



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:31 PM GMT

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
<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

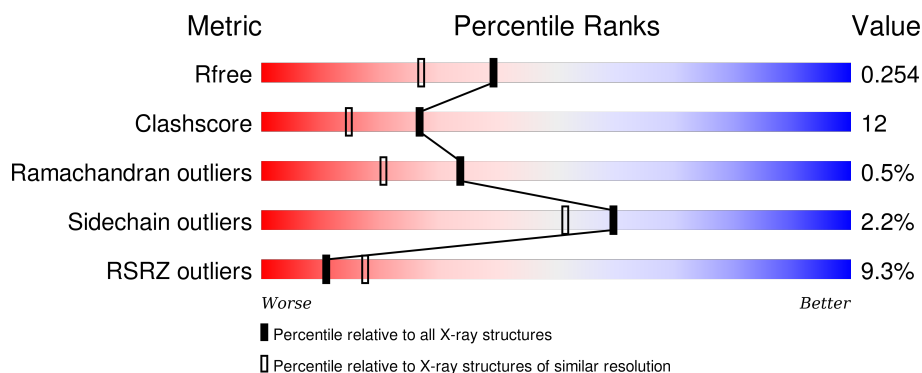
1 Overall quality at a glance

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}	91344	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (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 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 $\leq 5\%$. 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	<div> <div>9%</div> <div>70%</div> <div>25%</div> <div>• •</div> </div>
1	B	527	<div> <div>7%</div> <div>72%</div> <div>24%</div> <div>• •</div> </div>
2	C	389	<div> <div>2%</div> <div>80%</div> <div>19%</div> <div>•</div> </div>
2	D	389	<div> <div>14%</div> <div>65%</div> <div>34%</div> <div>•</div> </div>
3	E	170	<div> <div>0%</div> <div>82%</div> <div>14%</div> <div>• •</div> </div>

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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	EOH	B	9002	-	-	-	X

2 Entry composition

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			

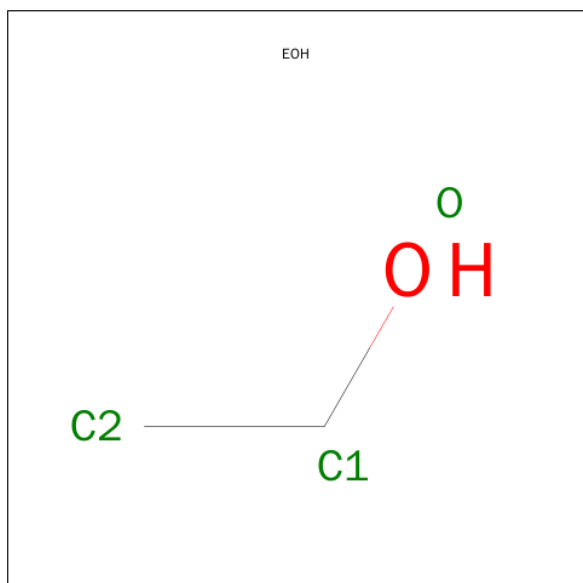
- Molecule 4 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

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

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

- Molecule 6 is ETHANOL (three-letter code: EOH) (formula: C₂H₆O).



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

- Molecule 7 is FORMIC ACID (three-letter code: FMT) (formula: CH₂O₂).



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

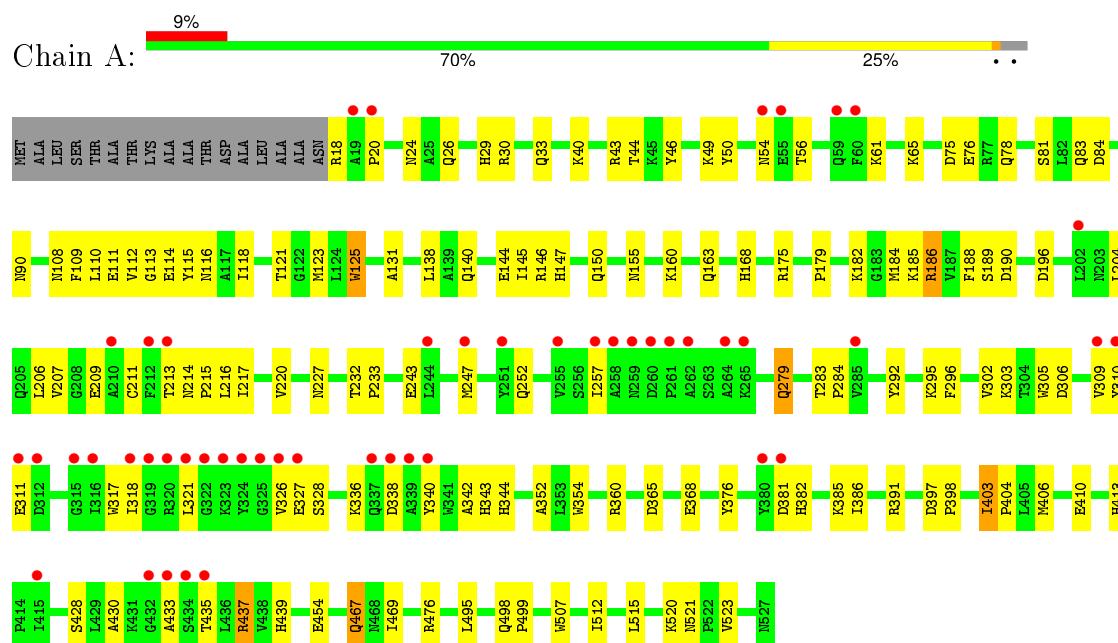
- Molecule 8 is water.

