Full wwPDB X-ray Structure Validation Report ⓘ

Jan 30, 2024 – 01:42 PM EST

PDB ID	:	1FZ7
Title	:	METHANE MONOOXYGENASE HYDROXYLASE, FORM III SOAKED IN 0.9 M ETHANOL
Authors	:	Whittington, D.A.; Sazinsky, M.H.; Lippard, S.J.
Deposited on	:	2000-10-03
Resolution	:	1.96 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:

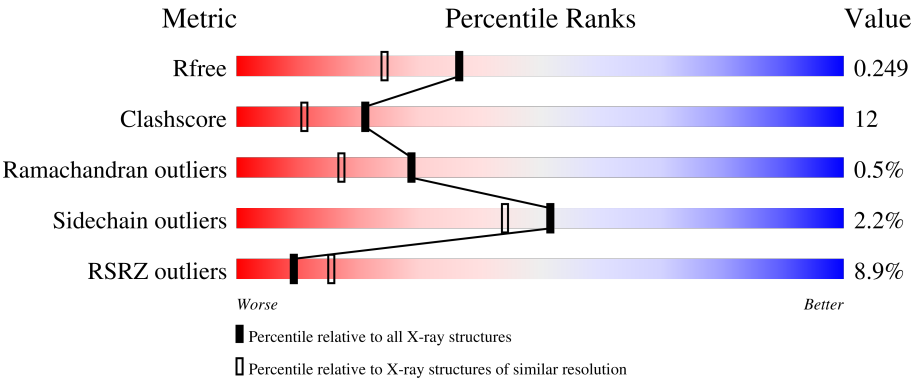
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.96 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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 <=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	9% 70% 25%
1	B	527	7% 72% 24%
2	C	389	2% 80% 19%
2	D	389	14% 65% 34%
3	E	170	82% 14%

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Mol	Chain	Length	Quality of chain
3	F	170	

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 18582 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
			4177	2673	719	767	18			
1	B	510	Total	C	N	O	S	0	0	0
			4177	2673	719	767	18			

- Molecule 2 is a protein called METHANE MONOOXYGENASE COMPONENT A, BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	388	Total	C	N	O	S	0	0	0
			3193	2054	551	580	8			
2	D	388	Total	C	N	O	S	7	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	0	0	0
			1368	867	246	250	5			
3	F	167	Total	C	N	O	S	0	0	0
			1377	872	248	252	5			

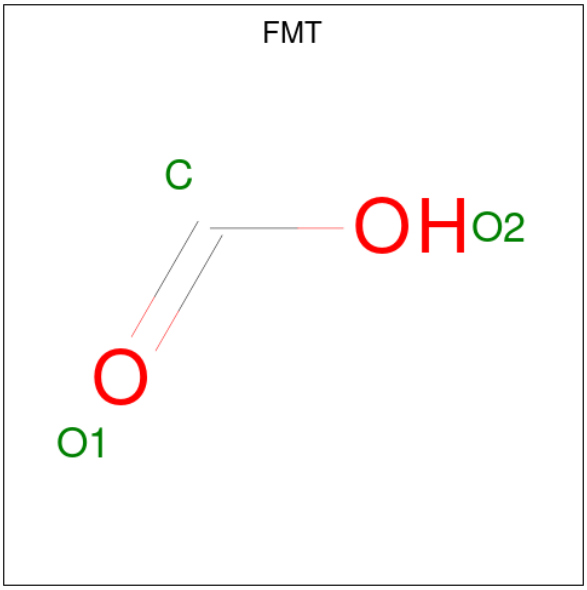
- Molecule 4 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

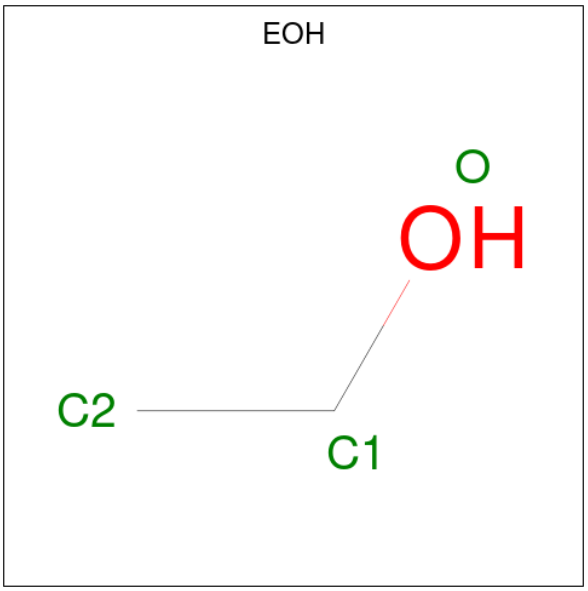
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Ca 1 1	0	0
5	C	2	Total Ca 2 2	0	0

- Molecule 6 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 3 1 2	0	0

- Molecule 7 is ETHANOL (three-letter code: EOH) (formula: C_2H_6O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C O 3 2 1	0	0

- Molecule 8 is water.

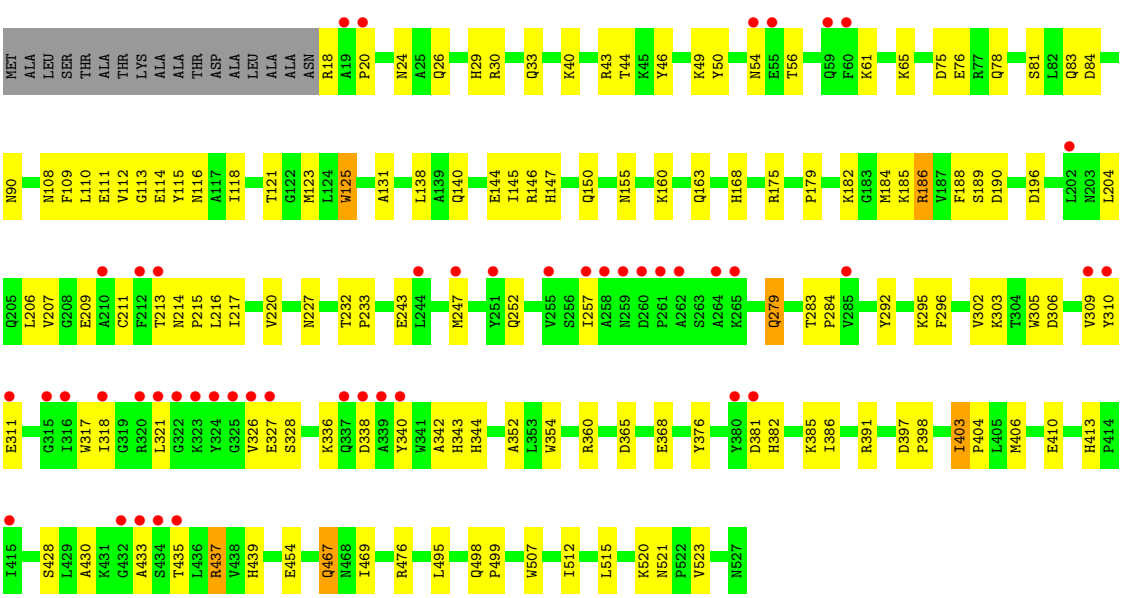
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	246	Total O 246 246	0	0
8	B	225	Total O 225 225	0	0
8	C	303	Total O 303 303	0	0
8	D	116	Total O 116 116	0	0
8	E	152	Total O 152 152	0	0
8	F	42	Total O 42 42	0	0

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.

