Full wwPDB X-ray Structure Validation Report (i)

Feb 4, 2024 – 08:56 PM EST

PDB ID	:	1XU5
Title	:	Soluble methane monooxygenase hydroxylase-phenol soaked
Authors	:	Sazinsky, M.H.; Lippard, S.J.
Deposited on	:	2004-10-25
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 (i) 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 (1)) were used in the production of this report:

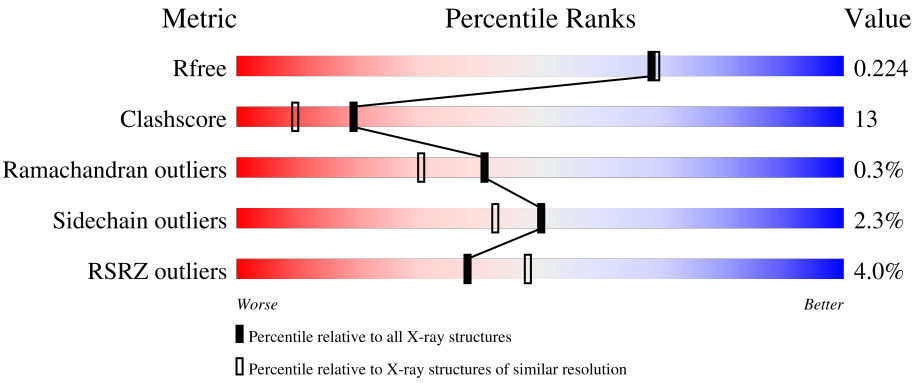
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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	2% 71% 25%
1	B	527	2% 70% 25%
2	C	389	% 81% 18%
2	D	389	8% 69% 29%
3	E	170	2% 79% 16%

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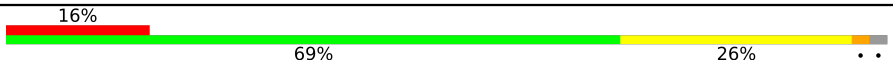
Mol	Chain	Length	Quality of chain
3	F	170	

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 18452 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Methane monooxygenase component A alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	510	Total	C	N	O	S	0	0	0
			4138	2649	709	762	18			
1	B	510	Total	C	N	O	S	0	0	0
			4137	2646	711	762	18			

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

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

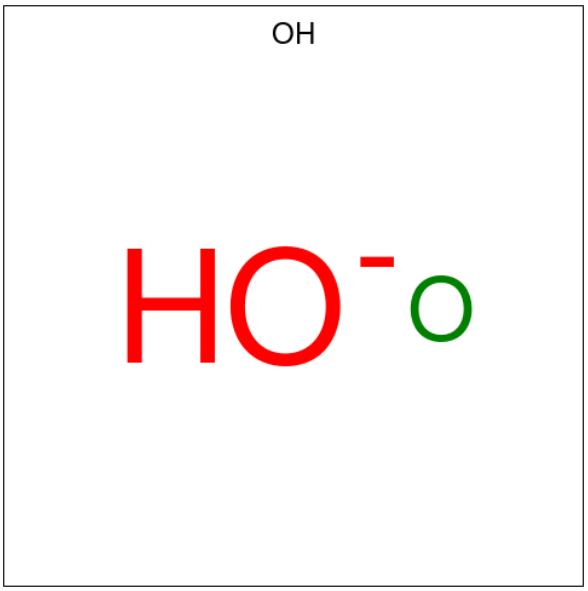
- Molecule 3 is a protein called Methane monooxygenase component A gamma chain.

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

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

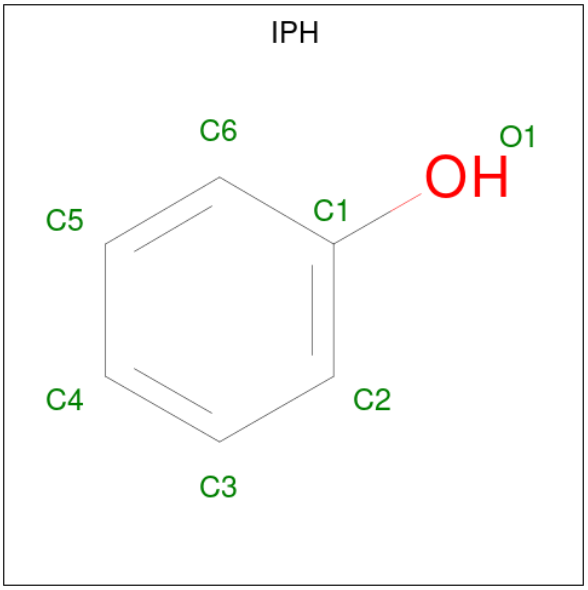
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Fe	0	0
			2	2		
4	B	2	Total	Fe	0	0
			2	2		

- Molecule 5 is HYDROXIDE ION (three-letter code: OH) (formula: HO).



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

- Molecule 6 is PHENOL (three-letter code: IPH) (formula: C_6H_6O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 7 6 1	0	0
6	B	1	Total C O 7 6 1	0	0

- Molecule 7 is water.

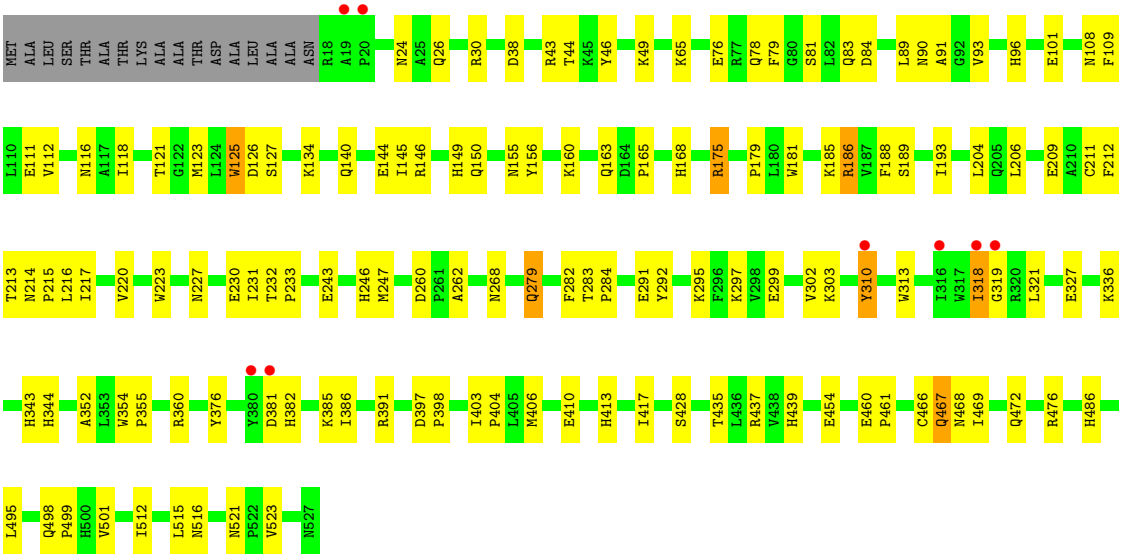
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	255	Total O 255 255	0	0
7	B	246	Total O 246 246	0	0
7	C	273	Total O 273 273	0	0
7	D	159	Total O 159 159	0	0
7	E	139	Total O 139 139	0	0
7	F	49	Total O 49 49	0	0

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.

