Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:32 PM GMT

PDB ID	:	1FZ6
Title	:	METHANE MONOOXYGENASE HYDROXYLASE, FORM II SOAKED IN 1 M METHANOL
Authors	:	Whittington, D.A.; Sazinsky, M.H.; Lippard, S.J.
Deposited on	:	2000-10-03
Resolution	:	2.05 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

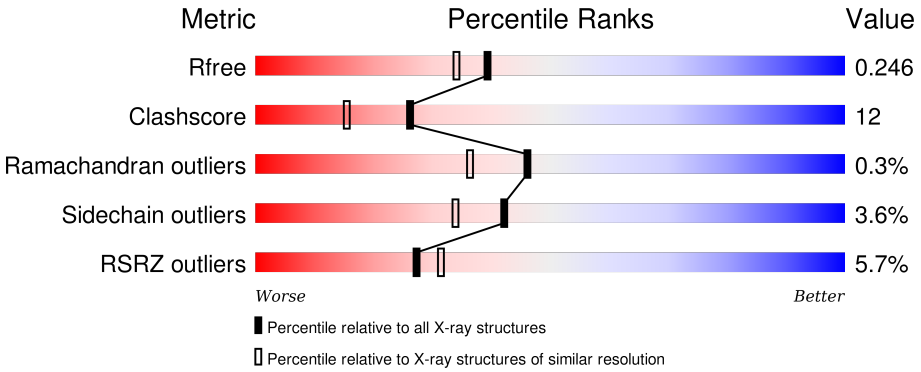
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.05 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}	91344	1192 (2.04-2.04)
Clashscore	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)
RSRZ outliers	91569	1194 (2.04-2.04)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	527	3% 72% 23%
1	B	527	4% 69% 26%
2	C	389	% 82% 16%
2	D	389	9% 70% 28%
3	E	170	4% 78% 15%

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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
6	MOH	B	9001	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 18586 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	40	0	0
			4177	2673	719	767	18			
1	B	510	Total	C	N	O	S	36	0	0
			4173	2671	718	766	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	30	0	0
			3193	2054	551	580	8			
2	D	388	Total	C	N	O	S	42	0	0
			3193	2054	551	580	8			

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	166	Total	C	N	O	S	4	0	0
			1368	867	246	250	5			
3	F	166	Total	C	N	O	S	8	0	0
			1366	866	245	250	5			

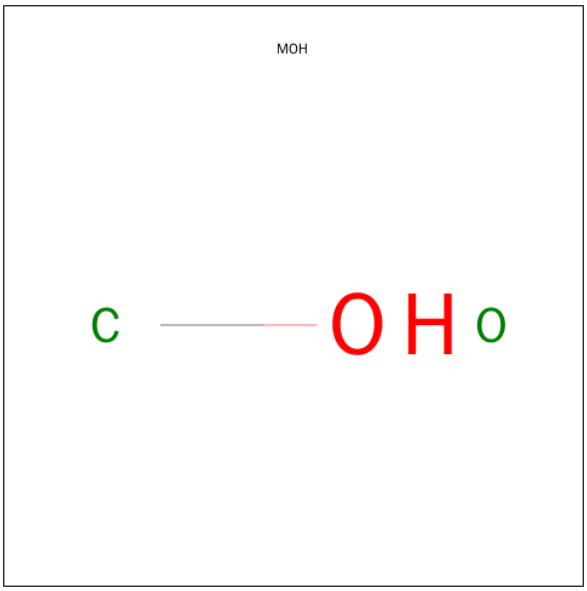
- Molecule 4 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 6 is METHANOL (three-letter code: MOH) (formula: CH_4O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C O 2 1 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	259	Total O 259 259	0	0

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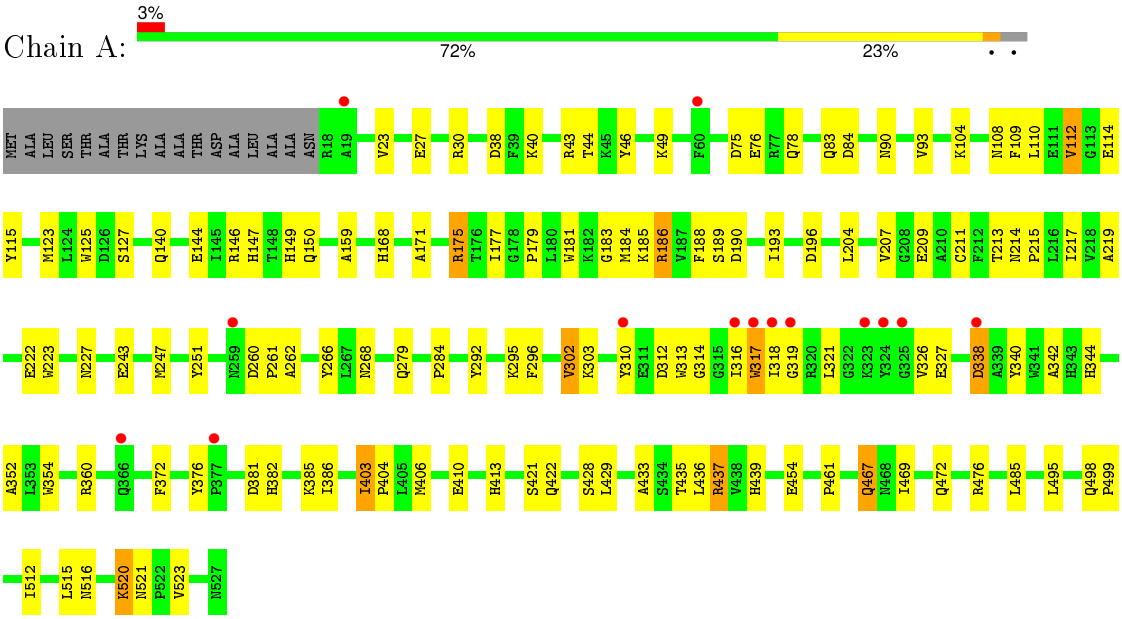
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	239	Total O 239 239	0	0
7	C	286	Total O 286 286	0	0
7	D	144	Total O 144 144	0	0
7	E	125	Total O 125 125	0	0
7	F	54	Total O 54 54	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

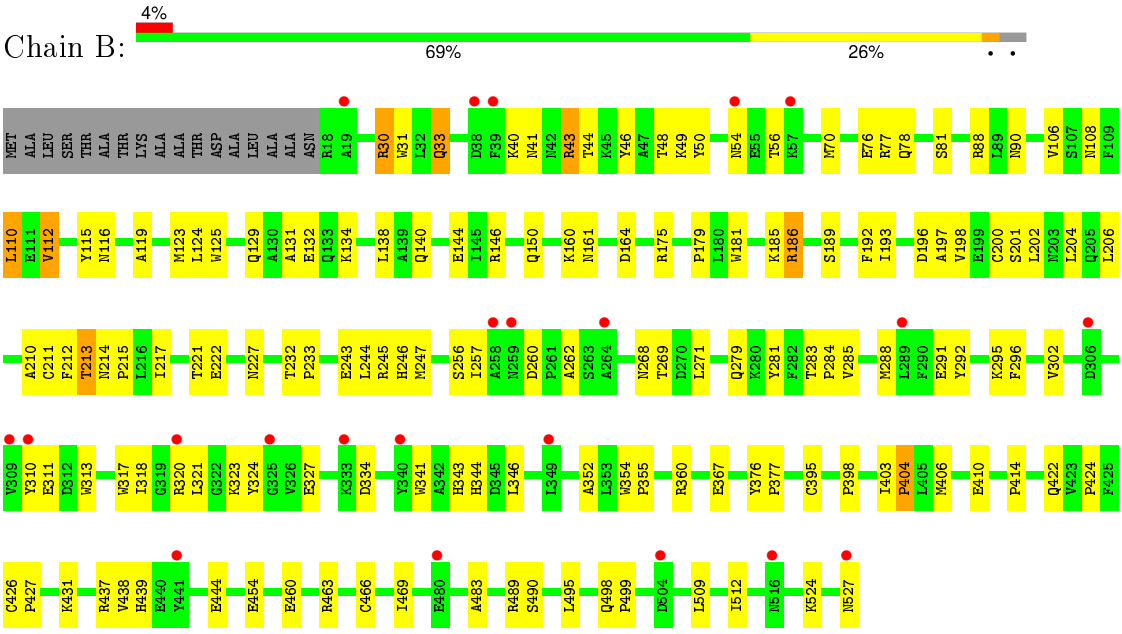
• Molecule 1: METHANE MONOOXYGENASE COMPONENT A, ALPHA CHAIN

