B:217:ILE:HG12	1.97	0.65
2:D:102:LEU:HD12	2:D:290:ILE:HG23	1.78	0.64
1:B:286:LEU:HD23	5:B:1305:3CL:CL5	2.34	0.64
1:A:213:THR:O	1:A:217:ILE:HG12	1.98	0.64
1:B:210:ALA:CA	1:B:247:MET:HE1	2.27	0.64
1:B:403:ILE:CD1	1:B:515:LEU:HD12	2.21	0.64
2:C:107:ALA:HB3	2:C:108:PRO:HD3	1.78	0.64
3:E:165:HIS:CE1	3:E:167:GLN:HE21	2.16	0.64
3:F:4:LEU:HD11	3:F:10:ASP:OD2	1.98	0.64
1:B:227:ASN:HD21	1:B:295:LYS:H	1.45	0.64
1:B:403:ILE:HD12	1:B:515:LEU:HD13	1.80	0.64
2:D:357:TYR:CE1	2:D:381:VAL:HG11	2.33	0.63
2:D:153:LEU:C	2:D:153:LEU:HD12	2.24	0.63
1:B:439:HIS:HD2	3:F:163:VAL:HA	1.63	0.63
1:A:188:PHE:CE2	5:A:2002[B]:3CL:CL5	2.88	0.63
1:B:160:LYS:HE3	1:B:161:ASN:OD1	1.99	0.63
1:A:108:ASN:HD21	1:A:175:ARG:HE	1.46	0.63
1:B:403:ILE:CD1	1:B:515:LEU:HD11	2.06	0.63
1:B:489:ARG:HD2	1:B:495:LEU:O	1.99	0.63
2:D:187:ILE:O	2:D:191:GLN:HG3	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:326:GLU:HB3	2:C:327:PRO:HD3	1.80	0.62
1:B:165:PRO:HG3	6:B:1478:HOH:O	1.98	0.62
2:C:261:ARG:HE	2:C:285:GLN:NE2	1.95	0.62
1:A:84:ASP:HB3	1:B:81:SER:OG	1.99	0.62
3:F:57:GLU:O	3:F:61:GLU:HG3	1.99	0.62
3:F:151:PRO:HB2	3:F:153:GLU:OE1	2.00	0.62
2:C:333:ARG:HD2	6:C:459:HOH:O	1.98	0.62
1:A:214:ASN:HB3	1:A:215:PRO:HD3	1.81	0.62
2:D:90:LEU:HD13	2:D:303:LEU:HD13	1.82	0.61
2:C:3:MET:HG3	2:C:4:LEU:N	2.14	0.61
2:D:61:ASP:OD1	3:F:7:HIS:HD2	1.83	0.61
1:A:76:GLU:HG2	1:B:76:GLU:OE2	2.01	0.61
1:A:260:ASP:OD2	1:A:262:ALA:HB3	2.01	0.61
2:C:336:MET:CE	2:C:385:LEU:HD23	2.31	0.61
3:F:44:ARG:NH2	6:F:849:HOH:O	2.21	0.61
2:D:261:ARG:HE	2:D:285:GLN:NE2	1.98	0.60
3:E:98:MET:HE2	3:E:138:ARG:CG	2.31	0.60
1:A:406:MET:O	1:A:410:GLU:HG3	2.01	0.60
3:F:44:ARG:HD3	3:F:47:TYR:CZ	2.36	0.60
1:A:495:LEU:HD11	1:A:512:ILE:HG13	1.83	0.60
1:B:210:ALA:N	1:B:247:MET:HE1	2.16	0.60
1:A:279:GLN:OE1	6:A:2104:HOH:O	2.17	0.60
2:C:213:VAL:HB	2:C:214:PRO:HD3	1.83	0.60
1:B:439:HIS:HB3	3:F:161:VAL:CG2	2.32	0.60
1:B:438:VAL:HB	3:F:164:VAL:HG22	1.83	0.59
2:C:247:SER:HG	2:C:324:TRP:CD1	2.20	0.59
1:B:405:LEU:HG	1:B:406:MET:N	2.17	0.59
3:E:98:MET:HE1	3:E:107:ALA:HB1	1.82	0.59
1:B:50:TYR:CD2	1:B:257:ILE:HD12	2.37	0.59
2:D:291:ALA:O	2:D:295:VAL:HG23	2.01	0.59
1:B:283:THR:HB	1:B:284:PRO:HD3	1.85	0.59
1:A:227:ASN:ND2	1:A:295:LYS:H	2.01	0.58
2:D:324:TRP:C	2:D:327:PRO:HD2	2.27	0.58
1:A:188:PHE:CZ	1:A:282:PHE:HZ	2.20	0.58
1:A:282:PHE:HD1	1:A:286:LEU:HD23	1.69	0.58
1:A:403:ILE:HD13	1:A:515:LEU:HD11	1.84	0.58
3:E:120:PRO:HD3	3:E:128:PHE:CG	2.39	0.58
1:A:155:ASN:HD22	1:A:168:HIS:HD2	1.51	0.58
3:F:144:ASN:O	6:F:862:HOH:O	2.16	0.58
3:E:98:MET:HE1	3:E:107:ALA:HB2	1.84	0.58
1:A:184:MET:HE3	1:A:184:MET:HA	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:302:VAL:HG13	1:B:376:TYR:HE2	1.68	0.58
1:A:175:ARG:HG3	1:A:181:TRP:CD2	2.38	0.58
1:B:465:GLU:OE2	6:B:1491:HOH:O	2.17	0.58
1:B:78:GLN:NE2	1:B:150:GLN:HE21	1.96	0.57
