



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 15, 2023 – 11:41 PM EDT

PDB ID : 1XVF
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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.35
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

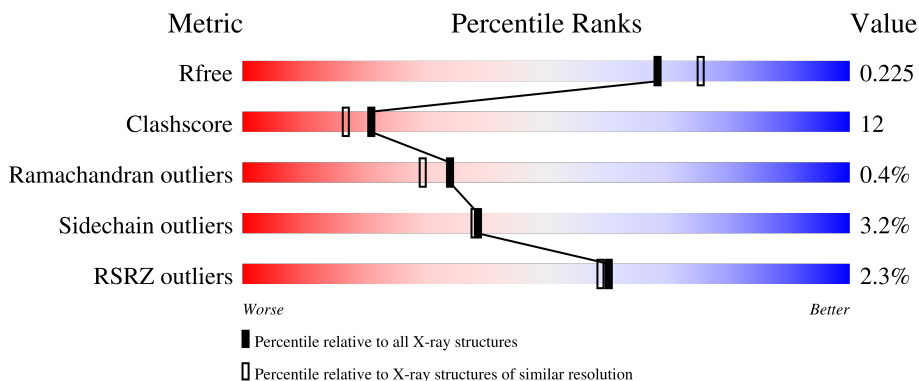
1 Overall quality at a glance i

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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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	 74% 21% . .
1	B	527	 69% 25% . .
2	C	389	 82% 17% .
2	D	389	 5% 71% 27% .
3	E	170	 85% 9% . . .

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Mol	Chain	Length	Quality of chain
3	F	170	

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	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
			Total	C	N	O	S			
1	A	510	4138	2649	709	762	18	0	0	0
1	B	510	4137	2646	711	762	18	0	0	0

- Molecule 2 is a protein called Methane monooxygenase component A beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	388	3163	2036	545	574	8	0	0	0
2	D	388	3151	2028	543	572	8	0	0	0

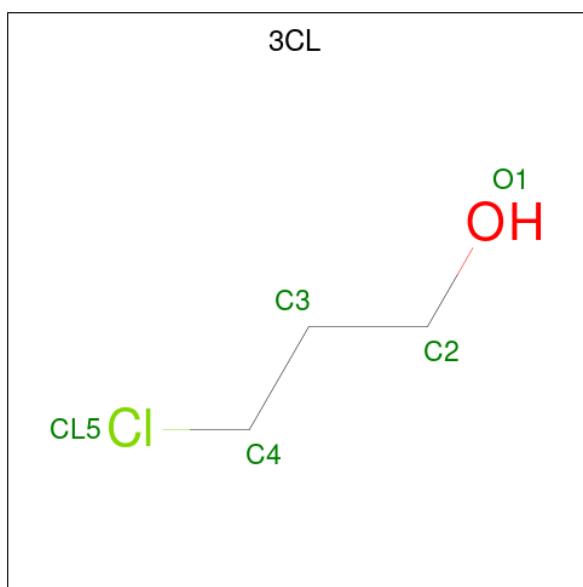
- Molecule 3 is a protein called Methane monooxygenase component A gamma chain.