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

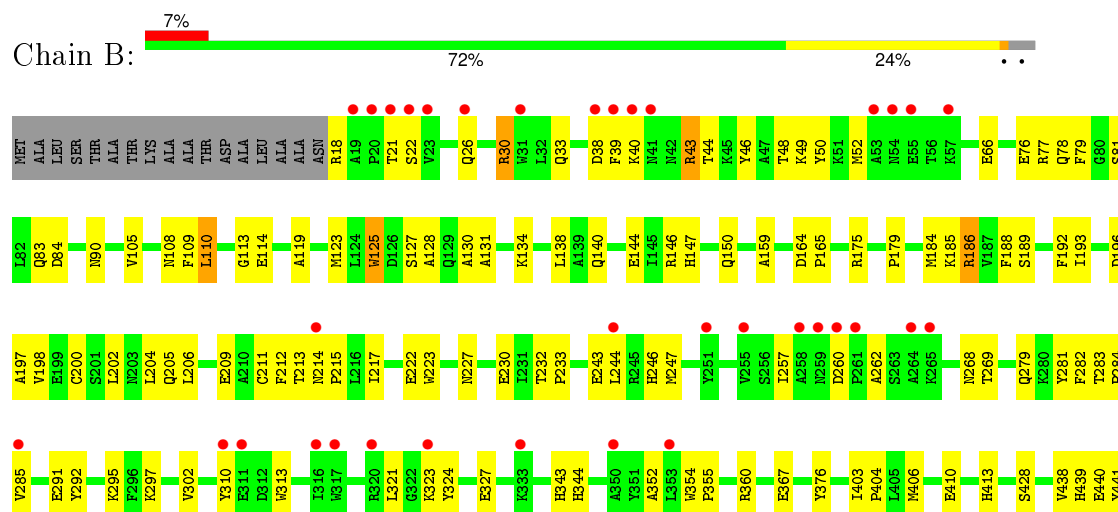
3 Residue-property plots

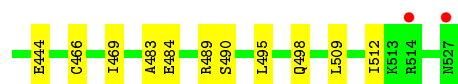
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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

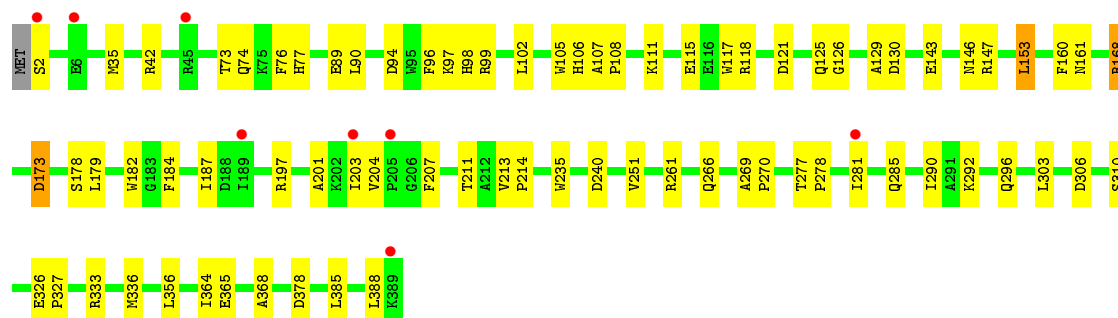
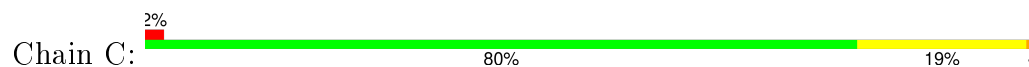


