



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2017 – 07:47 AM EDT

PDB ID : 1XMF
Title : Structure of Mn(II)-Soaked Apo Methane Monooxygenase Hydroxylase Crystals from *M. capsulatus* (Bath)
Authors : Sazinsky, M.H.; Merckx, M.; Cadieux, E.; Tang, S.; Lippard, S.J.
Deposited on : unknown
Resolution : 2.32 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
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	rb-20030345

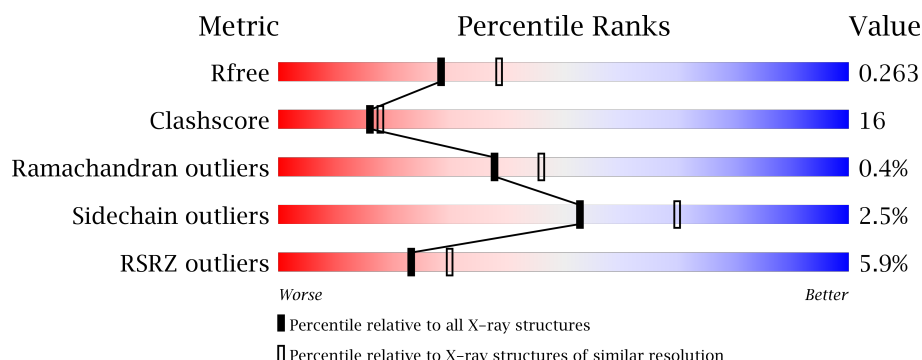
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.32 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}	100719	4787 (2.34-2.30)
Clashscore	112137	5439 (2.34-2.30)
Ramachandran outliers	110173	5386 (2.34-2.30)
Sidechain outliers	110143	5385 (2.34-2.30)
RSRZ outliers	101464	4814 (2.34-2.30)

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>7%</div> <div>61%</div> <div>33%</div> <div>..</div> </div>
1	B	527	<div> <div>6%</div> <div>63%</div> <div>32%</div> <div>..</div> </div>
2	C	388	<div> <div>%</div> <div>75%</div> <div>24%</div> <div>.</div> </div>
2	D	388	<div> <div>9%</div> <div>72%</div> <div>27%</div> <div>.</div> </div>
3	E	169	<div> <div>%</div> <div>78%</div> <div>20%</div> <div>..</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	169	<div><div></div><div>7%</div><div>76%</div><div>22%</div><div>..</div></div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 18436 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
			3167	2038	545	576	8			
2	D	388	Total	C	N	O	S	0	0	0
			3151	2028	543	572	8			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	18	GLU	ALA	CONFLICT	UNP P18798
C	370	ARG	ALA	CONFLICT	UNP P18798
D	18	GLU	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
			1364	864	245	250	5			
3	F	166	Total	C	N	O	S	0	0	0
			1358	860	243	250	5			

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	Ca 1	0	0
5	C	3	Total 3	Ca 3	0	0

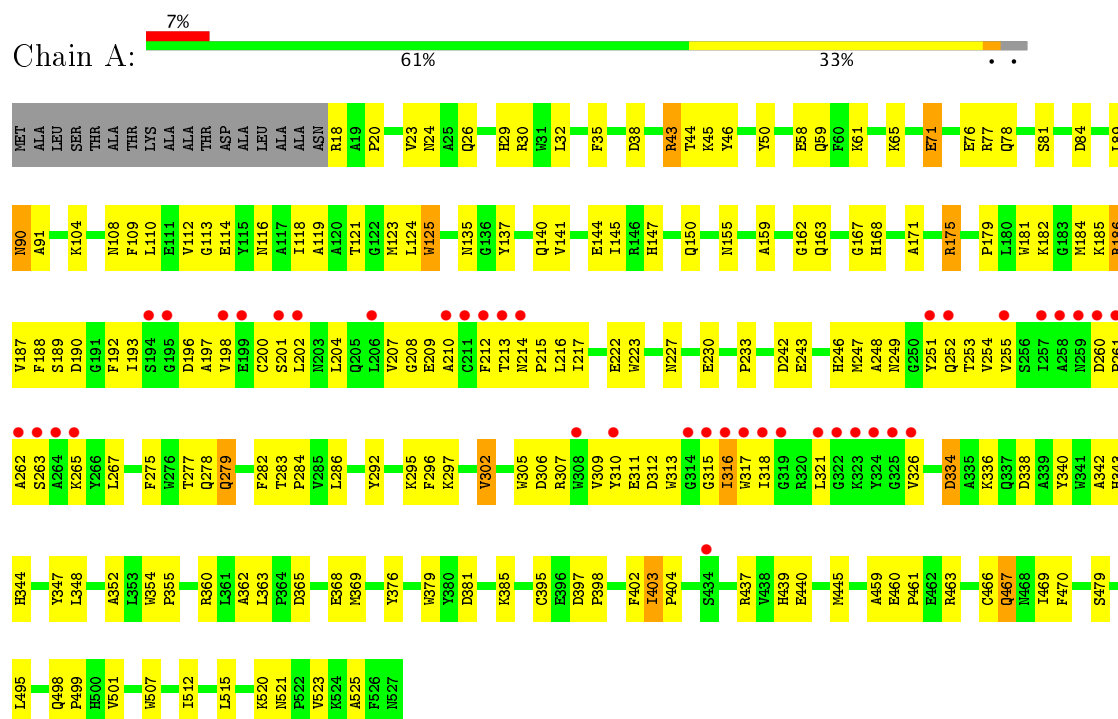
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	235	Total 235	O 235	0	0
6	B	212	Total 212	O 212	0	0
6	C	290	Total 290	O 290	0	0
6	D	150	Total 150	O 150	0	0
6	E	156	Total 156	O 156	0	0
6	F	70	Total 70	O 70	0	0