Chain A:



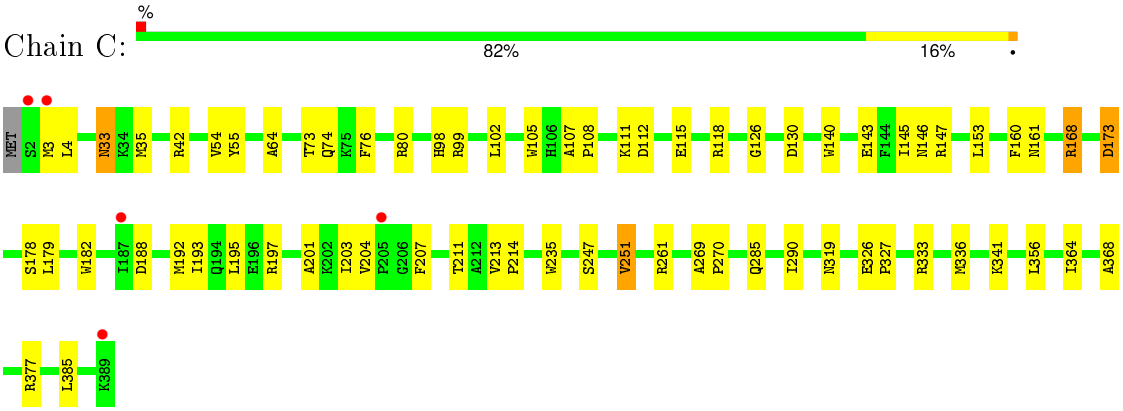
• Molecule 1: METHANE MONOOXYGENASE COMPONENT A, ALPHA CHAIN

Chain B:



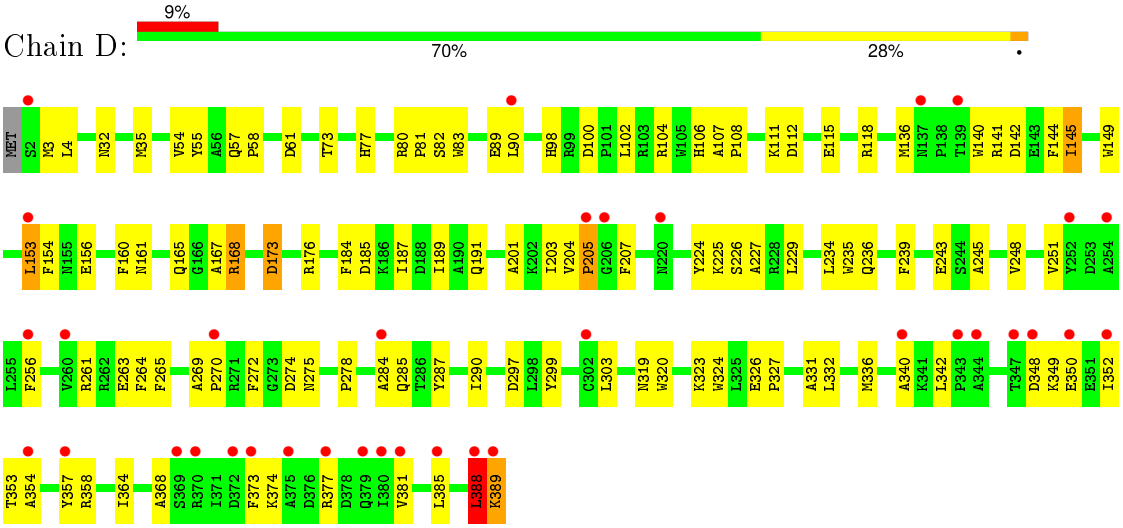
• Molecule 2: METHANE MONOOXYGENASE COMPONENT A, BETA CHAIN

Chain C:



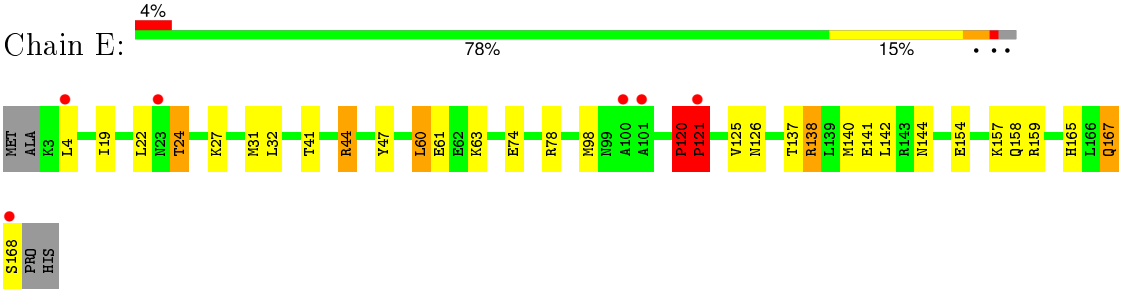
• Molecule 2: METHANE MONOOXYGENASE COMPONENT A, BETA CHAIN

Chain D:



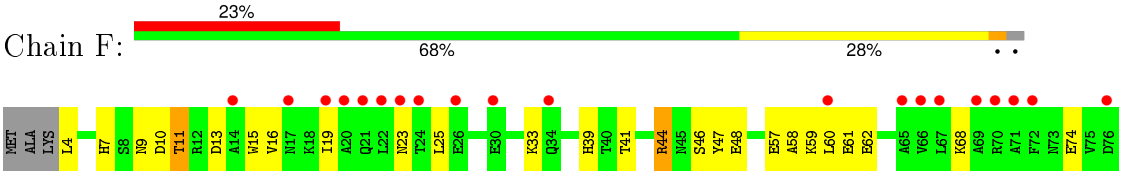
• Molecule 3: METHANE MONOOXYGENASE COMPONENT A, GAMMA CHAIN

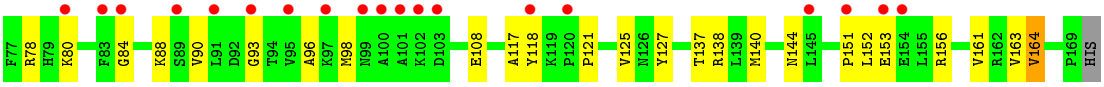
Chain E:



• Molecule 3: METHANE MONOOXYGENASE COMPONENT A, GAMMA CHAIN

Chain F:




F77
R78
H79
K80
F83
G84
K88
S89
V90
L91
D92
G93
T94
V95
A96
K97
N98
N99
A100
A101
K102
D103
E108
A117
Y118
K119
P120
P121
V125
N126
Y127
T137
R138
L139
M140
N144
L145
P151
L152
E153
E154
L155
R156
V161
R162
V163
V164
P169
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	70.67Å 171.29Å 221.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.90 – 2.05 29.87 – 2.05	Depositor EDS
% Data completeness (in resolution range)	89.0 (29.90-2.05) 89.1 (29.87-2.05)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.72 (at 2.04Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.218 , 0.244 0.220 , 0.246	Depositor DCC
R_{free} test set	5330 reflections (3.54%)	DCC
Wilson B-factor (Å^2)	28.2	Xtriage
Anisotropy	0.249	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 49.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 163529 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	18586	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.25% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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, MOH, 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	0.39	1/4302 (0.0%)	0.61	1/5842 (0.0%)
1	B	0.40	0/4298	0.60	0/5837
2	C	0.40	0/3289	0.60	0/4464
2	D	1.03	9/3289 (0.3%)	0.85	11/4464 (0.2%)
3	E	0.82	7/1396 (0.5%)	1.08	7/1880 (0.4%)
3	F	0.34	0/1395	0.57	1/1881 (0.1%)
All	All	0.60	17/17969 (0.1%)	0.70	20/24368 (0.1%)