1:B:211:CYS:HB2	1:B:313:TRP:CD1	2.39	0.57
2:C:112:ASP:OD1	2:D:118:ARG:NH2	2.38	0.57
2:C:146:ASN:ND2	2:C:197:ARG:HH21	2.02	0.57
2:C:59:ASN:ND2	6:C:603:HOH:O	2.15	0.57
3:F:98:MET:HG3	3:F:138:ARG:HG2	1.87	0.57
1:B:495:LEU:HD11	1:B:512:ILE:HG13	1.88	0.56
2:C:3:MET:HE2	2:C:4:LEU:HD13	1.88	0.56
1:B:43:ARG:HD2	1:B:43:ARG:C	2.30	0.56
2:D:107:ALA:HB3	2:D:108:PRO:HD3	1.86	0.56
1:A:439:HIS:HE1	1:A:454:GLU:OE1	1.88	0.56
2:D:349:LYS:HA	2:D:352:ILE:HG12	1.87	0.56
3:F:9:ASN:OD1	3:F:11:THR:HG23	2.05	0.56
2:C:201:ALA:HA	2:C:207:PHE:HB3	1.88	0.56
1:B:292:TYR:OH	1:B:344:HIS:HD2	1.89	0.56
1:A:186:ARG:HA	2:C:73:THR:OG1	2.06	0.55
1:B:123:MET:HE1	1:B:200:CYS:SG	2.46	0.55
1:B:461:PRO:HG2	3:F:159:ARG:CZ	2.36	0.55
1:A:140:GLN:O	1:A:144:GLU:HG2	2.07	0.55
1:B:344:HIS:HE1	1:B:376:TYR:CD2	2.24	0.55
3:E:41:THR:O	3:E:44:ARG:CD	2.51	0.55
1:B:164:ASP:OD1	1:B:489:ARG:NH2	2.40	0.55
1:B:206:LEU:HD23	1:B:271:LEU:HD13	1.88	0.55
2:C:3:MET:CG	2:C:4:LEU:H	2.17	0.55
2:D:140:TRP:NE1	2:D:145:ILE:HD11	2.22	0.55
1:B:291:GLU:OE1	1:B:343:HIS:HE1	1.89	0.55
1:B:490:SER:OG	2:D:32:ASN:HB2	2.06	0.55
1:A:413:HIS:HD2	1:A:428:SER:OG	1.89	0.55
1:A:49:LYS:HD3	3:E:144:ASN:HD22	1.72	0.54
1:B:33:GLN:HE21	1:B:33:GLN:HA	1.71	0.54
1:B:198:VAL:O	1:B:202:LEU:HG	2.07	0.54
2:C:111:LYS:O	2:C:115:GLU:HG3	2.07	0.54
2:C:116:GLU:HG2	2:D:119:TYR:CE1	2.43	0.54
1:A:286:LEU:HD22	5:A:1300:3CL:CL5	2.45	0.54
1:B:138:LEU:HD22	2:D:160:PHE:CZ	2.43	0.54
2:D:348:ASP:OD2	2:D:350:GLU:HB2	2.07	0.53
2:C:116:GLU:HG2	2:D:119:TYR:HE1	1.72	0.53
2:D:111:LYS:O	2:D:115:GLU:HG3	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:192:MET:HE2	2:D:192:MET:CA	2.38	0.53
1:B:134:LYS:HD3	2:D:161:ASN:HD21	1.74	0.53
1:B:281:TYR:CZ	1:B:285:VAL:HG21	2.43	0.53
2:D:105:TRP:O	2:D:108:PRO:HD2	2.08	0.53
1:B:49:LYS:HD3	3:F:140:MET:HB3	1.91	0.53
1:B:230:GLU:C	1:B:233:PRO:HD2	2.34	0.53
1:A:184:MET:HE2	1:A:188:PHE:CD2	2.44	0.53
1:A:230:GLU:C	1:A:233:PRO:HD2	2.35	0.52
1:A:461:PRO:HG2	3:E:159:ARG:CZ	2.39	0.52
1:B:398:PRO:HG3	1:B:507:TRP:CD1	2.44	0.52
1:A:243:GLU:O	1:A:247:MET:HG2	2.09	0.52
1:B:184:MET:HE2	1:B:188:PHE:CG	2.43	0.52
2:D:323:LYS:HB2	3:F:78:ARG:HH11	1.72	0.52
1:B:186:ARG:HD3	1:B:186:ARG:C	2.34	0.52
1:A:268:ASN:ND2	1:A:327:GLU:H	2.08	0.52
2:C:153:LEU:C	2:C:153:LEU:HD12	2.34	0.52
2:C:269:ALA:HB3	2:C:270:PRO:HD3	1.91	0.52
3:F:90:VAL:HG11	3:F:118:TYR:CZ	2.45	0.52
1:A:123:MET:HB2	2:C:168:ARG:HD3	1.91	0.52
1:A:185:LYS:O	1:A:189:SER:HB2	2.10	0.52
2:D:82:SER:O	2:D:168:ARG:NH2	2.40	0.52
3:F:19:ILE:HG21	3:F:60:LEU:HD12	1.92	0.52
1:B:466:CYS:HB2	2:D:73:THR:HA	1.92	0.51
2:D:275:ASN:C	2:D:278:PRO:HD2	2.35	0.51
1:B:108:ASN:HD21	1:B:175:ARG:HD3	1.75	0.51
2:D:243:GLU:HB2	2:D:320:TRP:CZ2	2.45	0.51
2:C:3:MET:HG3	2:C:4:LEU:HD13	1.92	0.51
2:C:336:MET:HE2	2:C:385:LEU:HD23	1.93	0.51