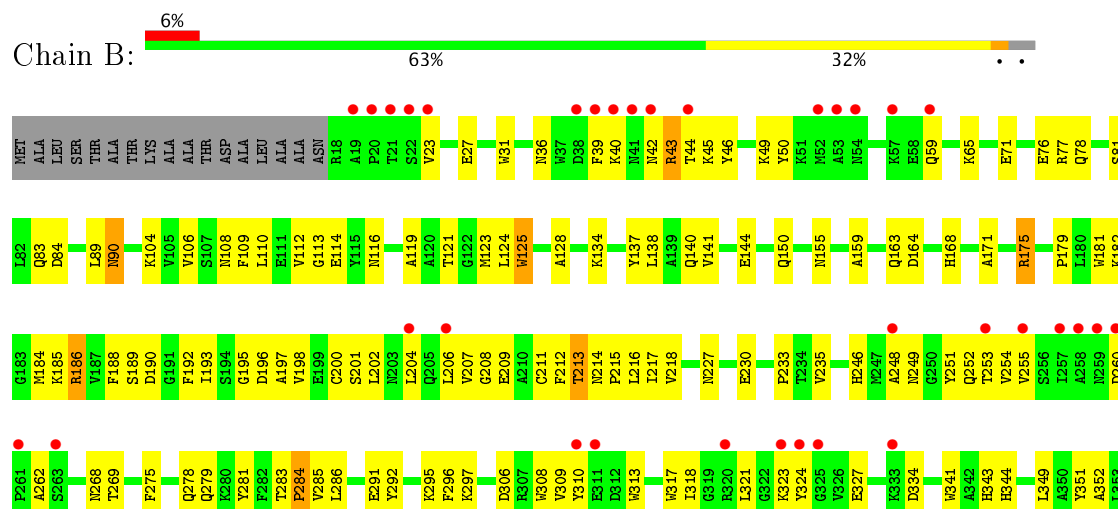
3 Residue-property plots

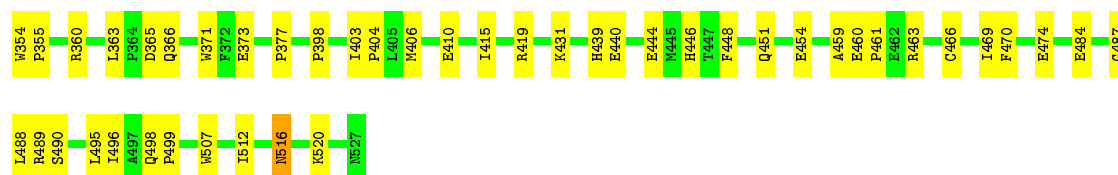
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

