Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:31 PM GMT

PDB ID	:	1FZ8
Title	:	METHANE MONOOXYGENASE HYDROXYLASE, FORM II COCRYSTALLIZED WITH DIBROMOMETHANE
Authors	:	Whittington, D.A.; Rosenzweig, A.C.; Frederick, C.A.; Lippard, S.J.
Deposited on	:	2000-10-03
Resolution	:	2.10 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

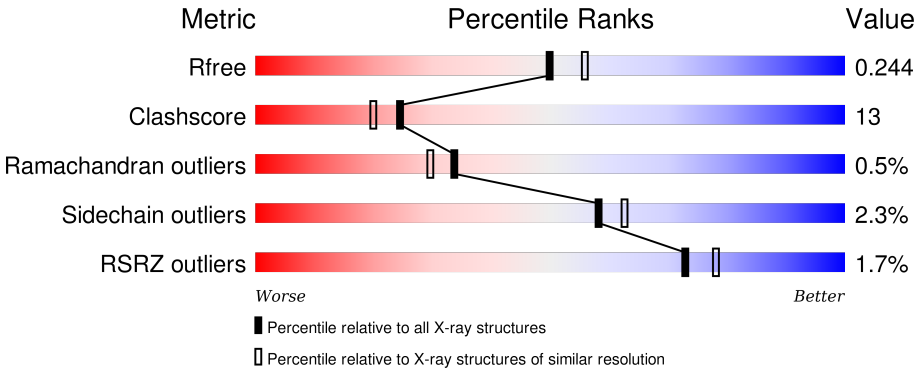
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	527	71% 25%
1	B	527	71% 24%
2	C	389	79% 19%
2	D	389	66% 33%
3	E	170	78% 19%

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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	2BM	B	9002	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 18611 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	511	Total	C	N	O	S	0	0	0
			4185	2677	721	769	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	0	0	0
			3189	2051	550	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	167	Total	C	N	O	S	0	0	0
			1375	872	247	251	5			
3	F	168	Total	C	N	O	S	0	0	0
			1386	878	250	253	5			

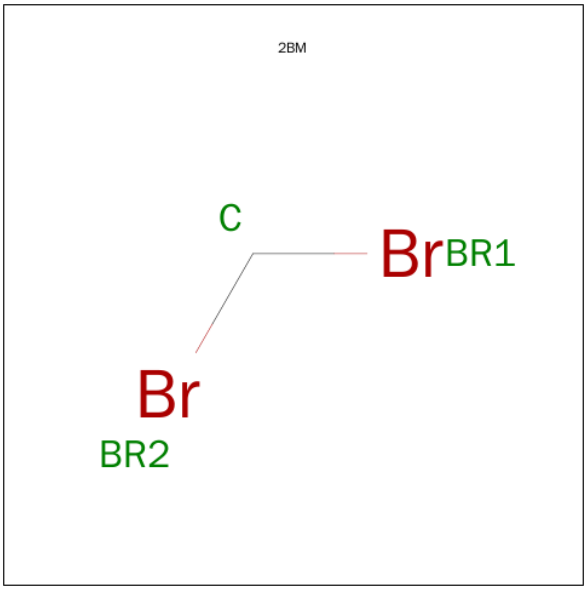
- Molecule 4 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

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

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

- Molecule 6 is DIBROMOMETHANE (three-letter code: 2BM) (formula: CH_2Br_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total Br C 3 2 1	0	0
6	B	1	Total Br C 3 2 1	0	0
6	B	1	Total Br C 3 2 1	0	0
6	D	1	Total Br C 3 2 1	0	0
6	C	1	Total Br C 3 2 1	0	0
6	A	1	Total Br C 3 2 1	0	0

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

- Molecule 7 is water.

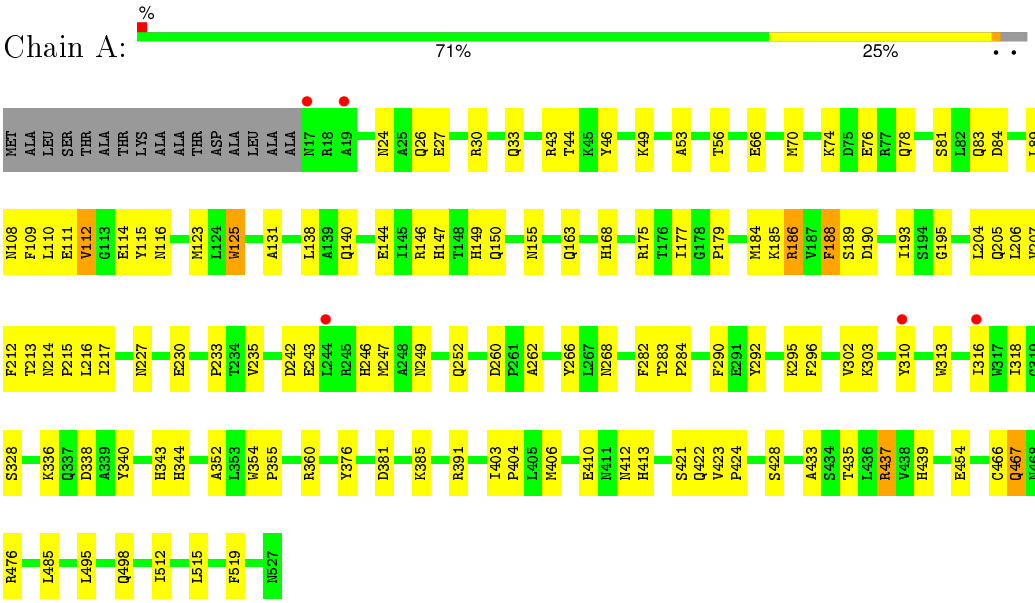
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	245	Total O 245 245	0	0
7	B	247	Total O 247 247	0	0
7	C	268	Total O 268 268	0	0
7	D	140	Total O 140 140	0	0
7	E	123	Total O 123 123	0	0
7	F	46	Total O 46 46	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

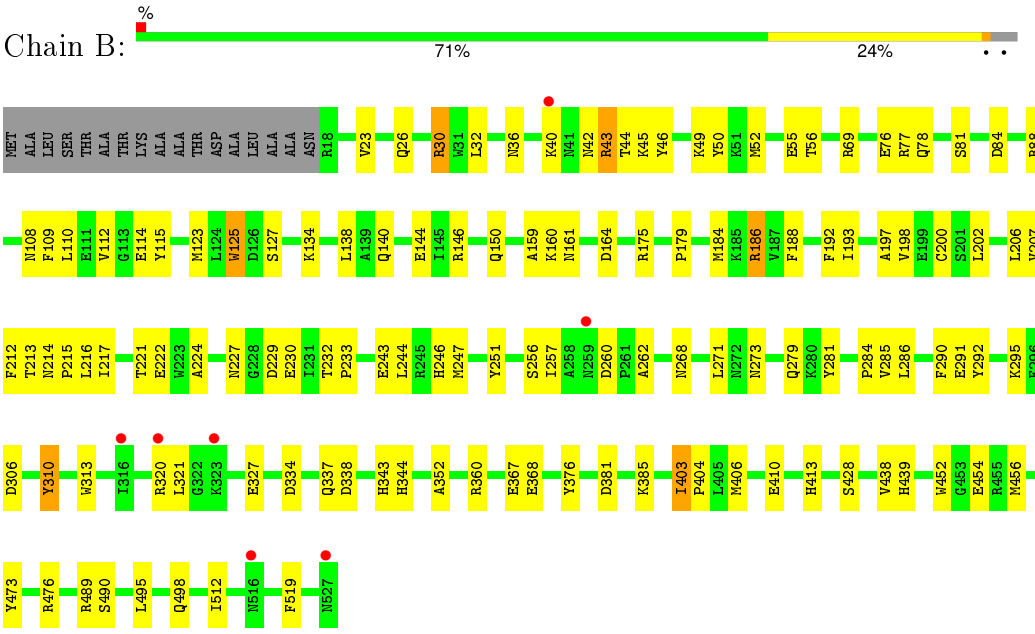
- Molecule 1: METHANE MONOOXYGENASE COMPONENT A, ALPHA CHAIN