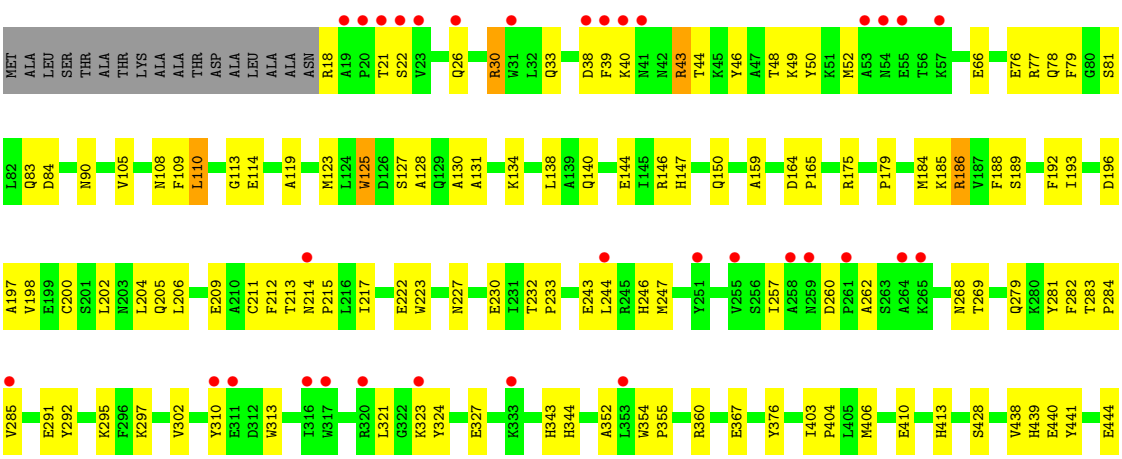
• Molecule 1: METHANE MONOOXYGENASE COMPONENT A, ALPHA CHAIN

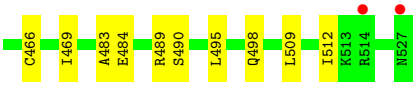
Chain A:



• Molecule 1: METHANE MONOOXYGENASE COMPONENT A, ALPHA CHAIN

Chain B:



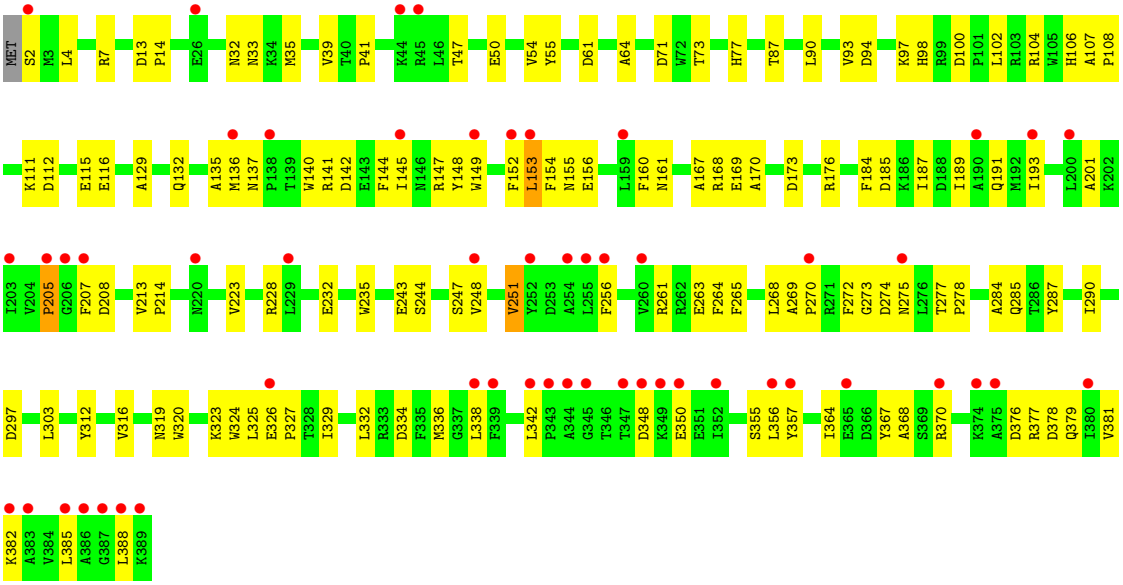


• Molecule 2: METHANE MONOOXYGENASE COMPONENT A, BETA CHAIN

Chain C:

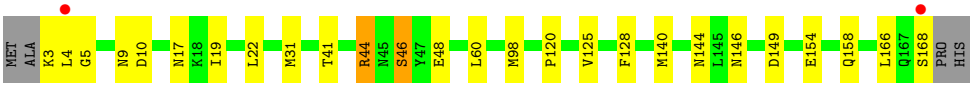
• Molecule 2: METHANE MONOOXYGENASE COMPONENT A, BETA CHAIN

Chain D:



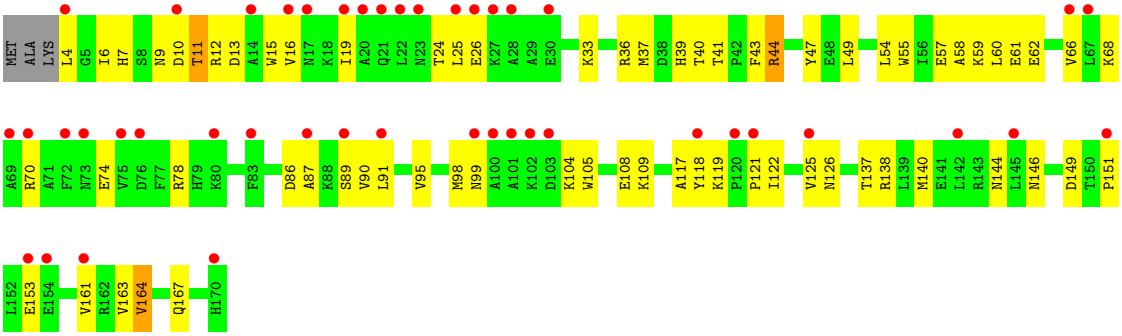
• Molecule 3: METHANE MONOOXYGENASE COMPONENT A, GAMMA CHAIN

Chain E:



• Molecule 3: METHANE MONOOXYGENASE COMPONENT A, GAMMA CHAIN

Chain F:


MET ALA LYS L4 G5 I6 H7 S8 N9 D10 T11 R12 D13 A14 W15 V16 N17 K18 I19 A20 Q21 L22 N23 T24 L25 E26 K27 A28 A29 E30 K33 R36 M37 D38 H39 T40 T41 P42 F43 R44 Y47 E48 L49 L54 W55 I56 E57 A58 K59 L60 E61 E62 V66 L67 K68
A69 R70 A71 F72 N73 E74 V75 D76 F77 R78 H79 K80 F83 D86 A87 K88 S89 V90 L91 V95 M98 N99 A100 A101 K102 D103 K104 W105 E108 K109 A117 Y118 K119 P120 P121 I122 V125 N126 T137 R138 L139 M140 E141 L142 R143 N144 L145 N146 D149 T150 P151
L152 E153 E154 V161 R162 V163 V164 Q167 H170

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	71.40Å 172.37Å 221.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.96 29.99 – 1.96	Depositor EDS
% Data completeness (in resolution range)	90.1 (30.00-1.96) 90.2 (29.99-1.96)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.19 (at 1.96Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.214 , 0.255 0.208 , 0.249	Depositor DCC
R_{free} test set	6226 reflections (3.24%)	wwPDB-VP
Wilson B-factor (Å^2)	28.1	Xtriage
Anisotropy	0.260	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 58.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	18582	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.34% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, FMT, EOH, 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	0.33	0/4302	0.55	0/5842
1	B	0.33	0/4302	0.55	0/5842
2	C	0.38	0/3289	0.57	0/4464
2	D	0.31	0/3289	0.53	0/4464
3	E	0.34	0/1396	0.59	0/1880
3	F	0.28	0/1407	0.52	0/1896
All	All	0.33	0/17985	0.55	0/24388