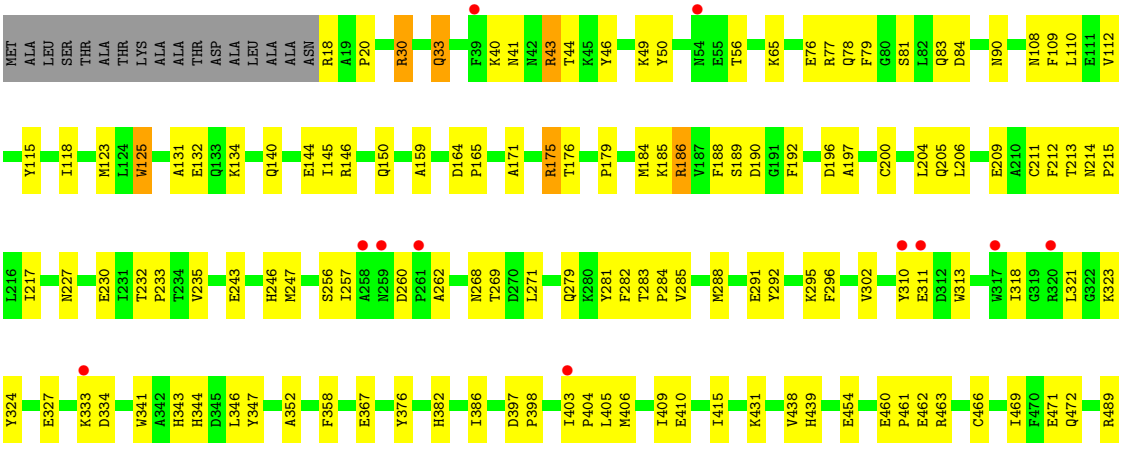
• Molecule 1: Methane monooxygenase component A alpha chain

Chain A:



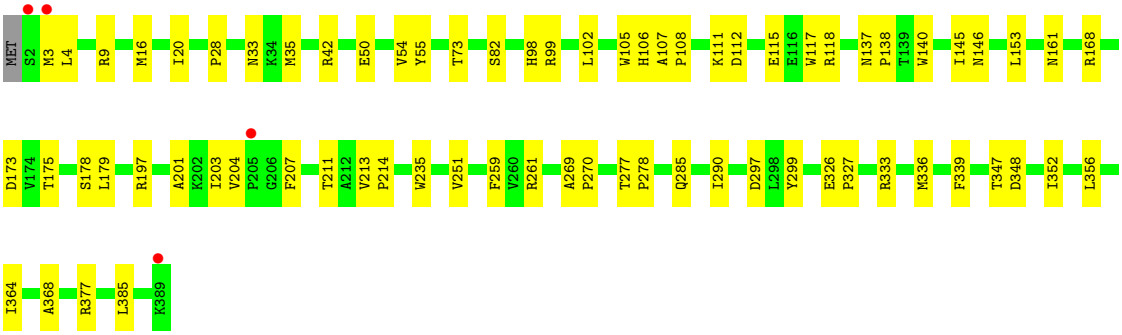
• Molecule 1: Methane monooxygenase component A alpha chain

Chain B:



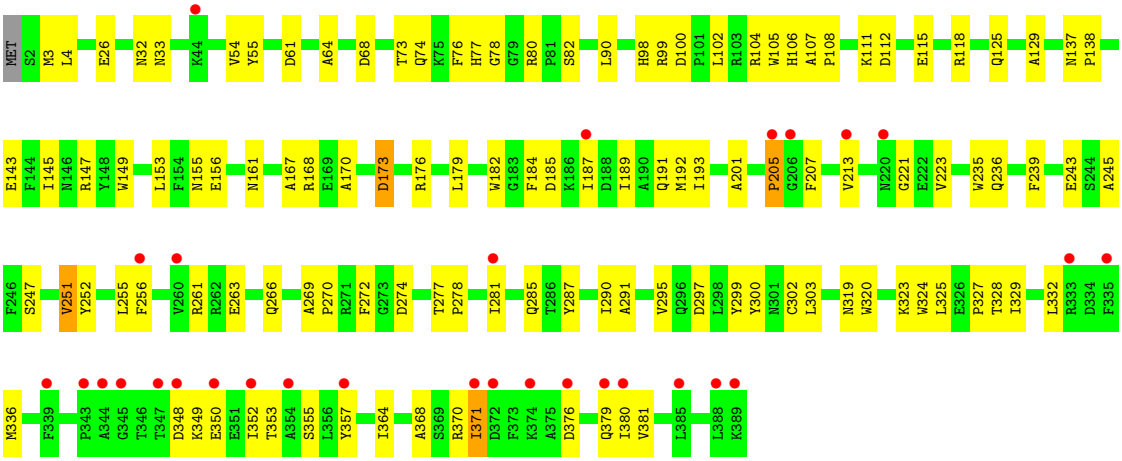
• Molecule 2: Methane monooxygenase component A beta chain

Chain C:



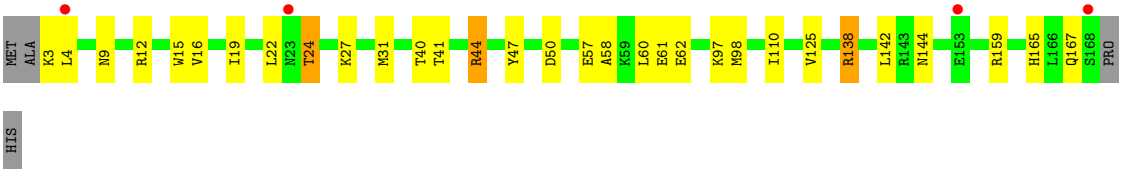
• Molecule 2: Methane monooxygenase component A beta chain

Chain D:



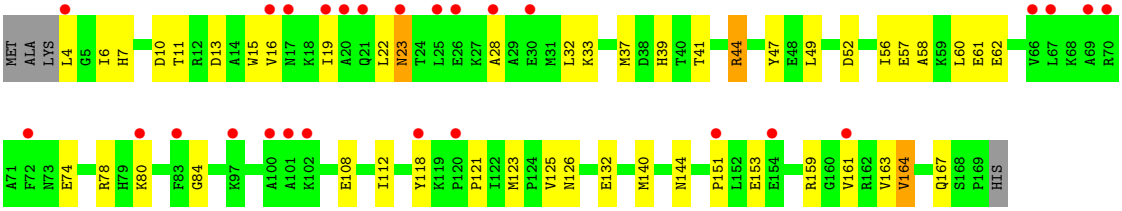
• Molecule 3: Methane monooxygenase component A gamma chain

Chain E:



• Molecule 3: Methane monooxygenase component A gamma chain

Chain F:


MET ALA LYS L4 G5 I6 H7 D10 T11 R12 D13 A14 W15 V16 N17 K18 I19 A20 Q21 L22 N23 T24 L25 E26 K27 A28 A29 E30 M31 L32 K33 M37 D38 H39 T40 T41 R44 Y47 E48 L49 D52 I56 E57 A58 K59 L60 E61 E62 V66 L67 K68 A69 R70
A71 F72 N73 E74 R78 H79 K80 F83 G84 K97 A100 A101 K102 E108 I112 Y118 K119 P120 P121 I122 M123 P124 V125 N126 E132 M140 N144 P151 L152 E153 E154 R159 G160 V161 R162 V163 V164 Q167 S168 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	71.19Å 171.56Å 221.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.94 – 1.96 29.94 – 1.96	Depositor EDS
% Data completeness (in resolution range)	92.4 (29.94-1.96) 92.5 (29.94-1.96)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	3.66 (at 1.96Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.200 , 0.228 0.196 , 0.224	Depositor DCC
R_{free} test set	8959 reflections (4.62%)	wwPDB-VP
Wilson B-factor (Å^2)	20.3	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 54.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	18452	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.39% 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: OH, FE, IPH