Chain A:



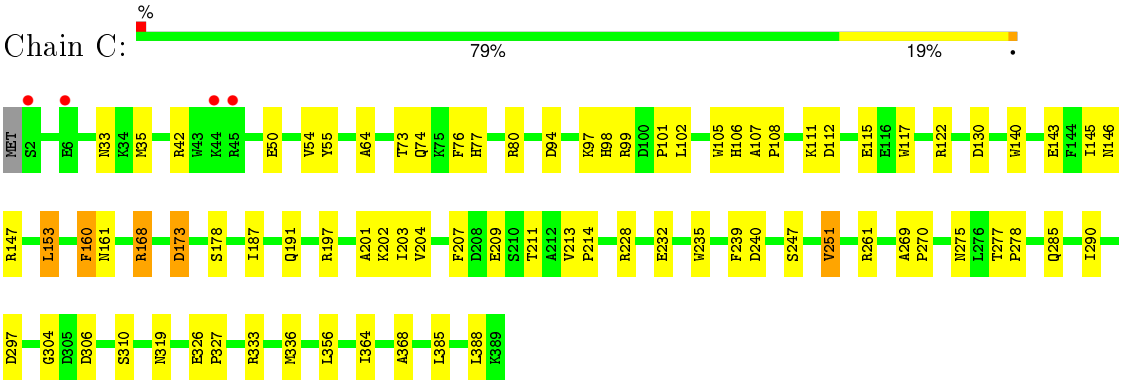
- Molecule 1: METHANE MONOOXYGENASE COMPONENT A, ALPHA CHAIN

Chain B:



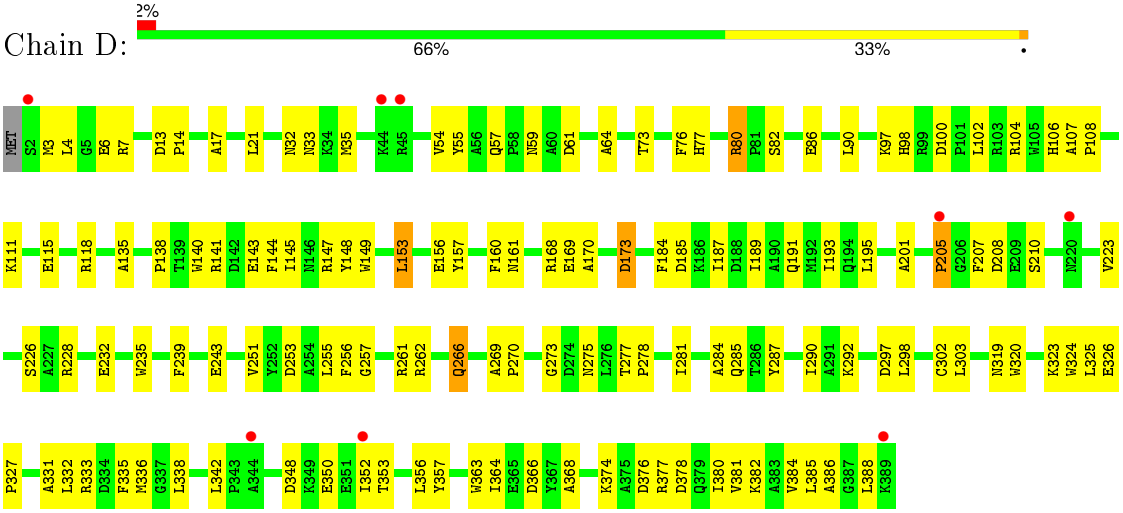
• Molecule 2: METHANE MONOOXYGENASE COMPONENT A, BETA CHAIN

Chain C:



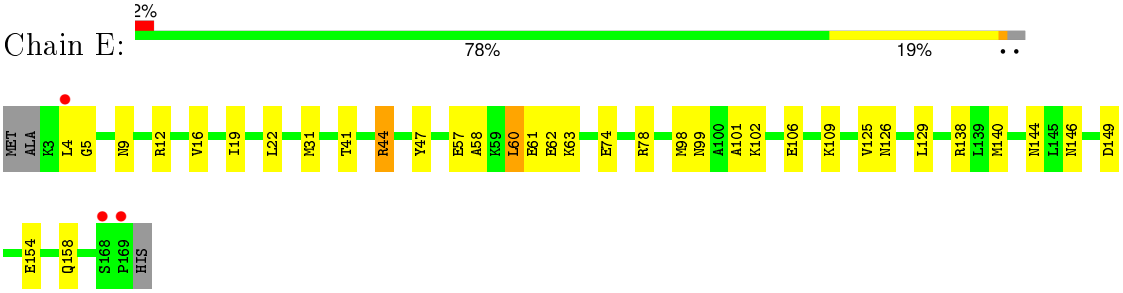
• Molecule 2: METHANE MONOOXYGENASE COMPONENT A, BETA CHAIN

Chain D:



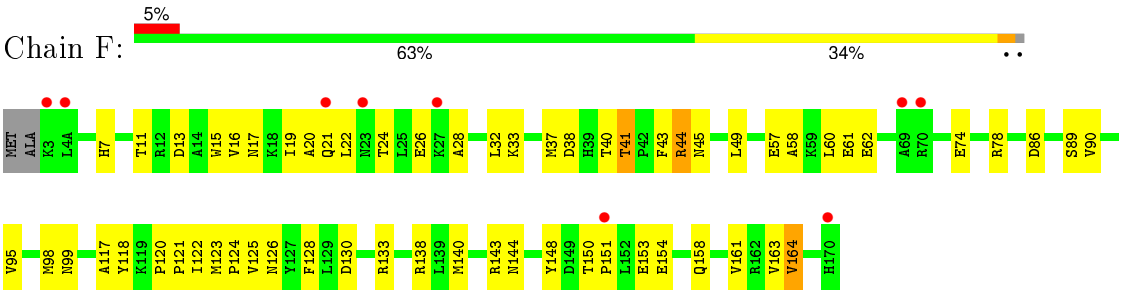
• Molecule 3: METHANE MONOOXYGENASE COMPONENT A, GAMMA CHAIN

Chain E:



• Molecule 3: METHANE MONOOXYGENASE COMPONENT A, GAMMA CHAIN

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	71.17Å 171.99Å 221.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	23.50 – 2.10 23.50 – 2.10	Depositor EDS
% Data completeness (in resolution range)	77.7 (23.50-2.10) 77.8 (23.50-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.56 (at 2.10Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.201 , 0.250 0.198 , 0.244	Depositor DCC
R_{free} test set	4359 reflections (3.66%)	DCC
Wilson B-factor (Å^2)	22.1	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 61.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 136816 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	18611	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, FE, 2BM

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	0/4310	0.55	0/5853
1	B	0.33	0/4302	0.56	0/5842
2	C	0.36	0/3289	0.57	0/4464
2	D	0.34	0/3285	0.54	0/4460
3	E	0.34	0/1404	0.57	0/1892
3	F	0.30	0/1416	0.50	0/1907
All	All	0.34	0/18006	0.55	0/24418