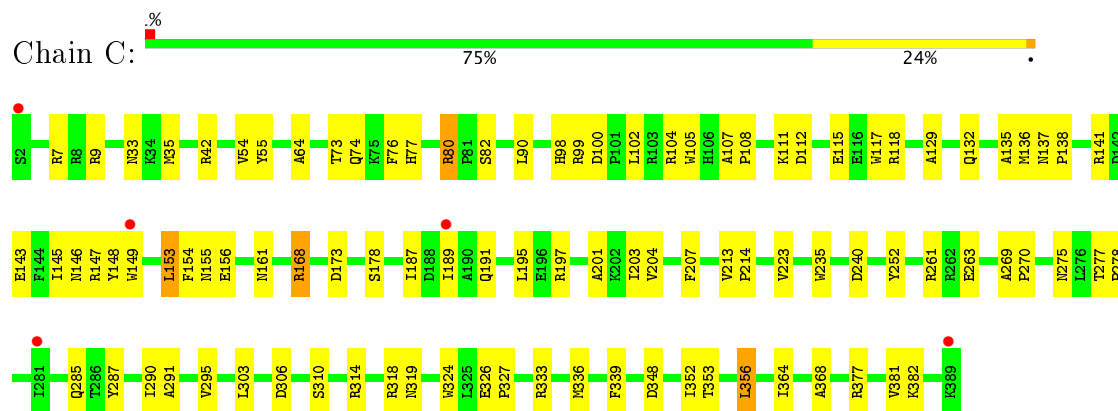


- Molecule 1: Methane monooxygenase component A alpha chain

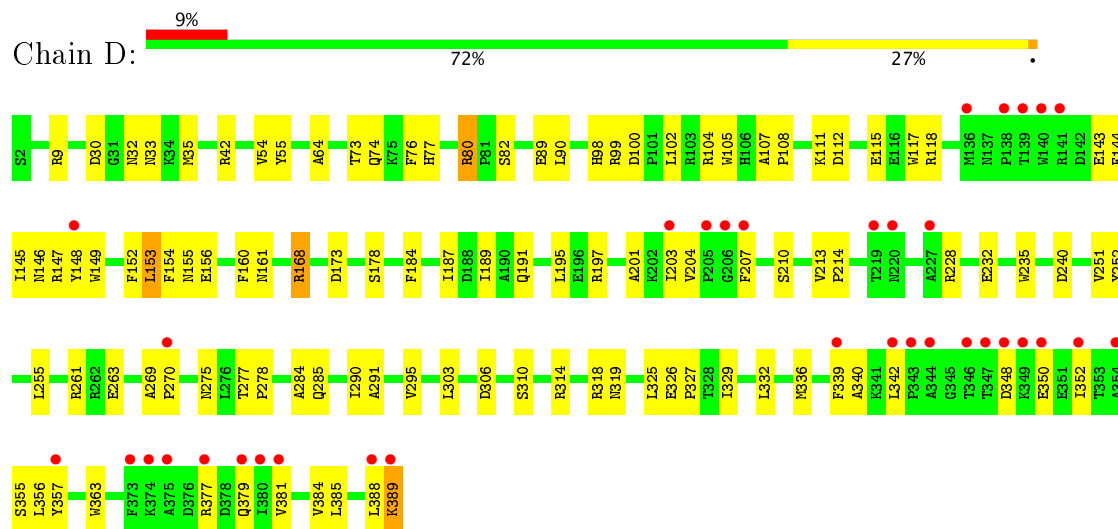




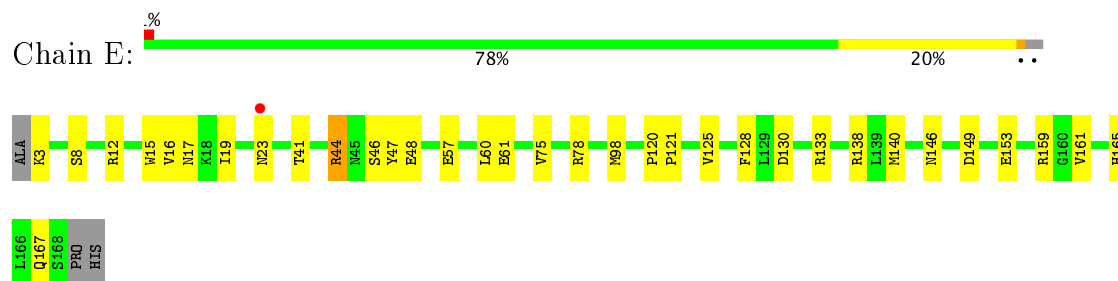
• Molecule 2: Methane monooxygenase component A beta chain



• Molecule 2: Methane monooxygenase component A beta chain

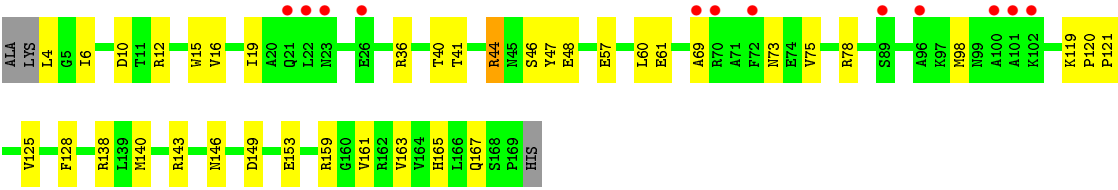


• Molecule 3: Methane monooxygenase component A gamma chain



• 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	70.82Å 171.68Å 220.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.76 – 2.32 28.76 – 2.15	Depositor EDS
% Data completeness (in resolution range)	84.3 (28.76-2.32) 80.3 (28.76-2.15)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.84 (at 2.16Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.219 , 0.263 0.218 , 0.263	Depositor DCC
R_{free} test set	3543 reflections (3.59%)	DCC
Wilson B-factor (Å ²)	31.9	Xtriage
Anisotropy	0.327	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	18436	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.35% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.36	0/4263	0.61	3/5797 (0.1%)
1	B	0.36	0/4262	0.61	3/5796 (0.1%)
2	C	0.36	0/3263	0.55	0/4435
2	D	0.37	0/3247	0.55	0/4417
3	E	0.34	0/1392	0.56	0/1876
3	F	0.35	0/1387	0.56	0/1873
All	All	0.36	0/17814	0.58	6/24194 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	77	ARG	NE-CZ-NH2	-13.35	113.62	120.30
1	B	77	ARG	NE-CZ-NH1	13.04	126.82	120.30
1	A	77	ARG	NE-CZ-NH1	-12.20	114.20	120.30
1	A	77	ARG	NE-CZ-NH2	11.92	126.26	120.30
1	B	77	ARG	CD-NE-CZ	6.55	132.77	123.60
1	A	77	ARG	CD-NE-CZ	6.06	132.08	123.60

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	4138	0	3897	179	0
1	B	4137	0	3888	169	0
2	C	3167	0	2987	99	0
2	D	3151	0	2957	105	0
3	E	1364	0	1352	34	0
3	F	1358	0	1335	40	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	1	0	0	0	0
5	C	3	0	0	0	0
6	A	235	0	0	9	0
6	B	212	0	0	11	0
6	C	290	0	0	14	0
6	D	150	0	0	7	0
6	E	156	0	0	6	0
6	F	70	0	0	2	0
All	All	18436	0	16416	548	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 16.