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

- Molecule 4 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

- Molecule 5 is 3-CHLOROPROPANOL (three-letter code: 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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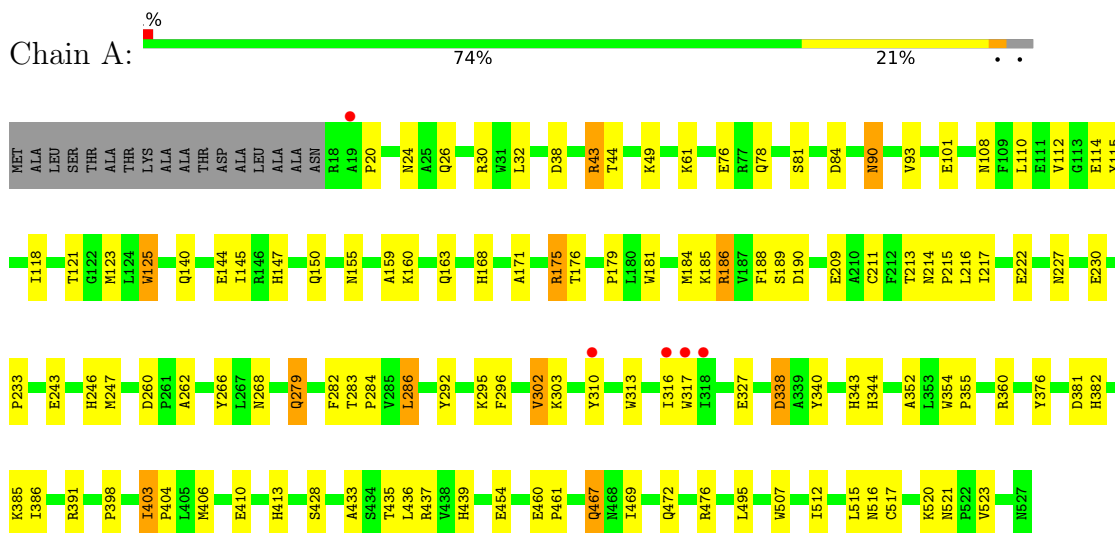
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	160	Total 160	O 160	0	0
6	F	66	Total 66	O 66	0	0

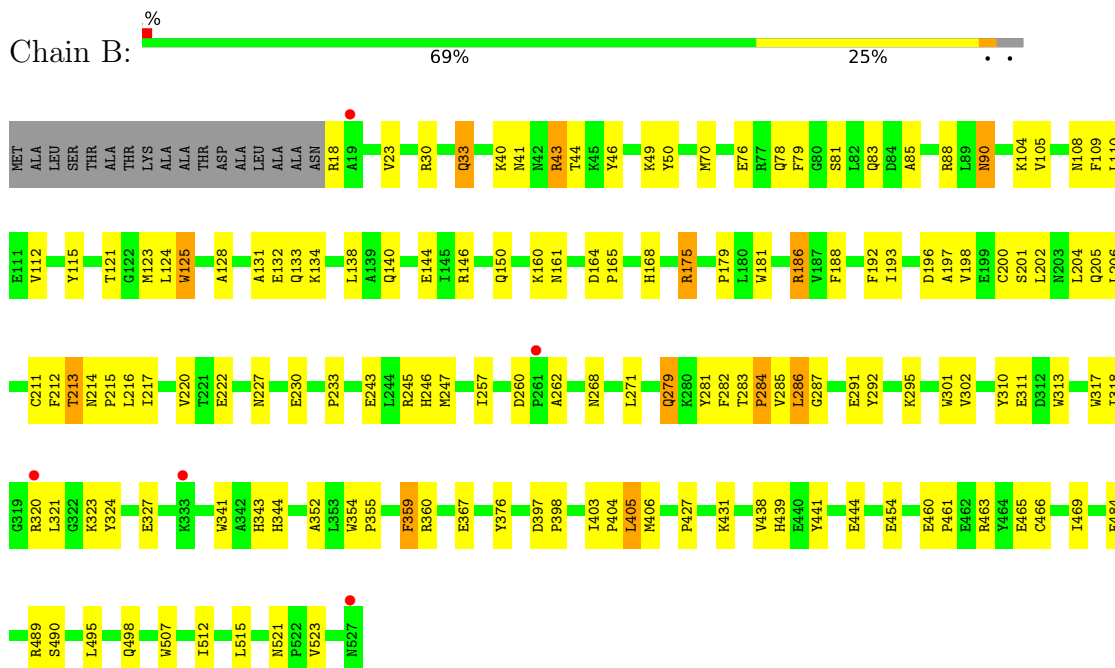
3 Residue-property plots [i](#)

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.