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	0/4263	0.57	0/5797
1	B	0.33	0/4262	0.59	1/5796 (0.0%)
2	C	0.36	0/3259	0.58	0/4430
2	D	0.32	0/3247	0.53	0/4417
3	E	0.33	0/1392	0.58	0/1876
3	F	0.28	0/1387	0.52	0/1873
All	All	0.33	0/17810	0.57	1/24189 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	175	ARG	C-N-CA	5.36	135.09	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	299	TYR	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4138	0	3897	122	0
1	B	4137	0	3888	134	0
2	C	3163	0	2986	64	0
2	D	3151	0	2960	101	0
3	E	1364	0	1352	28	0
3	F	1358	0	1335	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
6	A	7	0	6	0	0
6	B	7	0	6	0	0
7	A	255	0	0	6	0
7	B	246	0	0	6	0
7	C	273	0	0	3	0
7	D	159	0	0	4	0
7	E	139	0	0	0	0
7	F	49	0	0	4	0
All	All	18452	0	16430	436	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (436) 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:E:19:ILE:HD12	3:E:60:LEU:HD13	1.40	1.04
1:A:352:ALA:HA	1:A:404:PRO:HB2	1.46	0.95
1:A:78:GLN:HE22	1:A:150:GLN:HE21	1.05	0.93
1:A:118:ILE:HD13	1:A:145:ILE:HD13	1.49	0.93
1:B:78:GLN:HE22	1:B:150:GLN:HE21	1.04	0.93
1:B:118:ILE:HD13	1:B:145:ILE:HD13	1.49	0.91
1:A:155:ASN:HD22	1:A:168:HIS:HD2	1.18	0.90
1:B:217:ILE:HD12	7:B:2911:HOH:O	1.74	0.87
2:C:261:ARG:HE	2:C:285:GLN:HE22	1.25	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:467:GLN:HG3	7:A:2800:HOH:O	1.78	0.83
1:B:44:THR:HG22	1:B:46:TYR:H	1.42	0.83
1:B:108:ASN:HD21	1:B:175:ARG:HD3	1.43	0.83
1:B:352:ALA:HA	1:B:404:PRO:HB2	1.61	0.81
3:E:41:THR:O	3:E:44:ARG:HD2	1.79	0.81
3:E:15:TRP:O	3:E:19:ILE:HG12	1.80	0.81
2:C:102:LEU:HD12	2:C:290:ILE:HG23	1.61	0.81
3:F:80:LYS:HE2	3:F:84:GLY:HA2	1.63	0.81
1:B:439:HIS:HB3	3:F:161:VAL:HG21	1.63	0.81
3:F:41:THR:O	3:F:44:ARG:HD2	1.80	0.80
1:A:44:THR:HG22	1:A:46:TYR:H	1.47	0.78
2:D:352:ILE:HD12	2:D:353:THR:N	2.00	0.77
1:B:268:ASN:HD21	1:B:327:GLU:H	1.33	0.77
2:C:42:ARG:HB2	2:C:99:ARG:HH11	1.48	0.77
1:A:78:GLN:NE2	1:A:150:GLN:HE21	1.84	0.75
1:A:355:PRO:HG2	1:A:403:ILE:HD13	1.67	0.75
1:B:214:ASN:HB3	1:B:215:PRO:HD3	1.68	0.75
1:A:227:ASN:HD21	1:A:295:LYS:H	1.35	0.75
2:D:100:ASP:OD1	2:D:104:ARG:HD3	1.87	0.75
2:D:261:ARG:HE	2:D:285:GLN:HE22	1.32	0.75
1:B:403:ILE:HD12	1:B:404:PRO:HD2	1.69	0.75
2:D:90:LEU:HD13	2:D:303:LEU:HD13	1.69	0.74
1:B:382:HIS:O	1:B:386:ILE:HG12	1.88	0.74
2:D:371:ILE:HD13	2:D:371:ILE:H	1.53	0.74
3:E:19:ILE:CD1	3:E:60:LEU:HD13	2.17	0.73
1:B:209:GLU:HA	1:B:213:THR:OG1	1.88	0.73
1:B:439:HIS:HB3	3:F:161:VAL:CG2	2.19	0.73
3:E:22:LEU:HD11	3:E:31:MET:SD	2.28	0.73
2:C:3:MET:HG3	2:C:4:LEU:H	1.52	0.72
1:B:171:ALA:O	1:B:175:ARG:HG2	1.89	0.72
1:B:78:GLN:NE2	1:B:150:GLN:HE21	1.85	0.72
1:A:268:ASN:HD21	1:A:327:GLU:H	1.36	0.71
1:B:302:VAL:HG13	1:B:376:TYR:HE2	1.56	0.71
2:C:102:LEU:CD1	2:C:290:ILE:HG23	2.20	0.71
1:A:118:ILE:CD1	1:A:145:ILE:HD13	2.21	0.70
1:B:283:THR:HB	1:B:284:PRO:HD3	1.73	0.70
2:C:336:MET:CE	2:C:385:LEU:HD23	2.21	0.70
1:A:24:ASN:OD1	1:A:26:GLN:HG2	1.91	0.69
1:A:302:VAL:HG13	1:A:376:TYR:HE2	1.56	0.69
2:D:102:LEU:CD1	2:D:290:ILE:HG23	2.22	0.69
1:B:217:ILE:CD1	7:B:2911:HOH:O	2.37	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:167:ALA:O	2:D:176:ARG:NH1	2.25	0.69
1:B:227:ASN:HD21	1:B:295:LYS:H	1.41	0.68
1:A:214:ASN:HB3	1:A:215:PRO:HD3	1.74	0.68
2:C:42:ARG:HB2	2:C:99:ARG:NH1	2.08	0.68
3:F:153:GLU:H	3:F:153:GLU:CD	1.97	0.68
3:F:4:LEU:HD11	3:F:10:ASP:OD2	1.93	0.67
1:A:175:ARG:NH1	7:A:2802:HOH:O	2.10	0.67
2:C:333:ARG:HD2	7:C:552:HOH:O	1.94	0.67
2:D:319:ASN:OD1	3:F:78:ARG:HD3	1.94	0.67
3:F:13:ASP:O	3:F:16:VAL:HG22	1.94	0.67
2:C:107:ALA:HB3	2:C:108:PRO:HD3	1.78	0.66
1:A:96:HIS:HB2	2:C:20:ILE:HD12	1.78	0.66
1:B:33:GLN:HE22	1:B:132:GLU:H	1.42	0.66
1:B:33:GLN:NE2	1:B:132:GLU:H	1.93	0.65
3:F:58:ALA:O	3:F:62:GLU:HG3	1.97	0.65
1:A:417:ILE:CD1	1:A:468:ASN:HB2	2.26	0.64
2:C:146:ASN:HD21	2:C:197:ARG:HH21	1.44	0.64
1:A:76:GLU:HG2	1:B:76:GLU:OE2	1.97	0.64
1:A:175:ARG:HG3	1:A:181:TRP:CD2	2.33	0.64
1:A:382:HIS:O	1:A:386:ILE:HG12	1.97	0.64
1:B:288:MET:CE	1:B:346:LEU:HB3	2.27	0.64
3:F:52:ASP:O	3:F:56:ILE:HG12	1.98	0.64
1:B:134:LYS:HD3	2:D:161:ASN:HD21	1.61	0.64
2:D:189:ILE:O	2:D:193:ILE:HD13	1.98	0.64
2:D:364:ILE:HA	2:D:368:ALA:HB3	1.79	0.64
1:B:288:MET:HE1	1:B:346:LEU:CB	2.27	0.63
2:D:325:LEU:O	2:D:329:ILE:HG12	1.98	0.63
1:A:435:THR:CG2	1:A:437:ARG:HE	2.10	0.63
1:B:125:TRP:HE1	2:D:161:ASN:ND2	1.97	0.63
1:B:405:LEU:O	1:B:409:ILE:HD13	1.98	0.63
2:C:3:MET:HG3	2:C:4:LEU:HD13	1.80	0.63
1:B:367:GLU:HG3	7:B:2716:HOH:O	1.99	0.63
3:E:98:MET:O	3:E:98:MET:HE2	1.99	0.63
2:C:326:GLU:HB3	2:C:327:PRO:HD3	1.80	0.63
1:B:212:PHE:O	1:B:215:PRO:HD2	1.99	0.62
1:A:417:ILE:HD13	1:A:468:ASN:HB2	1.81	0.62
1:A:160:LYS:HE3	7:A:2854:HOH:O	1.98	0.62
1:A:268:ASN:ND2	1:A:327:GLU:H	1.98	0.62
1:A:352:ALA:CA	1:A:404:PRO:HB2	2.26	0.62
1:B:288:MET:HE1	1:B:346:LEU:C	2.19	0.62
1:A:118:ILE:HD13	1:A:145:ILE:CD1	2.24	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:TYR:OH	1:A:344:HIS:HD2	1.83	0.61
1:B:489:ARG:HD2	1:B:495:LEU:O	2.00	0.61
1:B:108:ASN:ND2	1:B:175:ARG:HD3	2.13	0.61