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4177	0	3975	110	0
1	B	4177	0	3975	113	0
2	C	3193	0	3042	66	0
2	D	3193	0	3042	106	0
3	E	1368	0	1363	19	0
3	F	1377	0	1364	59	0
4	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	2	0	0	0	0
5	A	1	0	0	0	0
5	C	2	0	0	0	0
6	A	3	0	1	0	0
7	B	3	0	5	0	0
8	A	246	0	0	8	0
8	B	225	0	0	4	0
8	C	303	0	0	5	0
8	D	116	0	0	3	0
8	E	152	0	0	1	0
8	F	42	0	0	2	0
All	All	18582	0	16767	414	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 (414) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:41:THR:HG23	3:F:43:PHE:H	1.21	1.06
2:C:270:PRO:HB3	2:D:270:PRO:HB3	1.37	1.05
1:A:78:GLN:HE22	1:A:150:GLN:HE21	1.05	0.95
1:A:352:ALA:HA	1:A:404:PRO:HB2	1.49	0.95
1:B:78:GLN:HE22	1:B:150:GLN:HE21	1.17	0.93
3:F:40:THR:O	3:F:41:THR:HG22	1.71	0.91
1:B:44:THR:HG22	1:B:46:TYR:H	1.37	0.86
1:B:352:ALA:HA	1:B:404:PRO:HB2	1.59	0.84
3:F:41:THR:O	3:F:44:ARG:HD2	1.77	0.84
1:B:244:LEU:HG	8:B:9096:HOH:O	1.78	0.83
1:A:44:THR:HG22	1:A:46:TYR:H	1.44	0.82
2:C:261:ARG:HE	2:C:285:GLN:HE22	1.23	0.82
1:A:209:GLU:HA	1:A:213:THR:HB	1.60	0.81
1:B:209:GLU:HA	1:B:213:THR:OG1	1.80	0.81
1:A:338:ASP:OD1	1:A:433:ALA:HB2	1.82	0.79
2:D:261:ARG:HE	2:D:285:GLN:HE22	1.28	0.79
1:A:155:ASN:HD22	1:A:168:HIS:HD2	1.31	0.79
1:A:403:ILE:HD13	1:A:515:LEU:HD11	1.64	0.79
2:D:319:ASN:OD1	3:F:78:ARG:HD3	1.83	0.79
2:D:100:ASP:OD1	2:D:104:ARG:HD3	1.84	0.78
3:F:13:ASP:O	3:F:16:VAL:HG22	1.83	0.78
1:A:227:ASN:HD21	1:A:295:LYS:H	1.33	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:102:LEU:HD12	2:D:290:ILE:HG23	1.68	0.76
2:C:146:ASN:HD21	2:C:197:ARG:HH21	1.31	0.76
1:B:268:ASN:HD21	1:B:327:GLU:H	1.32	0.75
1:A:467:GLN:HG3	8:A:9140:HOH:O	1.86	0.75
2:C:102:LEU:HD12	2:C:290:ILE:HG23	1.68	0.75
2:D:228:ARG:O	2:D:232:GLU:HG3	1.87	0.75
1:A:213:THR:O	1:A:217:ILE:HG12	1.87	0.74
3:E:41:THR:O	3:E:44:ARG:HD2	1.88	0.73
2:C:326:GLU:HB3	2:C:327:PRO:HD3	1.69	0.73
1:B:30:ARG:O	1:B:30:ARG:HD3	1.88	0.73
3:F:4:LEU:HD11	3:F:10:ASP:OD2	1.89	0.72
1:B:108:ASN:HD21	1:B:175:ARG:HH11	1.35	0.72
1:B:413:HIS:HD2	1:B:428:SER:OG	1.72	0.71
3:F:153:GLU:H	3:F:153:GLU:CD	1.94	0.70
1:B:179:PRO:HB3	1:B:469:ILE:HD13	1.73	0.70
1:B:439:HIS:HB3	3:F:161:VAL:HG21	1.72	0.70
3:F:146:ASN:HB3	3:F:149:ASP:OD2	1.91	0.70
2:C:333:ARG:HD3	8:C:5012:HOH:O	1.92	0.70
2:C:102:LEU:CD1	2:C:290:ILE:HG23	2.21	0.69
1:B:406:MET:O	1:B:410:GLU:HG3	1.92	0.69
1:B:18:ARG:O	2:D:129:ALA:HA	1.93	0.68
1:B:214:ASN:HB3	1:B:215:PRO:HD3	1.74	0.68
3:E:22:LEU:HD11	3:E:31:MET:SD	2.32	0.68
1:A:76:GLU:HG2	1:B:76:GLU:OE2	1.92	0.68
1:A:78:GLN:NE2	1:A:150:GLN:HE21	1.87	0.68
1:B:78:GLN:NE2	1:B:150:GLN:HE21	1.91	0.67
1:A:292:TYR:OH	1:A:344:HIS:HD2	1.78	0.67
1:B:292:TYR:OH	1:B:344:HIS:HD2	1.78	0.67
2:D:102:LEU:CD1	2:D:290:ILE:HG23	2.25	0.67
2:D:135:ALA:O	2:D:273:GLY:HA3	1.96	0.66
3:F:15:TRP:O	3:F:19:ILE:HG23	1.94	0.66
2:C:94:ASP:HB3	2:C:97:LYS:HG3	1.78	0.66
1:B:227:ASN:HD21	1:B:295:LYS:H	1.43	0.66
2:D:261:ARG:HE	2:D:285:GLN:NE2	1.94	0.65
3:F:41:THR:HG23	3:F:43:PHE:N	2.04	0.65
2:D:184:PHE:O	2:D:187:ILE:HG22	1.96	0.65
1:A:306:ASP:HB2	8:A:9217:HOH:O	1.96	0.65
2:C:269:ALA:HB3	2:C:270:PRO:HD3	1.78	0.65
3:F:9:ASN:OD1	3:F:11:THR:HG23	1.97	0.65
1:A:186:ARG:HA	2:C:73:THR:OG1	1.97	0.65
2:D:107:ALA:HB3	2:D:108:PRO:HD3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:MET:HE3	1:B:127:SER:HB3	1.79	0.65
1:A:20:PRO:HG3	2:C:129:ALA:HB2	1.79	0.64
1:A:108:ASN:HD21	1:A:175:ARG:HH11	1.45	0.64
3:E:98:MET:O	3:E:98:MET:HE2	1.97	0.64
1:B:52:MET:CE	1:B:127:SER:HB3	2.27	0.64
2:C:107:ALA:HB3	2:C:108:PRO:HD3	1.80	0.64
1:A:185:LYS:O	1:A:189:SER:HB2	1.98	0.63
1:A:310:TYR:CZ	1:A:336:LYS:HD2	2.33	0.63
2:D:269:ALA:HB1	2:D:274:ASP:OD2	1.99	0.63
1:A:227:ASN:ND2	1:A:295:LYS:H	1.96	0.63
1:B:243:GLU:O	1:B:247:MET:HG2	1.99	0.63
3:F:4:LEU:HD21	3:F:10:ASP:H	1.64	0.62
2:C:76:PHE:HZ	2:C:168:ARG:HH12	1.46	0.62
3:F:151:PRO:HB2	3:F:153:GLU:OE1	2.00	0.62
2:D:167:ALA:O	2:D:176:ARG:NH1	2.33	0.62
2:D:71:ASP:HB2	3:F:54:LEU:HD11	1.81	0.62
1:B:49:LYS:CE	3:F:144:ASN:HD22	2.13	0.62
2:C:96:PHE:O	2:C:99:ARG:NH2	2.32	0.62
3:F:105:TRP:O	3:F:109:LYS:HG3	2.00	0.61
1:A:279:GLN:HG2	1:A:283:THR:OG1	2.00	0.61
1:A:109:PHE:O	1:A:112:VAL:HG12	2.00	0.61
1:A:406:MET:O	1:A:410:GLU:HG3	1.99	0.61
3:F:57:GLU:O	3:F:61:GLU:HG3	2.00	0.60
3:F:58:ALA:O	3:F:62:GLU:HG3	2.01	0.60
1:A:108:ASN:HD21	1:A:175:ARG:HD3	1.66	0.60
1:B:119:ALA:HB1	2:D:168:ARG:HD2	1.83	0.60
1:B:269:THR:HG21	8:F:192:HOH:O	2.00	0.60
3:E:19:ILE:HG12	3:E:60:LEU:HD13	1.84	0.60
1:B:198:VAL:O	1:B:202:LEU:HG	2.02	0.60
1:A:84:ASP:HB3	1:B:81:SER:OG	2.01	0.59
2:C:365:GLU:HG2	8:C:5298:HOH:O	2.01	0.59
2:D:2:SER:HB2	8:D:488:HOH:O	2.02	0.59
2:D:324:TRP:C	2:D:327:PRO:HD2	2.23	0.59
1:B:302:VAL:HG13	1:B:376:TYR:HE2	1.68	0.59
1:A:439:HIS:HE1	1:A:454:GLU:OE1	1.86	0.59
3:F:61:GLU:O	3:F:121:PRO:HG2	2.03	0.59
2:D:102:LEU:HB2	2:D:104:ARG:HD2	1.85	0.59
2:D:187:ILE:O	2:D:191:GLN:HG3	2.02	0.59
1:B:164:ASP:OD1	1:B:489:ARG:NH2	2.36	0.59
3:F:44:ARG:HD3	3:F:47:TYR:CZ	2.37	0.59
1:A:214:ASN:HB3	1:A:215:PRO:HD3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:ARG:HD3	1:B:30:ARG:C	2.23	0.58
2:D:326:GLU:HB2	2:D:327:PRO:HD3	1.84	0.58
1:B:439:HIS:HD2	3:F:163:VAL:HA	1.69	0.57
1:B:206:LEU:HD11	1:B:321:LEU:HD11	1.86	0.57
1:B:213:THR:O	1:B:217:ILE:HG12	2.04	0.57
1:B:466:CYS:HB2	2:D:73:THR:HA	1.85	0.57
1:B:489:ARG:HD2	1:B:495:LEU:O	2.05	0.57
2:D:112:ASP:O	2:D:116:GLU:HG3	2.04	0.57
3:E:41:THR:O	3:E:44:ARG:CD	2.52	0.57
1:A:110:LEU:O	1:A:114:GLU:HG2	2.04	0.57
2:D:377:ARG:O	2:D:381:VAL:HG23	2.04	0.57
1:A:190:ASP:HB3	2:C:74:GLN:O	2.05	0.57
1:B:196:ASP:HB2	3:F:140:MET:SD	2.44	0.57
3:E:146:ASN:HB3	3:E:149:ASP:OD2	2.05	0.57
1:B:186:ARG:HD3	1:B:186:ARG:O	2.05	0.56
1:B:49:LYS:HE3	3:F:144:ASN:HD22	1.70	0.56
1:B:211:CYS:HB2	1:B:313:TRP:CD1	2.41	0.56
1:B:439:HIS:HB3	3:F:161:VAL:CG2	2.35	0.56
2:D:312:TYR:O	2:D:316:VAL:HG23	2.06	0.56
1:A:302:VAL:HG13	1:A:376:TYR:HE2	1.68	0.56
2:D:153:LEU:C	2:D:153:LEU:HD12	2.26	0.56
1:A:40:LYS:HD2	8:A:9119:HOH:O	2.06	0.56
1:A:403:ILE:HD13	1:A:515:LEU:CD1	2.35	0.56
2:C:146:ASN:ND2	2:C:197:ARG:HH21	2.02	0.56
2:D:269:ALA:HB3	2:D:270:PRO:HD3	1.88	0.56
3:F:91:LEU:O	3:F:95:VAL:HG23	2.05	0.56
1:B:291:GLU:OE1	1:B:343:HIS:HE1	1.89	0.55
1:B:495:LEU:HD11	1:B:512:ILE:HG13	1.88	0.55
2:C:211:THR:O	2:C:214:PRO:HD2	2.07	0.55