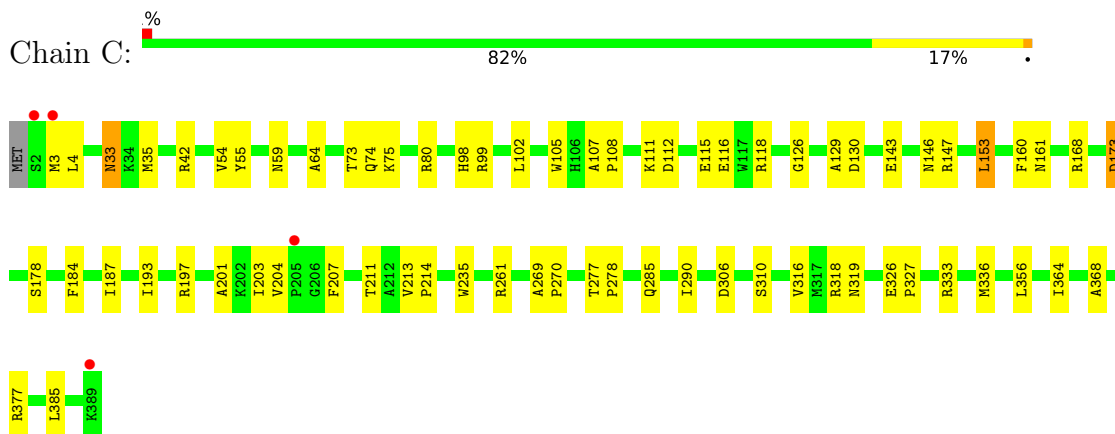
- Molecule 1: Methane monooxygenase component A alpha chain



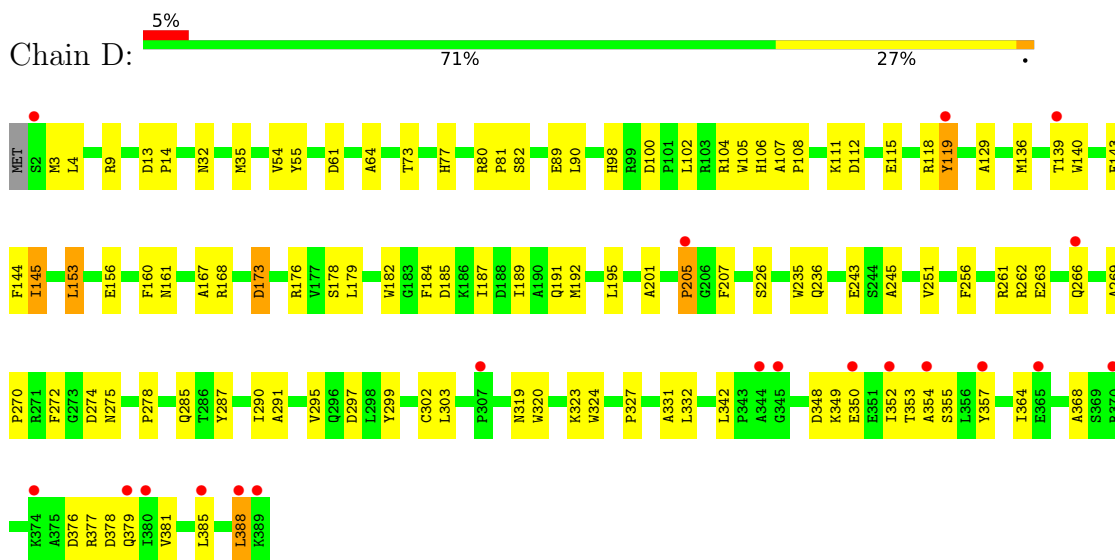
- Molecule 1: Methane monooxygenase component A alpha chain



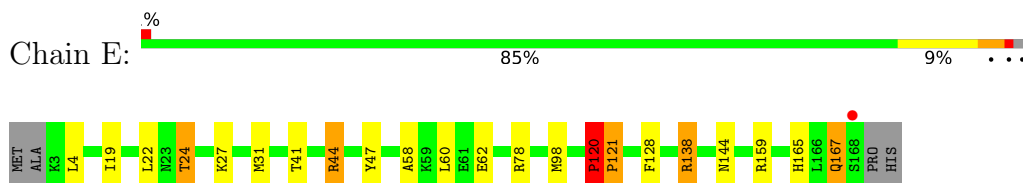
- Molecule 2: Methane monooxygenase component A beta chain