1:B:281:TYR:O	1:B:284:PRO:HD2	2.00	0.61
2:C:3:MET:HG3	2:C:4:LEU:N	2.15	0.61
1:A:381:ASP:HA	1:A:385:LYS:HE2	1.82	0.61
2:C:112:ASP:OD1	2:D:118:ARG:NH2	2.34	0.61
1:A:227:ASN:ND2	1:A:295:LYS:H	1.98	0.60
1:B:292:TYR:OH	1:B:344:HIS:HD2	1.84	0.60
1:B:49:LYS:HD3	3:F:144:ASN:HD22	1.67	0.60
2:D:348:ASP:OD2	2:D:350:GLU:HB2	2.01	0.60
3:E:24:THR:HG22	3:E:27:LYS:H	1.65	0.60
2:C:3:MET:CG	2:C:4:LEU:H	2.13	0.60
1:A:155:ASN:HD22	1:A:168:HIS:CD2	2.09	0.60
1:B:206:LEU:HD11	1:B:321:LEU:HD11	1.83	0.60
2:D:107:ALA:HB3	2:D:108:PRO:HD3	1.84	0.59
1:A:406:MET:O	1:A:410:GLU:HG3	2.02	0.59
2:D:201:ALA:HA	2:D:207:PHE:HB3	1.83	0.59
1:B:333:LYS:HG3	7:B:2868:HOH:O	2.02	0.59
3:F:151:PRO:HB2	3:F:153:GLU:OE1	2.02	0.58
1:A:83:GLN:HB3	1:B:77:ARG:HH12	1.67	0.58
3:F:44:ARG:HD3	3:F:47:TYR:CZ	2.38	0.58
1:A:495:LEU:HD11	1:A:512:ILE:HD13	1.85	0.58
1:B:179:PRO:HB3	1:B:469:ILE:HD13	1.85	0.58
1:A:213:THR:O	1:A:217:ILE:HG12	2.04	0.58
2:D:371:ILE:HD12	7:D:492:HOH:O	2.04	0.58
1:B:302:VAL:HG13	1:B:376:TYR:CE2	2.39	0.57
1:B:403:ILE:HD12	1:B:404:PRO:CD	2.33	0.57
1:B:243:GLU:O	1:B:247:MET:HG2	2.05	0.57
3:F:61:GLU:O	3:F:121:PRO:HG2	2.04	0.57
1:B:406:MET:O	1:B:410:GLU:HG3	2.04	0.57
1:A:231:ILE:HD12	1:A:231:ILE:N	2.20	0.57
1:B:398:PRO:HG3	1:B:507:TRP:CD1	2.40	0.57
1:B:118:ILE:HD13	1:B:145:ILE:CD1	2.28	0.57
2:D:153:LEU:C	2:D:153:LEU:HD12	2.25	0.57
1:B:288:MET:HE1	1:B:346:LEU:CG	2.35	0.56
2:D:76:PHE:HZ	2:D:168:ARG:HH12	1.52	0.56
3:E:165:HIS:CE1	3:E:167:GLN:HE21	2.22	0.56
1:A:243:GLU:O	1:A:247:MET:HG2	2.05	0.56
1:A:403:ILE:HD12	1:A:515:LEU:HD13	1.88	0.56
1:A:140:GLN:O	1:A:144:GLU:HG2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:ASN:ND2	1:B:295:LYS:H	2.02	0.56
2:C:339:PHE:CE2	2:C:352:ILE:HD12	2.41	0.56
2:C:348:ASP:O	2:C:352:ILE:HG12	2.05	0.56
2:D:277:THR:HG22	2:D:281:ILE:HD13	1.88	0.56
3:E:41:THR:O	3:E:44:ARG:CD	2.53	0.56
1:A:302:VAL:HG13	1:A:376:TYR:CE2	2.40	0.55
2:D:324:TRP:C	2:D:327:PRO:HD2	2.26	0.55
1:B:462:GLU:HG3	3:F:112:ILE:HD11	1.86	0.55
2:D:263:GLU:HB3	2:D:355:SER:HB2	1.88	0.55
1:B:20:PRO:HB2	2:D:125:GLN:HE21	1.71	0.55
1:B:192:PHE:O	1:B:200:CYS:HB3	2.07	0.55
1:B:118:ILE:CD1	1:B:145:ILE:HD13	2.29	0.55
2:D:277:THR:HB	2:D:278:PRO:HD3	1.89	0.55
2:D:332:LEU:O	2:D:336:MET:HG2	2.06	0.55
1:B:439:HIS:HD2	3:F:163:VAL:HA	1.72	0.55
3:E:165:HIS:HE1	3:E:167:GLN:HE21	1.54	0.55
1:B:269:THR:HG21	7:F:188:HOH:O	2.06	0.55
3:F:57:GLU:O	3:F:61:GLU:HG3	2.07	0.55
1:A:318:ILE:HD13	1:A:318:ILE:O	2.06	0.54
1:B:125:TRP:HE1	2:D:161:ASN:HD22	1.56	0.54
1:B:288:MET:HE1	1:B:346:LEU:HB3	1.89	0.54
1:B:344:HIS:HE1	1:B:376:TYR:CD2	2.25	0.54
1:A:179:PRO:HB3	1:A:469:ILE:HD13	1.88	0.54
2:D:187:ILE:O	2:D:191:GLN:HG3	2.07	0.54
1:B:108:ASN:HD21	1:B:175:ARG:HH21	1.55	0.54
1:B:495:LEU:HD11	1:B:512:ILE:CG1	2.38	0.54
3:E:138:ARG:NH2	3:E:142:LEU:HD21	2.23	0.54
1:A:49:LYS:HD3	3:E:144:ASN:HD22	1.73	0.54
1:A:486:HIS:HD2	7:A:2805:HOH:O	1.90	0.54
1:B:288:MET:HE1	1:B:346:LEU:HG	1.88	0.54
1:A:96:HIS:HB2	2:C:20:ILE:CD1	2.38	0.54
1:A:134:LYS:HD3	2:C:161:ASN:HD21	1.73	0.54
3:E:165:HIS:HE1	3:E:167:GLN:NE2	2.06	0.53
1:B:281:TYR:CZ	1:B:285:VAL:HG21	2.43	0.53
1:B:403:ILE:HG23	1:B:406:MET:HG3	1.89	0.53
3:E:4:LEU:O	3:E:4:LEU:HG	2.08	0.53
1:A:355:PRO:HG2	1:A:403:ILE:CD1	2.36	0.53
2:C:118:ARG:NH2	2:D:112:ASP:OD1	2.41	0.53
1:A:435:THR:HG21	1:A:437:ARG:HE	1.73	0.53
1:B:257:ILE:C	1:B:257:ILE:HD12	2.29	0.53
1:B:495:LEU:HD11	1:B:512:ILE:HG13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:57:GLU:O	3:E:61:GLU:HG3	2.09	0.53
2:C:175:THR:O	2:C:179:LEU:HD13	2.08	0.53
2:C:261:ARG:HE	2:C:285:GLN:NE2	2.01	0.53
3:F:19:ILE:HD12	3:F:19:ILE:C	2.28	0.53
1:B:438:VAL:HB	3:F:164:VAL:HG22	1.90	0.52
2:D:111:LYS:O	2:D:115:GLU:HG3	2.09	0.52
2:D:145:ILE:O	2:D:149:TRP:HB3	2.09	0.52
1:A:318:ILE:HD13	1:A:318:ILE:C	2.29	0.52
1:B:184:MET:HE2	1:B:188:PHE:HB2	1.90	0.52
1:B:211:CYS:HB2	1:B:313:TRP:CD1	2.45	0.52
1:B:490:SER:OG	2:D:32:ASN:HB2	2.09	0.52
2:C:269:ALA:HB3	2:C:270:PRO:HD3	1.90	0.52
3:F:80:LYS:HE2	3:F:84:GLY:CA	2.38	0.52
1:A:123:MET:HB2	2:C:168:ARG:HD3	1.91	0.52
1:B:164:ASP:OD1	1:B:489:ARG:NH2	2.42	0.52
1:B:288:MET:HE3	1:B:346:LEU:HD23	1.92	0.52
1:B:439:HIS:HE1	1:B:454:GLU:OE1	1.93	0.52
2:C:3:MET:SD	2:D:26:GLU:O	2.67	0.52
1:A:125:TRP:HE1	2:C:161:ASN:ND2	2.07	0.52
1:A:476:ARG:HD3	3:E:4:LEU:HG	1.92	0.52
2:C:146:ASN:ND2	2:C:197:ARG:HH21	2.08	0.52
2:D:102:LEU:HB2	2:D:104:ARG:HD2	1.92	0.52
1:A:439:HIS:HE1	1:A:454:GLU:OE1	1.93	0.52
3:F:15:TRP:O	3:F:19:ILE:HG23	2.10	0.51
1:A:260:ASP:OD2	1:A:262:ALA:HB3	2.10	0.51
1:B:164:ASP:CG	1:B:489:ARG:HH22	2.14	0.51
2:D:247:SER:O	2:D:251:VAL:HB	2.10	0.51
2:D:137:ASN:HB3	2:D:272:PHE:HB3	1.91	0.51
1:B:33:GLN:HA	1:B:131:ALA:HB3	1.93	0.51
3:F:33:LYS:O	3:F:37:MET:HG2	2.11	0.51
1:A:84:ASP:HB3	1:B:81:SER:OG	2.12	0.50
1:A:344:HIS:HE1	1:A:376:TYR:CD2	2.30	0.50
1:B:415:ILE:HD12	1:B:415:ILE:N	2.26	0.50
3:E:19:ILE:HD12	3:E:60:LEU:CD1	2.27	0.50
1:A:185:LYS:O	1:A:189:SER:HB2	2.11	0.50
2:C:161:ASN:HB3	2:C:235:TRP:CE2	2.46	0.50
2:D:239:PHE:HB2	3:F:126:ASN:HA	1.94	0.50
3:E:97:LYS:HE3	3:E:110:ILE:HD12	1.93	0.50