1:A:78:GLN:NE2	1:A:150:GLN:HE21	1.99	0.51
3:E:98:MET:HE3	3:E:98:MET:O	2.10	0.51
2:C:277:THR:HB	2:C:278:PRO:HD3	1.93	0.51
3:E:58:ALA:O	3:E:62:GLU:HG3	2.11	0.51
1:A:188:PHE:CZ	5:A:2002[B]:3CL:CL5	3.01	0.51
2:D:54:VAL:O	2:D:55:TYR:HB2	2.11	0.51
3:F:138:ARG:NE	6:F:833:HOH:O	2.13	0.51
1:A:184:MET:HE2	1:A:188:PHE:CG	2.45	0.51
3:F:61:GLU:O	3:F:121:PRO:HG2	2.11	0.51
1:B:403:ILE:CG1	1:B:515:LEU:HD13	2.41	0.50
2:D:185:ASP:O	2:D:189:ILE:HG12	2.11	0.50
1:B:146:ARG:HB2	2:D:106:HIS:CE1	2.46	0.50
1:B:196:ASP:HB2	3:F:140:MET:SD	2.51	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:189:ILE:HD11	2:D:287:TYR:CD1	2.46	0.50
1:A:282:PHE:CD1	1:A:286:LEU:HD23	2.46	0.50
1:A:472:GLN:NE2	6:A:2125:HOH:O	2.44	0.50
1:B:495:LEU:HD11	1:B:512:ILE:CG1	2.41	0.50
2:C:146:ASN:O	2:C:214:PRO:HG3	2.12	0.50
2:C:235:TRP:CD1	2:C:235:TRP:C	2.90	0.50
1:B:193:ILE:O	2:D:168:ARG:NH1	2.44	0.50
2:D:89:GLU:CD	3:F:125:VAL:HG13	2.36	0.50
1:A:61:LYS:NZ	6:A:2215:HOH:O	2.45	0.50
1:B:49:LYS:CE	3:F:144:ASN:HD22	2.24	0.50
1:B:44:THR:HG21	6:B:1395:HOH:O	2.11	0.49
1:A:110:LEU:HD12	5:A:2002[B]:3CL:CL5	2.49	0.49
1:B:43:ARG:HD2	1:B:43:ARG:O	2.12	0.49
1:B:108:ASN:HD21	1:B:175:ARG:CD	2.25	0.49
2:C:192:MET:HE2	2:C:192:MET:HA	1.94	0.49
1:A:32:LEU:HD13	1:A:32:LEU:O	2.10	0.49
1:A:216:LEU:CD1	1:A:286:LEU:HD11	2.43	0.49
1:A:302:VAL:HG22	1:A:376:TYR:CZ	2.47	0.49
1:B:164:ASP:CG	1:B:489:ARG:HH22	2.21	0.49
1:A:32:LEU:HD13	1:A:32:LEU:C	2.37	0.49
3:F:46:SER:OG	3:F:48:GLU:HG2	2.13	0.49
1:B:186:ARG:HD3	1:B:186:ARG:O	2.12	0.49
2:C:161:ASN:HB3	2:C:235:TRP:CE2	2.47	0.49
2:D:118:ARG:O	2:D:119:TYR:C	2.55	0.49
2:D:179:LEU:HD23	2:D:182:TRP:CE3	2.48	0.49
1:A:121:THR:HG21	1:A:140:GLN:CG	2.43	0.49
2:C:98:HIS:HE1	2:C:178:SER:OG	1.95	0.49
2:C:3:MET:CE	2:C:4:LEU:HD13	2.43	0.49
1:B:18:ARG:O	2:D:129:ALA:HA	2.13	0.49
1:B:260:ASP:OD2	1:B:262:ALA:HB3	2.13	0.49
2:D:324:TRP:O	2:D:327:PRO:HD2	2.12	0.49
1:A:114:GLU:CD	1:A:147:HIS:HB3	2.38	0.48
1:A:186:ARG:HD3	1:A:186:ARG:C	2.37	0.48
2:D:235:TRP:CD1	2:D:235:TRP:C	2.91	0.48
1:B:140:GLN:HG3	1:B:246:HIS:CD2	2.48	0.48
1:B:227:ASN:ND2	1:B:295:LYS:H	2.11	0.48
1:A:209:GLU:HG3	5:A:1302[A]:3CL:CL5	2.51	0.48
1:A:521:ASN:OD1	1:A:523:VAL:HG12	2.14	0.48
3:F:23:ASN:C	3:F:23:ASN:HD22	2.21	0.48
1:A:43:ARG:C	1:A:43:ARG:HD2	2.39	0.48
2:C:118:ARG:NH2	2:D:112:ASP:OD1	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:SER:HB3	1:B:85:ALA:HB2	1.96	0.48
1:A:171:ALA:O	1:A:175:ARG:HB3	2.14	0.48
1:B:125:TRP:HE1	2:D:161:ASN:ND2	2.12	0.48
1:B:188:PHE:CE1	1:B:282:PHE:HZ	2.32	0.48
1:B:354:TRP:CG	1:B:355:PRO:HD3	2.49	0.48
2:D:184:PHE:O	2:D:187:ILE:HG22	2.14	0.48
1:A:184:MET:HE2	1:A:188:PHE:HB2	1.94	0.47
1:A:398:PRO:HG3	1:A:507:TRP:CD1	2.48	0.47
1:A:175:ARG:HG2	1:A:176:THR:N	2.27	0.47
1:A:381:ASP:HA	1:A:385:LYS:HE2	1.96	0.47
1:B:33:GLN:HA	1:B:131:ALA:HB3	1.97	0.47