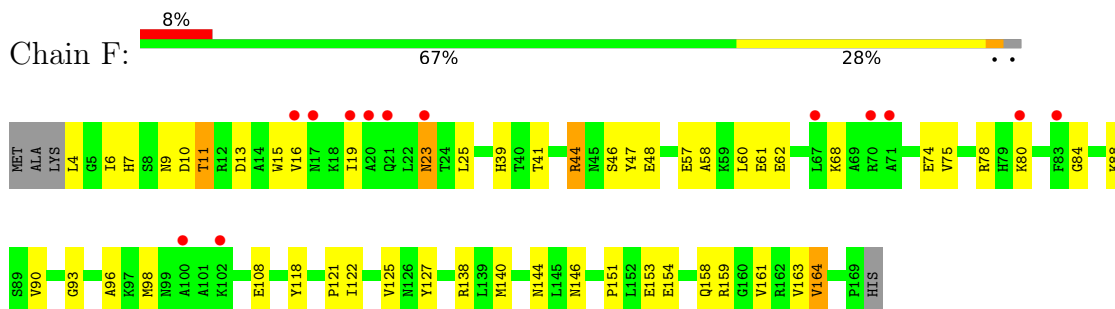
- Molecule 2: Methane monooxygenase component A beta chain



- 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) 94.0 (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)	Xtrriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.202 , 0.230 0.197 , 0.225	Depositor DCC
R_{free} test set	16940 reflections (9.37%)	wwPDB-VP
Wilson B-factor (Å ²)	24.2	Xtrriage
Anisotropy	0.218	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 56.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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: 3CL, FE

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	0/4263	0.58	0/5797
1	B	0.34	0/4262	0.59	1/5796 (0.0%)
2	C	0.37	0/3259	0.59	0/4430
2	D	0.36	0/3247	0.69	3/4417 (0.1%)
3	E	0.39	0/1392	0.86	4/1876 (0.2%)
3	F	0.29	0/1387	0.53	0/1873
All	All	0.35	0/17810	0.63	8/24189 (0.0%)

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 (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	120	PRO	C-N-CD	-19.66	77.35	120.60
2	D	119	TYR	CB-CG-CD1	-16.96	110.83	121.00
2	D	119	TYR	CB-CG-CD2	16.29	130.77	121.00
3	E	120	PRO	C-N-CA	13.70	179.55	122.00
1	B	359	PHE	CB-CG-CD1	-8.33	114.97	120.80
2	D	119	TYR	O-C-N	7.81	135.20	122.70
3	E	121	PRO	CA-N-CD	-6.50	102.40	111.50
3	E	167	GLN	N-CA-C	-5.07	97.32	111.00

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 [i](#)