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	4185	0	3981	110	0
1	B	4177	0	3975	128	0
2	C	3193	0	3042	73	0
2	D	3189	0	3031	103	0
3	E	1375	0	1370	30	0
3	F	1386	0	1377	57	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	9	0	0	2	0
6	B	9	0	0	2	0
6	C	9	0	0	1	0
6	D	3	0	0	0	0
7	A	245	0	0	6	0
7	B	247	0	0	8	0
7	C	268	0	0	8	0
7	D	140	0	0	3	0
7	E	123	0	0	2	0
7	F	46	0	0	1	0
All	All	18611	0	16776	443	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 (443) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:GLU:HA	1:A:213:THR:HG22	1.23	1.12
1:A:78:GLN:HE22	1:A:150:GLN:HE21	1.05	0.98
1:B:352:ALA:HA	1:B:404:PRO:HB2	1.45	0.97
1:B:44:THR:HG22	1:B:46:TYR:H	1.30	0.94
1:B:78:GLN:HE22	1:B:150:GLN:HE21	1.11	0.93
3:F:41:THR:HG22	3:F:43:PHE:H	1.31	0.91
1:A:467:GLN:HG3	7:E:219:HOH:O	1.71	0.89
1:A:209:GLU:HA	1:A:213:THR:CG2	2.02	0.88
3:E:19:ILE:HG12	3:E:60:LEU:HD13	1.55	0.87
3:F:150:THR:HG21	3:F:158:GLN:HE22	1.39	0.86
1:A:44:THR:HG22	1:A:46:TYR:H	1.42	0.84
2:C:261:ARG:HE	2:C:285:GLN:HE22	1.22	0.83
1:A:109:PHE:HB3	1:A:184:MET:HE3	1.62	0.82
1:B:209:GLU:HA	1:B:213:THR:OG1	1.81	0.81
3:F:154:GLU:HG3	3:F:158:GLN:HE21	1.43	0.80
1:A:352:ALA:HA	1:A:404:PRO:HB2	1.61	0.80
1:A:338:ASP:OD1	1:A:433:ALA:HB2	1.81	0.80
1:A:268:ASN:HD21	1:A:327:GLU:H	1.28	0.80
3:E:41:THR:O	3:E:44:ARG:HD2	1.82	0.79
2:D:100:ASP:OD1	2:D:104:ARG:HD3	1.82	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:150:THR:HG21	3:F:158:GLN:NE2	1.97	0.78
2:C:270:PRO:HB3	2:D:270:PRO:HB3	1.66	0.78
2:C:102:LEU:HD12	2:C:290:ILE:HG23	1.64	0.77
2:D:319:ASN:OD1	3:F:78:ARG:HD3	1.85	0.76
2:D:102:LEU:HD13	2:D:290:ILE:HG23	1.68	0.76
2:D:261:ARG:HE	2:D:285:GLN:HE22	1.33	0.76
2:D:228:ARG:O	2:D:232:GLU:HG3	1.86	0.75
2:C:326:GLU:HB3	2:C:327:PRO:HD3	1.68	0.75
2:D:102:LEU:CD1	2:D:290:ILE:HG23	2.16	0.75
3:F:41:THR:CG2	3:F:43:PHE:H	2.00	0.75
1:A:155:ASN:HD22	1:A:168:HIS:HD2	1.35	0.74
2:C:102:LEU:CD1	2:C:290:ILE:HG23	2.15	0.74
1:B:179:PRO:HB3	1:B:469:ILE:HD13	1.69	0.74
1:B:268:ASN:HD21	1:B:327:GLU:H	1.36	0.74
3:F:41:THR:O	3:F:44:ARG:HD2	1.87	0.73
1:A:403:ILE:HD13	1:A:515:LEU:HD11	1.70	0.73
2:C:146:ASN:HD21	2:C:197:ARG:HH21	1.34	0.73
2:D:76:PHE:HZ	2:D:168:ARG:HH12	1.35	0.73
1:A:406:MET:O	1:A:410:GLU:HG3	1.88	0.72
2:D:90:LEU:HD13	2:D:303:LEU:HD13	1.71	0.72
1:A:83:GLN:HB3	1:B:77:ARG:HH22	1.56	0.71
1:B:227:ASN:HD21	1:B:295:LYS:H	1.39	0.70
1:B:214:ASN:HB3	1:B:215:PRO:HD3	1.72	0.70
3:F:57:GLU:O	3:F:61:GLU:HG3	1.92	0.70
2:D:107:ALA:HB3	2:D:108:PRO:HD3	1.73	0.70
1:A:217:ILE:HG13	7:A:9221:HOH:O	1.91	0.70
1:A:214:ASN:HB3	1:A:215:PRO:HD3	1.73	0.70
2:C:333:ARG:HD3	7:C:9196:HOH:O	1.90	0.70
1:A:310:TYR:CZ	1:A:336:LYS:HD2	2.27	0.69
3:F:58:ALA:O	3:F:62:GLU:HG3	1.92	0.69
1:B:406:MET:O	1:B:410:GLU:HG3	1.92	0.69
1:B:251:TYR:HE2	1:B:320:ARG:HH12	1.40	0.69
1:A:78:GLN:NE2	1:A:150:GLN:HE21	1.87	0.68
1:A:227:ASN:HD21	1:A:295:LYS:H	1.39	0.68
3:E:146:ASN:HB3	3:E:149:ASP:OD2	1.93	0.67
1:B:403:ILE:HG23	1:B:406:MET:HG3	1.76	0.67
1:B:495:LEU:HD11	1:B:512:ILE:HG13	1.75	0.67
1:B:30:ARG:O	1:B:30:ARG:HD3	1.94	0.67
1:B:108:ASN:HD21	1:B:175:ARG:HH11	1.43	0.67
1:B:439:HIS:HD2	3:F:163:VAL:HA	1.60	0.66
1:B:78:GLN:NE2	1:B:150:GLN:HE21	1.88	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:146:ASN:ND2	2:C:197:ARG:HH21	1.94	0.65
1:B:292:TYR:OH	1:B:344:HIS:HD2	1.80	0.65
1:A:76:GLU:HG2	1:B:76:GLU:OE2	1.96	0.65
1:B:489:ARG:HD2	1:B:495:LEU:O	1.97	0.65
3:F:22:LEU:HD13	3:F:28:ALA:HA	1.78	0.64
1:B:206:LEU:HD23	1:B:271:LEU:HD13	1.78	0.64
3:F:15:TRP:O	3:F:19:ILE:HG23	1.97	0.64
2:D:61:ASP:OD1	3:F:7:HIS:HD2	1.81	0.64
1:B:49:LYS:HD3	3:F:144:ASN:HD22	1.63	0.64
1:B:110:LEU:O	1:B:114:GLU:HG2	1.98	0.64
1:B:211:CYS:HB2	1:B:313:TRP:CD1	2.33	0.64
3:E:58:ALA:O	3:E:62:GLU:HG3	1.96	0.63
1:B:144:GLU:HA	1:B:144:GLU:OE2	1.99	0.63
1:A:179:PRO:HB3	1:A:469:ILE:HD13	1.81	0.63
1:A:403:ILE:HD13	1:A:515:LEU:CD1	2.28	0.63
2:C:42:ARG:HB2	2:C:99:ARG:HH11	1.64	0.63
1:A:83:GLN:CB	1:B:77:ARG:HH12	2.11	0.63
2:C:42:ARG:HB2	2:C:99:ARG:NH1	2.14	0.63
3:E:99:ASN:HA	3:E:138:ARG:NH1	2.13	0.62
1:A:108:ASN:HD21	1:A:175:ARG:HH11	1.45	0.62
2:D:140:TRP:NE1	2:D:145:ILE:HD11	2.14	0.62
1:A:83:GLN:HB2	1:B:77:ARG:HH12	1.64	0.62
1:B:413:HIS:HD2	1:B:428:SER:OG	1.83	0.62
3:F:13:ASP:O	3:F:16:VAL:HG22	2.00	0.62
3:F:61:GLU:O	3:F:121:PRO:HG2	1.99	0.62
1:B:243:GLU:O	1:B:247:MET:HG2	1.99	0.62
2:D:111:LYS:O	2:D:115:GLU:HG3	1.99	0.61
1:A:381:ASP:O	1:A:385:LYS:HD2	2.00	0.61
3:F:150:THR:CG2	3:F:158:GLN:HE22	2.10	0.61
1:B:212:PHE:O	1:B:215:PRO:HD2	1.99	0.61
1:B:160:LYS:HE3	1:B:161:ASN:HD21	1.65	0.61
1:A:140:GLN:O	1:A:144:GLU:HG2	2.00	0.61
2:D:208:ASP:OD2	2:D:210:SER:HB3	2.00	0.61
1:B:213:THR:O	1:B:217:ILE:HG12	2.01	0.61
1:A:268:ASN:ND2	1:A:327:GLU:H	1.97	0.61
1:B:55:GLU:HG3	7:B:9229:HOH:O	2.01	0.61
1:A:318:ILE:HD12	1:A:328:SER:HA	1.81	0.61
1:A:292:TYR:OH	1:A:344:HIS:HD2	1.84	0.60
2:D:223:VAL:HG13	2:D:335:PHE:HA	1.82	0.60
1:A:216:LEU:HD21	6:A:9007:2BM:BR1	2.57	0.60
1:A:56:THR:HG23	1:A:252:GLN:HE21	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:261:ARG:HE	2:D:285:GLN:NE2	1.98	0.59