1:A:196:ASP:HB2	3:E:140:MET:SD	2.46	0.54
3:F:98:MET:HG3	3:F:138:ARG:HG2	1.88	0.54
1:A:56:THR:HG23	1:A:252:GLN:HE21	1.72	0.54
2:D:263:GLU:HB3	2:D:355:SER:HB2	1.88	0.54
3:E:46:SER:OG	3:E:48:GLU:HG2	2.07	0.54
2:D:357:TYR:CE2	2:D:381:VAL:HG21	2.42	0.54
3:F:61:GLU:HB3	3:F:121:PRO:HD3	1.88	0.54
3:E:5:GLY:H	3:E:9:ASN:HB3	1.72	0.54
2:D:323:LYS:HB2	3:F:78:ARG:NH1	2.23	0.54
1:A:305:TRP:CE2	1:A:309:VAL:HG21	2.43	0.54
2:D:140:TRP:NE1	2:D:145:ILE:HD11	2.22	0.54
3:F:4:LEU:CD2	3:F:10:ASP:H	2.20	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:PHE:O	1:B:215:PRO:HD2	2.08	0.54
2:D:111:LYS:O	2:D:115:GLU:HG3	2.07	0.54
1:B:483:ALA:HB2	1:B:509:LEU:HD21	1.90	0.54
2:C:213:VAL:HB	2:C:214:PRO:HD3	1.90	0.54
2:D:256:PHE:HA	2:D:332:LEU:HD21	1.90	0.54
2:C:98:HIS:HE1	2:C:178:SER:OG	1.92	0.53
2:D:141:ARG:CG	2:D:142:ASP:N	2.71	0.53
2:D:275:ASN:C	2:D:278:PRO:HD2	2.28	0.53
1:A:204:LEU:O	1:A:209:GLU:HG3	2.08	0.53
2:D:376:ASP:OD2	2:D:379:GLN:HB2	2.08	0.53
2:D:367:TYR:O	2:D:370:ARG:HB2	2.07	0.53
1:B:193:ILE:HB	2:D:168:ARG:CZ	2.39	0.53
1:B:140:GLN:HG3	1:B:246:HIS:CD2	2.43	0.53
2:C:261:ARG:HE	2:C:285:GLN:NE2	2.00	0.53
1:B:48:THR:O	3:F:137:THR:HG23	2.09	0.52
3:F:36:ARG:NH1	3:F:119:LYS:HB3	2.24	0.52
1:B:50:TYR:CD2	1:B:257:ILE:HD12	2.45	0.52
1:B:185:LYS:O	1:B:189:SER:HB2	2.10	0.52
1:B:367:GLU:HG3	8:B:9015:HOH:O	2.09	0.52
1:B:354:TRP:CG	1:B:355:PRO:HD3	2.45	0.52
1:A:18:ARG:O	2:C:129:ALA:HA	2.10	0.52
1:B:108:ASN:ND2	1:B:175:ARG:HH11	2.06	0.52
1:A:476:ARG:HD3	3:E:4:LEU:HG	1.92	0.52
2:D:378:ASP:O	2:D:382:LYS:HG3	2.10	0.51
1:B:49:LYS:HD3	3:F:140:MET:HB3	1.92	0.51
1:A:437:ARG:HG2	1:A:437:ARG:HH11	1.75	0.51
2:C:89:GLU:CD	3:E:125:VAL:HG13	2.31	0.51
2:D:137:ASN:HB3	2:D:272:PHE:HB3	1.93	0.51
1:A:76:GLU:OE1	1:B:76:GLU:HG2	2.10	0.51
1:B:192:PHE:O	1:B:200:CYS:HB3	2.11	0.51
2:C:333:ARG:HD2	8:C:5192:HOH:O	2.10	0.51
2:D:61:ASP:OD1	3:F:7:HIS:HD2	1.94	0.51
2:D:357:TYR:CE1	2:D:381:VAL:HG11	2.46	0.51
3:F:104:LYS:O	3:F:108:GLU:HG2	2.10	0.51
3:F:33:LYS:O	3:F:37:MET:HG2	2.10	0.50
1:A:29:HIS:CD2	1:A:61:LYS:HA	2.47	0.50
1:A:114:GLU:CD	1:A:147:HIS:HB3	2.32	0.50
1:A:140:GLN:O	1:A:144:GLU:HG2	2.12	0.50
1:B:227:ASN:ND2	1:B:295:LYS:H	2.09	0.50
2:D:201:ALA:HA	2:D:207:PHE:HB3	1.93	0.50
2:C:42:ARG:HB2	2:C:99:ARG:HG3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:265:PHE:O	2:D:269:ALA:HB2	2.12	0.50
3:F:19:ILE:HG22	3:F:60:LEU:HD21	1.94	0.50
1:B:184:MET:HE3	1:B:188:PHE:HB2	1.93	0.50
1:B:222:GLU:OE1	2:D:7:ARG:HD3	2.11	0.50
1:B:438:VAL:HB	3:F:164:VAL:HG22	1.92	0.50
2:C:266:GLN:HE22	2:D:132:GLN:CD	2.15	0.50
3:F:24:THR:HG22	3:F:26:GLU:H	1.77	0.49
1:A:113:GLY:HA3	1:A:188:PHE:CD2	2.47	0.49
1:B:26:GLN:HG3	8:B:9084:HOH:O	2.12	0.49
2:C:90:LEU:HD13	2:C:303:LEU:HD13	1.94	0.49
2:C:111:LYS:O	2:C:115:GLU:HG3	2.12	0.49
2:C:211:THR:C	2:C:214:PRO:HD2	2.33	0.49
2:D:147:ARG:HD2	2:D:148:TYR:CE1	2.47	0.49
1:B:138:LEU:HD22	2:D:160:PHE:CZ	2.47	0.49
1:B:441:TYR:HB2	3:F:161:VAL:HG23	1.93	0.49
2:C:336:MET:HE3	2:C:388:LEU:HG	1.94	0.49
1:A:206:LEU:HD12	1:A:317:TRP:HH2	1.77	0.49
1:B:186:ARG:HD3	1:B:186:ARG:C	2.33	0.49
1:B:33:GLN:HA	1:B:131:ALA:HB3	1.95	0.49
3:F:95:VAL:HG12	3:F:99:ASN:HD21	1.77	0.49
2:C:292:LYS:O	2:C:296:GLN:HG3	2.13	0.49
2:D:77:HIS:CD2	3:F:140:MET:HG2	2.48	0.49
1:B:108:ASN:HD21	1:B:175:ARG:HD3	1.78	0.49
1:B:186:ARG:HA	2:D:73:THR:OG1	2.12	0.49
2:D:94:ASP:HB3	2:D:97:LYS:HG3	1.94	0.49
2:D:156:GLU:HA	2:D:156:GLU:OE2	2.12	0.49
3:F:39:HIS:CD2	3:F:49:LEU:HD12	2.47	0.49
1:B:110:LEU:O	1:B:114:GLU:HG2	2.13	0.48
1:A:413:HIS:HD2	1:A:428:SER:OG	1.97	0.48
1:B:323:LYS:HE2	1:B:324:TYR:CE1	2.49	0.48
2:C:97:LYS:HD2	8:C:5101:HOH:O	2.12	0.48
1:A:83:GLN:HB3	1:B:77:ARG:NH1	2.29	0.48
2:C:143:GLU:O	2:C:147:ARG:HB3	2.13	0.48
1:A:125:TRP:HE1	2:C:161:ASN:ND2	2.12	0.48
1:B:43:ARG:HD2	1:B:43:ARG:C	2.34	0.48
2:C:336:MET:CE	2:C:385:LEU:HD23	2.43	0.48
1:B:144:GLU:OE2	1:B:144:GLU:HA	2.14	0.48
2:C:306:ASP:O	2:C:310:SER:HB2	2.13	0.48
2:D:54:VAL:O	2:D:55:TYR:HB2	2.14	0.48
2:D:324:TRP:O	2:D:327:PRO:HD2	2.14	0.48
1:A:49:LYS:HD3	3:E:144:ASN:HD22	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:136:MET:HA	2:D:273:GLY:O	2.14	0.48
1:A:186:ARG:HD3	1:A:186:ARG:C	2.34	0.47
1:B:164:ASP:CG	1:B:489:ARG:HH22	2.18	0.47
2:D:269:ALA:O	2:D:274:ASP:HB3	2.14	0.47
2:D:323:LYS:HB2	3:F:78:ARG:HH11	1.78	0.47
1:A:83:GLN:HB3	1:B:77:ARG:HH12	1.79	0.47
2:D:325:LEU:O	2:D:329:ILE:HG13	2.14	0.47
3:F:16:VAL:O	3:F:19:ILE:HG12	2.15	0.47
1:B:268:ASN:ND2	1:B:327:GLU:H	2.07	0.47
1:A:81:SER:OG	1:B:84:ASP:HB3	2.14	0.47
1:A:108:ASN:ND2	1:A:175:ARG:HH11	2.12	0.47
1:A:365:ASP:OD2	1:A:368:GLU:HG3	2.15	0.47
1:B:184:MET:HE1	1:B:282:PHE:CZ	2.48	0.47
2:D:90:LEU:HD13	2:D:303:LEU:HD13	1.97	0.47
1:B:490:SER:OG	2:D:32:ASN:HB2	2.14	0.47
2:D:145:ILE:O	2:D:149:TRP:HB3	2.15	0.47
2:D:213:VAL:HB	2:D:214:PRO:CD	2.45	0.47
1:A:398:PRO:HG3	1:A:507:TRP:CD1	2.50	0.47
1:B:123:MET:HE3	1:B:197:ALA:HA	1.97	0.47
1:B:260:ASP:OD2	1:B:262:ALA:HB3	2.15	0.47
2:C:2:SER:HB2	8:C:5038:HOH:O	2.14	0.47
2:D:364:ILE:HA	2:D:368:ALA:HB3	1.96	0.47
1:A:24:ASN:OD1	1:A:26:GLN:HG2	2.15	0.47
1:B:33:GLN:HE22	1:B:130:ALA:HB1	1.80	0.47
1:A:284:PRO:HB3	1:A:342:ALA:HB1	1.98	0.46
1:A:116:ASN:CG	1:A:189:SER:HA	2.36	0.46
2:D:274:ASP:OD2	2:D:277:THR:HB	2.15	0.46
2:C:336:MET:HE1	2:C:356:LEU:HD11	1.97	0.46
3:F:40:THR:O	3:F:41:THR:CG2	2.55	0.46
1:A:65:LYS:HB3	2:C:117:TRP:CG	2.50	0.46
1:A:243:GLU:O	1:A:247:MET:HG2	2.15	0.46
1:B:125:TRP:HE1	2:D:161:ASN:ND2	2.14	0.46
1:B:165:PRO:HG3	8:B:9114:HOH:O	2.16	0.46
1:A:118:ILE:HD13	1:A:145:ILE:HG12	1.97	0.46
1:A:144:GLU:HA	1:A:144:GLU:OE2	2.15	0.46
1:A:360:ARG:HG2	1:A:498:GLN:HB2	1.98	0.46
2:C:179:LEU:HD12	2:C:182:TRP:CZ3	2.51	0.46
2:D:161:ASN:HB3	2:D:235:TRP:CE2	2.50	0.46
1:A:50:TYR:CD2	1:A:257:ILE:HD12	2.51	0.46
1:A:138:LEU:HD22	2:C:160:PHE:CZ	2.50	0.46
1:B:204:LEU:HG	1:B:205:GLN:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:153:LEU:HD12	2:D:154:PHE:N	2.31	0.46
1:B:302:VAL:HG13	1:B:376:TYR:CE2	2.50	0.46
2:D:98:HIS:HD2	2:D:297:ASP:OD1	1.99	0.46
1:B:113:GLY:HA3	1:B:188:PHE:CD2	2.51	0.45
1:B:360:ARG:HG2	1:B:498:GLN:HB2	1.98	0.45
2:D:356:LEU:HD12	2:D:385:LEU:HD13	1.98	0.45
3:F:90:VAL:HG11	3:F:118:TYR:CE2	2.51	0.45
1:B:21:THR:HG22	1:B:22:SER:N	2.31	0.45
1:A:186:ARG:HD3	1:A:186:ARG:O	2.17	0.45
2:C:201:ALA:HA	2:C:207:PHE:HB3	1.98	0.45