1:B:206:LEU:HD23	1:B:271:LEU:HD13	1.92	0.50
2:C:3:MET:CE	2:C:4:LEU:HD13	2.42	0.50
1:A:44:THR:HG23	1:A:126:ASP:OD1	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:THR:HG21	1:B:256:SER:OG	2.10	0.50
3:E:3:LYS:HG2	3:E:9:ASN:HA	1.94	0.50
3:F:132:GLU:HG3	7:F:194:HOH:O	2.10	0.50
1:A:156:TYR:HE1	1:A:160:LYS:HZ3	1.60	0.50
1:A:193:ILE:HD11	2:C:82:SER:HB3	1.93	0.50
2:C:211:THR:O	2:C:214:PRO:HD2	2.12	0.50
2:D:352:ILE:HD12	2:D:352:ILE:C	2.31	0.50
1:A:232:THR:HB	1:A:233:PRO:HD3	1.93	0.49
2:D:324:TRP:O	2:D:327:PRO:HD2	2.12	0.49
1:B:206:LEU:HD11	1:B:321:LEU:CD1	2.42	0.49
2:C:111:LYS:O	2:C:115:GLU:HG3	2.12	0.49
2:D:98:HIS:CD2	2:D:99:ARG:N	2.80	0.49
2:D:102:LEU:HD13	2:D:290:ILE:HG23	1.93	0.49
2:C:213:VAL:HB	2:C:214:PRO:HD3	1.95	0.49
2:D:368:ALA:O	2:D:371:ILE:HD13	2.12	0.49
3:E:58:ALA:O	3:E:62:GLU:HG3	2.13	0.49
2:D:170:ALA:O	2:D:176:ARG:NH2	2.46	0.49
2:D:261:ARG:HE	2:D:285:GLN:NE2	2.06	0.49
1:A:279:GLN:HG2	1:A:283:THR:OG1	2.13	0.49
2:D:266:GLN:HB2	2:D:281:ILE:HG21	1.93	0.49
1:A:186:ARG:HA	2:C:73:THR:OG1	2.13	0.49
2:D:78:GLY:O	3:F:112:ILE:HD13	2.12	0.49
3:F:61:GLU:HB3	3:F:121:PRO:HD3	1.95	0.48
1:A:223:TRP:CZ3	1:A:297:LYS:HA	2.48	0.48
1:B:227:ASN:HD21	1:B:296:PHE:H	1.61	0.48
2:C:98:HIS:HE1	2:C:178:SER:OG	1.96	0.48
7:C:547:HOH:O	3:E:125:VAL:HG22	2.13	0.48
2:D:256:PHE:HA	2:D:332:LEU:HD21	1.95	0.48
7:D:506:HOH:O	3:F:125:VAL:HG22	2.13	0.48
1:B:140:GLN:O	1:B:144:GLU:HG2	2.14	0.48
1:B:302:VAL:CG1	1:B:376:TYR:HE2	2.24	0.48
1:A:44:THR:OG1	1:A:127:SER:HA	2.14	0.48
1:B:144:GLU:OE2	1:B:144:GLU:HA	2.13	0.48
2:C:140:TRP:NE1	2:C:145:ILE:HD11	2.29	0.48
1:A:413:HIS:HD2	1:A:428:SER:OG	1.97	0.47
2:D:245:ALA:HB3	2:D:299:TYR:OH	2.13	0.47
3:E:44:ARG:HD3	3:E:47:TYR:CZ	2.49	0.47
2:C:98:HIS:HD2	2:C:297:ASP:OD1	1.96	0.47
2:D:61:ASP:OD1	3:F:7:HIS:HD2	1.96	0.47
2:D:102:LEU:HD12	2:D:290:ILE:HG23	1.97	0.47
2:D:269:ALA:HB3	2:D:270:PRO:HD3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:ASP:HB2	3:F:140:MET:SD	2.55	0.47
2:C:153:LEU:C	2:C:153:LEU:HD12	2.35	0.47
1:A:354:TRP:CG	1:A:355:PRO:HD3	2.50	0.47
1:A:403:ILE:HD12	1:A:515:LEU:CD1	2.44	0.47
1:B:288:MET:HE1	1:B:347:TYR:N	2.30	0.47
2:C:203:ILE:HG13	2:C:204:VAL:HG23	1.95	0.47
1:A:417:ILE:HD12	1:A:468:ASN:HB2	1.96	0.47
1:A:521:ASN:OD1	1:A:523:VAL:HG12	2.15	0.47
1:A:165:PRO:HG3	7:A:2807:HOH:O	2.15	0.47
1:A:268:ASN:HD21	1:A:327:GLU:N	2.08	0.47
1:A:461:PRO:HG2	3:E:159:ARG:CZ	2.45	0.47
2:D:357:TYR:CE1	2:D:381:VAL:HG11	2.50	0.47
2:D:54:VAL:O	2:D:55:TYR:HB2	2.14	0.47
1:B:185:LYS:O	1:B:189:SER:HB2	2.15	0.47
1:B:79:PHE:O	1:B:83:GLN:HG3	2.14	0.47
1:B:33:GLN:HA	1:B:33:GLN:HE21	1.79	0.46
1:A:109:PHE:O	1:A:112:VAL:HG12	2.15	0.46
1:B:65:LYS:HE2	2:D:192:MET:HE2	1.97	0.46
1:B:323:LYS:HE2	1:B:324:TYR:CE1	2.50	0.46
2:C:211:THR:C	2:C:214:PRO:HD2	2.36	0.46
1:B:30:ARG:HD3	1:B:30:ARG:C	2.36	0.46
1:A:101:GLU:CD	1:A:360:ARG:HD3	2.36	0.46
1:A:163:GLN:O	2:C:28:PRO:HA	2.16	0.46
1:A:417:ILE:HD11	1:A:469:ILE:HG12	1.97	0.46
1:A:91:ALA:C	1:A:231:ILE:HD11	2.36	0.46
2:D:277:THR:HG22	2:D:281:ILE:CD1	2.45	0.46
3:F:39:HIS:HD2	7:F:191:HOH:O	1.97	0.46
2:C:54:VAL:O	2:C:55:TYR:HB2	2.15	0.46
2:D:324:TRP:HA	2:D:327:PRO:HD2	1.98	0.46
1:A:65:LYS:HB3	2:C:117:TRP:CG	2.51	0.46
1:B:115:TYR:OH	2:D:173:ASP:HA	2.16	0.46
1:B:460:GLU:N	1:B:461:PRO:HD3	2.30	0.46
2:D:329:ILE:CD1	2:D:380:ILE:HG23	2.46	0.46
1:A:211:CYS:HB2	1:A:313:TRP:CD1	2.50	0.46
1:B:472:GLN:NE2	7:B:2843:HOH:O	2.49	0.45
2:D:161:ASN:HB3	2:D:235:TRP:CE2	2.51	0.45
1:A:291:GLU:OE1	1:A:343:HIS:HE1	2.00	0.45
1:B:175:ARG:HA	1:B:358:PHE:CD2	2.52	0.45
1:B:176:THR:HG22	2:D:68:ASP:CG	2.35	0.45
2:C:364:ILE:HA	2:C:368:ALA:HB3	1.98	0.45
1:A:79:PHE:O	1:A:83:GLN:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:235:TRP:CD1	2:C:235:TRP:C	2.90	0.45
3:F:39:HIS:CD2	3:F:49:LEU:HD12	2.52	0.45
1:B:288:MET:CE	1:B:347:TYR:N	2.80	0.45
1:A:206:LEU:HD11	1:A:321:LEU:HD11	1.99	0.45
1:A:318:ILE:HG23	1:A:319:GLY:N	2.32	0.45
2:D:223:VAL:HG23	7:D:489:HOH:O	2.16	0.44
1:B:344:HIS:HE1	1:B:376:TYR:CE2	2.36	0.44
1:B:461:PRO:HG2	3:F:159:ARG:CZ	2.48	0.44
2:C:118:ARG:NH2	2:D:111:LYS:HD3	2.31	0.44
1:B:343:HIS:H	1:B:343:HIS:CD2	2.36	0.44
2:D:153:LEU:HB3	2:D:193:ILE:HG21	2.00	0.44
2:D:349:LYS:O	2:D:352:ILE:HG13	2.17	0.44
3:F:32:LEU:HA	3:F:60:LEU:HD23	1.99	0.44
1:B:281:TYR:CE1	1:B:285:VAL:HG21	2.52	0.44
2:D:77:HIS:CD2	3:F:140:MET:HG2	2.53	0.44
2:D:243:GLU:HB2	2:D:320:TRP:CZ2	2.53	0.44
2:D:235:TRP:CD1	2:D:235:TRP:C	2.91	0.44
3:F:4:LEU:HD21	3:F:10:ASP:H	1.81	0.44
1:A:24:ASN:OD1	1:A:26:GLN:CG	2.63	0.44
1:B:268:ASN:ND2	1:B:327:GLU:H	2.08	0.44
3:F:108:GLU:O	3:F:112:ILE:HG12	2.18	0.44
1:A:343:HIS:CD2	1:A:343:HIS:H	2.35	0.44
2:C:201:ALA:HA	2:C:207:PHE:HB3	1.99	0.44
1:A:188:PHE:CE1	1:A:282:PHE:HZ	2.35	0.44
1:A:246:HIS:N	1:A:246:HIS:CD2	2.86	0.44
1:B:230:GLU:C	1:B:233:PRO:HD2	2.38	0.44
2:D:98:HIS:HD2	2:D:297:ASP:OD1	2.00	0.44
2:D:184:PHE:O	2:D:187:ILE:HG22	2.18	0.44
2:D:277:THR:O	2:D:281:ILE:HD13	2.18	0.44
1:A:89:LEU:HD21	1:B:230:GLU:HG3	2.00	0.43
1:B:471:GLU:HB3	7:F:201:HOH:O	2.18	0.43
1:A:125:TRP:HE1	2:C:161:ASN:HD22	1.66	0.43