1:B:367:GLU:HG3	6:B:1383:HOH:O	2.13	0.47
2:C:211:THR:C	2:C:214:PRO:HD2	2.40	0.47
2:D:102:LEU:HB2	2:D:104:ARG:HD2	1.95	0.47
2:C:319:ASN:OD1	3:E:78:ARG:HD3	2.14	0.47
2:C:333:ARG:HD3	6:C:533:HOH:O	2.14	0.47
2:D:80:ARG:HD2	2:D:81:PRO:O	2.14	0.47
1:A:101:GLU:CD	1:A:360:ARG:HD3	2.39	0.47
1:B:246:HIS:CD2	1:B:246:HIS:N	2.82	0.47
2:C:211:THR:O	2:C:214:PRO:HD2	2.14	0.47
1:A:344:HIS:HE1	1:A:376:TYR:CD2	2.33	0.47
1:B:23:VAL:HB	2:D:195:LEU:HD11	1.96	0.47
1:B:344:HIS:HE1	1:B:376:TYR:CE2	2.33	0.47
1:A:211:CYS:HB2	1:A:313:TRP:CD1	2.50	0.47
1:A:76:GLU:OE1	1:B:76:GLU:HG2	2.15	0.47
1:B:313:TRP:CZ2	1:B:318:ILE:HD11	2.50	0.47
1:A:115:TYR:OH	2:C:173:ASP:HA	2.15	0.46
2:C:105:TRP:O	2:C:108:PRO:HD2	2.15	0.46
3:F:74:GLU:O	3:F:78:ARG:HG3	2.16	0.46
1:A:382:HIS:O	1:A:386:ILE:HG13	2.15	0.46
1:B:184:MET:HE3	1:B:184:MET:HA	1.98	0.46
3:F:88:LYS:HB2	3:F:127:TYR:CE2	2.51	0.46
1:A:125:TRP:HE1	2:C:161:ASN:ND2	2.12	0.46
1:B:144:GLU:OE2	1:B:144:GLU:HA	2.16	0.46
1:A:24:ASN:OD1	1:A:26:GLN:HG2	2.15	0.46
1:A:216:LEU:HD13	1:A:286:LEU:HD11	1.98	0.46
1:B:175:ARG:NE	1:B:181:TRP:CZ2	2.83	0.46
2:D:385:LEU:O	2:D:388:LEU:HD12	2.16	0.46
1:A:209:GLU:CG	5:A:1302[A]:3CL:CL5	3.01	0.46
2:C:306:ASP:O	2:C:310:SER:HB2	2.16	0.46
3:E:4:LEU:HG	3:E:4:LEU:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:GLU:HA	1:A:222:GLU:OE1	2.16	0.45
2:C:203:ILE:HG13	2:C:204:VAL:HG23	1.97	0.45
2:D:226:SER:HB2	2:D:331:ALA:HA	1.98	0.45
1:B:192:PHE:CE2	1:B:204:LEU:HA	2.51	0.45
1:A:159:ALA:O	2:C:33:ASN:HB2	2.16	0.45
1:B:484:GLU:OE1	3:F:6:ILE:HB	2.17	0.45
1:B:302:VAL:HG13	1:B:376:TYR:CE2	2.49	0.45
1:B:317:TRP:CE3	1:B:320:ARG:NH2	2.85	0.45
1:B:403:ILE:CG1	1:B:515:LEU:CD1	2.92	0.45
2:C:146:ASN:HB2	2:C:207:PHE:CZ	2.52	0.45
2:D:349:LYS:HG3	2:D:352:ILE:HD11	1.98	0.45
1:A:108:ASN:HD21	1:A:175:ARG:NE	2.12	0.45
1:A:266:TYR:HB3	6:A:2141:HOH:O	2.16	0.45
1:B:230:GLU:OE2	2:D:9:ARG:HD3	2.17	0.45
1:B:403:ILE:HG13	1:B:515:LEU:HD13	1.99	0.45
2:D:156:GLU:HA	2:D:156:GLU:OE2	2.16	0.45
1:A:44:THR:HG22	6:A:2053:HOH:O	2.16	0.45
1:A:354:TRP:CG	1:A:355:PRO:HD3	2.52	0.45
2:D:376:ASP:OD2	2:D:379:GLN:HG2	2.16	0.45
1:B:184:MET:HE2	1:B:188:PHE:CD2	2.52	0.45
1:B:186:ARG:HA	2:D:73:THR:OG1	2.16	0.45
3:F:75:VAL:HG23	6:F:1171:HOH:O	2.17	0.45
1:A:20:PRO:HG3	2:C:129:ALA:HB2	1.99	0.45
2:D:313:ASN:HB3	2:D:317:MET:HE2	1.98	0.45
1:B:41:ASN:O	2:D:236:GLN:HB3	2.17	0.45
2:D:201:ALA:HA	2:D:207:PHE:HB3	1.99	0.45
1:A:303:LYS:HE3	1:A:303:LYS:HB2	1.79	0.44
1:A:495:LEU:HD11	1:A:512:ILE:CG1	2.46	0.44
2:C:54:VAL:O	2:C:55:TYR:HB2	2.17	0.44
1:B:115:TYR:OH	2:D:173:ASP:HA	2.17	0.44
2:C:299:TYR:O	2:C:317:MET:HE1	2.17	0.44
1:A:118:ILE:HD13	1:A:145:ILE:HG12	1.99	0.44
2:C:126:GLY:O	2:C:130:ASP:HB2	2.17	0.44
1:B:108:ASN:HD21	1:B:175:ARG:NH1	2.08	0.44
1:B:140:GLN:O	1:B:144:GLU:HG2	2.18	0.44
1:A:24:ASN:OD1	1:A:26:GLN:CG	2.66	0.44