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
3	E	0	1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	389	LYS	CB-CG	35.74	2.49	1.52
2	D	389	LYS	CA-C	32.22	2.36	1.52
3	E	167	GLN	C-N	-18.30	0.92	1.34
2	D	389	LYS	CA-CB	14.82	1.86	1.53
2	D	388	LEU	CA-C	13.22	1.87	1.52
3	E	167	GLN	CA-C	10.67	1.80	1.52
3	E	167	GLN	C-O	-10.08	1.04	1.23
2	D	389	LYS	N-CA	7.73	1.61	1.46
3	E	121	PRO	CG-CD	6.68	1.72	1.50
2	D	389	LYS	CG-CD	6.66	1.75	1.52
2	D	388	LEU	C-N	6.45	1.48	1.34
1	A	317	TRP	CB-CG	-6.25	1.39	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	121	PRO	N-CD	6.11	1.56	1.47
2	D	388	LEU	N-CA	5.86	1.58	1.46
2	D	388	LEU	C-O	-5.40	1.13	1.23
3	E	120	PRO	C-N	5.07	1.43	1.34
3	E	121	PRO	CA-C	5.04	1.62	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	120	PRO	C-N-CD	-27.86	59.30	120.60
2	D	389	LYS	N-CA-CB	-20.98	72.84	110.60
2	D	389	LYS	N-CA-C	16.70	156.10	111.00
2	D	389	LYS	CA-C-O	15.21	152.04	120.10
3	E	121	PRO	CA-N-CD	-14.31	91.47	111.50
2	D	389	LYS	CA-CB-CG	13.78	143.71	113.40
3	E	167	GLN	O-C-N	12.73	143.07	122.70
2	D	388	LEU	CA-C-N	12.16	143.95	117.20
2	D	388	LEU	CA-C-O	-9.59	99.96	120.10
3	E	121	PRO	N-CA-C	-9.39	87.69	112.10
3	E	167	GLN	CA-C-O	-9.09	101.00	120.10
2	D	389	LYS	CB-CA-C	7.87	126.14	110.40
2	D	389	LYS	CB-CG-CD	7.45	130.97	111.60
2	D	373	PHE	N-CA-C	-6.86	92.48	111.00
3	E	120	PRO	C-N-CA	6.39	148.83	122.00
1	A	317	TRP	N-CA-CB	-6.22	99.40	110.60
2	D	374	LYS	N-CA-C	-5.60	95.87	111.00
2	D	388	LEU	C-N-CA	5.37	135.13	121.70
3	E	121	PRO	CA-CB-CG	-5.25	94.02	104.00
3	F	39	HIS	N-CA-C	5.18	124.98	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	E	120	PRO	Mainchain