2:D:152:PHE:O	2:D:155:ASN:HB3	2.16	0.45
2:D:263:GLU:OE2	2:D:263:GLU:HA	2.17	0.45
1:A:381:ASP:HA	1:A:385:LYS:HE2	1.99	0.45
1:B:495:LEU:HD11	1:B:512:ILE:CG1	2.46	0.45
2:D:148:TYR:HE2	2:D:223:VAL:HG21	1.82	0.45
2:D:336:MET:CE	2:D:356:LEU:HD11	2.47	0.45
1:A:125:TRP:HE1	2:C:161:ASN:HD22	1.64	0.45
1:A:397:ASP:HA	1:A:398:PRO:HD3	1.78	0.45
2:D:47:THR:OG1	2:D:50:GLU:HG3	2.17	0.45
1:A:227:ASN:HD21	1:A:296:PHE:H	1.64	0.44
1:A:318:ILE:HD11	1:A:327:GLU:O	2.16	0.44
1:A:216:LEU:O	1:A:220:VAL:HG23	2.17	0.44
1:A:302:VAL:CG1	1:A:376:TYR:HE2	2.29	0.44
2:D:348:ASP:OD2	2:D:350:GLU:HB3	2.17	0.44
1:B:184:MET:CE	1:B:188:PHE:HB2	2.47	0.44
1:B:484:GLU:OE1	3:F:6:ILE:HB	2.17	0.44
3:E:3:LYS:HB3	3:E:10:ASP:OD1	2.17	0.44
3:E:154:GLU:O	3:E:158:GLN:HG3	2.17	0.44
3:F:74:GLU:O	3:F:78:ARG:HG3	2.18	0.44
1:B:403:ILE:HG23	1:B:403:ILE:O	2.17	0.44
1:A:321:LEU:N	1:A:321:LEU:HD12	2.31	0.44
1:A:354:TRP:CH2	1:A:499:PRO:HD3	2.53	0.44
1:B:202:LEU:HD22	1:B:206:LEU:HD23	1.98	0.44
1:A:207:VAL:O	1:A:211:CYS:HB3	2.17	0.44
2:D:247:SER:O	2:D:251:VAL:HB	2.17	0.44
3:F:33:LYS:HE3	3:F:117:ALA:HA	2.00	0.44
2:C:105:TRP:O	2:C:108:PRO:HD2	2.17	0.44
2:C:184:PHE:O	2:C:187:ILE:HG22	2.18	0.44
2:D:176:ARG:HG3	2:D:176:ARG:HH11	1.83	0.44
3:F:12:ARG:O	3:F:16:VAL:HG13	2.18	0.44
1:A:495:LEU:HD11	1:A:512:ILE:CG1	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:208:ASP:HA	8:D:497:HOH:O	2.17	0.44
2:C:364:ILE:HA	2:C:368:ALA:HB3	2.00	0.43
1:A:185:LYS:HA	1:A:189:SER:HB2	1.99	0.43
2:C:266:GLN:NE2	2:D:132:GLN:CD	2.72	0.43
1:A:26:GLN:HG2	8:A:9192:HOH:O	2.18	0.43
1:A:318:ILE:HD13	1:A:328:SER:HA	1.99	0.43
2:D:189:ILE:HD11	2:D:284:ALA:HA	2.01	0.43
2:D:264:PHE:O	2:D:268:LEU:HG	2.18	0.43
1:B:114:GLU:CD	1:B:147:HIS:HB3	2.39	0.43
3:F:95:VAL:HG12	3:F:99:ASN:ND2	2.33	0.43
1:A:33:GLN:HA	1:A:131:ALA:HB3	2.01	0.43
1:B:283:THR:HB	1:B:284:PRO:HD3	2.01	0.43
3:F:36:ARG:CZ	3:F:119:LYS:HB3	2.48	0.43
1:B:79:PHE:O	1:B:83:GLN:HG3	2.18	0.43
2:C:77:HIS:CD2	3:E:140:MET:HG2	2.53	0.43
1:B:66:GLU:HA	1:B:66:GLU:OE2	2.19	0.43
1:B:444:GLU:OE2	1:B:444:GLU:HA	2.18	0.43
2:C:203:ILE:HG13	2:C:204:VAL:HG23	2.00	0.43
1:A:182:LYS:O	2:C:73:THR:HG21	2.19	0.42
1:B:140:GLN:HG3	1:B:246:HIS:CE1	2.54	0.42
1:B:159:ALA:O	2:D:33:ASN:HB2	2.19	0.42
1:A:186:ARG:HB3	8:A:9153:HOH:O	2.19	0.42
1:B:128:ALA:O	1:B:134:LYS:HE2	2.19	0.42
1:B:140:GLN:HG3	1:B:246:HIS:NE2	2.34	0.42
1:B:146:ARG:HB2	2:D:106:HIS:CE1	2.54	0.42
1:B:230:GLU:C	1:B:233:PRO:HD2	2.39	0.42
2:C:266:GLN:HB2	2:C:281:ILE:HG21	2.01	0.42
2:D:185:ASP:O	2:D:189:ILE:HG12	2.19	0.42
1:A:303:LYS:HE3	1:A:303:LYS:HB2	1.85	0.42
1:A:306:ASP:O	1:A:310:TYR:HB2	2.19	0.42
1:A:521:ASN:OD1	1:A:523:VAL:HG12	2.20	0.42
2:C:240:ASP:HB2	3:E:125:VAL:CG2	2.49	0.42
2:D:244:SER:O	2:D:248:VAL:HG23	2.19	0.42
3:E:17:ASN:HB3	8:E:907:HOH:O	2.18	0.42
2:C:235:TRP:CD1	2:C:235:TRP:C	2.92	0.42
1:B:281:TYR:CZ	1:B:285:VAL:HG21	2.54	0.42
2:D:153:LEU:HA	2:D:193:ILE:HD12	2.02	0.42
3:F:25:LEU:HD22	3:F:68:LYS:HA	2.02	0.42
2:D:54:VAL:HG12	2:D:55:TYR:CD2	2.54	0.42
1:A:179:PRO:HB3	1:A:469:ILE:HD13	2.02	0.42
2:D:336:MET:HE1	2:D:356:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:55:TRP:CZ2	3:F:59:LYS:HE2	2.55	0.42
1:B:202:LEU:HD22	1:B:206:LEU:CD2	2.50	0.42
1:B:232:THR:HB	1:B:233:PRO:HD3	2.02	0.42
1:B:344:HIS:HE1	1:B:376:TYR:CD2	2.37	0.42
1:A:44:THR:HG21	8:A:9204:HOH:O	2.18	0.41
1:A:163:GLN:HG2	8:A:9037:HOH:O	2.19	0.41
1:B:105:VAL:O	1:B:109:PHE:HB2	2.20	0.41
2:C:336:MET:HE2	2:C:385:LEU:HA	2.02	0.41
2:D:277:THR:N	2:D:278:PRO:CD	2.83	0.41
1:A:123:MET:HB2	2:C:168:ARG:HD3	2.03	0.41
1:B:38:ASP:O	1:B:39:PHE:HB3	2.20	0.41
1:B:52:MET:HE1	1:B:127:SER:HB3	1.99	0.41
2:D:169:GLU:O	2:D:170:ALA:C	2.57	0.41
2:D:235:TRP:CD1	2:D:235:TRP:C	2.91	0.41
2:D:243:GLU:HB2	2:D:320:TRP:CZ2	2.54	0.41
3:F:125:VAL:HG23	3:F:126:ASN:N	2.35	0.41
1:A:118:ILE:HD11	1:A:145:ILE:HA	2.03	0.41
2:D:93:VAL:HG13	8:D:478:HOH:O	2.19	0.41
2:D:144:PHE:CZ	2:D:342:LEU:HD23	2.56	0.41
2:D:189:ILE:HD11	2:D:287:TYR:CD1	2.55	0.41
1:A:113:GLY:HA3	1:A:188:PHE:HD2	1.84	0.41
1:A:292:TYR:OH	1:A:344:HIS:CD2	2.65	0.41
3:F:66:VAL:HG12	3:F:70:ARG:NH2	2.36	0.41
1:A:125:TRP:CD1	1:A:125:TRP:C	2.94	0.41
1:B:223:TRP:CZ3	1:B:297:LYS:HA	2.55	0.41
2:C:121:ASP:O	2:C:125:GLN:HG3	2.20	0.41
2:C:261:ARG:NE	2:C:285:GLN:HE22	2.04	0.41
2:D:357:TYR:CD2	2:D:381:VAL:HG21	2.56	0.41
1:A:146:ARG:HB2	2:C:106:HIS:CE1	2.55	0.41
1:B:50:TYR:CD1	1:B:50:TYR:N	2.89	0.41
2:D:357:TYR:CD2	2:D:377:ARG:NH2	2.89	0.41
1:A:184:MET:HE3	1:A:188:PHE:HB2	2.03	0.41
2:D:39:VAL:O	2:D:41:PRO:HD3	2.21	0.41
1:A:65:LYS:HB3	2:C:117:TRP:CD2	2.56	0.41
1:A:75:ASP:OD2	1:A:146:ARG:NH1	2.54	0.41
1:A:121:THR:HG21	1:A:140:GLN:CG	2.50	0.41
1:A:382:HIS:O	1:A:386:ILE:HG13	2.20	0.41
1:B:123:MET:SD	2:D:168:ARG:NH1	2.94	0.41
1:B:283:THR:HB	1:B:284:PRO:CD	2.50	0.41
2:C:153:LEU:C	2:C:153:LEU:HD12	2.41	0.41
2:C:161:ASN:HB3	2:C:235:TRP:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:120:PRO:HD3	3:E:128:PHE:CG	2.56	0.41
1:A:321:LEU:O	1:A:326:VAL:HB	2.21	0.41
1:A:343:HIS:H	1:A:343:HIS:CD2	2.39	0.41
2:C:277:THR:N	2:C:278:PRO:CD	2.84	0.41
2:D:213:VAL:HB	2:D:214:PRO:HD3	2.02	0.41
1:A:344:HIS:HE1	1:A:376:TYR:CD2	2.39	0.40
2:D:87:THR:HG21	2:D:169:GLU:OE1	2.21	0.40
1:A:232:THR:HB	1:A:233:PRO:HD3	2.02	0.40
1:A:430:ALA:HA	8:A:9170:HOH:O	2.20	0.40
2:D:228:ARG:HH11	2:D:228:ARG:HG2	1.86	0.40
1:A:108:ASN:O	1:A:111:GLU:HB3	2.20	0.40
2:C:126:GLY:O	2:C:130:ASP:HB2	2.21	0.40
2:D:148:TYR:CE2	2:D:338:LEU:HD13	2.56	0.40
3:F:39:HIS:HD2	8:F:189:HOH:O	2.04	0.40
1:A:184:MET:CE	1:A:188:PHE:HB2	2.52	0.40
1:A:435:THR:HG22	3:E:168:SER:HA	2.03	0.40
1:A:439:HIS:CE1	1:A:454:GLU:OE1	2.71	0.40
2:C:118:ARG:NH2	2:D:112:ASP:OD1	2.53	0.40
2:C:146:ASN:O	2:C:214:PRO:HG3	2.22	0.40
3:F:86:ASP:HB3	3:F:89:SER:OG	2.21	0.40
1:A:115:TYR:OH	2:C:173:ASP:HA	2.22	0.40
2:D:13:ASP:HA	2:D:14:PRO:HD3	1.96	0.40
2:D:261:ARG:NE	2:D:285:GLN:HE22	2.07	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%)	486 (96%)	20 (4%)	2 (0%)	34 22
1	B	508/527 (96%)	483 (95%)	24 (5%)	1 (0%)	47 38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	C	386/389 (99%)	377 (98%)	8 (2%)	1 (0%)	41 30
2	D	386/389 (99%)	357 (92%)	25 (6%)	4 (1%)	15 6
3	E	164/170 (96%)	162 (99%)	2 (1%)	0	100 100
3	F	165/170 (97%)	156 (94%)	7 (4%)	2 (1%)	13 4
All	All	2117/2172 (98%)	2021 (96%)	86 (4%)	10 (0%)	29 17