• Molecule 1: METHANE MONOOXYGENASE COMPONENT A, ALPHA CHAIN

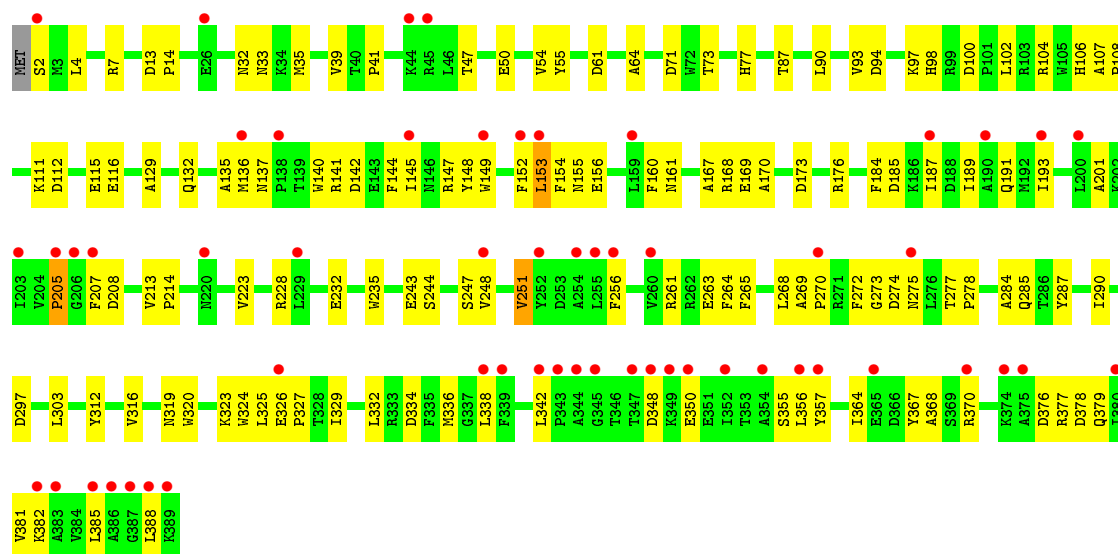




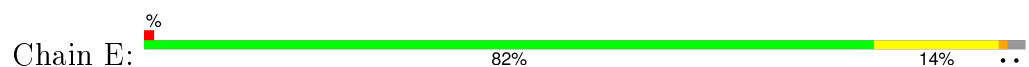
• Molecule 2: METHANE MONOOXYGENASE COMPONENT A, BETA CHAIN