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	107	0
1	B	4137	0	3888	136	0
2	C	3163	0	2986	65	0
2	D	3151	0	2960	86	0
3	E	1364	0	1352	19	0
3	F	1358	0	1335	49	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	409	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 (409) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:F:13:ASP:O	3:F:16:VAL:HG22	1.86	0.74
2:D:100:ASP:OD1	2:D:104:ARG:HD3	1.89	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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
3:F:153:GLU:H	3:F:153:GLU:CD	1.95	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: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
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
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: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
1:B:405:LEU:HG	1:B:406:MET:N	2.17	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
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
2:D:153:LEU:C	2:D:153:LEU:HD12	2.24	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:70:MET:HE1	1:B:245:ARG:NH1	2.22	0.54
1:B:138:LEU:HD22	2:D:160:PHE:CZ	2.43	0.54
2:D:324:TRP:C	2:D:327:PRO:HD2	2.27	0.54
1:B:123:MET:HE3	1:B:197:ALA:HA	1.90	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
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
3:E:98:MET:HE2	3:E:138:ARG:HG2	1.92	0.52
1:A:461:PRO:HG2	3:E:159:ARG:CZ	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:323:LYS:HB2	3:F:78:ARG:HH11	1.72	0.52
1:A:268:ASN:ND2	1:A:327:GLU:H	2.08	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:A:184:MET:HE2	1:A:188:PHE:HB2	1.92	0.51
1:B:466:CYS:HB2	2:D:73:THR:HA	1.92	0.51
1:B:43:ARG:HD2	1:B:43:ARG:C	2.30	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
1:A:78:GLN:NE2	1:A:150:GLN:HE21	1.99	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
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
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
1:B:193:ILE:O	2:D:168:ARG:NH1	2.44	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:VAL:HG22	1:A:376:TYR:CZ	2.47	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: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: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
2:C:118:ARG:NH2	2:D:112:ASP:OD1	2.45	0.48
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:A:230:GLU:C	1:A:233:PRO:HD2	2.35	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:C:153:LEU:C	2:C:153:LEU:HD12	2.34	0.48
2:D:184:PHE:O	2:D:187:ILE:HG22	2.14	0.48
1:B:230:GLU:C	1:B:233:PRO:HD2	2.34	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:D:102:LEU:HB2	2:D:104:ARG:HD2	1.95	0.47
2:D:136:MET:HE2	2:D:274:ASP:HA	1.95	0.47
1:B:186:ARG:HD3	1:B:186:ARG:C	2.34	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:CYS:HB2	1:A:313:TRP:CD1	2.50	0.47
2:C:336:MET:HE1	2:C:385:LEU:HD23	1.96	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
2:D:275:ASN:C	2:D:278:PRO:HD2	2.35	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
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:192:MET:HA	2:D:192:MET:CE	2.46	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
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
2:C:235:TRP:CD1	2:C:235:TRP:C	2.90	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:89:GLU:CD	3:F:125:VAL:HG13	2.36	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:186:ARG:HD3	1:A:186:ARG:C	2.37	0.45
1:A:354:TRP:CG	1:A:355:PRO:HD3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:376:ASP:OD2	2:D:379:GLN:HG2	2.16	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
1:B:41:ASN:O	2:D:236:GLN:HB3	2.17	0.45
1:B:164:ASP:CG	1:B:489:ARG:HH22	2.21	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
2:D:118:ARG:O	2:D:119:TYR:C	2.55	0.44
1:A:32:LEU:HD13	1:A:32:LEU:C	2.37	0.44
1:A:184:MET:HE1	1:A:188:PHE:CD2	2.52	0.44
1:B:115:TYR:OH	2:D:173:ASP:HA	2.17	0.44
3:F:23:ASN:C	3:F:23:ASN:HD22	2.21	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
1:A:114:GLU:CD	1:A:147:HIS:HB3	2.38	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:D:235:TRP:CD1	2:D:235:TRP:C	2.91	0.43
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
2:D:291:ALA:HB2	6:D:1323:HOH:O	2.18	0.43
1:A:43:ARG:HD2	1:A:43:ARG:C	2.39	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
2:D:263:GLU:OE2	2:D:263:GLU:HA	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:179:PRO:HB3	1:A:469:ILE:HD13	2.01	0.42
2:C:211:THR:C	2:C:214:PRO:HD2	2.40	0.42
1:A:101:GLU:CD	1:A:360:ARG:HD3	2.39	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
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
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
2:D:192:MET:HA	2:D:192:MET:HE2	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
3:F:90:VAL:HG11	3:F:118:TYR:CE2	2.55	0.41
1:A:460:GLU:N	1:A:461:PRO:HD3	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:VAL:O	1:B:109:PHE:HB2	2.21	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
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: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
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:364:ILE:HA	2:C:368:ALA:HB3	2.03	0.41
1:A:190:ASP:HB3	2:C:74:GLN:O	2.21	0.41
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: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
1:B:70:MET:CE	1:B:245:ARG:NH1	2.85	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%)	47	44
1	B	508/527 (96%)	480 (94%)	26 (5%)	2 (0%)	34	30
2	C	386/389 (99%)	375 (97%)	10 (3%)	1 (0%)	41	37
2	D	386/389 (99%)	365 (95%)	18 (5%)	3 (1%)	19	13
3	E	164/170 (96%)	160 (98%)	3 (2%)	1 (1%)	25	19
3	F	164/170 (96%)	157 (96%)	6 (4%)	1 (1%)	25	19
All	All	2116/2172 (97%)	2020 (96%)	87 (4%)	9 (0%)	34	30