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	4177	0	3975	99	0
1	B	4173	0	3969	125	0
2	C	3193	0	3042	56	0
2	D	3193	0	3042	107	0
3	E	1368	0	1362	33	0
3	F	1366	0	1357	44	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
6	B	2	0	0	0	0
7	A	259	0	0	6	0
7	B	239	0	0	6	0
7	C	286	0	0	3	0
7	D	144	0	0	0	0
7	E	125	0	0	2	0
7	F	54	0	0	0	0
All	All	18586	0	16747	415	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 (415) 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)
2:D:389:LYS:CD	2:D:389:LYS:CG	1.75	1.59
2:D:389:LYS:CA	2:D:389:LYS:CB	1.86	1.50
3:E:167:GLN:C	3:E:167:GLN:CA	1.80	1.49
2:D:388:LEU:C	2:D:388:LEU:CA	1.87	1.42
2:D:389:LYS:N	2:D:389:LYS:CB	2.07	1.17
3:E:165:HIS:CE1	3:E:167:GLN:HE21	1.66	1.13
3:E:165:HIS:HE1	3:E:167:GLN:NE2	1.48	1.12
3:F:80:LYS:HE2	3:F:84:GLY:HA2	1.49	0.94
2:D:389:LYS:C	2:D:389:LYS:HA	1.87	0.93
2:D:389:LYS:CA	2:D:389:LYS:C	2.36	0.93
2:D:261:ARG:HE	2:D:285:GLN:HE22	1.17	0.92
2:D:389:LYS:CB	2:D:389:LYS:CG	2.49	0.91
1:A:44:THR:HG22	1:A:46:TYR:H	1.35	0.90
1:A:78:GLN:HE22	1:A:150:GLN:HE21	1.16	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:167:GLN:CA	3:E:168:SER:N	2.32	0.88
2:C:261:ARG:HE	2:C:285:GLN:HE22	1.19	0.88
1:B:352:ALA:HA	1:B:404:PRO:HB2	1.58	0.86
3:F:41:THR:O	3:F:44:ARG:HD2	1.76	0.85
1:B:44:THR:HG22	1:B:46:TYR:H	1.42	0.85
3:E:22:LEU:HD11	3:E:31:MET:SD	2.18	0.84
3:E:167:GLN:O	3:E:167:GLN:CA	2.24	0.83
1:B:78:GLN:HE22	1:B:150:GLN:HE21	1.28	0.81
2:D:90:LEU:HD13	2:D:303:LEU:HD13	1.63	0.81
1:A:352:ALA:HA	1:A:404:PRO:HB2	1.61	0.80
3:F:4:LEU:HD21	3:F:10:ASP:H	1.47	0.80
3:E:165:HIS:HE1	3:E:167:GLN:HE21	0.79	0.79
3:E:165:HIS:CE1	3:E:167:GLN:NE2	2.38	0.79
3:F:58:ALA:O	3:F:62:GLU:HG3	1.83	0.78
2:D:319:ASN:OD1	3:F:78:ARG:HD3	1.84	0.78
2:D:389:LYS:H	2:D:389:LYS:CB	1.95	0.78
1:A:338:ASP:OD2	1:A:433:ALA:HB2	1.84	0.77
1:A:313:TRP:CD1	1:A:317:TRP:CD1	2.72	0.77
2:D:261:ARG:HE	2:D:285:GLN:NE2	1.83	0.75
2:C:3:MET:HG3	2:C:4:LEU:H	1.52	0.75
1:A:268:ASN:HD21	1:A:327:GLU:H	1.34	0.75
2:D:256:PHE:HA	2:D:332:LEU:HD21	1.69	0.75
1:B:33:GLN:HE22	1:B:132:GLU:H	1.34	0.74
3:F:153:GLU:CD	3:F:153:GLU:H	1.90	0.74
1:B:302:VAL:HG13	1:B:376:TYR:HE2	1.53	0.74
2:D:100:ASP:OD1	2:D:104:ARG:HD3	1.88	0.73
3:F:13:ASP:O	3:F:16:VAL:HG22	1.86	0.73
1:A:213:THR:O	1:A:217:ILE:HG12	1.88	0.73
3:E:24:THR:HG22	3:E:27:LYS:H	1.51	0.73
1:A:467:GLN:HG3	7:A:5223:HOH:O	1.89	0.72
2:D:388:LEU:O	2:D:388:LEU:CA	2.34	0.72
1:A:227:ASN:HD21	1:A:295:LYS:H	1.36	0.72
2:C:102:LEU:HD12	2:C:290:ILE:HG23	1.70	0.72
2:C:326:GLU:HB3	2:C:327:PRO:HD3	1.71	0.71
1:B:355:PRO:HG2	1:B:403:ILE:CD1	2.20	0.71
3:E:41:THR:O	3:E:44:ARG:HD2	1.91	0.70
1:B:291:GLU:OE1	1:B:343:HIS:HE1	1.76	0.69
2:C:146:ASN:HD21	2:C:197:ARG:HH21	1.40	0.69
3:F:151:PRO:HB2	3:F:153:GLU:OE1	1.93	0.69
2:D:364:ILE:HA	2:D:368:ALA:HB3	1.72	0.69
2:D:107:ALA:HB3	2:D:108:PRO:HD3	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:323:LYS:HB2	3:F:78:ARG:NH1	2.07	0.69
2:C:146:ASN:ND2	2:C:197:ARG:HH21	1.91	0.68
1:B:160:LYS:HE3	1:B:161:ASN:OD1	1.94	0.68
2:C:102:LEU:CD1	2:C:290:ILE:HG23	2.23	0.68
1:A:435:THR:HG21	1:A:437:ARG:HE	1.60	0.67
1:A:243:GLU:O	1:A:247:MET:HG2	1.95	0.67
2:D:357:TYR:CE1	2:D:381:VAL:HG11	2.30	0.66
1:B:214:ASN:HB3	1:B:215:PRO:HD3	1.76	0.66
1:B:355:PRO:HG2	1:B:403:ILE:HD11	1.78	0.66
2:C:105:TRP:O	2:C:108:PRO:HD2	1.96	0.66
1:B:213:THR:O	1:B:217:ILE:HG12	1.95	0.66
1:A:476:ARG:HD3	3:E:4:LEU:HG	1.78	0.65
2:C:76:PHE:HZ	2:C:168:ARG:HH12	1.45	0.65
1:B:489:ARG:HD2	1:B:495:LEU:O	1.97	0.65
1:B:422:GLN:O	1:B:424:PRO:HD3	1.96	0.65
1:B:33:GLN:NE2	1:B:132:GLU:H	1.93	0.65
1:B:439:HIS:HD2	3:F:163:VAL:HA	1.63	0.64
1:A:429:LEU:O	1:A:429:LEU:HG	1.96	0.64
1:A:108:ASN:HD21	1:A:175:ARG:HE	1.46	0.64
1:B:206:LEU:HD11	1:B:321:LEU:HD11	1.79	0.64
1:A:214:ASN:HB3	1:A:215:PRO:HD3	1.80	0.63
1:B:108:ASN:HD21	1:B:175:ARG:HD3	1.62	0.63
3:E:61:GLU:HB3	3:E:121:PRO:HG2	1.81	0.63
1:B:33:GLN:HE21	1:B:33:GLN:HA	1.62	0.63
2:D:153:LEU:HD12	2:D:153:LEU:C	2.20	0.62
2:D:385:LEU:HD12	2:D:388:LEU:CD1	2.30	0.62
1:A:260:ASP:OD2	1:A:262:ALA:HB3	2.00	0.62
1:B:179:PRO:HB3	1:B:469:ILE:HD13	1.82	0.62
2:D:275:ASN:C	2:D:278:PRO:HD2	2.20	0.62
1:B:164:ASP:OD1	1:B:489:ARG:NH2	2.33	0.61
1:A:175:ARG:HG3	1:A:181:TRP:CD2	2.36	0.61
2:C:261:ARG:HE	2:C:285:GLN:NE2	1.94	0.61
3:F:57:GLU:O	3:F:61:GLU:HG3	2.00	0.61
3:E:19:ILE:HG12	3:E:60:LEU:HD13	1.83	0.60
1:B:268:ASN:HD21	1:B:327:GLU:H	1.47	0.60
1:B:439:HIS:HB3	3:F:161:VAL:HG21	1.83	0.60
1:B:49:LYS:CE	3:F:144:ASN:HD22	2.13	0.60
3:E:167:GLN:C	3:E:167:GLN:CB	2.68	0.60
1:B:227:ASN:HD21	1:B:295:LYS:H	1.49	0.60
1:A:76:GLU:HG2	1:B:76:GLU:OE2	2.01	0.60
1:A:227:ASN:ND2	1:A:295:LYS:H	1.99	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:349:LYS:HA	2:D:352:ILE:HG12	1.84	0.59