• Molecule 2: METHANE MONOOXYGENASE COMPONENT A, BETA CHAIN

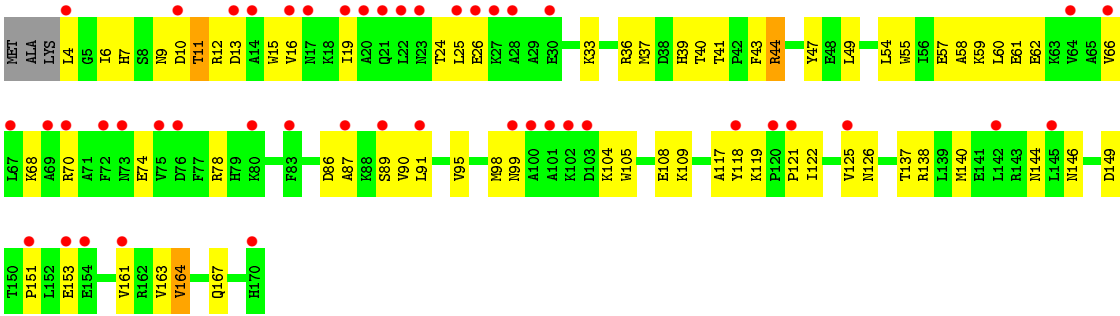


• Molecule 3: METHANE MONOOXYGENASE COMPONENT A, GAMMA CHAIN



• 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	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
$\langle I/\sigma(I) \rangle$ ¹	5.19 (at 1.96Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.214 , 0.255 0.214 , 0.254	Depositor DCC
R_{free} test set	6226 reflections (3.52%)	DCC
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
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 192171 reflections	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FMT, EOH, CA, 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 [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	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	B	3	0	5	0	0
7	A	3	0	1	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:CD	3:F:153:GLU:H	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
3:E:22:LEU:HD11	3:E:31:MET:SD	2.32	0.68
1:B:214:ASN:HB3	1:B:215:PRO:HD3	1.74	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
3:F:15:TRP:O	3:F:19:ILE:HG23	1.94	0.66
2:D:135:ALA:O	2:D:273:GLY:HA3	1.96	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
3:F:41:THR:HG23	3:F:43:PHE:N	2.04	0.65
2:D:261:ARG:HE	2:D:285:GLN:NE2	1.94	0.65
2:D:184:PHE:O	2:D:187:ILE:HG22	1.96	0.65
2:C:269:ALA:HB3	2:C:270:PRO:HD3	1.78	0.65
1:A:306:ASP:HB2	8:A:9217:HOH:O	1.96	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:310:TYR:CZ	1:A:336:LYS:HD2	2.33	0.63
1:A:185:LYS:O	1:A:189:SER:HB2	1.98	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
2:C:96:PHE:O	2:C:99:ARG:NH2	2.32	0.62
1:B:49:LYS:CE	3:F:144:ASN:HD22	2.13	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:58:ALA:O	3:F:62:GLU:HG3	2.01	0.60
3:F:57:GLU:O	3:F:61:GLU:HG3	2.00	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
3:F:44:ARG:HD3	3:F:47:TYR:CZ	2.37	0.59
1:B:164:ASP:OD1	1:B:489:ARG:NH2	2.36	0.59
1:B:30:ARG:HD3	1:B:30:ARG:C	2.23	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:ASN:HB3	1:A:215:PRO:HD3	1.85	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:213:THR:O	1:B:217:ILE:HG12	2.04	0.57
1:B:206:LEU:HD11	1:B:321:LEU:HD11	1.86	0.57
1:B:489:ARG:HD2	1:B:495:LEU:O	2.05	0.57
1:B:466:CYS:HB2	2:D:73:THR:HA	1.85	0.57
3:E:41:THR:O	3:E:44:ARG:CD	2.52	0.57
2:D:112:ASP:O	2:D:116:GLU:HG3	2.04	0.57
2:D:377:ARG:O	2:D:381:VAL:HG23	2.04	0.57
1:A:110:LEU:O	1:A:114:GLU:HG2	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:439:HIS:HB3	3:F:161:VAL:CG2	2.35	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
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:HD12	2:D:153:LEU:C	2.26	0.56
1:A:403:ILE:HD13	1:A:515:LEU:CD1	2.35	0.56
1:A:40:LYS:HD2	8:A:9119:HOH:O	2.06	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
2:C:211:THR:O	2:C:214:PRO:HD2	2.07	0.55
1:B:495:LEU:HD11	1:B:512:ILE:HG13	1.88	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
3:F:61:GLU:HB3	3:F:121:PRO:HD3	1.88	0.54
2:D:357:TYR:CE2	2:D:381:VAL:HG21	2.42	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
3:F:4:LEU:CD2	3:F:10:ASP:H	2.20	0.54
2:D:140:TRP:NE1	2:D:145:ILE:HD11	2.22	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
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
1:B:483:ALA:HB2	1:B:509:LEU:HD21	1.90	0.54
2:D:275:ASN:C	2:D:278:PRO:HD2	2.28	0.53
2:D:141:ARG:CG	2:D:142:ASP:N	2.71	0.53
2:C:98:HIS:HE1	2:C:178:SER:OG	1.92	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
2:C:261:ARG:HE	2:C:285:GLN:NE2	2.00	0.53
1:B:140:GLN:HG3	1:B:246:HIS:CD2	2.43	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:B:108:ASN:ND2	1:B:175:ARG:HH11	2.06	0.52
1:A:18:ARG:O	2:C:129:ALA:HA	2.10	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
2:C:333:ARG:HD2	8:C:5192:HOH:O	2.10	0.51