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	40	LYS
1	A	311	GLU
2	D	64	ALA
3	F	122	ILE
1	A	340	TYR
2	D	205	PRO
2	D	251	VAL
3	F	87	ALA
2	D	388	LEU
2	C	251	VAL

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%)	419 (97%)	13 (3%)	41 30
1	B	432/442 (98%)	423 (98%)	9 (2%)	53 46
2	C	322/323 (100%)	317 (98%)	5 (2%)	62 58
2	D	322/323 (100%)	316 (98%)	6 (2%)	57 50
3	E	144/147 (98%)	141 (98%)	3 (2%)	53 46
3	F	145/147 (99%)	141 (97%)	4 (3%)	43 33
All	All	1797/1824 (98%)	1757 (98%)	40 (2%)	52 44

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ARG
1	A	43	ARG
1	A	54	ASN
1	A	90	ASN
1	A	125	TRP
1	A	160	LYS
1	A	186	ARG
1	A	279	GLN
1	A	391	ARG
1	A	403	ILE
1	A	437	ARG
1	A	467	GLN
1	A	520	LYS
1	B	30	ARG
1	B	43	ARG
1	B	90	ASN
1	B	110	LEU
1	B	125	TRP
1	B	186	ARG
1	B	279	GLN
1	B	310	TYR
1	B	440	GLU
2	C	35	MET
2	C	153	LEU
2	C	168	ARG
2	C	173	ASP
2	C	378	ASP
2	D	4	LEU
2	D	35	MET
2	D	153	LEU
2	D	173	ASP
2	D	205	PRO
2	D	334	ASP
3	E	44	ARG
3	E	46	SER
3	E	166	LEU
3	F	11	THR
3	F	44	ARG
3	F	164	VAL
3	F	167	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	54	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	203	ASN
1	A	227	ASN
1	A	249	ASN
1	A	252	GLN
1	A	268	ASN
1	A	273	ASN
1	A	279	GLN
1	A	343	HIS
1	A	344	HIS
1	A	382	HIS
1	A	412	ASN
1	A	413	HIS
1	A	439	HIS
1	A	442	ASN
1	A	472	GLN
1	B	33	GLN
1	B	42	ASN
1	B	78	GLN
1	B	90	ASN
1	B	100	ASN
1	B	108	ASN
1	B	133	GLN
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