2:D:389:LYS:CE	2:D:389:LYS:CG	2.77	0.59
1:B:302:VAL:HG13	1:B:376:TYR:CE2	2.36	0.59
1:B:288:MET:CE	1:B:346:LEU:HB3	2.31	0.59
1:B:198:VAL:O	1:B:202:LEU:HG	2.02	0.59
1:A:104:LYS:HG2	1:A:168:HIS:CD2	2.37	0.59
2:D:140:TRP:NE1	2:D:145:ILE:HD11	2.18	0.59
1:A:185:LYS:O	1:A:189:SER:HB2	2.04	0.58
2:C:107:ALA:HB3	2:C:108:PRO:HD3	1.84	0.58
2:D:348:ASP:OD2	2:D:350:GLU:HB2	2.03	0.58
2:D:389:LYS:OXT	2:D:389:LYS:HA	2.03	0.58
1:B:438:VAL:HB	3:F:164:VAL:HG22	1.86	0.58
1:A:222:GLU:OE1	1:A:222:GLU:HA	2.04	0.58
3:F:44:ARG:HD3	3:F:47:TYR:CZ	2.39	0.57
2:C:3:MET:HG3	2:C:4:LEU:N	2.18	0.57
2:D:323:LYS:HB2	3:F:78:ARG:HH11	1.68	0.57
1:A:435:THR:CG2	1:A:437:ARG:HE	2.17	0.57
1:B:206:LEU:HD23	1:B:271:LEU:HD13	1.86	0.57
2:D:340:ALA:CB	2:D:389:LYS:HD3	2.35	0.57
1:A:268:ASN:ND2	1:A:327:GLU:H	2.02	0.57
2:D:187:ILE:O	2:D:191:GLN:HG3	2.04	0.57
2:C:111:LYS:O	2:C:115:GLU:HG3	2.05	0.56
3:F:98:MET:HG3	3:F:138:ARG:HG2	1.87	0.56
1:A:78:GLN:NE2	1:A:150:GLN:HE21	1.95	0.56
1:A:209:GLU:HA	1:A:213:THR:HB	1.87	0.56
1:A:186:ARG:HA	2:C:73:THR:OG1	2.06	0.56
2:D:324:TRP:C	2:D:327:PRO:HD2	2.26	0.56
1:B:50:TYR:CD2	1:B:257:ILE:HD12	2.40	0.56
2:C:364:ILE:HA	2:C:368:ALA:HB3	1.87	0.56
1:A:44:THR:OG1	1:A:127:SER:HA	2.06	0.56
1:B:439:HIS:HB3	3:F:161:VAL:CG2	2.36	0.56
2:D:82:SER:O	2:D:168:ARG:NH2	2.34	0.56
1:B:43:ARG:HD2	1:B:43:ARG:O	2.06	0.56
2:C:270:PRO:HB3	2:D:270:PRO:HB3	1.88	0.55
1:A:207:VAL:O	1:A:211:CYS:HB3	2.06	0.55
1:B:354:TRP:CG	1:B:355:PRO:HD3	2.42	0.55
1:A:313:TRP:CD1	1:A:317:TRP:HD1	2.25	0.55
3:F:9:ASN:OD1	3:F:11:THR:HG23	2.06	0.55
2:C:201:ALA:HA	2:C:207:PHE:HB3	1.88	0.55
3:E:167:GLN:O	3:E:167:GLN:N	2.39	0.55
2:D:224:TYR:O	2:D:227:ALA:HB3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:ILE:O	2:D:168:ARG:NH1	2.40	0.55
2:C:118:ARG:NH2	2:D:112:ASP:OD1	2.39	0.55
1:A:382:HIS:O	1:A:386:ILE:HG13	2.07	0.55
1:B:175:ARG:CZ	1:B:181:TRP:CH2	2.90	0.54
1:B:291:GLU:OE1	1:B:343:HIS:CE1	2.59	0.54
3:F:15:TRP:O	3:F:19:ILE:HG23	2.08	0.54
1:A:84:ASP:HB3	1:B:81:SER:OG	2.08	0.54
3:F:74:GLU:O	3:F:78:ARG:HG3	2.08	0.54
3:E:167:GLN:C	3:E:167:GLN:N	2.57	0.53
1:A:140:GLN:O	1:A:144:GLU:HG2	2.08	0.53
1:B:355:PRO:HG2	1:B:403:ILE:HD12	1.91	0.53
2:D:243:GLU:HB2	2:D:320:TRP:CZ2	2.43	0.53
3:E:22:LEU:O	3:E:63:LYS:HE2	2.09	0.53
2:D:102:LEU:HD12	2:D:290:ILE:HG23	1.91	0.53
3:F:25:LEU:HD22	3:F:68:LYS:HA	1.91	0.53
2:C:333:ARG:HD2	7:C:5166:HOH:O	2.09	0.53
1:B:283:THR:HB	1:B:284:PRO:HD3	1.91	0.53
2:D:336:MET:HE3	2:D:388:LEU:HD11	1.90	0.53
1:B:288:MET:HE1	1:B:346:LEU:C	2.29	0.52
2:D:385:LEU:HD12	2:D:388:LEU:HD11	1.92	0.52
2:D:140:TRP:HB2	2:D:272:PHE:CD2	2.45	0.52
1:B:44:THR:HG21	7:B:9009:HOH:O	2.09	0.52
2:D:102:LEU:HB2	2:D:104:ARG:HD2	1.91	0.52
1:A:292:TYR:OH	1:A:344:HIS:HD2	1.93	0.52
2:D:89:GLU:CD	3:F:125:VAL:HG13	2.31	0.52
1:B:246:HIS:N	1:B:246:HIS:CD2	2.76	0.52
1:A:406:MET:O	1:A:410:GLU:HG3	2.10	0.52
1:B:212:PHE:O	1:B:215:PRO:HD2	2.10	0.51
1:A:123:MET:HB2	2:C:168:ARG:HD3	1.91	0.51
1:B:43:ARG:HD2	1:B:43:ARG:C	2.30	0.51
3:E:98:MET:HE2	3:E:138:ARG:HG2	1.92	0.51
2:D:102:LEU:CD1	2:D:290:ILE:HG23	2.40	0.51
1:B:164:ASP:CG	1:B:489:ARG:HH22	2.14	0.51
2:D:263:GLU:OE2	2:D:263:GLU:HA	2.08	0.51
1:B:490:SER:OG	2:D:32:ASN:HB2	2.09	0.51
2:D:269:ALA:HB3	2:D:270:PRO:HD3	1.92	0.51
1:B:269:THR:HG23	7:B:9185:HOH:O	2.10	0.51
1:A:413:HIS:HD2	1:A:428:SER:OG	1.94	0.51
2:D:167:ALA:O	2:D:176:ARG:NH1	2.43	0.51
1:A:314:GLY:C	1:A:318:ILE:HG21	2.30	0.51
2:D:58:PRO:HD2	2:D:83:TRP:HZ3	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:TRP:CZ2	1:A:403:ILE:HD11	2.46	0.51
1:A:314:GLY:O	1:A:318:ILE:HG21	2.10	0.51
2:C:188:ASP:O	2:C:192:MET:HG2	2.11	0.51
1:B:211:CYS:HB2	1:B:313:TRP:CD1	2.46	0.51
1:B:123:MET:HE3	1:B:197:ALA:HA	1.93	0.51
1:A:413:HIS:CD2	1:A:429:LEU:HB2	2.47	0.50
1:B:186:ARG:HA	2:D:73:THR:OG1	2.11	0.50
1:A:302:VAL:HG22	1:A:376:TYR:CZ	2.46	0.50
2:D:156:GLU:OE2	2:D:156:GLU:HA	2.12	0.50
2:C:211:THR:O	2:C:214:PRO:HD2	2.11	0.50
2:D:269:ALA:HB1	2:D:274:ASP:OD2	2.10	0.50
1:B:260:ASP:OD2	1:B:262:ALA:HB3	2.12	0.50
3:F:90:VAL:HG11	3:F:118:TYR:CZ	2.46	0.50
1:B:119:ALA:HA	2:D:167:ALA:O	2.11	0.50
2:C:213:VAL:HB	2:C:214:PRO:HD3	1.93	0.50
1:A:437:ARG:NH1	1:A:454:GLU:OE2	2.43	0.50
1:B:70:MET:HE3	7:B:9140:HOH:O	2.11	0.50
1:A:159:ALA:O	2:C:33:ASN:HB2	2.12	0.50
1:B:49:LYS:HD3	3:F:140:MET:HB3	1.94	0.50
1:A:49:LYS:HD3	3:E:144:ASN:HD22	1.77	0.50
2:D:61:ASP:OD1	3:F:7:HIS:HD2	1.94	0.50
1:B:106:VAL:O	1:B:110:LEU:HB2	2.12	0.50
2:C:3:MET:CG	2:C:4:LEU:H	2.24	0.49
1:A:76:GLU:OE1	1:B:76:GLU:HG2	2.12	0.49
2:D:389:LYS:HG3	2:D:389:LYS:CD	2.20	0.49
1:A:520:LYS:HZ2	1:A:520:LYS:HB3	1.75	0.49
2:C:235:TRP:CD1	2:C:235:TRP:C	2.86	0.49
3:E:44:ARG:HD3	3:E:47:TYR:CZ	2.48	0.49