1:B:192:PHE:O	1:B:200:CYS:HB3	2.11	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:B:227:ASN:ND2	1:B:295:LYS:H	2.09	0.50
1:A:114:GLU:CD	1:A:147:HIS:HB3	2.32	0.50
2:D:201:ALA:HA	2:D:207:PHE:HB3	1.93	0.50
1:A:140:GLN:O	1:A:144:GLU:HG2	2.12	0.50
2:D:265:PHE:O	2:D:269:ALA:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:42:ARG:HB2	2:C:99:ARG:HG3	1.92	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
2:C:211:THR:C	2:C:214:PRO:HD2	2.33	0.49
2:C:90:LEU:HD13	2:C:303:LEU:HD13	1.94	0.49
1:B:26:GLN:HG3	8:B:9084:HOH:O	2.12	0.49
2:D:147:ARG:HD2	2:D:148:TYR:CE1	2.47	0.49
1:A:113:GLY:HA3	1:A:188:PHE:CD2	2.47	0.49
2:C:111:LYS:O	2:C:115:GLU:HG3	2.12	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:B:138:LEU:HD22	2:D:160:PHE:CZ	2.47	0.49
1:B:186:ARG:HD3	1:B:186:ARG:C	2.33	0.49
1:A:206:LEU:HD12	1:A:317:TRP:HH2	1.77	0.49
3:F:95:VAL:HG12	3:F:99:ASN:HD21	1.77	0.49
1:B:33:GLN:HA	1:B:131:ALA:HB3	1.95	0.49
2:D:77:HIS:CD2	3:F:140:MET:HG2	2.48	0.49
2:C:292:LYS:O	2:C:296:GLN:HG3	2.13	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
3:F:39:HIS:CD2	3:F:49:LEU:HD12	2.47	0.49
2:D:156:GLU:OE2	2:D:156:GLU:HA	2.12	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
2:C:97:LYS:HD2	8:C:5101:HOH:O	2.12	0.48
1:B:323:LYS:HE2	1:B:324:TYR:CE1	2.49	0.48
2:C:143:GLU:O	2:C:147:ARG:HB3	2.13	0.48
1:A:83:GLN:HB3	1:B:77:ARG:NH1	2.29	0.48
2:C:336:MET:CE	2:C:385:LEU:HD23	2.43	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:D:324:TRP:O	2:D:327:PRO:HD2	2.14	0.48
2:C:306:ASP:O	2:C:310:SER:HB2	2.13	0.48
1:B:144:GLU:HA	1:B:144:GLU:OE2	2.14	0.48
2:D:54:VAL:O	2:D:55:TYR:HB2	2.14	0.48
2:D:136:MET:HA	2:D:273:GLY:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:LYS:HD3	3:E:144:ASN:HD22	1.77	0.48
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: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
1:A:83:GLN:HB3	1:B:77:ARG:HH12	1.79	0.47
3:F:16:VAL:O	3:F:19:ILE:HG12	2.15	0.47
2:D:325:LEU:O	2:D:329:ILE:HG13	2.14	0.47
1:B:268:ASN:ND2	1:B:327:GLU:H	2.07	0.47
1:A:108:ASN:ND2	1:A:175:ARG:HH11	2.12	0.47
1:B:184:MET:HE1	1:B:282:PHE:CZ	2.48	0.47
1:A:365:ASP:OD2	1:A:368:GLU:HG3	2.15	0.47
2:D:90:LEU:HD13	2:D:303:LEU:HD13	1.97	0.47
1:A:81:SER:OG	1:B:84:ASP:HB3	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:B:490:SER:OG	2:D:32:ASN:HB2	2.14	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
1:A:398:PRO:HG3	1:A:507:TRP:CD1	2.50	0.47
2:D:364:ILE:HA	2:D:368:ALA:HB3	1.96	0.47
2:C:2:SER:HB2	8:C:5038:HOH:O	2.14	0.47
1:B:33:GLN:HE22	1:B:130:ALA:HB1	1.80	0.47
1:A:24:ASN:OD1	1:A:26:GLN:HG2	2.15	0.47
1:A:284:PRO:HB3	1:A:342:ALA:HB1	1.98	0.46
2:D:274:ASP:OD2	2:D:277:THR:HB	2.15	0.46
1:A:116:ASN:CG	1:A:189:SER:HA	2.36	0.46
3:F:40:THR:O	3:F:41:THR:CG2	2.55	0.46
2:C:336:MET:HE1	2:C:356:LEU:HD11	1.97	0.46
1:B:165:PRO:HG3	8:B:9114:HOH:O	2.16	0.46
1:B:125:TRP:HE1	2:D:161:ASN:ND2	2.14	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:A:144:GLU:HA	1:A:144:GLU:OE2	2.15	0.46
2:C:179:LEU:HD12	2:C:182:TRP:CZ3	2.51	0.46
1:A:118:ILE:HD13	1:A:145:ILE:HG12	1.97	0.46
1:A:360:ARG:HG2	1:A:498:GLN:HB2	1.98	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
2:D:153:LEU:HD12	2:D:154:PHE:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:LEU:HG	1:B:205:GLN:HG3	1.97	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
2:D:356:LEU:HD12	2:D:385:LEU:HD13	1.98	0.45
1:B:360:ARG:HG2	1:B:498:GLN:HB2	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:D:152:PHE:O	2:D:155:ASN:HB3	2.16	0.45
2:C:201:ALA:HA	2:C:207:PHE:HB3	1.98	0.45
2:D:263:GLU:OE2	2:D:263:GLU:HA	2.17	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:381:ASP:HA	1:A:385:LYS:HE2	1.99	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: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:A:216:LEU:O	1:A:220:VAL:HG23	2.17	0.44