1:B:439:HIS:HB3	3:F:161:VAL:CG2	2.33	0.59
1:B:123:MET:CE	1:B:197:ALA:HA	2.32	0.59
1:A:109:PHE:O	1:A:112:VAL:HG12	2.02	0.59
1:B:23:VAL:HB	2:D:195:LEU:HD21	1.83	0.59
1:B:291:GLU:OE1	1:B:343:HIS:HE1	1.84	0.59
1:B:206:LEU:HD11	1:B:321:LEU:HD11	1.84	0.58
3:E:98:MET:O	3:E:98:MET:HE2	2.02	0.58
2:C:211:THR:O	2:C:214:PRO:HD2	2.03	0.58
1:B:302:VAL:HG13	1:B:376:TYR:HE2	1.66	0.58
1:A:435:THR:HG21	1:A:437:ARG:HE	1.68	0.58
2:C:261:ARG:HE	2:C:285:GLN:NE2	1.97	0.58
2:C:50:GLU:OE1	2:C:99:ARG:NH1	2.36	0.58
3:E:41:THR:O	3:E:44:ARG:CD	2.51	0.58
1:B:244:LEU:HG	7:B:9178:HOH:O	2.03	0.57
2:D:324:TRP:O	2:D:327:PRO:HD2	2.04	0.57
1:B:192:PHE:O	1:B:200:CYS:HB3	2.05	0.57
3:F:153:GLU:CD	3:F:153:GLU:H	2.07	0.57
2:C:111:LYS:O	2:C:115:GLU:HG3	2.04	0.57
1:A:243:GLU:O	1:A:247:MET:HG2	2.03	0.57
2:C:336:MET:HE1	2:C:356:LEU:HD11	1.87	0.57
2:C:209:GLU:HG2	7:C:9215:HOH:O	2.05	0.57
1:A:204:LEU:O	1:A:209:GLU:HG3	2.04	0.57
1:B:337:GLN:HG3	1:B:338:ASP:N	2.19	0.57
3:F:98:MET:HG3	3:F:138:ARG:HG2	1.87	0.57
1:B:159:ALA:O	2:D:33:ASN:HB2	2.05	0.56
3:F:61:GLU:HB3	3:F:121:PRO:HD3	1.87	0.56
1:A:227:ASN:ND2	1:A:295:LYS:H	2.03	0.56
2:C:105:TRP:O	2:C:108:PRO:HD2	2.05	0.56
3:F:40:THR:O	3:F:41:THR:HB	2.06	0.56
1:A:213:THR:O	1:A:217:ILE:HG12	2.06	0.55
1:A:439:HIS:HE1	1:A:454:GLU:OE1	1.89	0.55
1:A:108:ASN:HD21	1:A:175:ARG:HD3	1.71	0.55
1:B:281:TYR:CZ	1:B:285:VAL:HG21	2.41	0.55
2:D:153:LEU:C	2:D:153:LEU:HD12	2.27	0.55
2:C:333:ARG:HD2	7:C:9271:HOH:O	2.05	0.55
1:B:108:ASN:HD21	1:B:175:ARG:HD3	1.71	0.55
2:C:336:MET:CE	2:C:385:LEU:HD23	2.36	0.55
3:E:101:ALA:HA	3:E:106:GLU:OE2	2.06	0.55
2:D:262:ARG:HA	2:D:266:GLN:HB3	1.89	0.55
1:A:83:GLN:HB2	1:B:77:ARG:NH1	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:107:ALA:HB3	2:C:108:PRO:HD3	1.89	0.55
2:D:364:ILE:HA	2:D:368:ALA:HB3	1.88	0.55
2:C:319:ASN:OD1	3:E:78:ARG:HD3	2.07	0.55
1:B:164:ASP:CG	1:B:489:ARG:HH22	2.10	0.55
3:F:41:THR:HG22	3:F:43:PHE:N	2.11	0.54
1:B:439:HIS:HB3	3:F:161:VAL:HG21	1.89	0.54
3:E:57:GLU:O	3:E:61:GLU:HG3	2.05	0.54
2:C:187:ILE:O	2:C:191:GLN:HG3	2.07	0.54
2:D:138:PRO:HA	2:D:141:ARG:NH1	2.22	0.54
3:E:109:LYS:HE2	7:E:289:HOH:O	2.08	0.54
1:A:381:ASP:HA	1:A:385:LYS:HE2	1.89	0.54
1:B:123:MET:HE2	1:B:197:ALA:HA	1.90	0.54
1:B:439:HIS:HE1	1:B:454:GLU:OE1	1.90	0.54
1:A:360:ARG:HG2	1:A:498:GLN:HB2	1.89	0.54
1:B:290:PHE:CD2	6:B:9002:2BM:BR1	3.16	0.54
1:B:209:GLU:HA	1:B:213:THR:HG1	1.73	0.54
2:D:266:GLN:HA	2:D:266:GLN:HE21	1.73	0.54
2:D:98:HIS:HD2	2:D:297:ASP:OD1	1.91	0.54
1:A:84:ASP:HB3	1:B:81:SER:OG	2.07	0.54
1:A:211:CYS:HB2	1:A:313:TRP:CD1	2.43	0.54
7:C:9035:HOH:O	3:E:125:VAL:HG22	2.06	0.54
1:B:227:ASN:ND2	1:B:295:LYS:H	2.06	0.53
1:A:114:GLU:CD	1:A:147:HIS:HB3	2.28	0.53
3:F:33:LYS:HE3	3:F:117:ALA:CB	2.38	0.53
1:A:24:ASN:OD1	1:A:26:GLN:HG2	2.08	0.53
1:A:495:LEU:HD11	1:A:512:ILE:CG1	2.39	0.53
1:B:232:THR:HB	1:B:233:PRO:HD3	1.91	0.53
2:C:269:ALA:HB3	2:C:270:PRO:HD3	1.89	0.53
1:B:302:VAL:HG13	1:B:376:TYR:CE2	2.42	0.53
1:B:495:LEU:HD11	1:B:512:ILE:CG1	2.38	0.53
1:A:110:LEU:O	1:A:114:GLU:HG2	2.09	0.53
1:B:50:TYR:CD2	1:B:257:ILE:HD12	2.43	0.53
2:D:275:ASN:C	2:D:278:PRO:HD2	2.29	0.53
2:D:292:LYS:HE3	2:D:366:ASP:OD2	2.08	0.53
2:D:348:ASP:OD2	2:D:350:GLU:HB3	2.08	0.53
1:B:134:LYS:HD3	2:D:161:ASN:HD21	1.74	0.52
3:F:24:THR:HG22	3:F:26:GLU:H	1.74	0.52
1:B:164:ASP:OD1	1:B:489:ARG:NH2	2.42	0.52
2:D:336:MET:CE	2:D:356:LEU:HD11	2.39	0.52
2:D:54:VAL:O	2:D:55:TYR:HB2	2.08	0.52
1:A:27:GLU:CD	2:C:202:LYS:HZ1	2.12	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:213:VAL:HB	2:C:214:PRO:HD3	1.92	0.52
1:B:108:ASN:ND2	1:B:175:ARG:HH11	2.08	0.52
2:D:80:ARG:HG2	2:D:86:GLU:OE1	2.09	0.52
2:D:145:ILE:O	2:D:149:TRP:HB3	2.09	0.52
2:D:357:TYR:CE1	2:D:381:VAL:HG11	2.45	0.52
1:A:78:GLN:HE21	1:A:235:VAL:HA	1.74	0.52
2:D:185:ASP:O	2:D:189:ILE:HG12	2.10	0.52
2:D:201:ALA:HA	2:D:207:PHE:HB3	1.92	0.51
1:B:367:GLU:HG3	7:B:9024:HOH:O	2.10	0.51
1:A:186:ARG:HA	2:C:73:THR:OG1	2.10	0.51
2:C:306:ASP:O	2:C:310:SER:HB2	2.10	0.51
1:A:260:ASP:OD2	1:A:262:ALA:HB3	2.11	0.51
1:B:49:LYS:CD	3:F:144:ASN:HD22	2.23	0.51
3:E:154:GLU:O	3:E:158:GLN:HG3	2.10	0.51
2:C:153:LEU:HD12	2:C:153:LEU:C	2.31	0.51
2:D:326:GLU:HB3	2:D:327:PRO:HD3	1.91	0.51
1:A:495:LEU:HD11	1:A:512:ILE:HG13	1.92	0.51
2:D:6:GLU:HG3	7:D:9049:HOH:O	2.10	0.51
3:F:74:GLU:O	3:F:78:ARG:HG3	2.11	0.50
1:B:473:TYR:O	1:B:519:PHE:HB2	2.09	0.50
1:B:360:ARG:HG2	1:B:498:GLN:HB2	1.94	0.50
2:D:336:MET:HE2	2:D:384:VAL:HG12	1.94	0.50
1:A:227:ASN:HD21	1:A:296:PHE:H	1.58	0.50
1:B:49:LYS:CE	3:F:144:ASN:HD22	2.25	0.50
2:D:323:LYS:HB2	3:F:78:ARG:NH1	2.26	0.50
2:D:189:ILE:HD11	2:D:287:TYR:CD1	2.46	0.50
2:D:324:TRP:C	2:D:327:PRO:HD2	2.32	0.50
2:D:352:ILE:HG13	2:D:353:THR:N	2.26	0.50
2:D:352:ILE:HD11	2:D:388:LEU:HD11	1.93	0.50
3:F:130:ASP:OD1	3:F:133:ARG:NH1	2.42	0.50
3:F:41:THR:O	3:F:44:ARG:CD	2.59	0.50
1:B:207:VAL:HG22	1:B:313:TRP:CZ2	2.46	0.50
1:B:84:ASP:OD1	1:B:88:ARG:NH2	2.45	0.50
2:D:378:ASP:O	2:D:382:LYS:HG3	2.11	0.50
1:B:244:LEU:HB2	7:B:9030:HOH:O	2.10	0.49
2:D:97:LYS:HD2	7:D:9142:HOH:O	2.12	0.49