3:E:165:HIS:CE1	3:E:167:GLN:NE2	2.79	0.44
1:A:43:ARG:HD2	1:A:43:ARG:O	2.18	0.44
2:D:377:ARG:O	2:D:381:VAL:HG23	2.18	0.44
2:C:33:ASN:HD22	2:C:33:ASN:H	1.66	0.43
2:C:316:VAL:O	2:C:319:ASN:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:291:ALA:HB2	6:D:1323:HOH:O	2.18	0.43
3:F:153:GLU:CD	3:F:153:GLU:N	2.72	0.43
1:A:313:TRP:CD1	1:A:317:TRP:CD1	3.06	0.43
1:B:79:PHE:O	1:B:83:GLN:HG3	2.17	0.43
1:B:140:GLN:HG3	1:B:246:HIS:CE1	2.54	0.43
1:B:427:PRO:HD2	6:B:1431:HOH:O	2.17	0.43
3:E:40:THR:C	3:E:41:THR:HG23	2.43	0.43
1:A:93:VAL:HG11	2:D:3:MET:HG2	1.99	0.43
1:A:163:GLN:HG2	6:A:2153:HOH:O	2.19	0.43
1:A:246:HIS:N	1:A:246:HIS:CD2	2.86	0.43
2:C:33:ASN:HD22	2:C:33:ASN:N	2.14	0.43
2:C:143:GLU:O	2:C:147:ARG:HB3	2.19	0.43
3:E:44:ARG:HD3	3:E:47:TYR:CZ	2.54	0.43
1:A:435:THR:HG22	1:A:436:LEU:N	2.34	0.43
1:B:116:ASN:CG	1:B:189:SER:HA	2.44	0.43
1:B:291:GLU:OE1	1:B:343:HIS:CE1	2.70	0.43
1:B:360:ARG:HG2	1:B:498:GLN:HB2	2.01	0.43
3:F:4:LEU:HD23	3:F:9:ASN:HB2	2.01	0.43
1:B:49:LYS:HD3	3:F:144:ASN:HD22	1.84	0.43
1:B:521:ASN:OD1	1:B:523:VAL:HG12	2.19	0.43
2:C:261:ARG:NE	2:C:285:GLN:HE22	2.06	0.43
2:D:77:HIS:CG	3:F:140:MET:HG2	2.53	0.43
1:A:216:LEU:HD13	1:A:286:LEU:HD21	2.01	0.43
1:B:104:LYS:HG2	1:B:168:HIS:CG	2.54	0.43
1:B:192:PHE:O	1:B:200:CYS:HB3	2.19	0.43
1:B:209:GLU:C	1:B:247:MET:HE1	2.44	0.43
1:A:179:PRO:HB3	1:A:469:ILE:HD13	2.01	0.42
1:B:245:ARG:HG3	1:B:245:ARG:HH11	1.84	0.42
2:D:161:ASN:HB3	2:D:235:TRP:CE2	2.54	0.42
2:D:263:GLU:OE2	2:D:263:GLU:HA	2.18	0.42
1:A:125:TRP:HE1	2:C:161:ASN:HD22	1.67	0.42
1:A:302:VAL:HG22	1:A:376:TYR:OH	2.20	0.42
2:D:140:TRP:HB2	2:D:272:PHE:CD2	2.55	0.42
1:A:302:VAL:HG11	1:A:340:TYR:CE1	2.54	0.42
1:B:460:GLU:OE1	1:B:463:ARG:HD3	2.20	0.42
1:A:227:ASN:HD21	1:A:296:PHE:H	1.66	0.42
1:B:216:LEU:O	1:B:220:VAL:HG23	2.20	0.42
2:D:262:ARG:HA	2:D:266:GLN:HB3	2.02	0.42
3:F:93:GLY:O	3:F:96:ALA:HB3	2.19	0.42
1:B:124:LEU:HD21	1:B:201:SER:HB2	2.02	0.42
1:B:128:ALA:HB1	1:B:133:GLN:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:PHE:O	1:B:215:PRO:HD2	2.20	0.42
1:A:90:ASN:HD22	1:A:90:ASN:HA	1.62	0.42
1:B:439:HIS:HE1	1:B:454:GLU:OE1	2.03	0.42
2:D:245:ALA:HB3	2:D:299:TYR:OH	2.19	0.42
3:F:138:ARG:NH2	6:F:833:HOH:O	2.46	0.42
1:A:343:HIS:CD2	1:A:343:HIS:H	2.37	0.42
1:B:397:ASP:HA	1:B:398:PRO:HD3	1.85	0.42
2:C:153:LEU:HA	2:C:193:ILE:HD12	2.01	0.42
1:A:283:THR:HB	1:A:284:PRO:HD3	2.01	0.41
1:B:175:ARG:NE	1:B:181:TRP:CH2	2.88	0.41
3:F:15:TRP:O	3:F:19:ILE:HG23	2.20	0.41
1:B:206:LEU:HD11	1:B:321:LEU:CD1	2.48	0.41
2:D:63:ILE:O	2:D:64:ALA:C	2.62	0.41
3:F:90:VAL:HG11	3:F:118:TYR:CE2	2.55	0.41
1:A:116:ASN:CG	1:A:189:SER:HA	2.46	0.41
1:A:460:GLU:N	1:A:461:PRO:HD3	2.35	0.41
1:B:105:VAL:O	1:B:109:PHE:HB2	2.21	0.41
2:D:80:ARG:HG2	2:D:81:PRO:HD2	2.03	0.41
1:A:512:ILE:O	1:A:515:LEU:HB2	2.19	0.41
1:B:243:GLU:O	1:B:247:MET:HG2	2.21	0.41