All (548) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:340:ALA:HB2	2:D:389:LYS:HB2	1.31	1.06
2:C:270:PRO:HB3	2:D:270:PRO:HB3	1.46	0.95
1:B:44:THR:HG22	1:B:46:TYR:H	1.33	0.93
1:B:209:GLU:HA	1:B:213:THR:HB	1.51	0.93
1:A:44:THR:HG22	1:A:46:TYR:H	1.34	0.92
1:A:78:GLN:HE22	1:A:150:GLN:HE21	1.12	0.91
1:A:403:ILE:HD13	1:A:515:LEU:HD11	1.51	0.90
1:A:352:ALA:HA	1:A:404:PRO:HB2	1.55	0.88
1:A:209:GLU:HA	1:A:213:THR:HB	1.55	0.88
2:D:102:LEU:HD12	2:D:290:ILE:HG23	1.56	0.87
2:C:102:LEU:HD12	2:C:290:ILE:HG23	1.57	0.87
1:B:78:GLN:HE22	1:B:150:GLN:HE21	1.21	0.86
1:B:283:THR:HB	1:B:284:PRO:HD3	1.59	0.84
1:B:59:GLN:NE2	1:B:248:ALA:HB1	1.92	0.83
2:D:261:ARG:HE	2:D:285:GLN:HE22	1.26	0.82
1:A:185:LYS:O	1:A:189:SER:HB2	1.80	0.81
1:A:216:LEU:HD13	1:A:286:LEU:HD13	1.63	0.80
2:C:261:ARG:HE	2:C:285:GLN:HE22	1.24	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:GLU:HG2	1:B:76:GLU:HG2	1.64	0.80
1:B:352:ALA:HA	1:B:404:PRO:HB2	1.62	0.80
1:A:292:TYR:OH	1:A:344:HIS:HD2	1.65	0.79
1:B:268:ASN:HD21	1:B:327:GLU:H	1.28	0.79
1:B:185:LYS:O	1:B:189:SER:HB2	1.83	0.79
3:E:48:GLU:HB3	6:E:229:HOH:O	1.81	0.78
1:A:227:ASN:HD21	1:A:295:LYS:H	1.31	0.78
2:C:102:LEU:CD1	2:C:290:ILE:HG23	2.13	0.78
1:A:59:GLN:NE2	1:A:248:ALA:HB1	1.99	0.77
2:D:102:LEU:CD1	2:D:290:ILE:HG23	2.16	0.76
2:D:76:PHE:HZ	2:D:168:ARG:HH12	1.35	0.74
1:B:227:ASN:HD21	1:B:295:LYS:H	1.35	0.74
1:A:190:ASP:HB3	2:C:74:GLN:O	1.88	0.74
2:C:76:PHE:HZ	2:C:168:ARG:HH12	1.36	0.74
3:F:41:THR:O	3:F:44:ARG:HD2	1.88	0.72
1:A:196:ASP:HB2	3:E:140:MET:SD	2.30	0.72
2:D:385:LEU:O	2:D:388:LEU:HB2	1.89	0.72
1:A:113:GLY:HA2	1:A:188:PHE:HB3	1.72	0.71
3:E:41:THR:O	3:E:44:ARG:HD2	1.90	0.71
1:A:108:ASN:HD21	1:A:175:ARG:HE	1.37	0.71
1:A:198:VAL:O	1:A:202:LEU:HG	1.90	0.71
1:A:495:LEU:HD11	1:A:512:ILE:HG13	1.72	0.71
1:B:198:VAL:O	1:B:202:LEU:HG	1.90	0.71
1:B:439:HIS:HD2	3:F:163:VAL:HA	1.55	0.70
2:D:389:LYS:HD2	2:D:389:LYS:OXT	1.91	0.70
2:D:388:LEU:HD23	2:D:389:LYS:HG3	1.75	0.69
3:F:98:MET:HG3	3:F:138:ARG:HG2	1.74	0.69
1:B:108:ASN:HD21	1:B:175:ARG:HE	1.40	0.69
1:A:175:ARG:HG3	1:A:181:TRP:CD2	2.28	0.69
1:A:439:HIS:HB3	3:E:161:VAL:HG21	1.75	0.69
1:B:179:PRO:HB3	1:B:469:ILE:HD13	1.74	0.69
2:D:107:ALA:HB3	2:D:108:PRO:HD3	1.75	0.69
1:A:192:PHE:O	1:A:200:CYS:HB3	1.92	0.69
1:B:192:PHE:O	1:B:200:CYS:HB3	1.94	0.68
1:B:175:ARG:HG3	1:B:181:TRP:CD2	2.28	0.68
3:F:4:LEU:HB3	6:F:226:HOH:O	1.92	0.68
1:B:190:ASP:HB3	2:D:74:GLN:O	1.94	0.67
2:C:107:ALA:HB3	2:C:108:PRO:HD3	1.76	0.67
1:B:213:THR:O	1:B:217:ILE:HG12	1.94	0.67
1:B:439:HIS:HB3	3:F:161:VAL:HG21	1.77	0.66