2:D:256:PHE:HA	2:D:332:LEU:HD21	1.94	0.49
2:D:187:ILE:O	2:D:191:GLN:HG3	2.12	0.49
1:A:78:GLN:HE22	1:A:150:GLN:NE2	1.90	0.49
2:C:336:MET:HE1	2:C:385:LEU:HD23	1.94	0.49
3:E:74:GLU:O	3:E:78:ARG:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:333:ARG:NH2	2:D:386:ALA:HB3	2.28	0.49
3:F:19:ILE:HG13	3:F:20:ALA:N	2.25	0.49
1:B:146:ARG:HB2	2:D:106:HIS:CE1	2.47	0.49
2:C:143:GLU:O	2:C:147:ARG:HB3	2.13	0.49
2:C:112:ASP:OD1	2:D:118:ARG:NH2	2.46	0.49
1:A:230:GLU:C	1:A:233:PRO:HD2	2.33	0.49
1:B:286:LEU:HD22	6:B:9002:2BM:BR2	2.68	0.49
1:A:290:PHE:CD2	6:A:9008:2BM:BR1	3.21	0.48
1:A:163:GLN:HG2	7:A:9054:HOH:O	2.12	0.48
1:B:160:LYS:HE3	1:B:161:ASN:ND2	2.27	0.48
1:A:435:THR:CG2	1:A:437:ARG:HE	2.26	0.48
2:D:102:LEU:HB2	2:D:104:ARG:HD2	1.96	0.48
1:A:147:HIS:CE1	7:A:9253:HOH:O	2.66	0.48
2:D:143:GLU:O	2:D:147:ARG:HB3	2.12	0.48
1:A:316:ILE:O	1:A:320:ARG:HG3	2.14	0.48
1:B:32:LEU:C	1:B:32:LEU:HD23	2.33	0.48
1:B:44:THR:HG21	7:B:9119:HOH:O	2.14	0.48
1:B:211:CYS:HB2	1:B:313:TRP:CG	2.49	0.48
2:D:235:TRP:CD1	2:D:235:TRP:C	2.87	0.48
2:C:201:ALA:HA	2:C:207:PHE:HB3	1.96	0.48
2:D:157:TYR:O	2:D:160:PHE:HB3	2.14	0.48
1:A:108:ASN:ND2	1:A:175:ARG:HH11	2.11	0.48
1:A:310:TYR:CE2	1:A:336:LYS:HD2	2.49	0.48
2:D:189:ILE:HD12	2:D:284:ALA:HB2	1.94	0.48
3:E:22:LEU:HD11	3:E:31:MET:SD	2.54	0.48
2:D:243:GLU:HB2	2:D:320:TRP:CZ2	2.48	0.48
1:A:190:ASP:HB3	2:C:74:GLN:O	2.13	0.47
1:A:115:TYR:OH	2:C:173:ASP:HA	2.14	0.47
2:C:203:ILE:HG13	2:C:204:VAL:HG23	1.95	0.47
1:B:476:ARG:HG3	1:B:476:ARG:HH11	1.80	0.47
1:A:89:LEU:HD21	1:B:230:GLU:HG3	1.96	0.47
1:B:138:LEU:HD22	2:D:160:PHE:CZ	2.49	0.47
3:F:118:TYR:HB3	3:F:123:MET:HB2	1.96	0.47
2:D:17:ALA:O	2:D:21:LEU:HG	2.14	0.47
1:B:206:LEU:HD11	1:B:321:LEU:CD1	2.45	0.47
2:D:140:TRP:CE2	2:D:145:ILE:HD11	2.50	0.47
1:B:23:VAL:HB	2:D:195:LEU:CD2	2.44	0.47
2:C:94:ASP:HB3	2:C:97:LYS:HG3	1.96	0.47
2:C:235:TRP:CD1	2:C:235:TRP:C	2.87	0.47
1:B:344:HIS:HE1	1:B:376:TYR:CD2	2.32	0.47
1:B:43:ARG:C	1:B:43:ARG:HD2	2.36	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:ARG:O	1:B:43:ARG:HD2	2.14	0.47
3:E:138:ARG:HH11	3:E:138:ARG:HG2	1.80	0.47
2:D:353:THR:O	2:D:357:TYR:HD1	1.98	0.47
2:C:364:ILE:HA	2:C:368:ALA:HB3	1.97	0.47
2:D:298:LEU:O	2:D:302:CYS:HB2	2.14	0.47
1:A:109:PHE:HD2	1:A:184:MET:HE2	1.80	0.46
1:A:125:TRP:HE1	2:C:161:ASN:ND2	2.13	0.46
2:D:269:ALA:HB3	2:D:270:PRO:HD3	1.97	0.46
2:D:223:VAL:CG1	2:D:335:PHE:HA	2.45	0.46
3:F:151:PRO:HB2	3:F:153:GLU:OE1	2.14	0.46
2:C:76:PHE:HZ	2:C:168:ARG:HH12	1.63	0.46
1:B:123:MET:HE3	1:B:197:ALA:HA	1.97	0.46
1:A:302:VAL:HG13	1:A:303:LYS:N	2.31	0.46
1:B:140:GLN:HG3	1:B:246:HIS:CD2	2.50	0.46
1:B:193:ILE:HD11	2:D:82:SER:HB3	1.97	0.46
3:E:5:GLY:H	3:E:9:ASN:HB3	1.81	0.46
1:A:24:ASN:OD1	1:A:26:GLN:CG	2.63	0.46
1:A:138:LEU:HD22	2:C:160:PHE:CZ	2.50	0.46
2:D:140:TRP:O	2:D:145:ILE:HD13	2.15	0.46
2:C:97:LYS:HD2	7:C:9232:HOH:O	2.15	0.46
7:B:9055:HOH:O	3:F:143:ARG:HG2	2.16	0.46
1:B:36:ASN:HD21	1:B:42:ASN:HD21	1.64	0.46
1:B:108:ASN:HD21	1:B:175:ARG:CD	2.29	0.46
2:D:77:HIS:CD2	3:F:140:MET:HG2	2.50	0.46
1:A:49:LYS:HD3	3:E:144:ASN:HD22	1.81	0.46
2:C:240:ASP:HB2	3:E:125:VAL:CG2	2.45	0.46
2:D:380:ILE:O	2:D:384:VAL:HG23	2.15	0.46
2:C:54:VAL:O	2:C:55:TYR:HB2	2.15	0.46
2:C:42:ARG:HB2	2:C:99:ARG:HG3	1.98	0.45
2:D:195:LEU:O	2:D:195:LEU:HD23	2.16	0.45
2:D:266:GLN:HB2	2:D:281:ILE:HG21	1.98	0.45
3:F:17:ASN:O	3:F:21:GLN:HG2	2.16	0.45
2:C:261:ARG:NE	2:C:285:GLN:HE22	2.03	0.45
2:D:82:SER:O	2:D:168:ARG:NH2	2.47	0.45
1:A:53:ALA:HB3	1:A:56:THR:OG1	2.15	0.45
3:E:102:LYS:HD2	3:E:102:LYS:N	2.31	0.45
1:B:439:HIS:HB3	3:F:161:VAL:HG22	1.98	0.45
1:B:291:GLU:OE1	1:B:343:HIS:CE1	2.67	0.45
2:D:77:HIS:CG	3:F:140:MET:HG2	2.52	0.45
2:D:148:TYR:CD1	2:D:338:LEU:HD11	2.51	0.45
2:D:385:LEU:HD22	2:D:388:LEU:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:95:VAL:HG12	3:F:99:ASN:ND2	2.31	0.45
2:D:325:LEU:HD12	2:D:325:LEU:O	2.16	0.45
1:B:52:MET:CE	1:B:127:SER:HB3	2.47	0.45
2:D:336:MET:HE2	2:D:356:LEU:HD11	1.99	0.45
1:A:466:CYS:HB2	2:C:73:THR:HA	1.98	0.45
1:A:177:ILE:HG12	1:A:485:LEU:HB2	1.98	0.45
2:D:144:PHE:CE2	2:D:342:LEU:HD23	2.51	0.45
1:A:205:GLN:NE2	1:A:249:ASN:HB3	2.31	0.45
1:B:30:ARG:HD3	1:B:30:ARG:C	2.37	0.45
1:A:193:ILE:HD12	2:C:168:ARG:HH21	1.81	0.45
1:A:185:LYS:O	1:A:189:SER:HB2	2.17	0.45
1:A:343:HIS:H	1:A:343:HIS:CD2	2.33	0.45
2:D:156:GLU:OE2	2:D:156:GLU:HA	2.17	0.45
1:A:66:GLU:O	1:A:70:MET:HG2	2.15	0.45
1:B:381:ASP:HA	1:B:385:LYS:HE2	1.99	0.45
1:A:212:PHE:O	1:A:215:PRO:HD2	2.16	0.45
1:A:207:VAL:O	1:A:211:CYS:HB3	2.17	0.45
1:A:188:PHE:CE1	1:A:282:PHE:HZ	2.34	0.45
2:C:277:THR:HB	2:C:278:PRO:HD3	1.98	0.45
1:B:302:VAL:CG1	1:B:376:TYR:HE2	2.29	0.44
2:C:240:ASP:HB2	3:E:125:VAL:HG21	1.98	0.44
1:B:297:LYS:NZ	1:B:368:GLU:OE2	2.49	0.44
1:A:206:LEU:HD21	1:A:321:LEU:HD13	1.98	0.44
1:A:44:THR:HG21	7:A:9147:HOH:O	2.17	0.44
3:E:44:ARG:HD3	3:E:47:TYR:CZ	2.52	0.44
1:B:268:ASN:HD21	1:B:327:GLU:N	2.11	0.44
1:A:83:GLN:HB3	1:B:77:ARG:NH2	2.29	0.44
1:B:251:TYR:HE2	1:B:320:ARG:NH1	2.11	0.44
1:A:437:ARG:NH1	1:A:454:GLU:OE2	2.49	0.44