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Mol	Chain	Res	Type
1	B	451	GLN
1	B	516	ASN
1	B	527	ASN
2	C	98	HIS
2	C	146	ASN
2	C	161	ASN
2	C	266	GLN
2	C	285	GLN
2	C	296	GLN
2	C	301	ASN
2	D	98	HIS
2	D	161	ASN
2	D	285	GLN
3	E	45	ASN
3	E	144	ASN
3	F	7	HIS
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 9 ligands modelled in this entry, 7 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
7	EOH	B	9002	4	2,2,2	0.50	0	1,1,1	0.14	0
6	FMT	A	9001	4	2,2,2	0.65	0	1,1,1	0.62	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%)	0.50	48 (9%) 8 13	22, 36, 62, 78	0
1	B	510/527 (96%)	0.32	35 (6%) 16 25	22, 36, 63, 78	0
2	C	388/389 (99%)	-0.01	7 (1%) 68 76	18, 26, 46, 62	0
2	D	388/389 (99%)	0.83	54 (13%) 2 4	26, 46, 68, 82	2 (0%)
3	E	166/170 (97%)	-0.04	2 (1%) 79 84	20, 29, 46, 69	0
3	F	167/170 (98%)	1.47	44 (26%) 0 0	37, 56, 75, 86	0
All	All	2129/2172 (98%)	0.46	190 (8%) 9 15	18, 37, 66, 86	2 (0%)