3:E:98:MET:HG3	3:E:138:ARG:HG2	1.77	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:TYR:O	1:B:284:PRO:HD2	1.95	0.66
1:B:45:LYS:HE3	6:D:497:HOH:O	1.94	0.66
1:B:309:VAL:O	1:B:309:VAL:HG12	1.95	0.66
1:A:24:ASN:OD1	1:A:26:GLN:HG2	1.96	0.66
1:A:284:PRO:HB3	1:A:342:ALA:HB1	1.78	0.66
1:A:78:GLN:NE2	1:A:150:GLN:HE21	1.89	0.66
1:A:227:ASN:ND2	1:A:295:LYS:H	1.93	0.65
1:B:406:MET:O	1:B:410:GLU:HG3	1.97	0.65
1:B:360:ARG:HG2	1:B:498:GLN:HB2	1.79	0.65
1:B:214:ASN:HB2	1:B:215:PRO:HD3	1.79	0.65
1:B:306:ASP:O	1:B:310:TYR:HB2	1.97	0.65
2:C:333:ARG:HD3	6:C:5134:HOH:O	1.97	0.65
3:E:19:ILE:HG12	3:E:60:LEU:HD13	1.78	0.64
1:A:213:THR:O	1:A:217:ILE:HG12	1.96	0.64
3:F:57:GLU:O	3:F:61:GLU:HG3	1.98	0.64
1:B:439:HIS:HB3	3:F:161:VAL:CG2	2.27	0.64
2:C:333:ARG:HD2	6:C:5040:HOH:O	1.98	0.64
2:C:80:ARG:HB2	6:E:174:HOH:O	1.99	0.63
1:A:116:ASN:CG	1:A:189:SER:HA	2.19	0.62
1:A:18:ARG:O	2:C:129:ALA:HA	1.99	0.62
2:D:269:ALA:HB3	2:D:270:PRO:HD3	1.81	0.62
1:A:467:GLN:HG3	6:A:5123:HOH:O	1.98	0.62
1:B:113:GLY:HA2	1:B:188:PHE:HB3	1.80	0.62
1:B:206:LEU:HD11	1:B:321:LEU:HD11	1.80	0.62
3:E:12:ARG:O	3:E:16:VAL:HG23	1.99	0.62
1:B:23:VAL:HG13	1:B:27:GLU:OE2	2.00	0.62
2:C:269:ALA:HB3	2:C:270:PRO:HD3	1.79	0.62
1:A:204:LEU:O	1:A:209:GLU:HG3	1.99	0.62
3:F:12:ARG:O	3:F:16:VAL:HG23	2.00	0.62
1:A:193:ILE:HD12	2:C:168:ARG:HH21	1.63	0.61
1:A:140:GLN:HG3	1:A:246:HIS:CE1	2.36	0.61
1:B:254:VAL:HG11	1:B:321:LEU:HD22	1.83	0.61
2:C:201:ALA:HA	2:C:207:PHE:HB3	1.82	0.61
2:C:100:ASP:OD1	2:C:104:ARG:NH1	2.34	0.61
3:F:4:LEU:HD21	3:F:10:ASP:CG	2.21	0.61
1:B:196:ASP:HB2	3:F:140:MET:SD	2.41	0.60
1:B:398:PRO:HG3	1:B:507:TRP:CD1	2.37	0.60
1:B:50:TYR:CG	1:B:198:VAL:HG21	2.35	0.60
1:B:292:TYR:OH	1:B:344:HIS:HD2	1.83	0.60
1:B:489:ARG:NH1	1:B:496:ILE:HA	2.16	0.60
1:A:302:VAL:HG13	1:A:376:TYR:HE2	1.66	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:THR:HG21	1:B:140:GLN:HG2	1.82	0.60
2:D:263:GLU:HB3	2:D:355:SER:HB2	1.83	0.60
2:C:348:ASP:O	2:C:352:ILE:HG12	2.02	0.60
2:D:201:ALA:HA	2:D:207:PHE:HB3	1.83	0.60
2:D:213:VAL:HG23	6:D:397:HOH:O	2.01	0.60
1:A:23:VAL:HB	2:C:195:LEU:CD1	2.32	0.60
1:B:140:GLN:O	1:B:144:GLU:HG2	2.01	0.60
2:D:350:GLU:HG2	6:D:432:HOH:O	2.01	0.60
1:A:121:THR:HG21	1:A:140:GLN:HG2	1.82	0.60
2:C:261:ARG:HE	2:C:285:GLN:NE2	1.99	0.60
1:B:193:ILE:HD12	2:D:168:ARG:HH21	1.67	0.59
2:D:340:ALA:HB2	2:D:389:LYS:CB	2.20	0.59
2:D:348:ASP:O	2:D:352:ILE:HG12	2.02	0.59
1:A:140:GLN:O	1:A:144:GLU:HG2	2.03	0.59
1:B:140:GLN:HG3	1:B:246:HIS:CE1	2.37	0.59
2:D:100:ASP:OD1	2:D:104:ARG:NH1	2.35	0.59