2:C:42:ARG:HB2	2:C:99:ARG:HG3	2.02	0.41
2:D:139:THR:O	2:D:143:GLU:HB3	2.19	0.41
2:D:144:PHE:CE2	2:D:342:LEU:HD23	2.56	0.41
2:D:169:GLU:O	2:D:170:ALA:C	2.62	0.41
1:A:175:ARG:HG3	1:A:181:TRP:CE2	2.55	0.41
1:B:441:TYR:HB2	3:F:161:VAL:HG23	2.01	0.41
2:C:75:LYS:HB3	2:C:80:ARG:O	2.20	0.41
1:A:160:LYS:HE3	6:A:2187:HOH:O	2.21	0.41
1:B:184:MET:HE3	1:B:187:VAL:CG2	2.51	0.41
1:B:279:GLN:HE21	1:B:279:GLN:HB2	1.68	0.41
3:E:24:THR:HG23	6:E:190:HOH:O	2.20	0.41
1:B:341:TRP:CE2	1:B:431:LYS:HD3	2.56	0.41
2:D:98:HIS:HE1	2:D:178:SER:OG	2.03	0.41
3:E:98:MET:HE2	3:E:138:ARG:HG2	2.03	0.41
1:A:160:LYS:HA	2:C:33:ASN:HB2	2.03	0.41
2:D:263:GLU:HB3	2:D:355:SER:HB2	2.02	0.41
2:C:269:ALA:N	2:C:270:PRO:CD	2.84	0.41
2:C:324:TRP:C	2:C:327:PRO:HD2	2.46	0.41
2:C:364:ILE:HA	2:C:368:ALA:HB3	2.03	0.41
2:D:153:LEU:C	2:D:153:LEU:CD1	2.94	0.41
1:A:190:ASP:HB3	2:C:74:GLN:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:323:LYS:HE2	1:B:324:TYR:CE1	2.57	0.41
2:D:98:HIS:HA	2:D:302:CYS:SG	2.60	0.41
2:D:352:ILE:HG13	2:D:353:THR:N	2.35	0.41
3:F:86:ASP:O	3:F:87:ALA:C	2.64	0.41
3:F:154:GLU:O	3:F:158:GLN:HG3	2.21	0.41
2:D:98:HIS:HD2	2:D:297:ASP:OD1	2.04	0.40
2:D:269:ALA:HB3	2:D:270:PRO:HD3	2.03	0.40
3:F:25:LEU:HD22	3:F:68:LYS:HA	2.03	0.40
1:A:283:THR:HB	1:A:284:PRO:CD	2.52	0.40
1:B:204:LEU:HG	1:B:205:GLN:HG3	2.02	0.40
1:B:444:GLU:OE2	1:B:444:GLU:HA	2.21	0.40
1:B:460:GLU:N	1:B:461:PRO:HD3	2.36	0.40
2:C:54:VAL:HG12	2:C:55:TYR:CD2	2.56	0.40
2:C:184:PHE:O	2:C:187:ILE:HG22	2.21	0.40
2:D:13:ASP:HA	2:D:14:PRO:HD3	1.98	0.40
1:B:90:ASN:HD22	1:B:90:ASN:HA	1.64	0.40
1:B:121:THR:HG21	1:B:140:GLN:HB3	2.03	0.40
1:B:287:GLY:HA3	1:B:301:TRP:CD1	2.57	0.40
2:D:136:MET:HE2	2:D:274:ASP:OD1	2.20	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	508/527 (96%)	483 (95%)	24 (5%)	1 (0%)	43	42
1	B	508/527 (96%)	480 (94%)	26 (5%)	2 (0%)	30	27
2	C	386/389 (99%)	375 (97%)	10 (3%)	1 (0%)	36	35
2	D	386/389 (99%)	365 (95%)	18 (5%)	3 (1%)	16	11
3	E	164/170 (96%)	160 (98%)	3 (2%)	1 (1%)	21	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	F	164/170 (96%)	157 (96%)	6 (4%)	1 (1%)	21	17
All	All	2116/2172 (97%)	2020 (96%)	87 (4%)	9 (0%)	30	27

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	121	PRO
2	D	205	PRO
1	B	40	LYS
2	D	64	ALA
2	C	64	ALA
1	B	284	PRO
2	D	251	VAL
3	F	122	ILE
1	A	316	ILE

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	423/442 (96%)	412 (97%)	11 (3%)	40	44
1	B	422/442 (96%)	409 (97%)	13 (3%)	35	37
2	C	315/323 (98%)	308 (98%)	7 (2%)	45	50
2	D	312/323 (97%)	307 (98%)	5 (2%)	55	62
3	E	143/147 (97%)	140 (98%)	3 (2%)	47	52
3	F	142/147 (97%)	137 (96%)	5 (4%)	32	32
All	All	1757/1824 (96%)	1713 (98%)	44 (2%)	42	45

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ARG
1	A	38	ASP

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Mol	Chain	Res	Type