1:A:303:LYS:HE3	1:A:303:LYS:HB2	1.87	0.43
1:B:78:GLN:HE21	1:B:235:VAL:HA	1.84	0.43
2:C:336:MET:HE1	2:C:385:LEU:HD23	1.96	0.43
2:D:349:LYS:HA	2:D:352:ILE:HG13	2.01	0.43
1:A:83:GLN:HB3	1:B:77:ARG:NH1	2.31	0.43
1:A:209:GLU:HA	1:A:213:THR:HB	2.00	0.43
1:B:186:ARG:HA	2:D:73:THR:OG1	2.18	0.43
2:C:3:MET:CG	2:C:4:LEU:N	2.75	0.43
2:D:323:LYS:HB2	3:F:78:ARG:HH11	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:ILE:HG21	1:B:145:ILE:HD11	2.01	0.43
1:B:123:MET:SD	2:D:168:ARG:NH1	2.91	0.43
3:F:23:ASN:N	3:F:23:ASN:HD22	2.17	0.43
1:A:360:ARG:HG2	1:A:498:GLN:HB2	2.01	0.43
1:A:437:ARG:NH1	1:A:454:GLU:OE2	2.50	0.43
1:A:81:SER:OG	1:B:84:ASP:HB3	2.18	0.43
1:A:495:LEU:HD11	1:A:512:ILE:CD1	2.47	0.43
1:B:50:TYR:CD1	1:B:50:TYR:N	2.87	0.43
2:C:137:ASN:HA	2:C:138:PRO:HD3	1.88	0.43
1:A:310:TYR:CZ	1:A:336:LYS:HD2	2.53	0.43
1:B:341:TRP:CE2	1:B:431:LYS:HD3	2.54	0.43
2:D:156:GLU:HA	2:D:156:GLU:OE2	2.19	0.43
1:B:291:GLU:OE1	1:B:343:HIS:HE1	2.01	0.43
2:C:259:PHE:CE1	2:C:356:LEU:HD22	2.54	0.43
2:D:349:LYS:HA	2:D:352:ILE:CG1	2.49	0.43
3:F:22:LEU:HD13	3:F:28:ALA:HA	2.00	0.43
1:B:43:ARG:HD2	1:B:43:ARG:C	2.39	0.43
2:C:277:THR:HB	2:C:278:PRO:HD3	2.01	0.43
3:F:125:VAL:HG23	3:F:126:ASN:N	2.33	0.43
1:A:216:LEU:O	1:A:220:VAL:HG23	2.18	0.42
1:A:360:ARG:NH2	1:A:501:VAL:O	2.52	0.42
1:A:466:CYS:HB2	2:C:73:THR:HA	2.00	0.42
1:A:472:GLN:NE2	7:A:2800:HOH:O	2.52	0.42
2:C:50:GLU:OE1	2:C:99:ARG:NH1	2.52	0.42
2:D:189:ILE:HD11	2:D:287:TYR:CD1	2.54	0.42
3:F:118:TYR:HB3	3:F:123:MET:HB2	2.00	0.42
1:A:116:ASN:CG	1:A:189:SER:HA	2.40	0.42
1:B:260:ASP:OD2	1:B:262:ALA:HB3	2.19	0.42
1:B:397:ASP:HA	1:B:398:PRO:HD3	1.85	0.42
2:D:291:ALA:O	2:D:295:VAL:HG23	2.20	0.42
1:B:140:GLN:HG3	1:B:246:HIS:CE1	2.54	0.42
2:D:145:ILE:HD11	2:D:274:ASP:OD2	2.19	0.42
1:A:108:ASN:HD21	1:A:175:ARG:HE	1.67	0.42
2:D:82:SER:O	2:D:168:ARG:NH2	2.50	0.42
2:D:98:HIS:CD2	2:D:99:ARG:H	2.37	0.42
3:F:74:GLU:O	3:F:78:ARG:HG3	2.19	0.42
1:A:149:HIS:CE1	2:C:105:TRP:HB2	2.55	0.42
1:B:204:LEU:HG	1:B:205:GLN:HG3	2.02	0.42
2:D:185:ASP:O	2:D:189:ILE:HG12	2.20	0.42
3:E:40:THR:C	3:E:41:THR:HG23	2.39	0.42
1:B:123:MET:HE3	1:B:197:ALA:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:376:ASP:OD2	2:D:379:GLN:HG2	2.20	0.42
1:A:435:THR:HG21	1:A:437:ARG:NE	2.34	0.42
1:B:466:CYS:HB2	2:D:73:THR:HA	2.02	0.42
3:F:32:LEU:HD13	3:F:60:LEU:HB3	2.02	0.42
1:B:159:ALA:O	2:D:33:ASN:HB2	2.20	0.42
1:A:204:LEU:O	1:A:209:GLU:HG3	2.19	0.42
1:B:18:ARG:O	2:D:129:ALA:HA	2.19	0.42
1:A:283:THR:HB	1:A:284:PRO:HD3	2.01	0.41
1:A:352:ALA:HA	1:A:404:PRO:CB	2.34	0.41
1:B:188:PHE:CE1	1:B:282:PHE:HZ	2.39	0.41
1:B:232:THR:HB	1:B:233:PRO:HD3	2.02	0.41
2:C:347:THR:HG21	2:C:352:ILE:HD11	2.02	0.41
2:D:213:VAL:HG23	7:D:502:HOH:O	2.20	0.41
1:A:108:ASN:O	1:A:111:GLU:HB3	2.20	0.41
1:B:246:HIS:CD2	1:B:246:HIS:N	2.87	0.41
1:B:292:TYR:OH	1:B:344:HIS:CD2	2.71	0.41
2:D:90:LEU:CD1	2:D:303:LEU:HD13	2.45	0.41
1:B:313:TRP:CZ2	1:B:318:ILE:HD11	2.55	0.41
1:A:146:ARG:HB2	2:C:106:HIS:CE1	2.55	0.41
1:B:41:ASN:O	2:D:236:GLN:HB3	2.21	0.41
2:C:336:MET:HE2	2:C:385:LEU:HA	2.02	0.41
2:D:300:TYR:CE1	2:D:370:ARG:HG3	2.55	0.41
2:C:16:MET:O	2:C:20:ILE:HG12	2.20	0.41
2:D:143:GLU:O	2:D:147:ARG:HB3	2.20	0.41
3:E:165:HIS:CE1	3:E:167:GLN:HG3	2.56	0.41
1:A:121:THR:HG21	1:A:140:GLN:CG	2.51	0.41
1:B:108:ASN:ND2	1:B:175:ARG:HH21	2.19	0.41
3:E:12:ARG:O	3:E:16:VAL:HG23	2.21	0.41
1:A:230:GLU:C	1:A:233:PRO:HD2	2.41	0.41
1:A:302:VAL:CG1	1:A:376:TYR:HE2	2.28	0.41
1:B:521:ASN:OD1	1:B:523:VAL:HG12	2.20	0.41
2:D:98:HIS:HA	2:D:302:CYS:SG	2.60	0.41
1:A:212:PHE:O	1:A:215:PRO:HD2	2.20	0.41
3:E:44:ARG:NH2	3:E:50:ASP:OD1	2.54	0.41
1:A:93:VAL:HG11	2:D:3:MET:HG2	2.02	0.41
1:A:299:GLU:CG	1:A:303:LYS:HD3	2.51	0.41
1:B:460:GLU:OE1	1:B:463:ARG:HD3	2.21	0.41
2:C:9:ARG:NH2	7:C:591:HOH:O	2.48	0.41
2:C:99:ARG:HH11	2:C:99:ARG:HG3	1.86	0.41
2:D:155:ASN:ND2	2:D:252:TYR:OH	2.53	0.41
1:A:279:GLN:HG2	1:A:283:THR:HG1	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:347:THR:CG2	2:C:352:ILE:HD11	2.51	0.41
1:A:354:TRP:CH2	1:A:499:PRO:HD3	2.56	0.40
1:A:435:THR:CG2	1:A:437:ARG:NE	2.81	0.40
1:A:460:GLU:N	1:A:461:PRO:HD3	2.36	0.40
1:B:109:PHE:O	1:B:112:VAL:HG12	2.21	0.40
1:B:165:PRO:HG3	7:B:2850:HOH:O	2.21	0.40
2:D:137:ASN:HA	2:D:138:PRO:HD3	1.92	0.40
2:D:179:LEU:HD23	2:D:182:TRP:CE3	2.56	0.40
1:A:118:ILE:HG21	1:A:145:ILE:HD11	2.03	0.40
1:A:397:ASP:HA	1:A:398:PRO:HD3	1.80	0.40
2:D:105:TRP:O	2:D:108:PRO:HD2	2.20	0.40
2:D:263:GLU:OE2	2:D:263:GLU:HA	2.21	0.40
1:B:146:ARG:HB2	2:D:106:HIS:CE1	2.56	0.40
1:B:190:ASP:HB3	2:D:74:GLN:O	2.21	0.40
3:F:23:ASN:N	3:F:23:ASN:ND2	2.69	0.40
2:D:255:LEU:HB2	2:D:328:THR:HG21	2.03	0.40
3:E:98:MET:HE2	3:E:138:ARG:HG2	2.03	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%)	484 (95%)	24 (5%)	0	100 100
1	B	508/527 (96%)	484 (95%)	23 (4%)	1 (0%)	47 38
2	C	386/389 (99%)	375 (97%)	10 (3%)	1 (0%)	41 30
2	D	386/389 (99%)	366 (95%)	16 (4%)	4 (1%)	15 6
3	E	164/170 (96%)	161 (98%)	3 (2%)	0	100 100
3	F	164/170 (96%)	157 (96%)	6 (4%)	1 (1%)	25 14
All	All	2116/2172 (97%)	2027 (96%)	82 (4%)	7 (0%)	41 30