1:B:291:GLU:OE1	1:B:343:HIS:HE1	1.86	0.59
2:D:111:LYS:O	2:D:115:GLU:HG3	2.02	0.59
1:B:207:VAL:HG11	1:B:275:PHE:HA	1.84	0.59
1:B:39:PHE:CE2	2:D:232:GLU:HG2	2.38	0.59
1:A:214:ASN:HB2	1:A:215:PRO:HD3	1.84	0.58
2:C:213:VAL:HG23	6:C:5035:HOH:O	2.03	0.58
1:A:171:ALA:O	1:A:175:ARG:HB3	2.03	0.58
1:B:171:ALA:O	1:B:175:ARG:HB3	2.04	0.58
1:A:186:ARG:HD3	1:A:186:ARG:O	2.03	0.58
1:A:313:TRP:HA	1:A:317:TRP:HB3	1.85	0.58
1:B:163:GLN:HG2	6:B:5034:HOH:O	2.01	0.58
1:A:279:GLN:HG2	1:A:283:THR:OG1	2.04	0.58
2:D:332:LEU:HB3	2:D:384:VAL:HG13	1.86	0.58
2:C:111:LYS:O	2:C:115:GLU:HG3	2.03	0.58
1:A:23:VAL:HB	2:C:195:LEU:HD11	1.85	0.58
2:D:187:ILE:O	2:D:191:GLN:HG3	2.04	0.57
1:B:255:VAL:HG22	1:B:324:TYR:CE2	2.39	0.57
2:D:9:ARG:NH2	6:D:487:HOH:O	2.37	0.57
1:B:186:ARG:HD3	1:B:186:ARG:O	2.04	0.57
2:D:143:GLU:O	2:D:147:ARG:HB3	2.05	0.57
1:A:439:HIS:HB3	3:E:161:VAL:CG2	2.34	0.57
3:E:57:GLU:O	3:E:61:GLU:HG3	2.04	0.57
3:F:61:GLU:HB3	3:F:121:PRO:HD3	1.87	0.57
3:F:165:HIS:CE1	3:F:167:GLN:HE21	2.23	0.57
1:A:262:ALA:HA	1:A:265:LYS:NZ	2.20	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:135:ALA:HB3	6:C:5268:HOH:O	2.05	0.57
2:C:104:ARG:NE	6:C:5234:HOH:O	2.38	0.56
1:A:460:GLU:HB3	1:A:463:ARG:HG3	1.87	0.56
1:A:305:TRP:CH2	1:A:336:LYS:HA	2.40	0.56
3:E:17:ASN:HB3	6:E:194:HOH:O	2.04	0.56
1:A:398:PRO:HG3	1:A:507:TRP:CD1	2.41	0.56
1:A:230:GLU:HG3	1:B:89:LEU:HD21	1.86	0.56
1:A:113:GLY:CA	1:A:188:PHE:HB3	2.36	0.56
1:A:89:LEU:HD21	1:B:230:GLU:HG3	1.88	0.56
1:B:78:GLN:NE2	1:B:150:GLN:HE21	1.98	0.56
1:B:201:SER:OG	1:B:253:THR:HG21	2.05	0.56
1:B:269:THR:HB	6:B:5192:HOH:O	2.05	0.56
2:C:143:GLU:O	2:C:147:ARG:HB3	2.06	0.56
2:D:261:ARG:HE	2:D:285:GLN:NE2	2.00	0.56
1:A:50:TYR:CG	1:A:198:VAL:HG21	2.41	0.56
3:F:19:ILE:HG12	3:F:60:LEU:HD13	1.87	0.56
1:A:208:GLY:HA2	1:A:278:GLN:HE21	1.70	0.55
1:A:182:LYS:O	2:C:73:THR:HG21	2.06	0.55
2:D:153:LEU:HD12	2:D:153:LEU:C	2.26	0.55
1:A:76:GLU:OE2	1:B:76:GLU:HG2	2.06	0.55
2:C:339:PHE:CE2	2:C:352:ILE:HD12	2.41	0.55
1:A:186:ARG:HA	2:C:73:THR:OG1	2.07	0.55
1:A:227:ASN:HD21	1:A:295:LYS:N	2.04	0.55
1:A:18:ARG:HG2	2:C:129:ALA:O	2.06	0.55
2:D:102:LEU:HD11	2:D:290:ILE:HG12	1.89	0.55
2:D:332:LEU:HB3	2:D:384:VAL:CG1	2.37	0.55
3:E:19:ILE:HG12	3:E:60:LEU:CD1	2.37	0.55
3:F:165:HIS:HE1	3:F:167:GLN:HG3	1.71	0.55
2:C:270:PRO:HB3	2:D:270:PRO:CB	2.30	0.54
1:B:466:CYS:HB2	2:D:73:THR:HA	1.89	0.54
3:E:165:HIS:CE1	3:E:167:GLN:HE21	2.25	0.54
1:A:306:ASP:O	1:A:310:TYR:HB2	2.08	0.54
1:B:520:LYS:HD2	6:B:5190:HOH:O	2.07	0.54
1:A:18:ARG:N	6:A:5188:HOH:O	2.39	0.54