3:F:74:GLU:O	3:F:78:ARG:HG3	2.18	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
1:B:403:ILE:O	1:B:403:ILE:HG23	2.17	0.44
1:B:202:LEU:HD22	1:B:206:LEU:HD23	1.98	0.44
1:A:354:TRP:CH2	1:A:499:PRO:HD3	2.53	0.44
1:A:321:LEU:N	1:A:321:LEU:HD12	2.31	0.44
3:F:33:LYS:HE3	3:F:117:ALA:HA	2.00	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:12:ARG:O	3:F:16:VAL:HG13	2.18	0.44
2:C:105:TRP:O	2:C:108:PRO:HD2	2.17	0.44
2:D:176:ARG:HH11	2:D:176:ARG:HG3	1.83	0.44
2:C:184:PHE:O	2:C:187:ILE:HG22	2.18	0.44
2:D:208:ASP:HA	8:D:497:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:495:LEU:HD11	1:A:512:ILE:CG1	2.47	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
3:F:95:VAL:HG12	3:F:99:ASN:ND2	2.33	0.43
1:B:114:GLU:CD	1:B:147:HIS:HB3	2.39	0.43
3:F:36:ARG:CZ	3:F:119:LYS:HB3	2.48	0.43
1:B:283:THR:HB	1:B:284:PRO:HD3	2.01	0.43
1:A:33:GLN:HA	1:A:131:ALA:HB3	2.01	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:HA	1:B:444:GLU:OE2	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:140:GLN:HG3	1:B:246:HIS:NE2	2.34	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:B:128:ALA:O	1:B:134:LYS:HE2	2.19	0.42
1:B:230:GLU:C	1:B:233:PRO:HD2	2.39	0.42
1:B:146:ARG:HB2	2:D:106:HIS:CE1	2.54	0.42
1:A:306:ASP:O	1:A:310:TYR:HB2	2.19	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
1:A:303:LYS:HE3	1:A:303:LYS:HB2	1.85	0.42
1:A:521:ASN:OD1	1:A:523:VAL:HG12	2.20	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
2:D:336:MET:HE1	2:D:356:LEU:HD11	2.01	0.42
3:F:55:TRP:CZ2	3:F:59:LYS:HE2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:PRO:HB3	1:A:469:ILE:HD13	2.02	0.42
1:B:344:HIS:HE1	1:B:376:TYR:CD2	2.37	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
2:D:277:THR:N	2:D:278:PRO:CD	2.83	0.41
1:A:44:THR:HG21	8:A:9204:HOH:O	2.18	0.41
2:C:336:MET:HE2	2:C:385:LEU:HA	2.02	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
1:B:52:MET:HE1	1:B:127:SER:HB3	1.99	0.41
1:A:123:MET:HB2	2:C:168:ARG:HD3	2.03	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
1:B:38:ASP:O	1:B:39:PHE:HB3	2.20	0.41
2:D:169:GLU:O	2:D:170:ALA:C	2.57	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:189:ILE:HD11	2:D:287:TYR:CD1	2.55	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
1:A:292:TYR:OH	1:A:344:HIS:CD2	2.65	0.41
1:A:113:GLY:HA3	1:A:188:PHE:HD2	1.84	0.41
3:F:66:VAL:HG12	3:F:70:ARG:NH2	2.36	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:125:TRP:C	1:A:125:TRP:CD1	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:D:357:TYR:CD2	2:D:377:ARG:NH2	2.89	0.41
1:B:50:TYR:CD1	1:B:50:TYR:N	2.89	0.41
1:A:146:ARG:HB2	2:C:106:HIS:CE1	2.55	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:B:123:MET:SD	2:D:168:ARG:NH1	2.94	0.41
1:A:121:THR:HG21	1:A:140:GLN:CG	2.50	0.41
2:C:161:ASN:HB3	2:C:235:TRP:CE2	2.56	0.41
1:A:65:LYS:HB3	2:C:117:TRP:CD2	2.56	0.41
1:B:283:THR:HB	1:B:284:PRO:CD	2.50	0.41
1:A:75:ASP:OD2	1:A:146:ARG:NH1	2.54	0.41
3:E:120:PRO:HD3	3:E:128:PHE:CG	2.56	0.41
1:A:382:HIS:O	1:A:386:ILE:HG13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:153:LEU:HD12	2:C:153:LEU:C	2.41	0.41
2:D:213:VAL:HB	2:D:214:PRO:HD3	2.02	0.41
1:A:321:LEU:O	1:A:326:VAL:HB	2.21	0.41
2:C:277:THR:N	2:C:278:PRO:CD	2.84	0.41
1:A:343:HIS:H	1:A:343:HIS:CD2	2.39	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
2:D:228:ARG:HH11	2:D:228:ARG:HG2	1.86	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
1:A:108:ASN:O	1:A:111:GLU:HB3	2.20	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
2:C:126:GLY:O	2:C:130:ASP:HB2	2.21	0.40
2:C:146:ASN:O	2:C:214:PRO:HG3	2.22	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
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
3:F:86:ASP:HB3	3:F:89:SER:OG	2.21	0.40
2:D:261:ARG:NE	2:D:285:GLN:HE22	2.07	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