2:C:161:ASN:HB3	2:C:235:TRP:CE2	2.52	0.44
1:B:438:VAL:O	3:F:164:VAL:HG13	2.18	0.44
1:B:217:ILE:O	1:B:221:THR:HG23	2.17	0.44
3:E:99:ASN:HA	3:E:138:ARG:HH11	1.79	0.44
2:C:130:ASP:OD2	2:D:262:ARG:HD3	2.17	0.44
1:A:93:VAL:HG11	2:D:3:MET:HG2	2.00	0.44
1:A:109:PHE:HD2	1:A:184:MET:CE	2.31	0.44
1:B:198:VAL:O	1:B:202:LEU:HG	2.18	0.44
1:B:140:GLN:HG3	1:B:246:HIS:CE1	2.52	0.44
1:B:105:VAL:O	1:B:109:PHE:HB2	2.18	0.44
2:C:77:HIS:CD2	3:E:140:MET:HG2	2.53	0.44
1:B:466:CYS:HB2	2:D:73:THR:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:125:VAL:HG23	3:F:126:ASN:N	2.32	0.44
1:A:206:LEU:HD11	1:A:321:LEU:HD11	2.00	0.44
2:D:135:ALA:O	2:D:273:GLY:HA3	2.18	0.44
3:F:33:LYS:O	3:F:37:MET:HG2	2.18	0.43
3:F:123:MET:HG2	3:F:124:PRO:N	2.33	0.43
1:B:56:THR:HG21	1:B:256:SER:OG	2.17	0.43
1:B:306:ASP:O	1:B:310:TYR:HB2	2.18	0.43
1:A:283:THR:HB	1:A:284:PRO:HD3	1.99	0.43
1:B:88:ARG:HD3	7:B:9208:HOH:O	2.17	0.43
2:D:255:LEU:HD21	2:D:363:TRP:CG	2.54	0.43
2:C:211:THR:C	2:C:214:PRO:HD2	2.39	0.43
3:F:33:LYS:HE3	3:F:117:ALA:HA	2.00	0.43
2:D:377:ARG:O	2:D:381:VAL:HG23	2.19	0.43
2:D:184:PHE:O	2:D:187:ILE:HG22	2.18	0.43
1:B:184:MET:O	1:B:188:PHE:HB2	2.18	0.43
2:D:376:ASP:O	2:D:380:ILE:HG13	2.18	0.43
1:A:344:HIS:HE1	1:A:376:TYR:CD2	2.37	0.43
1:B:246:HIS:N	1:B:246:HIS:CD2	2.85	0.43
3:F:86:ASP:HB3	3:F:89:SER:OG	2.18	0.43
2:D:193:ILE:HA	7:D:9135:HOH:O	2.18	0.43
1:A:413:HIS:HD2	1:A:428:SER:OG	2.01	0.43
1:B:222:GLU:OE1	2:D:7:ARG:HD3	2.19	0.43
1:B:344:HIS:HE1	1:B:376:TYR:CE2	2.36	0.43
1:B:334:ASP:HA	1:B:337:GLN:HG2	2.01	0.43
1:A:81:SER:OG	1:B:84:ASP:HB3	2.19	0.43
3:F:49:LEU:HA	7:F:194:HOH:O	2.17	0.43
2:D:226:SER:HB2	2:D:331:ALA:HA	2.00	0.43
1:A:74:LYS:NZ	1:A:242:ASP:OD2	2.52	0.42
1:A:108:ASN:O	1:A:111:GLU:HB3	2.18	0.42
2:D:336:MET:HE1	2:D:356:LEU:HD11	2.01	0.42
1:B:186:ARG:HA	2:D:73:THR:OG1	2.19	0.42
2:C:247:SER:O	2:C:251:VAL:HB	2.19	0.42
3:E:12:ARG:O	3:E:16:VAL:HG23	2.18	0.42
2:D:169:GLU:O	2:D:170:ALA:C	2.56	0.42
2:C:336:MET:HE2	2:C:385:LEU:HA	2.01	0.42
2:D:189:ILE:HD11	2:D:284:ALA:HA	2.01	0.42
3:F:32:LEU:HA	3:F:60:LEU:HD23	2.01	0.42
1:B:206:LEU:HB2	7:B:9187:HOH:O	2.19	0.42
2:D:239:PHE:HB2	3:F:126:ASN:HA	2.01	0.42
2:D:277:THR:N	2:D:278:PRO:CD	2.83	0.42
1:B:268:ASN:ND2	1:B:327:GLU:H	2.08	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:243:GLU:HB2	2:D:320:TRP:CE2	2.55	0.42
2:C:168:ARG:HG2	2:C:168:ARG:HH11	1.84	0.42
2:C:140:TRP:NE1	2:C:145:ILE:HD11	2.34	0.42
2:D:57:GLN:NE2	2:D:59:ASN:HD21	2.17	0.42
3:F:90:VAL:HG11	3:F:118:TYR:CE2	2.55	0.42
1:A:266:TYR:HB3	7:A:9016:HOH:O	2.20	0.42
1:B:44:THR:HG22	1:B:45:LYS:N	2.35	0.42
2:C:98:HIS:HE1	2:C:178:SER:OG	2.02	0.42
1:A:146:ARG:HB2	2:C:106:HIS:CE1	2.54	0.42
1:A:476:ARG:HD3	3:E:4:LEU:HG	2.01	0.41
1:A:423:VAL:HA	1:A:424:PRO:HD3	1.92	0.41
1:A:149:HIS:CE1	2:C:105:TRP:HB2	2.56	0.41
1:A:123:MET:HB2	2:C:168:ARG:HD3	2.01	0.41
2:C:228:ARG:O	2:C:232:GLU:HG3	2.21	0.41
1:B:224:ALA:HB1	1:B:229:ASP:HB3	2.02	0.41
2:C:146:ASN:O	2:C:214:PRO:HG3	2.20	0.41
1:A:354:TRP:N	1:A:355:PRO:CD	2.84	0.41
2:C:122:ARG:HG3	6:C:9010:2BM:BR2	2.75	0.41
2:C:304:GLY:HA3	7:C:9088:HOH:O	2.19	0.41
3:F:98:MET:HG3	3:F:138:ARG:CG	2.49	0.41
1:B:273:ASN:ND2	3:F:148:TYR:OH	2.53	0.41
1:B:216:LEU:HD13	1:B:286:LEU:HD13	2.03	0.41
1:A:246:HIS:N	1:A:246:HIS:CD2	2.88	0.41
3:F:120:PRO:HD3	3:F:128:PHE:CD2	2.56	0.41
2:C:269:ALA:N	2:C:270:PRO:CD	2.84	0.41
2:D:138:PRO:HA	2:D:141:ARG:HH12	1.83	0.41
2:C:239:PHE:O	3:E:129:LEU:HD12	2.21	0.41
1:B:125:TRP:CD1	1:B:125:TRP:C	2.94	0.41
3:E:22:LEU:O	3:E:63:LYS:HE2	2.21	0.41
3:F:90:VAL:HG11	3:F:118:TYR:CZ	2.56	0.41
1:B:52:MET:HE3	1:B:127:SER:HB3	2.03	0.41
2:C:98:HIS:HD2	2:C:297:ASP:OD1	2.04	0.41
1:B:260:ASP:OD2	1:B:262:ALA:HB3	2.20	0.41
1:A:195:GLY:HA2	7:C:9044:HOH:O	2.20	0.41
2:D:253:ASP:OD1	2:D:257:GLY:HA3	2.21	0.41
1:B:69:ARG:HH11	1:B:69:ARG:HG2	1.85	0.41
1:A:33:GLN:HA	1:A:131:ALA:HB3	2.03	0.41
3:E:125:VAL:HG23	3:E:126:ASN:N	2.36	0.40
1:B:452:TRP:O	1:B:456:MET:HG3	2.21	0.40
1:B:490:SER:OG	2:D:32:ASN:HB2	2.21	0.40
1:B:115:TYR:OH	2:D:173:ASP:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:99:ARG:O	2:C:101:PRO:HD3	2.21	0.40
2:C:336:MET:CE	2:C:388:LEU:HG	2.51	0.40
1:B:184:MET:HE2	1:B:188:PHE:HB2	2.02	0.40
3:F:38:ASP:OD1	3:F:45:ASN:OD1	2.39	0.40
1:A:186:ARG:HD3	1:A:186:ARG:O	2.21	0.40
3:F:123:MET:HG2	3:F:124:PRO:CD	2.52	0.40
2:C:168:ARG:CG	2:C:168:ARG:HH11	2.34	0.40
1:A:116:ASN:CG	1:A:189:SER:HA	2.42	0.40
1:A:473:TYR:HB3	1:A:519:PHE:CD1	2.57	0.40
7:A:9016:HOH:O	3:E:144:ASN:HB3	2.21	0.40
2:D:13:ASP:HA	2:D:14:PRO:HD3	1.96	0.40
2:C:275:ASN:HB2	7:C:9011:HOH:O	2.21	0.40
1:A:421:SER:O	1:A:422:GLN:HB2	2.21	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	509/527 (97%)	487 (96%)	21 (4%)	1 (0%)	52	53
1	B	508/527 (96%)	475 (94%)	31 (6%)	2 (0%)	39	37
2	C	386/389 (99%)	376 (97%)	8 (2%)	2 (0%)	34	30
2	D	386/389 (99%)	364 (94%)	18 (5%)	4 (1%)	19	13
3	E	165/170 (97%)	163 (99%)	2 (1%)	0	100	100
3	F	166/170 (98%)	158 (95%)	7 (4%)	1 (1%)	30	24
All	All	2120/2172 (98%)	2023 (95%)	87 (4%)	10 (0%)	34	30