1:A:439:HIS:HE1	1:A:454:GLU:OE1	1.95	0.49
1:B:227:ASN:HD21	1:B:296:PHE:H	1.60	0.49
1:A:360:ARG:HG2	1:A:498:GLN:HB2	1.95	0.49
2:D:324:TRP:O	2:D:327:PRO:HD2	2.12	0.49
1:B:41:ASN:O	2:D:236:GLN:HB3	2.12	0.49
1:A:284:PRO:HB3	1:A:342:ALA:HB1	1.94	0.49
3:F:80:LYS:HE3	3:F:84:GLY:O	2.12	0.49
2:C:336:MET:HE1	2:C:385:LEU:HD23	1.95	0.49
2:C:341:LYS:HE3	7:C:5020:HOH:O	2.12	0.49
1:A:421:SER:O	1:A:422:GLN:HB2	2.13	0.49
1:B:495:LEU:HD11	1:B:512:ILE:CG1	2.41	0.49
1:B:302:VAL:CG1	1:B:376:TYR:HE2	2.24	0.49
3:E:157:LYS:HD2	7:E:295:HOH:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:377:ARG:O	2:D:381:VAL:HG23	2.13	0.48
1:B:112:VAL:CG2	2:D:58:PRO:HG3	2.43	0.48
1:A:196:ASP:HB2	3:E:140:MET:SD	2.53	0.48
2:C:319:ASN:OD1	3:E:78:ARG:HD3	2.12	0.48
2:C:3:MET:CE	2:C:4:LEU:HD13	2.43	0.48
1:B:112:VAL:HG21	1:B:181:TRP:HH2	1.78	0.48
1:A:403:ILE:HD12	7:A:5094:HOH:O	2.12	0.48
1:A:495:LEU:HD11	1:A:512:ILE:HG13	1.95	0.48
1:A:302:VAL:HG13	1:A:376:TYR:HE2	1.78	0.48
2:D:111:LYS:O	2:D:115:GLU:HG3	2.13	0.48
2:C:3:MET:HE2	2:C:4:LEU:HD13	1.96	0.48
1:B:146:ARG:HG2	1:B:150:GLN:OE1	2.14	0.48
1:B:138:LEU:HD22	2:D:160:PHE:CZ	2.49	0.48
1:B:406:MET:O	1:B:410:GLU:HG3	2.13	0.48
1:A:110:LEU:O	1:A:114:GLU:HG2	2.14	0.48
1:A:193:ILE:HD12	2:C:168:ARG:HH21	1.79	0.48
3:F:46:SER:OG	3:F:48:GLU:HG2	2.14	0.48
1:B:367:GLU:HG3	7:B:9131:HOH:O	2.13	0.48
1:B:344:HIS:HE1	1:B:376:TYR:CD2	2.32	0.47
2:D:326:GLU:HB2	2:D:327:PRO:HD3	1.96	0.47
1:B:466:CYS:HB2	2:D:73:THR:HA	1.95	0.47
1:A:219:ALA:O	1:A:223:TRP:HD1	1.97	0.47
1:B:78:GLN:NE2	1:B:150:GLN:HE21	2.05	0.47
2:D:234:LEU:HD13	2:D:248:VAL:HG22	1.95	0.47
2:D:54:VAL:HG12	2:D:55:TYR:CD2	2.49	0.47
3:F:61:GLU:HB3	3:F:121:PRO:HD3	1.95	0.47
1:A:83:GLN:HB3	1:B:77:ARG:HH12	1.80	0.47
3:E:138:ARG:NH2	3:E:142:LEU:HD21	2.30	0.47
2:D:226:SER:HB2	2:D:331:ALA:HA	1.96	0.47
1:B:124:LEU:HD21	1:B:201:SER:HB2	1.95	0.47
2:C:333:ARG:HD3	7:C:5024:HOH:O	2.13	0.47
1:B:48:THR:O	3:F:137:THR:HG23	2.14	0.47
1:B:414:PRO:O	1:B:426:CYS:SG	2.70	0.47
2:C:146:ASN:O	2:C:214:PRO:HG3	2.15	0.47
2:D:349:LYS:HE2	2:D:385:LEU:HD21	1.96	0.47
1:B:146:ARG:HB2	2:D:106:HIS:CE1	2.49	0.47
1:B:355:PRO:CG	1:B:403:ILE:HD11	2.44	0.47
1:A:520:LYS:NZ	1:A:520:LYS:HB3	2.30	0.47
1:B:140:GLN:O	1:B:144:GLU:HG2	2.15	0.47
1:B:193:ILE:HB	2:D:168:ARG:CZ	2.45	0.47
1:B:193:ILE:HD11	2:D:82:SER:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:336:MET:CE	2:C:385:LEU:HD23	2.45	0.47
1:B:288:MET:HE1	1:B:346:LEU:HG	1.97	0.46
1:A:211:CYS:HB2	1:A:313:TRP:CD1	2.50	0.46
2:C:146:ASN:HB2	2:C:207:PHE:CZ	2.51	0.46
1:A:171:ALA:O	1:A:175:ARG:HD2	2.15	0.46
1:B:444:GLU:HA	1:B:444:GLU:OE2	2.15	0.46
3:F:19:ILE:HG21	3:F:60:LEU:HD12	1.98	0.46
1:B:192:PHE:O	1:B:200:CYS:HB3	2.16	0.46
2:D:185:ASP:O	2:D:189:ILE:HG12	2.16	0.46
1:A:302:VAL:HG11	1:A:340:TYR:CE1	2.50	0.46
1:A:108:ASN:HD21	1:A:175:ARG:NE	2.12	0.46
1:A:302:VAL:HG22	1:A:376:TYR:OH	2.16	0.46
3:E:125:VAL:HG23	3:E:126:ASN:N	2.31	0.46
1:A:227:ASN:HD21	1:A:296:PHE:H	1.63	0.46
1:B:288:MET:HE1	1:B:346:LEU:CB	2.46	0.46
2:D:189:ILE:HD11	2:D:287:TYR:CD1	2.51	0.46
2:C:54:VAL:O	2:C:55:TYR:HB2	2.16	0.46
1:B:49:LYS:HE3	3:F:144:ASN:HD22	1.79	0.45
1:A:321:LEU:O	1:A:326:VAL:HB	2.16	0.45
1:B:175:ARG:CZ	1:B:181:TRP:CZ2	2.99	0.45
1:B:227:ASN:ND2	1:B:295:LYS:H	2.14	0.45
1:B:144:GLU:HA	1:B:144:GLU:OE2	2.16	0.45
2:D:349:LYS:HG3	2:D:352:ILE:HD11	1.97	0.45
1:B:495:LEU:HD11	1:B:512:ILE:HG13	1.98	0.45
2:C:269:ALA:N	2:C:270:PRO:CD	2.80	0.45
1:B:334:ASP:HB2	7:B:9103:HOH:O	2.16	0.45
1:A:109:PHE:O	1:A:112:VAL:HG12	2.17	0.45
2:C:247:SER:O	2:C:251:VAL:HB	2.17	0.45
3:E:154:GLU:O	3:E:158:GLN:HG3	2.17	0.45
2:C:269:ALA:HB3	2:C:270:PRO:HD3	1.99	0.45
2:D:189:ILE:HD11	2:D:284:ALA:HA	1.99	0.45
1:B:192:PHE:CE2	1:B:204:LEU:HA	2.52	0.45
3:F:152:LEU:O	3:F:156:ARG:HG3	2.16	0.45
1:A:303:LYS:HE3	1:A:303:LYS:HB2	1.83	0.44
1:A:435:THR:HG22	1:A:436:LEU:N	2.32	0.44
1:B:313:TRP:CZ2	1:B:318:ILE:HD11	2.52	0.44
2:C:98:HIS:HE1	2:C:178:SER:OG	1.99	0.44
2:D:388:LEU:CB	2:D:388:LEU:C	2.78	0.44
3:F:4:LEU:HD11	3:F:10:ASP:OD2	2.17	0.44
1:B:524:LYS:O	1:B:527:ASN:HB2	2.18	0.44
1:B:341:TRP:CE2	1:B:431:LYS:HD3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:203:ILE:HG13	2:C:204:VAL:HG23	1.99	0.44
1:B:115:TYR:OH	2:D:173:ASP:HA	2.17	0.44
2:D:352:ILE:HD12	2:D:388:LEU:HD11	1.99	0.44
2:C:179:LEU:HD12	2:C:182:TRP:CZ3	2.52	0.44
1:A:512:ILE:O	1:A:515:LEU:HB2	2.17	0.44
3:F:88:LYS:HB2	3:F:127:TYR:CE2	2.53	0.44
2:D:235:TRP:CD1	2:D:235:TRP:C	2.90	0.44
1:B:317:TRP:CE3	1:B:320:ARG:NH2	2.85	0.44
2:D:80:ARG:HD2	2:D:81:PRO:O	2.18	0.44
2:D:225:LYS:O	2:D:229:LEU:HG	2.18	0.44
2:D:201:ALA:HA	2:D:207:PHE:HB3	1.99	0.44
1:A:472:GLN:NE2	7:A:5223:HOH:O	2.51	0.44
3:F:61:GLU:O	3:F:121:PRO:HG2	2.17	0.44
3:F:33:LYS:HE3	3:F:117:ALA:CB	2.47	0.44