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%)	39 27
1	B	508/527 (96%)	483 (95%)	24 (5%)	1 (0%)	52 43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	386/389 (99%)	377 (98%)	8 (2%)	1 (0%)	46	35
2	D	386/389 (99%)	357 (92%)	25 (6%)	4 (1%)	19	8
3	E	164/170 (96%)	162 (99%)	2 (1%)	0	100	100
3	F	165/170 (97%)	156 (94%)	7 (4%)	2 (1%)	16	5
All	All	2117/2172 (98%)	2021 (96%)	86 (4%)	10 (0%)	34	21

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 ⓘ

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%)	48	36
1	B	432/442 (98%)	423 (98%)	9 (2%)	61	53
2	C	322/323 (100%)	317 (98%)	5 (2%)	70	66
2	D	322/323 (100%)	316 (98%)	6 (2%)	65	58
3	E	144/147 (98%)	141 (98%)	3 (2%)	61	53
3	F	145/147 (99%)	141 (97%)	4 (3%)	51	39
All	All	1797/1824 (98%)	1757 (98%)	40 (2%)	60	51

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

Some 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 carbohydrates 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	FMT	A	9001	4	0,2,2	0.00	-	0,1,1	0.00	-
6	EOH	B	9002	4	2,2,2	0.47	0	1,1,1	0.15	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
7	FMT	A	9001	4	-	0/0/0/0	0/0/0/0
6	EOH	B	9002	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, 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%)	0.54	50 (9%)	10 15	22, 36, 62, 78	0
1	B	510/527 (96%)	0.36	37 (7%)	18 28	22, 36, 63, 78	0
2	C	388/389 (99%)	0.02	8 (2%)	67 75	18, 26, 46, 62	0
2	D	388/389 (99%)	0.88	56 (14%)	3 6	26, 46, 68, 82	2 (0%)
3	E	166/170 (97%)	-0.01	2 (1%)	81 87	20, 29, 46, 69	0
3	F	167/170 (98%)	1.52	46 (27%)	1 0	37, 56, 75, 86	0
All	All	2129/2172 (98%)	0.50	199 (9%)	11 17	18, 37, 66, 86	2 (0%)

All (199) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	244	LEU	6.3
1	A	19	ALA	5.8
2	D	205	PRO	5.6
1	A	316	ILE	5.6
1	B	316	ILE	5.6
1	A	310	TYR	5.3
1	A	326	VAL	5.2
3	F	101	ALA	5.1
2	D	207	PHE	5.0
1	A	433	ALA	5.0
1	B	55	GLU	4.8
1	B	244	LEU	4.6
3	F	72	PHE	4.5
3	F	102	LYS	4.5
1	B	39	PHE	4.4
1	A	260	ASP	4.3
2	D	389	LYS	4.3
3	F	83	PHE	4.3
2	D	375	ALA	4.2