1	A	90	ASN
1	A	112	VAL
1	A	125	TRP
1	A	175	ARG
1	A	286	LEU
1	A	302	VAL
1	A	310	TYR
1	A	403	ILE
1	A	467	GLN
1	B	30	ARG
1	B	43	ARG
1	B	90	ASN
1	B	110	LEU
1	B	112	VAL
1	B	125	TRP
1	B	213	THR
1	B	222	GLU
1	B	279	GLN
1	B	286	LEU
1	B	310	TYR
1	B	311	GLU
1	B	405	LEU
2	C	33	ASN
2	C	153	LEU
2	C	173	ASP
2	C	179	LEU
2	C	195	LEU
2	C	356	LEU
2	C	377	ARG
2	D	4	LEU
2	D	145	ILE
2	D	153	LEU
2	D	173	ASP
2	D	205	PRO
3	E	24	THR
3	E	44	ARG
3	E	120	PRO
3	F	11	THR
3	F	23	ASN
3	F	74	GLU
3	F	108	GLU
3	F	164	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) 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	155	ASN
1	A	161	ASN
1	A	168	HIS
1	A	203	ASN
1	A	227	ASN
1	A	249	ASN
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	411	ASN
1	A	413	HIS
1	A	422	GLN
1	A	439	HIS
1	A	442	ASN
1	A	472	GLN
1	A	486	HIS
1	A	516	ASN
1	B	33	GLN
1	B	78	GLN
1	B	90	ASN
1	B	100	ASN
1	B	108	ASN
1	B	168	HIS
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	278	GLN
1	B	279	GLN
1	B	343	HIS
1	B	344	HIS

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Mol	Chain	Res	Type
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	146	ASN
2	C	161	ASN
2	C	266	GLN
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	285	GLN
2	D	289	GLN
2	D	293	GLN
2	D	296	GLN
2	D	301	ASN
3	E	45	ASN
3	E	111	HIS
3	E	144	ASN
3	E	158	GLN
3	E	165	HIS
3	E	167	GLN
3	F	7	HIS
3	F	23	ASN
3	F	45	ASN
3	F	99	ASN
3	F	144	ASN
3	F	167	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	3CL	A	1301	-	4,4,4	0.24	0	3,3,3	0.62	0
5	3CL	A	1302[A]	4	4,4,4	0.60	0	3,3,3	1.11	0
5	3CL	A	2002[B]	4	4,4,4	0.56	0	3,3,3	1.41	0
5	3CL	B	1305	-	4,4,4	0.36	0	3,3,3	0.69	0
5	3CL	D	1306	-	4,4,4	1.07	1 (25%)	3,3,3	0.92	0
5	3CL	B	1304	-	4,4,4	0.66	0	3,3,3	0.40	0
5	3CL	B	1303	4	4,4,4	2.17	2 (50%)	3,3,3	2.13	2 (66%)
5	3CL	A	1300	-	4,4,4	1.87	1 (25%)	3,3,3	1.61	1 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	3CL	A	1301	-	-	0/2/2/2	-
5	3CL	A	1302[A]	4	-	2/2/2/2	-
5	3CL	A	2002[B]	4	-	0/2/2/2	-
5	3CL	B	1305	-	-	0/2/2/2	-
5	3CL	D	1306	-	-	0/2/2/2	-
5	3CL	B	1304	-	-	0/2/2/2	-
5	3CL	B	1303	4	-	0/2/2/2	-
5	3CL	A	1300	-	-	2/2/2/2	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1303	3CL	C3-C2	-3.59	1.31	1.51
5	A	1300	3CL	C4-CL5	-3.08	1.52	1.78
5	B	1303	3CL	C3-C4	2.38	1.63	1.50
5	D	1306	3CL	O1-C2	2.10	1.52	1.42

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1300	3CL	C4-C3-C2	-2.52	106.70	113.31
5	B	1303	3CL	C3-C4-CL5	-2.24	100.09	112.51
5	B	1303	3CL	C4-C3-C2	-2.21	107.53	113.31

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1302[A]	3CL	O1-C2-C3-C4
5	A	1302[A]	3CL	C2-C3-C4-CL5
5	A	1300	3CL	C2-C3-C4-CL5
5	A	1300	3CL	O1-C2-C3-C4

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1302[A]	3CL	2	0
5	A	2002[B]	3CL	3	0
5	B	1305	3CL	1	0
5	B	1303	3CL	1	0