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	40	LYS
2	D	64	ALA
2	D	205	PRO
2	C	251	VAL
2	D	251	VAL
2	D	221	GLY
3	F	6	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	423/442 (96%)	410 (97%)	13 (3%)	40	28
1	B	422/442 (96%)	411 (97%)	11 (3%)	46	36
2	C	315/323 (98%)	311 (99%)	4 (1%)	69	65
2	D	312/323 (97%)	307 (98%)	5 (2%)	62	58
3	E	143/147 (97%)	140 (98%)	3 (2%)	53	46
3	F	142/147 (97%)	137 (96%)	5 (4%)	36	24
All	All	1757/1824 (96%)	1716 (98%)	41 (2%)	50	42

All (41) 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	125	TRP
1	A	175	ARG
1	A	186	ARG
1	A	279	GLN
1	A	310	TYR
1	A	318	ILE

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Mol	Chain	Res	Type
1	A	391	ARG
1	A	467	GLN
1	A	516	ASN
1	B	30	ARG
1	B	33	GLN
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	311	GLU
1	B	334	ASP
2	C	33	ASN
2	C	35	MET
2	C	173	ASP
2	C	377	ARG
2	D	4	LEU
2	D	80	ARG
2	D	173	ASP
2	D	205	PRO
2	D	371	ILE
3	E	24	THR
3	E	44	ARG
3	E	138	ARG
3	F	11	THR
3	F	23	ASN
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 (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	78	GLN
1	A	90	ASN
1	A	100	ASN
1	A	108	ASN
1	A	116	ASN
1	A	168	HIS