1:A:193:ILE:HB	2:C:168:ARG:CZ	2.37	0.54
2:C:318:ARG:HD2	6:C:5165:HOH:O	2.07	0.54
1:A:403:ILE:HD13	1:A:515:LEU:CD1	2.32	0.54
1:B:495:LEU:HD11	1:B:512:ILE:HG13	1.89	0.54
1:B:211:CYS:HB2	1:B:313:TRP:CD1	2.43	0.54
3:E:3:LYS:N	6:E:300:HOH:O	2.40	0.54
1:A:124:LEU:HD21	1:A:201:SER:HB2	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:TRP:CH2	2:D:210:SER:HA	2.42	0.54
1:B:489:ARG:NH1	1:B:496:ILE:O	2.41	0.53
3:E:165:HIS:HE1	3:E:167:GLN:HG3	1.73	0.53
1:A:302:VAL:CG1	1:A:340:TYR:HA	2.39	0.53
2:C:54:VAL:HG12	2:C:55:TYR:CD2	2.43	0.53
1:B:207:VAL:HG22	1:B:313:TRP:CZ2	2.43	0.53
2:C:306:ASP:O	2:C:310:SER:HB2	2.08	0.53
2:D:291:ALA:O	2:D:295:VAL:HG23	2.09	0.53
2:D:275:ASN:C	2:D:278:PRO:HD2	2.28	0.53
3:F:165:HIS:CE1	3:F:167:GLN:HG3	2.44	0.53
1:A:29:HIS:CD2	1:A:61:LYS:HA	2.43	0.53
1:B:488:LEU:HB2	6:B:5167:HOH:O	2.08	0.53
1:A:84:ASP:HB3	1:B:81:SER:OG	2.08	0.53
1:A:110:LEU:O	1:A:114:GLU:HG2	2.08	0.53
1:A:354:TRP:CH2	1:A:499:PRO:HD3	2.43	0.53
2:C:326:GLU:HB3	2:C:327:PRO:HD3	1.90	0.53
1:B:268:ASN:ND2	1:B:327:GLU:H	2.01	0.53
2:C:90:LEU:HD13	2:C:303:LEU:HD13	1.90	0.53
6:B:5208:HOH:O	3:F:143:ARG:HG2	2.07	0.53
1:B:193:ILE:HB	2:D:168:ARG:CZ	2.39	0.53
2:C:104:ARG:NH2	6:C:5234:HOH:O	2.39	0.53
1:A:305:TRP:CE2	1:A:309:VAL:HG21	2.44	0.53
1:A:495:LEU:HD11	1:A:512:ILE:CG1	2.38	0.53
1:A:123:MET:HE2	1:A:197:ALA:HB2	1.90	0.53
1:B:208:GLY:HA2	1:B:278:GLN:HE21	1.73	0.53
2:C:54:VAL:O	2:C:55:TYR:HB2	2.09	0.53
1:A:302:VAL:HG11	1:A:340:TYR:CD1	2.44	0.52
1:B:186:ARG:HD3	1:B:186:ARG:C	2.30	0.52
1:A:466:CYS:HB2	2:C:73:THR:HA	1.91	0.52
1:A:207:VAL:HG11	1:A:275:PHE:HA	1.90	0.52
1:B:460:GLU:N	1:B:461:PRO:HD3	2.25	0.52
2:D:54:VAL:HG12	2:D:55:TYR:CD2	2.44	0.52
2:D:153:LEU:HD12	2:D:154:PHE:N	2.23	0.52
2:C:153:LEU:HD12	2:C:153:LEU:C	2.30	0.52
1:A:251:TYR:O	1:A:255:VAL:HG23	2.10	0.52
1:A:312:ASP:HA	1:A:316:ILE:CG2	2.40	0.52
1:B:251:TYR:O	1:B:255:VAL:HG23	2.08	0.52
1:B:459:ALA:C	1:B:461:PRO:HD3	2.30	0.52
1:A:186:ARG:HD3	1:A:186:ARG:C	2.29	0.52
2:D:310:SER:O	2:D:314:ARG:HG3	2.10	0.52
1:A:81:SER:OG	1:B:84:ASP:HB3	2.08	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:GLU:HG2	1:B:76:GLU:OE2	2.10	0.52
1:B:159:ALA:O	2:D:33:ASN:HB2	2.10	0.52
3:E:146:ASN:HB3	3:E:149:ASP:OD2	2.10	0.51
1:A:307:ARG:HG3	1:A:307:ARG:HH11	1.75	0.51
2:C:146:ASN:HD21	2:C:197:ARG:HH21	1.58	0.51
2:D:105:TRP:O	2:D:108:PRO:HD2	2.10	0.51
2:D:306:ASP:O	2:D:310:SER:HB2	2.10	0.51
1:A:243:GLU:O	1:A:247:MET:HG2	2.10	0.51
1:A:292:TYR:OH	1:A:344:HIS:CD2	2.55	0.51
1:B:349:LEU:HD22	1:B:415:ILE:HD13	1.91	0.51
1:B:123:MET:HB2	2:D:168:ARG:HD3	1.92	0.51