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Mol	Chain	Res	Type	RSRZ
3	F	21	GLN	4.2
1	A	322	GLY	4.2
1	B	310	TYR	4.2
3	F	26	GLU	4.2
1	B	40	LYS	4.1
1	A	20	PRO	4.0
2	D	374	LYS	4.0
1	A	60	PHE	4.0
3	F	100	ALA	4.0
3	F	23	ASN	4.0
3	F	80	LYS	4.0
2	D	229	LEU	3.9
1	A	320	ARG	3.9
1	A	259	ASN	3.8
2	D	388	LEU	3.7
1	B	54	ASN	3.7
1	B	527	ASN	3.7
2	D	344	ALA	3.7
2	D	220	ASN	3.7
3	F	27	LYS	3.6
2	C	2	SER	3.6
2	D	44	LYS	3.6
3	F	170	HIS	3.6
1	B	53	ALA	3.6
2	D	382	LYS	3.5
1	B	21	THR	3.5
3	F	69	ALA	3.5
1	B	320	ARG	3.5
2	D	349	LYS	3.5
2	D	45	ARG	3.5
1	B	259	ASN	3.5
2	C	205	PRO	3.5
2	D	153	LEU	3.4
3	F	161	VAL	3.4
1	A	54	ASN	3.4
1	B	19	ALA	3.4
1	A	59	GLN	3.4
1	B	311	GLU	3.3
1	B	20	PRO	3.3
3	E	4	LEU	3.3
1	A	434	SER	3.3
3	F	121	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
2	D	2	SER	3.3
3	F	66	VAL	3.3
1	A	251	TYR	3.2
1	A	318	ILE	3.2
2	C	203	ILE	3.2
1	A	257	ILE	3.2
2	D	356	LEU	3.1
3	F	118	TYR	3.1
1	B	38	ASP	3.1
3	F	89	SER	3.1
2	D	260	VAL	3.1
3	F	76	ASP	3.1
1	A	338	ASP	3.0
1	A	315	GLY	3.0
3	F	20	ALA	3.0
2	D	380	ILE	3.0
3	F	120	PRO	3.0
2	D	348	ASP	3.0
3	F	14	ALA	2.9
3	F	19	ILE	2.9
3	F	154	GLU	2.9
3	F	67	LEU	2.9
2	D	256	PHE	2.8
2	D	343	PRO	2.8
2	D	159	LEU	2.8
3	F	16	VAL	2.8
2	C	6	GLU	2.8
2	D	255	LEU	2.8
1	A	262	ALA	2.8
1	B	23	VAL	2.8
3	F	22	LEU	2.8
2	D	347	THR	2.8
2	D	270	PRO	2.8
2	D	385	LEU	2.7
1	A	285	VAL	2.7
1	A	340	TYR	2.7
1	A	255	VAL	2.7
2	D	342	LEU	2.7
1	A	435	THR	2.6
2	D	152	PHE	2.6
3	F	4	LEU	2.6
3	F	91	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
3	F	28	ALA	2.6
1	A	261	PRO	2.6
3	F	73	ASN	2.6
1	A	325	GLY	2.6
3	F	103	ASP	2.6
1	B	264	ALA	2.6
2	C	45	ARG	2.5
3	F	10	ASP	2.5
1	A	247	MET	2.5
1	B	514	ARG	2.5
1	A	321	LEU	2.5
3	F	142	LEU	2.5
2	C	389	LYS	2.5
2	D	275	ASN	2.5
3	F	17	ASN	2.5
2	D	350	GLU	2.5
1	B	261	PRO	2.5
1	B	333	LYS	2.5
1	A	264	ALA	2.5
3	F	145	LEU	2.5
2	D	145	ILE	2.4
2	D	352	ILE	2.4
3	F	87	ALA	2.4
2	D	206	GLY	2.4
1	B	323	LYS	2.4
1	B	26	GLN	2.4
2	D	338	LEU	2.4
2	D	26	GLU	2.4
1	A	265	LYS	2.4
1	A	337	GLN	2.4
3	F	30	GLU	2.4
1	B	57	LYS	2.4
1	B	317	TRP	2.4
1	B	41	ASN	2.4
1	A	309	VAL	2.4
2	D	248	VAL	2.4
1	A	202	LEU	2.3
1	A	212	PHE	2.3
2	D	326	GLU	2.3
1	A	339	ALA	2.3
1	B	285	VAL	2.3
2	D	387	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	55	GLU	2.3
2	D	138	PRO	2.3
1	B	31	TRP	2.3
1	B	265	LYS	2.3
1	B	22	SER	2.3
3	E	168	SER	2.3
1	A	381	ASP	2.3
3	F	25	LEU	2.3
1	A	323	LYS	2.3
1	A	311	GLU	2.3
3	F	151	PRO	2.3
2	D	254	ALA	2.3
1	A	324	TYR	2.3
1	B	251	TYR	2.3
2	D	357	TYR	2.3
1	A	432	GLY	2.2
1	A	213	THR	2.2
1	A	210	ALA	2.2
1	A	258	ALA	2.2
1	A	415	ILE	2.2
2	D	203	ILE	2.2
3	F	70	ARG	2.2
1	B	353	LEU	2.2
2	D	193	ILE	2.2
2	D	252	TYR	2.2
1	B	255	VAL	2.2
3	F	125	VAL	2.2
2	D	136	MET	2.2
2	D	383	ALA	2.2
2	C	189	ILE	2.2
1	A	380	TYR	2.2
2	D	345	GLY	2.2
2	D	365	GLU	2.2
2	D	370	ARG	2.2
2	D	386	ALA	2.2
2	D	200	LEU	2.2
1	B	258	ALA	2.1
2	D	339	PHE	2.1
3	F	75	VAL	2.1
3	F	153	GLU	2.1
2	C	281	ILE	2.1
2	D	149	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	190	ALA	2.1
3	F	64	VAL	2.1
1	B	214	ASN	2.1
1	A	327	GLU	2.1
1	B	350	ALA	2.1
3	F	99	ASN	2.1
1	B	260	ASP	2.1
1	A	319	GLY	2.0
3	F	13	ASP	2.0
2	D	354	ALA	2.0
1	A	312	ASP	2.0
2	D	187	ILE	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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, 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	LLDF	B-factors(Å ²)	Q<0.9
6	EOH	B	9002	3/3	0.86	0.21	3.54	46,46,47,49	0
7	FMT	A	9001	3/3	0.93	0.12	-0.34	51,51,53,57	0
4	FE	B	5004	1/1	0.99	0.03	-2.75	44,44,44,44	0
4	FE	B	5003	1/1	0.99	0.03	-2.91	34,34,34,34	0
4	FE	A	5001	1/1	0.99	0.02	-3.83	42,42,42,42	0
5	CA	A	5005	1/1	0.99	0.06	-4.04	40,40,40,40	0
4	FE	A	5002	1/1	0.98	0.03	-4.14	49,49,49,49	0
5	CA	C	5006	1/1	0.94	0.04	-	65,65,65,65	0
5	CA	C	5007	1/1	0.99	0.06	-	40,40,40,40	0

6.5 Other polymers ⓘ

There are no such residues in this entry.