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	340	TYR
1	B	40	LYS
2	D	205	PRO
2	D	374	LYS
2	D	64	ALA
2	C	64	ALA
1	B	284	PRO
2	C	251	VAL
3	F	122	ILE
2	D	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	433/442 (98%)	422 (98%)	11 (2%)	55	59
1	B	432/442 (98%)	422 (98%)	10 (2%)	58	62
2	C	322/323 (100%)	314 (98%)	8 (2%)	55	59
2	D	321/323 (99%)	314 (98%)	7 (2%)	60	64
3	E	145/147 (99%)	143 (99%)	2 (1%)	74	80
3	F	146/147 (99%)	142 (97%)	4 (3%)	52	56
All	All	1799/1824 (99%)	1757 (98%)	42 (2%)	58	62

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ARG
1	A	43	ARG
1	A	90	ASN
1	A	112	VAL
1	A	125	TRP
1	A	186	ARG
1	A	188	PHE
1	A	391	ARG
1	A	412	ASN

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Mol	Chain	Res	Type
1	A	437	ARG
1	A	467	GLN
1	B	26	GLN
1	B	30	ARG
1	B	43	ARG
1	B	90	ASN
1	B	112	VAL
1	B	125	TRP
1	B	186	ARG
1	B	279	GLN
1	B	310	TYR
1	B	403	ILE
2	C	33	ASN
2	C	35	MET
2	C	80	ARG
2	C	117	TRP
2	C	153	LEU
2	C	160	PHE
2	C	168	ARG
2	C	173	ASP
2	D	4	LEU
2	D	35	MET
2	D	80	ARG
2	D	153	LEU
2	D	173	ASP
2	D	205	PRO
2	D	266	GLN
3	E	44	ARG
3	E	60	LEU
3	F	11	THR
3	F	41	THR
3	F	44	ARG
3	F	164	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