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 [i](#)

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%)	405 (96%)	18 (4%)	29	26
1	B	422/442 (96%)	407 (96%)	15 (4%)	35	34
2	C	315/323 (98%)	308 (98%)	7 (2%)	52	55
2	D	312/323 (97%)	305 (98%)	7 (2%)	52	55
3	E	143/147 (97%)	139 (97%)	4 (3%)	43	44
3	F	142/147 (97%)	137 (96%)	5 (4%)	36	35
All	All	1757/1824 (96%)	1701 (97%)	56 (3%)	39	38

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ARG
1	A	38	ASP
1	A	43	ARG
1	A	90	ASN
1	A	112	VAL
1	A	125	TRP
1	A	175	ARG
1	A	186	ARG
1	A	279	GLN
1	A	286	LEU
1	A	302	VAL
1	A	310	TYR
1	A	338	ASP
1	A	391	ARG
1	A	403	ILE
1	A	467	GLN
1	A	516	ASN
1	A	520	LYS
1	B	30	ARG
1	B	33	GLN
1	B	43	ARG
1	B	90	ASN
1	B	110	LEU
1	B	112	VAL
1	B	125	TRP
1	B	186	ARG
1	B	213	THR
1	B	222	GLU
1	B	279	GLN
1	B	286	LEU

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Mol	Chain	Res	Type
1	B	310	TYR
1	B	311	GLU
1	B	405	LEU
2	C	33	ASN
2	C	35	MET
2	C	153	LEU
2	C	160	PHE
2	C	173	ASP
2	C	356	LEU
2	C	377	ARG
2	D	4	LEU
2	D	35	MET
2	D	145	ILE
2	D	153	LEU
2	D	173	ASP
2	D	205	PRO
2	D	388	LEU
3	E	24	THR
3	E	44	ARG
3	E	120	PRO
3	E	138	ARG
3	F	11	THR
3	F	23	ASN
3	F	44	ARG
3	F	108	GLU
3	F	164	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) 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	116	ASN
1	A	168	HIS
1	A	227	ASN
1	A	249	ASN
1	A	268	ASN
1	A	273	ASN
1	A	278	GLN

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Mol	Chain	Res	Type
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	439	HIS
1	A	442	ASN
1	A	472	GLN
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	116	ASN
1	B	155	ASN
1	B	168	HIS
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	516	ASN
1	B	527	ASN
2	C	33	ASN
2	C	98	HIS
2	C	146	ASN
2	C	161	ASN
2	C	285	GLN
2	C	301	ASN
2	D	98	HIS
2	D	125	GLN
2	D	161	ASN
2	D	285	GLN
2	D	296	GLN

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Mol	Chain	Res	Type
2	D	301	ASN
3	E	45	ASN
3	E	111	HIS
3	E	144	ASN
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 [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 monosaccharides 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	0.60	0
5	3CL	B	1304	-	4,4,4	0.67	0	3,3,3	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	3CL	A	1300	-	4,4,4	1.83	1 (25%)	3,3,3	1.56	1 (33%)
5	3CL	D	1306	-	4,4,4	1.06	1 (25%)	3,3,3	0.91	0
5	3CL	B	1303	4	4,4,4	2.11	2 (50%)	3,3,3	2.13	2 (66%)
5	3CL	B	1305	-	4,4,4	0.38	0	3,3,3	0.67	0
5	3CL	A	2002[B]	4	4,4,4	0.54	0	3,3,3	1.45	1 (33%)
5	3CL	A	1302[A]	4	4,4,4	0.60	0	3,3,3	1.10	0

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	B	1304	-	-	0/2/2/2	-
5	3CL	A	1300	-	-	1/2/2/2	-
5	3CL	D	1306	-	-	0/2/2/2	-
5	3CL	B	1303	4	-	0/2/2/2	-
5	3CL	B	1305	-	-	0/2/2/2	-
5	3CL	A	2002[B]	4	-	0/2/2/2	-
5	3CL	A	1302[A]	4	-	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	-3.48	1.31	1.50
5	A	1300	3CL	C4-CL5	-3.00	1.52	1.78
5	B	1303	3CL	C3-C4	2.36	1.63	1.50
5	D	1306	3CL	O1-C2	2.07	1.52	1.42