1:B:196:ASP:HB2	3:F:140:MET:SD	2.58	0.43
1:A:251:TYR:CD2	1:A:321:LEU:HD21	2.53	0.43
1:B:281:TYR:CZ	1:B:285:VAL:HG21	2.52	0.43
1:A:521:ASN:OD1	1:A:523:VAL:HG12	2.18	0.43
1:A:184:MET:HE2	1:A:188:PHE:HB2	2.01	0.43
2:D:141:ARG:HG2	2:D:142:ASP:N	2.33	0.43
1:B:70:MET:HE1	1:B:245:ARG:NH1	2.33	0.43
2:D:189:ILE:HD12	2:D:284:ALA:HB2	2.00	0.43
1:B:134:LYS:HD3	2:D:161:ASN:HD21	1.81	0.43
2:C:126:GLY:O	2:C:130:ASP:HB2	2.19	0.43
1:A:354:TRP:CH2	1:A:499:PRO:HD3	2.53	0.43
2:C:54:VAL:HG12	2:C:55:TYR:CD2	2.54	0.43
1:B:54:ASN:HB3	1:B:129:GLN:HB2	2.00	0.43
1:A:372:PHE:O	1:A:376:TYR:N	2.45	0.43
2:D:98:HIS:HD2	2:D:297:ASP:OD1	2.02	0.43
1:A:177:ILE:HG12	1:A:485:LEU:HB2	2.01	0.43
1:B:360:ARG:HG2	1:B:498:GLN:HB2	2.00	0.43
1:B:292:TYR:OH	1:B:344:HIS:HD2	2.02	0.43
1:B:123:MET:CE	1:B:197:ALA:HA	2.49	0.43
2:D:144:PHE:CE2	2:D:342:LEU:HD23	2.54	0.43
1:B:483:ALA:HB2	1:B:509:LEU:HD21	2.00	0.43
2:D:203:ILE:HG13	2:D:204:VAL:HG23	2.01	0.43
2:C:112:ASP:OD1	2:D:118:ARG:NH2	2.52	0.43
2:D:57:GLN:HA	2:D:58:PRO:HD3	1.89	0.42
1:A:312:ASP:O	1:A:316:ILE:HB	2.19	0.42
2:C:211:THR:C	2:C:214:PRO:HD2	2.40	0.42
1:B:108:ASN:HD21	1:B:175:ARG:HH11	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:165:GLN:OE1	2:D:239:PHE:HA	2.20	0.42
1:A:186:ARG:HD3	1:A:186:ARG:C	2.40	0.42
1:B:30:ARG:HD3	1:B:31:TRP:CD1	2.55	0.42
1:B:56:THR:HG21	1:B:256:SER:OG	2.18	0.42
2:D:145:ILE:O	2:D:149:TRP:HB3	2.20	0.42
1:A:318:ILE:HG23	1:A:319:GLY:N	2.35	0.42
2:C:42:ARG:HB2	2:C:99:ARG:HG3	2.01	0.42
1:A:175:ARG:HG3	1:A:181:TRP:CE2	2.54	0.42
2:D:58:PRO:HD2	2:D:83:TRP:CZ3	2.54	0.42
2:C:143:GLU:O	2:C:147:ARG:HB3	2.20	0.42
1:A:260:ASP:OD1	1:A:261:PRO:HD2	2.20	0.42
1:A:190:ASP:HB3	2:C:74:GLN:O	2.20	0.42
1:A:93:VAL:HG11	2:D:3:MET:HG2	2.01	0.42
1:B:288:MET:HE3	1:B:346:LEU:HB3	2.01	0.42
1:A:125:TRP:HE1	2:C:161:ASN:ND2	2.17	0.42
1:B:437:ARG:NH1	1:B:454:GLU:OE2	2.52	0.42
1:B:33:GLN:HA	1:B:131:ALA:HB3	2.02	0.42
1:B:283:THR:HB	1:B:284:PRO:CD	2.49	0.42
1:B:244:LEU:HB2	7:B:9224:HOH:O	2.19	0.42
3:F:41:THR:O	3:F:44:ARG:CD	2.59	0.42
1:B:354:TRP:CH2	1:B:499:PRO:HD3	2.55	0.42
1:A:109:PHE:HB3	1:A:184:MET:SD	2.60	0.42
2:D:245:ALA:HB3	2:D:299:TYR:OH	2.20	0.42
1:A:149:HIS:CE1	2:C:105:TRP:HB2	2.55	0.42
2:D:184:PHE:O	2:D:187:ILE:HG22	2.20	0.42
1:B:317:TRP:HE3	1:B:320:ARG:NH2	2.17	0.42
1:A:179:PRO:HB3	1:A:469:ILE:HD13	2.02	0.42
2:C:33:ASN:HD22	2:C:33:ASN:N	2.17	0.41
3:E:4:LEU:CG	3:E:4:LEU:O	2.68	0.41
2:C:140:TRP:NE1	2:C:145:ILE:HD11	2.35	0.41
2:D:77:HIS:CG	3:F:140:MET:HG2	2.55	0.41
3:F:93:GLY:O	3:F:96:ALA:HB3	2.20	0.41
1:A:40:LYS:HD2	7:A:5122:HOH:O	2.20	0.41
3:F:59:LYS:HA	3:F:59:LYS:HD3	1.86	0.41
2:D:354:ALA:O	2:D:358:ARG:HG3	2.20	0.41
1:B:210:ALA:HA	1:B:247:MET:CE	2.50	0.41
1:A:266:TYR:HB3	7:A:5058:HOH:O	2.19	0.41
3:E:137:THR:O	3:E:141:GLU:HG3	2.21	0.41
2:D:349:LYS:CE	2:D:385:LEU:HD21	2.51	0.41
2:C:193:ILE:O	2:C:197:ARG:HG3	2.20	0.41
3:E:32:LEU:HD13	3:E:60:LEU:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:74:GLU:O	3:E:78:ARG:HG3	2.21	0.41
1:B:232:THR:HB	1:B:233:PRO:HD3	2.03	0.41
2:D:389:LYS:HG2	2:D:389:LYS:CD	2.20	0.41
1:B:460:GLU:OE1	1:B:463:ARG:HD3	2.21	0.41
2:D:264:PHE:HD2	2:D:265:PHE:CD1	2.39	0.41
2:D:389:LYS:CA	2:D:389:LYS:HB2	2.25	0.41
2:D:385:LEU:CD1	2:D:388:LEU:CD1	2.97	0.41
1:B:217:ILE:O	1:B:221:THR:HG23	2.21	0.41
3:E:4:LEU:HD12	3:E:4:LEU:O	2.20	0.41
1:B:288:MET:HE1	1:B:346:LEU:CG	2.50	0.41
1:B:30:ARG:HD3	1:B:31:TRP:NE1	2.36	0.41
1:A:461:PRO:HG2	3:E:159:ARG:CZ	2.51	0.41
1:B:116:ASN:CG	1:B:189:SER:HA	2.41	0.41
1:B:323:LYS:HE2	1:B:324:TYR:CE1	2.56	0.41
3:F:153:GLU:CD	3:F:153:GLU:N	2.67	0.41
2:D:153:LEU:HG	2:D:154:PHE:CD1	2.56	0.41
2:D:136:MET:HE2	2:D:274:ASP:HA	2.02	0.41
2:D:144:PHE:CD1	2:D:144:PHE:N	2.89	0.41
1:A:23:VAL:HA	1:A:27:GLU:OE2	2.20	0.41
1:A:381:ASP:HA	1:A:385:LYS:HE2	2.03	0.41
1:B:355:PRO:CD	1:B:403:ILE:HD11	2.51	0.40
1:B:243:GLU:O	1:B:247:MET:HG2	2.21	0.40
1:A:75:ASP:OD2	1:A:146:ARG:NH1	2.54	0.40
1:A:204:LEU:O	1:A:209:GLU:HG3	2.21	0.40
1:B:185:LYS:O	1:B:189:SER:HB2	2.22	0.40
1:A:147:HIS:CE1	7:A:5219:HOH:O	2.74	0.40
3:F:98:MET:HG3	3:F:138:ARG:CG	2.51	0.40
1:A:183:GLY:HA2	1:A:422:GLN:HB2	2.03	0.40
1:A:115:TYR:OH	2:C:173:ASP:HA	2.21	0.40
2:D:340:ALA:HA	2:D:389:LYS:HD3	2.03	0.40
2:D:352:ILE:HG13	2:D:353:THR:N	2.35	0.40
3:E:24:THR:HG23	7:E:183:HOH:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	508/527 (96%)	487 (96%)	21 (4%)	0	100	100
1	B	508/527 (96%)	479 (94%)	28 (6%)	1 (0%)	52	43
2	C	386/389 (99%)	372 (96%)	12 (3%)	2 (0%)	34	22
2	D	386/389 (99%)	362 (94%)	21 (5%)	3 (1%)	24	12
3	E	164/170 (96%)	159 (97%)	4 (2%)	1 (1%)	30	18
3	F	164/170 (96%)	153 (93%)	11 (7%)	0	100	100
All	All	2116/2172 (97%)	2012 (95%)	97 (5%)	7 (0%)	46	36