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

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Mol	Chain	Res	Type
1	A	116	ASN
1	A	168	HIS
1	A	214	ASN
1	A	227	ASN
1	A	249	ASN
1	A	252	GLN
1	A	268	ASN
1	A	273	ASN
1	A	278	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	36	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
1	B	451	GLN
1	B	516	ASN
1	B	527	ASN
2	C	33	ASN
2	C	98	HIS
2	C	146	ASN

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Mol	Chain	Res	Type
2	C	161	ASN
2	C	285	GLN
2	C	379	GLN
2	D	98	HIS
2	D	155	ASN
2	D	161	ASN
2	D	266	GLN
2	D	285	GLN
2	D	301	ASN
3	E	45	ASN
3	E	144	ASN
3	E	165	HIS
3	F	7	HIS
3	F	39	HIS
3	F	45	ASN
3	F	99	ASN
3	F	144	ASN
3	F	158	GLN
3	F	167	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 17 ligands modelled in this entry, 7 are monoatomic - leaving 10 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	2BM	A	9006	-	2,2,2	0.18	0	1,1,1	0.72	0
6	2BM	A	9007	-	2,2,2	0.12	0	1,1,1	0.45	0
6	2BM	A	9008	-	2,2,2	0.04	0	1,1,1	0.04	0
6	2BM	B	9001	-	2,2,2	0.16	0	1,1,1	0.44	0
6	2BM	B	9002	-	2,2,2	0.03	0	1,1,1	0.06	0
6	2BM	B	9003	-	2,2,2	0.13	0	1,1,1	0.25	0
6	2BM	C	9005	-	2,2,2	0.09	0	1,1,1	0.35	0
6	2BM	C	9009	-	2,2,2	0.06	0	1,1,1	0.26	0
6	2BM	C	9010	-	2,2,2	0.04	0	1,1,1	0.15	0
6	2BM	D	9004	-	2,2,2	0.02	0	1,1,1	0.02	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
6	2BM	A	9006	-	-	0/0/0/0	0/0/0/0
6	2BM	A	9007	-	-	0/0/0/0	0/0/0/0
6	2BM	A	9008	-	-	0/0/0/0	0/0/0/0
6	2BM	B	9001	-	-	0/0/0/0	0/0/0/0
6	2BM	B	9002	-	-	0/0/0/0	0/0/0/0
6	2BM	B	9003	-	-	0/0/0/0	0/0/0/0
6	2BM	C	9005	-	-	0/0/0/0	0/0/0/0
6	2BM	C	9009	-	-	0/0/0/0	0/0/0/0
6	2BM	C	9010	-	-	0/0/0/0	0/0/0/0
6	2BM	D	9004	-	-	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.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	9007	2BM	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	9008	2BM	1	0
6	B	9002	2BM	2	0
6	C	9010	2BM	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	511/527 (96%)	-0.28	6 (1%)	81	85	11, 27, 47, 64	0
1	B	510/527 (96%)	-0.31	7 (1%)	78	82	15, 27, 44, 60	0
2	C	388/389 (99%)	-0.56	4 (1%)	84	87	12, 19, 33, 53	0
2	D	388/389 (99%)	-0.11	8 (2%)	67	72	15, 30, 51, 68	0
3	E	167/170 (98%)	-0.40	3 (1%)	71	76	14, 23, 38, 68	0
3	F	168/170 (98%)	0.34	9 (5%)	29	38	27, 39, 55, 67	0
All	All	2132/2172 (98%)	-0.27	37 (1%)	73	78	11, 26, 48, 68	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	169	PRO	4.6
1	A	316	ILE	4.4
3	E	4	LEU	3.6
3	F	4(A)	LEU	3.5
1	A	19	ALA	3.4
2	C	6	GLU	3.2
1	B	527	ASN	3.2
1	A	17	ASN	3.0
3	F	170	HIS	2.9
1	A	310	TYR	2.9
3	E	168	SER	2.7
2	C	45	ARG	2.7
1	A	244	LEU	2.6
1	B	316	ILE	2.6
3	F	21	GLN	2.5
2	C	2	SER	2.5
3	F	3	LYS	2.5
3	F	151	PRO	2.4
2	D	389	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
2	D	44	LYS	2.4
2	D	45	ARG	2.3
3	F	69	ALA	2.2
3	F	27	LYS	2.2
2	D	352	ILE	2.2
1	B	516	ASN	2.2
3	F	23	ASN	2.2
1	A	320	ARG	2.1
1	B	320	ARG	2.1
2	D	2	SER	2.1
1	B	259	ASN	2.1
1	B	40	LYS	2.1
1	B	323	LYS	2.1
2	C	44	LYS	2.1
2	D	220	ASN	2.1
3	F	70	ARG	2.1
2	D	344	ALA	2.0
2	D	205	PRO	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
6	2BM	C	9010	3/3	0.90	0.15	1.34	38,38,40,42	3
6	2BM	C	9009	3/3	0.97	0.07	-0.54	34,34,37,38	3
6	2BM	B	9001	3/3	0.99	0.07	-1.81	25,25,29,34	3

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
6	2BM	C	9005	3/3	0.99	0.04	-2.03	28,28,29,32	3
6	2BM	A	9008	3/3	0.99	0.06	-2.31	28,28,29,30	3
6	2BM	D	9004	3/3	0.99	0.06	-2.54	28,28,33,34	3
4	FE	A	5002	1/1	0.98	0.05	-3.09	36,36,36,36	0
6	2BM	A	9006	3/3	0.99	0.04	-3.17	29,29,29,30	0
4	FE	A	5001	1/1	1.00	0.03	-3.21	27,27,27,27	0
6	2BM	A	9007	3/3	1.00	0.04	-3.28	30,30,33,35	3
5	CA	A	5005	1/1	0.98	0.04	-3.97	35,35,35,35	0
6	2BM	B	9003	3/3	1.00	0.04	-4.25	27,27,28,33	0
4	FE	B	5003	1/1	1.00	0.05	-4.87	25,25,25,25	0
6	2BM	B	9002	3/3	0.99	0.04	-5.62	27,27,29,33	3
4	FE	B	5004	1/1	0.99	0.03	-7.49	33,33,33,33	0
5	CA	C	5006	1/1	0.98	0.09	-	50,50,50,50	0
5	CA	C	5007	1/1	0.94	0.05	-	49,49,49,49	0

6.5 Other polymers (i)

There are no such residues in this entry.