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1300	3CL	C4-C3-C2	-2.42	106.70	113.29
5	B	1303	3CL	C3-C4-CL5	-2.36	100.09	112.23
5	B	1303	3CL	C4-C3-C2	-2.12	107.53	113.29
5	A	2002[B]	3CL	C3-C4-CL5	-2.09	101.49	112.23

There are no chirality outliers.

All (3) 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

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1300	3CL	1	0
5	B	1303	3CL	1	0
5	B	1305	3CL	1	0
5	A	2002[B]	3CL	3	0
5	A	1302[A]	3CL	2	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%)	-0.20	5 (0%) 82 81	17, 26, 47, 67	0
1	B	510/527 (96%)	-0.19	5 (0%) 82 81	17, 27, 47, 71	0
2	C	388/389 (99%)	-0.46	4 (1%) 82 81	14, 21, 39, 70	0
2	D	388/389 (99%)	0.22	20 (5%) 27 26	18, 35, 59, 104	0
3	E	166/170 (97%)	-0.32	1 (0%) 89 88	16, 24, 42, 96	0
3	F	166/170 (97%)	0.67	13 (7%) 13 12	31, 44, 65, 86	0
All	All	2128/2172 (97%)	-0.11	48 (2%) 60 59	14, 28, 53, 104	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	168	SER	6.2
2	D	389	LYS	6.0
1	A	316	ILE	4.2
2	D	352	ILE	4.2
2	C	2	SER	3.9
2	D	205	PRO	3.7
1	B	527	ASN	3.7
3	F	21	GLN	3.5
3	F	70	ARG	3.5
3	F	100	ALA	3.1
2	D	119	TYR	3.1
2	D	388	LEU	3.0
1	B	261	PRO	2.9
3	F	83	PHE	2.9
3	F	20	ALA	2.9
3	F	23	ASN	2.9
2	D	344	ALA	2.8
1	A	310	TYR	2.8
2	D	380	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
2	D	307	PRO	2.7
3	F	17	ASN	2.7
3	F	16	VAL	2.5
2	D	374	LYS	2.5
2	C	205	PRO	2.4
2	D	385	LEU	2.4
3	F	102	LYS	2.3
1	A	19	ALA	2.3
2	D	365	GLU	2.3
2	D	379	GLN	2.3
3	F	71	ALA	2.3
2	D	357	TYR	2.3
3	F	67	LEU	2.2
3	F	80	LYS	2.2
2	D	354	ALA	2.2
1	A	317	TRP	2.2
2	D	350	GLU	2.2
2	C	3	MET	2.2
3	F	19	ILE	2.2
1	B	333	LYS	2.1
2	D	139	THR	2.1
1	B	19	ALA	2.1
1	B	320	ARG	2.1
2	D	345	GLY	2.1
2	D	266	GLN	2.1
1	A	318	ILE	2.1
2	D	370	ARG	2.1
2	D	2	SER	2.0
2	C	389	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides 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	0.50	0.32	45,45,45,45	0
5	3CL	D	1306	5/5	0.56	0.31	53,53,53,53	0
5	3CL	A	1300	5/5	0.62	0.30	46,46,46,46	0
5	3CL	B	1305	5/5	0.72	0.29	40,40,40,40	0
5	3CL	A	2002[B]	5/5	0.82	0.48	62,62,62,62	5
5	3CL	A	1302[A]	5/5	0.86	0.46	63,63,63,63	5
5	3CL	A	1301	5/5	0.90	0.19	28,28,28,28	0
5	3CL	B	1304	5/5	0.94	0.15	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	0.03	28,28,28,28	0
4	FE	B	1174	1/1	0.99	0.02	28,28,28,28	0
4	FE	A	1171	1/1	1.00	0.03	23,23,23,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.