All (190) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	244	LEU	6.1
1	A	19	ALA	5.7
2	D	205	PRO	5.5
1	B	316	ILE	5.5
1	A	316	ILE	5.4
1	A	310	TYR	5.2
1	A	326	VAL	5.0
3	F	101	ALA	4.9
2	D	207	PHE	4.9
1	A	433	ALA	4.9
1	B	55	GLU	4.8
1	B	244	LEU	4.5
3	F	102	LYS	4.5
3	F	72	PHE	4.4
2	D	389	LYS	4.3
1	A	260	ASP	4.2
1	B	39	PHE	4.2
3	F	83	PHE	4.2
3	F	21	GLN	4.1

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Mol	Chain	Res	Type	RSRZ
2	D	375	ALA	4.1
1	B	310	TYR	4.1
1	A	322	GLY	4.1
3	F	26	GLU	4.1
1	B	40	LYS	4.1
2	D	374	LYS	4.0
1	A	20	PRO	3.9
3	F	23	ASN	3.9
3	F	80	LYS	3.9
1	A	60	PHE	3.9
3	F	100	ALA	3.9
1	A	320	ARG	3.8
2	D	229	LEU	3.8
1	A	259	ASN	3.7
1	B	54	ASN	3.6
1	B	527	ASN	3.6
3	F	27	LYS	3.6
2	D	220	ASN	3.6
2	D	388	LEU	3.6
2	D	44	LYS	3.6
2	D	344	ALA	3.6
2	C	2	SER	3.5
1	B	320	ARG	3.5
1	B	53	ALA	3.5
3	F	170	HIS	3.5
2	D	382	LYS	3.5
2	D	349	LYS	3.5
1	B	21	THR	3.5
2	D	45	ARG	3.4
3	F	69	ALA	3.4
1	B	259	ASN	3.4
2	C	205	PRO	3.4
2	D	153	LEU	3.4
1	A	54	ASN	3.3
3	F	161	VAL	3.3
1	A	59	GLN	3.3
1	B	311	GLU	3.3
1	B	19	ALA	3.3
1	B	20	PRO	3.3
1	A	434	SER	3.2
2	D	2	SER	3.2
3	F	121	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
3	E	4	LEU	3.2
1	A	251	TYR	3.2
1	A	318	ILE	3.2
2	C	203	ILE	3.2
3	F	66	VAL	3.1
3	F	118	TYR	3.1
1	B	38	ASP	3.0
2	D	356	LEU	3.0
1	A	257	ILE	3.0
3	F	89	SER	3.0
3	F	76	ASP	3.0
1	A	338	ASP	3.0
2	D	260	VAL	3.0
3	F	120	PRO	2.9
1	A	315	GLY	2.9
3	F	20	ALA	2.9
2	D	348	ASP	2.9
2	D	380	ILE	2.8
3	F	14	ALA	2.8
3	F	154	GLU	2.8
2	C	6	GLU	2.8
3	F	67	LEU	2.8
2	D	343	PRO	2.8
3	F	19	ILE	2.8
2	D	256	PHE	2.8
3	F	16	VAL	2.8
1	A	262	ALA	2.7
1	B	23	VAL	2.7
2	D	159	LEU	2.7
2	D	255	LEU	2.7
2	D	347	THR	2.7
2	D	270	PRO	2.7
3	F	22	LEU	2.7
1	A	340	TYR	2.6
2	D	385	LEU	2.6
1	A	285	VAL	2.6
1	A	435	THR	2.6
1	A	255	VAL	2.6
2	D	342	LEU	2.6
2	D	152	PHE	2.5
3	F	4	LEU	2.5
3	F	28	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
3	F	73	ASN	2.5
3	F	91	LEU	2.5
1	A	261	PRO	2.5
1	A	325	GLY	2.5
2	C	45	ARG	2.5
3	F	103	ASP	2.5
1	A	247	MET	2.5
3	F	10	ASP	2.5
2	D	275	ASN	2.5
1	B	514	ARG	2.5
2	C	389	LYS	2.5
2	D	350	GLU	2.5
1	B	264	ALA	2.5
1	B	333	LYS	2.5
3	F	17	ASN	2.5
1	A	321	LEU	2.4
1	A	264	ALA	2.4
3	F	142	LEU	2.4
1	B	261	PRO	2.4
1	B	323	LYS	2.4
2	D	206	GLY	2.4
1	A	265	LYS	2.4
1	B	57	LYS	2.4
1	B	26	GLN	2.4
3	F	87	ALA	2.4
2	D	26	GLU	2.4
3	F	30	GLU	2.4
2	D	145	ILE	2.4
2	D	338	LEU	2.3
3	F	145	LEU	2.3
1	A	337	GLN	2.3
2	D	352	ILE	2.3
1	B	41	ASN	2.3
1	B	317	TRP	2.3
1	A	55	GLU	2.3
2	D	326	GLU	2.3
2	D	248	VAL	2.3
1	A	202	LEU	2.3
2	D	387	GLY	2.2
1	A	309	VAL	2.2
1	A	339	ALA	2.2
1	B	265	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	31	TRP	2.2
3	E	168	SER	2.2
1	A	381	ASP	2.2
1	A	311	GLU	2.2
1	A	212	PHE	2.2
1	A	323	LYS	2.2
2	D	138	PRO	2.2
1	B	22	SER	2.2
1	B	285	VAL	2.2
1	B	251	TYR	2.2
2	D	357	TYR	2.2
3	F	151	PRO	2.2
1	A	432	GLY	2.2
3	F	25	LEU	2.2
3	F	70	ARG	2.2
1	A	324	TYR	2.2
2	D	254	ALA	2.2
1	A	213	THR	2.2
2	D	252	TYR	2.2
2	D	370	ARG	2.2
2	D	365	GLU	2.2
1	B	255	VAL	2.2
1	A	415	ILE	2.1
2	D	203	ILE	2.1
2	D	136	MET	2.1
1	A	210	ALA	2.1
1	A	258	ALA	2.1
1	A	380	TYR	2.1
2	D	193	ILE	2.1
2	D	345	GLY	2.1
1	B	353	LEU	2.1
2	D	383	ALA	2.1
3	F	125	VAL	2.1
2	C	189	ILE	2.1
2	D	386	ALA	2.1
3	F	153	GLU	2.1
1	B	258	ALA	2.1
2	D	200	LEU	2.1
1	A	327	GLU	2.0
1	B	214	ASN	2.0
2	D	339	PHE	2.0
3	F	75	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
2	D	190	ALA	2.0
2	D	149	TRP	2.0
3	F	99	ASN	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, 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	B-factors(Å^2)	Q<0.9
7	EOH	B	9002	3/3	0.86	0.21	46,46,47,49	0
6	FMT	A	9001	3/3	0.93	0.12	51,51,53,57	0
5	CA	C	5006	1/1	0.94	0.04	65,65,65,65	0
4	FE	A	5002	1/1	0.98	0.03	49,49,49,49	0
5	CA	A	5005	1/1	0.99	0.06	40,40,40,40	0
4	FE	A	5001	1/1	0.99	0.02	42,42,42,42	0
5	CA	C	5007	1/1	0.99	0.06	40,40,40,40	0
4	FE	B	5003	1/1	0.99	0.03	34,34,34,34	0
4	FE	B	5004	1/1	0.99	0.03	44,44,44,44	0

6.5 Other polymers (i)

There are no such residues in this entry.