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	121	PRO
1	B	40	LYS
2	D	388	LEU
2	C	64	ALA
2	D	251	VAL
2	C	251	VAL
2	D	205	PRO

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	432/442 (98%)	416 (96%)	16 (4%)	41	32
1	B	431/442 (98%)	412 (96%)	19 (4%)	35	26
2	C	322/323 (100%)	312 (97%)	10 (3%)	47	39
2	D	322/323 (100%)	314 (98%)	8 (2%)	55	48
3	E	144/147 (98%)	138 (96%)	6 (4%)	36	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	F	144/147 (98%)	139 (96%)	5 (4%)	43 35
All	All	1795/1824 (98%)	1731 (96%)	64 (4%)	42 34

All (64) 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	175	ARG
1	A	186	ARG
1	A	279	GLN
1	A	302	VAL
1	A	310	TYR
1	A	338	ASP
1	A	403	ILE
1	A	437	ARG
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	88	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	310	TYR
1	B	311	GLU
1	B	377	PRO
1	B	395	CYS
1	B	398	PRO
1	B	404	PRO
1	B	427	PRO
2	C	33	ASN

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Mol	Chain	Res	Type
2	C	35	MET
2	C	80	ARG
2	C	153	LEU
2	C	160	PHE
2	C	168	ARG
2	C	173	ASP
2	C	195	LEU
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	168	ARG
2	D	173	ASP
2	D	205	PRO
2	D	388	LEU
3	E	24	THR
3	E	44	ARG
3	E	60	LEU
3	E	120	PRO
3	E	121	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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) 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	168	HIS
1	A	227	ASN
1	A	249	ASN
1	A	268	ASN

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Mol	Chain	Res	Type
1	A	273	ASN
1	A	278	GLN
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	516	ASN
1	B	33	GLN
1	B	78	GLN
1	B	90	ASN
1	B	100	ASN
1	B	108	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	155	ASN
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	144	ASN
3	E	165	HIS
3	E	167	GLN
3	F	7	HIS
3	F	45	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

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 7 are monoatomic - leaving 1 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	$\#\|Z\| > 2$
6	MOH	B	9001	4	1,1,1	0.43	0	0,0,0	0.00	-

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
6	MOH	B	9001	4	-	0/0/0/0	0/0/0/0

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, 95^{th} 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%)	0.21	14 (2%) 58 64	21, 32, 49, 63	10 (1%)
1	B	510/527 (96%)	0.21	22 (4%) 39 44	20, 33, 50, 62	9 (1%)
2	C	388/389 (99%)	-0.12	5 (1%) 79 83	18, 25, 39, 54	7 (1%)
2	D	388/389 (99%)	0.67	36 (9%) 11 12	21, 40, 61, 79	10 (2%)
3	E	166/170 (97%)	0.11	6 (3%) 46 53	21, 30, 44, 59	1 (0%)
3	F	166/170 (97%)	1.22	39 (23%) 1 1	37, 49, 67, 75	2 (1%)
All	All	2128/2172 (97%)	0.31	122 (5%) 27 31	18, 33, 55, 79	39 (1%)

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	389	LYS	8.9
2	D	205	PRO	6.0
3	F	100	ALA	6.0
3	F	101	ALA	5.6
2	D	385	LEU	5.4
1	B	527	ASN	5.1
2	C	2	SER	4.9
1	A	310	TYR	4.9
1	A	319	GLY	4.8
3	F	19	ILE	4.8
3	F	23	ASN	4.5
2	D	354	ALA	4.4
3	F	21	GLN	4.4
2	D	220	ASN	4.3
3	E	4	LEU	4.3
1	B	259	ASN	4.3
2	D	381	VAL	4.3
2	D	380	ILE	4.2
2	D	344	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	323	LYS	3.9
2	C	3	MET	3.9
1	B	264	ALA	3.8
3	F	102	LYS	3.8
2	D	352	ILE	3.8
2	D	2	SER	3.8
2	D	388	LEU	3.8
2	D	350	GLU	3.7
3	F	26	GLU	3.7
1	A	338	ASP	3.6
3	F	84	GLY	3.6
3	F	103	ASP	3.4
3	F	22	LEU	3.3
2	D	137	ASN	3.3
1	A	317	TRP	3.2
3	F	120	PRO	3.2
1	A	316	ILE	3.2
2	D	379	GLN	3.1
1	B	289	LEU	3.1
3	F	20	ALA	3.1
3	F	72	PHE	3.0
3	E	100	ALA	3.0
1	B	54	ASN	3.0
3	E	168	SER	3.0
2	D	340	ALA	3.0
2	D	369	SER	2.9
2	D	348	ASP	2.9
2	D	357	TYR	2.8
3	E	121	PRO	2.8
1	B	325	GLY	2.8
3	F	30	GLU	2.8
1	B	258	ALA	2.7
3	F	17	ASN	2.7
3	F	93	GLY	2.7
2	D	372	ASP	2.6
3	F	80	LYS	2.6
2	D	284	ALA	2.6
3	F	71	ALA	2.6
1	B	504	ASP	2.6
3	F	83	PHE	2.6
2	D	343	PRO	2.6
2	D	375	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	441	TYR	2.6
1	B	19	ALA	2.6
1	A	366	GLN	2.6
1	B	39	PHE	2.6
2	D	270	PRO	2.6
2	D	260	VAL	2.6
2	D	153	LEU	2.5
3	F	67	LEU	2.5
3	F	95	VAL	2.5
2	D	139	THR	2.5
1	A	324	TYR	2.5
2	C	205	PRO	2.5
2	D	252	TYR	2.5
3	F	151	PRO	2.5
1	A	60	PHE	2.4
1	A	318	ILE	2.4
1	A	259	ASN	2.4
3	F	91	LEU	2.4
1	B	320	ARG	2.4
2	D	254	ALA	2.4
1	B	349	LEU	2.4
3	F	34	GLN	2.3
2	D	370	ARG	2.3
3	F	153	GLU	2.3
3	F	70	ARG	2.3
3	E	101	ALA	2.3
3	F	65	ALA	2.3
1	A	325	GLY	2.3
1	B	480	GLU	2.3
2	D	373	PHE	2.3
2	D	206	GLY	2.3
2	C	187	ILE	2.3
3	F	66	VAL	2.2
2	D	347	THR	2.2
3	F	118	TYR	2.2
3	F	69	ALA	2.2
3	F	89	SER	2.2
1	B	38	ASP	2.2
2	D	90	LEU	2.2
1	B	310	TYR	2.2
3	F	154	GLU	2.2
3	F	145	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	306	ASP	2.1
2	D	256	PHE	2.1
1	B	340	TYR	2.1
3	F	14	ALA	2.1
3	F	76	ASP	2.1
3	F	99	ASN	2.1
2	C	389	LYS	2.1
3	F	97	LYS	2.1
1	A	377	PRO	2.1
2	D	377	ARG	2.1
1	A	19	ALA	2.1
1	B	516	ASN	2.1
2	D	302	CYS	2.1
3	E	23	ASN	2.1
1	B	309	VAL	2.1
1	B	333	LYS	2.1
3	F	60	LEU	2.0
3	F	24	THR	2.0
1	B	57	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
6	MOH	B	9001	2/2	0.90	0.21	3.13	43,43,43,45	0
5	CA	A	5006	1/1	0.97	0.14	0.03	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	FE	B	5003	1/1	0.99	0.04	-2.47	30,30,30,30	0
4	FE	B	5004	1/1	0.99	0.02	-2.93	41,41,41,41	0
4	FE	A	5002	1/1	0.98	0.03	-4.47	42,42,42,42	0
4	FE	A	5001	1/1	0.99	0.02	-5.25	30,30,30,30	0
5	CA	C	5007	1/1	0.45	0.10	-	77,77,77,77	0
5	CA	B	5005	1/1	0.94	0.10	-	68,68,68,68	0

6.5 Other polymers

There are no such residues in this entry.