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Mol	Chain	Res	Type
1	A	227	ASN
1	A	249	ASN
1	A	268	ASN
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	413	HIS
1	A	439	HIS
1	A	442	ASN
1	A	472	GLN
1	A	486	HIS
1	A	516	ASN
1	B	33	GLN
1	B	78	GLN
1	B	90	ASN
1	B	100	ASN
1	B	108	ASN
1	B	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	411	ASN
1	B	413	HIS
1	B	439	HIS
1	B	451	GLN
1	B	472	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

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Mol	Chain	Res	Type
2	C	285	GLN
2	C	301	ASN
2	D	98	HIS
2	D	125	GLN
2	D	155	ASN
2	D	161	ASN
2	D	285	GLN
2	D	296	GLN
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	23	ASN
3	F	39	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 8 ligands modelled in this entry, 4 are monoatomic and 2 are modelled with single atom - 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	$\#\|Z\| > 2$
6	IPH	B	2666	-	7,7,7	2.08	3 (42%)	8,8,8	1.76	2 (25%)
6	IPH	A	2667	-	7,7,7	2.06	3 (42%)	8,8,8	1.73	2 (25%)

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	IPH	B	2666	-	-	-	0/1/1/1
6	IPH	A	2667	-	-	-	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	2666	IPH	C5-C6	3.19	1.45	1.38
6	A	2667	IPH	C5-C6	3.05	1.45	1.38
6	B	2666	IPH	C3-C2	2.80	1.44	1.38
6	A	2667	IPH	C3-C2	2.74	1.44	1.38
6	B	2666	IPH	C2-C1	2.45	1.43	1.38
6	A	2667	IPH	C2-C1	2.38	1.43	1.38

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	2666	IPH	C6-C1-C2	3.49	125.64	119.77
6	A	2667	IPH	C6-C1-C2	3.42	125.52	119.77
6	B	2666	IPH	C3-C2-C1	-2.40	115.93	119.31
6	A	2667	IPH	C3-C2-C1	-2.38	115.95	119.31

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%)	0.07	8 (1%) 72 79	12, 21, 37, 48	0
1	B	510/527 (96%)	0.09	13 (2%) 57 66	13, 23, 37, 49	0
2	C	388/389 (99%)	-0.22	4 (1%) 82 87	10, 16, 29, 44	0
2	D	388/389 (99%)	0.64	30 (7%) 13 21	17, 30, 49, 77	0
3	E	166/170 (97%)	-0.02	4 (2%) 59 68	13, 19, 31, 54	0
3	F	166/170 (97%)	1.09	27 (16%) 1 2	26, 39, 55, 64	0
All	All	2128/2172 (97%)	0.20	86 (4%) 38 48	10, 23, 44, 77	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	389	LYS	7.6
2	D	205	PRO	6.5
3	E	4	LEU	5.3
3	F	100	ALA	5.2
2	D	380	ILE	5.1
2	D	385	LEU	5.1
2	C	3	MET	4.2
2	D	352	ILE	4.0
2	D	379	GLN	3.8
2	D	388	LEU	3.6
3	F	102	LYS	3.5
2	C	205	PRO	3.5
2	D	357	TYR	3.5
3	F	19	ILE	3.4
3	F	23	ASN	3.4
1	B	310	TYR	3.4
1	A	318	ILE	3.4
3	F	26	GLU	3.3
1	B	54	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
2	D	348	ASP	3.2
3	F	80	LYS	3.2
1	B	39	PHE	3.2
1	A	310	TYR	3.1
2	D	220	ASN	3.1
3	E	168	SER	3.0
3	F	70	ARG	3.0
1	A	316	ILE	2.9
2	D	344	ALA	2.9
1	B	527	ASN	2.9
3	F	4	LEU	2.9
2	D	374	LYS	2.9
2	D	343	PRO	2.9
3	F	17	ASN	2.9
1	B	259	ASN	2.8
2	D	335	PHE	2.8
1	B	320	ARG	2.8
2	D	44	LYS	2.7
3	F	83	PHE	2.6
2	D	260	VAL	2.6
2	D	354	ALA	2.6
3	F	69	ALA	2.6
2	D	376	ASP	2.6
2	D	347	THR	2.6
3	F	20	ALA	2.5
3	F	101	ALA	2.5
1	B	258	ALA	2.5
2	C	2	SER	2.5
3	F	25	LEU	2.5
2	D	256	PHE	2.5
3	F	21	GLN	2.4
2	D	187	ILE	2.4
1	B	333	LYS	2.3
1	B	504	ASP	2.3
1	A	380	TYR	2.2
1	B	311	GLU	2.2
2	D	345	GLY	2.2
2	D	350	GLU	2.2
1	A	319	GLY	2.2
3	F	66	VAL	2.2
2	D	372	ASP	2.2
3	F	67	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
3	F	154	GLU	2.2
2	D	339	PHE	2.2
2	D	213	VAL	2.2
1	B	317	TRP	2.1
3	F	118	TYR	2.1
3	E	153	GLU	2.1
3	F	120	PRO	2.1
1	B	261	PRO	2.1
2	C	389	LYS	2.1
2	D	333	ARG	2.1
3	F	72	PHE	2.1
2	D	281	ILE	2.1
2	D	371	ILE	2.1
3	F	28	ALA	2.1
1	A	381	ASP	2.1
3	F	30	GLU	2.1
1	A	20	PRO	2.1
3	F	16	VAL	2.0
3	F	161	VAL	2.0
3	F	97	LYS	2.0
1	B	403	ILE	2.0
1	A	19	ALA	2.0
2	D	206	GLY	2.0
3	F	151	PRO	2.0
3	E	23	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
6	IPH	B	2666	7/7	0.92	0.18	26,27,29,32	0
6	IPH	A	2667	7/7	0.93	0.14	29,30,31,32	0
5	OH	A	1177	1/1	0.99	0.05	23,23,23,23	0
5	OH	B	1173	1/1	0.99	0.04	25,25,25,25	0
4	FE	A	1175	1/1	0.99	0.03	24,24,24,24	0
4	FE	B	1171	1/1	0.99	0.03	26,26,26,26	0
4	FE	B	1170	1/1	1.00	0.04	19,19,19,19	0
4	FE	A	1174	1/1	1.00	0.03	19,19,19,19	0

6.5 Other polymers (i)

There are no such residues in this entry.