5	A	1300	3CL	1	0

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	510/527 (96%)	0.02	10 (1%) 65 64	17, 26, 47, 67	0
1	B	510/527 (96%)	0.04	11 (2%) 62 61	17, 27, 47, 71	0
2	C	388/389 (99%)	-0.36	5 (1%) 75 74	14, 21, 39, 70	0
2	D	388/389 (99%)	0.61	33 (8%) 16 15	18, 35, 59, 104	0
3	E	166/170 (97%)	-0.08	5 (3%) 52 51	16, 24, 42, 96	0
3	F	166/170 (97%)	1.23	35 (21%) 2 2	31, 44, 65, 86	0
All	All	2128/2172 (97%)	0.15	99 (4%) 36 35	14, 28, 53, 104	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	168	SER	7.4
2	D	352	ILE	6.5
3	F	4	LEU	4.7
3	E	4	LEU	4.5
2	D	119	TYR	4.3
3	F	19	ILE	4.2
3	F	83	PHE	4.2
2	D	380	ILE	4.1
1	A	318	ILE	3.8
2	D	385	LEU	3.8
1	A	317	TRP	3.7
2	D	388	LEU	3.6
3	E	121	PRO	3.3
2	D	266	GLN	3.3
2	D	374	LYS	3.2
1	A	54	ASN	3.1
2	D	384	VAL	3.0
3	F	16	VAL	3.0
2	D	389	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
3	F	122	ILE	2.9
3	F	80	LYS	2.9
1	B	256	SER	2.8
2	C	3	MET	2.8
2	D	216	ALA	2.8
2	D	344	ALA	2.7
1	A	310	TYR	2.7
3	F	60	LEU	2.7
1	B	260	ASP	2.7
2	D	206	GLY	2.7
1	A	282	PHE	2.7
3	F	72	PHE	2.7
3	F	24	THR	2.7
3	F	67	LEU	2.7
2	D	229	LEU	2.7
3	F	70	ARG	2.6
2	D	357	TYR	2.6
3	F	17	ASN	2.6
2	D	339	PHE	2.5
2	D	372	ASP	2.5
2	D	375	ALA	2.5
2	D	370	ARG	2.5
1	B	309	VAL	2.5
2	C	2	SER	2.5
3	F	71	ALA	2.5
1	B	216	LEU	2.5
2	C	119	TYR	2.4
3	F	5	GLY	2.4
3	F	128	PHE	2.4
1	B	54	ASN	2.4
2	D	223	VAL	2.4
2	D	320	TRP	2.4
1	B	213	THR	2.4
1	B	310	TYR	2.4
3	F	39	HIS	2.4
2	D	338	LEU	2.4
3	F	84	GLY	2.3
3	F	161	VAL	2.3
1	A	392	ALA	2.3
3	F	100	ALA	2.3
3	E	23	ASN	2.3
3	F	20	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	308	TRP	2.3
3	F	127	TYR	2.3
2	D	333	ARG	2.3
1	A	338	ASP	2.3
2	D	376	ASP	2.3
3	F	118	TYR	2.3
1	B	39	PHE	2.2
3	F	63	LYS	2.2
1	B	44	THR	2.2
2	C	389	LYS	2.2
2	D	311	ASP	2.2
3	F	93	GLY	2.2
3	F	69	ALA	2.2
3	F	82	ALA	2.2
1	B	317	TRP	2.2
3	E	167	GLN	2.2
1	A	517	CYS	2.2
3	F	78	ARG	2.2
3	F	77	PHE	2.1
3	F	75	VAL	2.1
2	D	379	GLN	2.1
3	F	145	LEU	2.1
3	F	96	ALA	2.1
2	D	275	ASN	2.1
1	A	302	VAL	2.1
2	D	316	VAL	2.1
3	F	66	VAL	2.1
2	D	343	PRO	2.1
2	D	345	GLY	2.1
1	A	403	ILE	2.1
2	D	381	VAL	2.1
3	F	163	VAL	2.1
3	F	73	ASN	2.0
2	D	348	ASP	2.0
2	D	148	TYR	2.0
2	C	308	GLU	2.0
3	F	154	GLU	2.0
2	D	332	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(Å ²)	Q<0.9
5	3CL	B	1303	5/5	0.46	0.25	45,45,45,45	0
5	3CL	D	1306	5/5	0.58	0.22	53,53,53,53	0
5	3CL	A	1300	5/5	0.61	0.27	46,46,46,46	0
5	3CL	B	1305	5/5	0.73	0.23	40,40,40,40	0
5	3CL	A	2002[B]	5/5	0.82	0.37	62,62,62,62	5
5	3CL	A	1302[A]	5/5	0.86	0.33	63,63,63,63	5
5	3CL	A	1301	5/5	0.90	0.14	28,28,28,28	0
5	3CL	B	1304	5/5	0.93	0.13	20,20,20,20	0
4	FE	B	1175	1/1	0.99	0.03	22,22,22,22	0
4	FE	A	1170	1/1	0.99	0.04	28,28,28,28	0
4	FE	B	1174	1/1	0.99	0.03	28,28,28,28	0
4	FE	A	1171	1/1	1.00	0.01	23,23,23,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.