2:D:54:VAL:O	2:D:55:TYR:HB2	2.10	0.51
2:C:104:ARG:CZ	6:C:5234:HOH:O	2.57	0.51
2:C:104:ARG:HH11	2:C:104:ARG:HG3	1.75	0.51
3:E:165:HIS:CE1	3:E:167:GLN:HG3	2.45	0.51
1:B:36:ASN:HD21	1:B:42:ASN:HD21	1.58	0.51
2:C:161:ASN:HB3	2:C:235:TRP:CE2	2.45	0.51
2:D:104:ARG:HH11	2:D:104:ARG:HG3	1.74	0.51
2:D:82:SER:O	2:D:168:ARG:NH2	2.43	0.51
1:A:163:GLN:HG2	6:A:5011:HOH:O	2.11	0.51
3:F:4:LEU:CD2	3:F:10:ASP:H	2.24	0.51
1:B:209:GLU:HA	1:B:213:THR:CB	2.34	0.51
1:B:297:LYS:HG2	1:B:371:TRP:CE2	2.45	0.51
3:E:3:LYS:HE2	3:E:8:SER:OG	2.11	0.51
1:A:65:LYS:HD2	2:C:117:TRP:HB2	1.93	0.50
2:C:146:ASN:ND2	2:C:197:ARG:HH21	2.09	0.50
3:E:23:ASN:HB2	6:E:216:HOH:O	2.12	0.50
1:B:50:TYR:CD1	1:B:50:TYR:N	2.79	0.50
2:D:339:PHE:CE2	2:D:352:ILE:HD12	2.46	0.50
1:A:137:TYR:O	1:A:141:VAL:HG23	2.12	0.50
1:A:76:GLU:HG2	1:B:76:GLU:CG	2.39	0.50
2:C:187:ILE:O	2:C:191:GLN:HG3	2.11	0.50
2:D:379:GLN:HB3	6:D:528:HOH:O	2.11	0.50
1:A:155:ASN:HD22	1:A:168:HIS:HD2	1.58	0.50
1:A:222:GLU:OE1	2:C:7:ARG:HD3	2.11	0.50
1:B:260:ASP:OD2	1:B:262:ALA:HB3	2.11	0.50
3:F:46:SER:OG	3:F:48:GLU:HG2	2.10	0.50
1:A:50:TYR:CD1	1:A:50:TYR:N	2.79	0.50
1:B:351:TYR:CE2	1:B:363:LEU:HD21	2.47	0.50
1:A:76:GLU:CG	1:B:76:GLU:HG2	2.37	0.50
3:E:46:SER:OG	3:E:48:GLU:HG2	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:61:GLU:HB3	3:E:121:PRO:HD3	1.94	0.50
1:A:108:ASN:HD21	1:A:175:ARG:NE	2.09	0.50
1:A:297:LYS:HD2	1:A:297:LYS:N	2.27	0.50
2:C:324:TRP:C	2:C:327:PRO:HD2	2.33	0.50
1:A:310:TYR:OH	1:A:336:LYS:HD2	2.10	0.49
1:A:116:ASN:CB	1:A:189:SER:HA	2.42	0.49
2:C:82:SER:O	2:C:168:ARG:NH2	2.44	0.49
1:A:260:ASP:OD2	1:A:262:ALA:HB3	2.13	0.49
1:B:137:TYR:O	1:B:141:VAL:HG23	2.13	0.49
1:B:218:VAL:HG12	6:B:5171:HOH:O	2.13	0.49
2:D:336:MET:HB3	2:D:388:LEU:HA	1.93	0.49
1:A:159:ALA:O	2:C:33:ASN:HB2	2.12	0.49
1:A:381:ASP:HA	1:A:385:LYS:HE2	1.93	0.49
1:B:227:ASN:ND2	1:B:295:LYS:H	2.06	0.49
2:C:153:LEU:HD12	2:C:154:PHE:N	2.28	0.49
2:D:388:LEU:HD23	2:D:389:LYS:N	2.27	0.49
1:A:210:ALA:HA	1:A:247:MET:CE	2.42	0.49
1:A:334:ASP:OD2	1:A:334:ASP:N	2.46	0.49
1:A:440:GLU:HG3	1:A:445:MET:SD	2.53	0.49
1:B:175:ARG:HG3	1:B:181:TRP:CE2	2.48	0.49
2:C:270:PRO:CB	2:D:270:PRO:HB3	2.33	0.49
2:D:90:LEU:HD13	2:D:303:LEU:HD13	1.95	0.49
1:A:369:MET:HG2	1:A:379:TRP:CH2	2.49	0.48
1:A:109:PHE:O	1:A:112:VAL:HG12	2.13	0.48
1:A:175:ARG:HG3	1:A:181:TRP:CE2	2.48	0.48
2:C:105:TRP:O	2:C:108:PRO:HD2	2.13	0.48
2:D:263:GLU:OE2	2:D:263:GLU:HA	2.13	0.48
1:B:439:HIS:HE1	1:B:454:GLU:OE1	1.97	0.48
3:F:165:HIS:HE1	3:F:167:GLN:HE21	1.61	0.48
1:A:216:LEU:HD11	1:A:286:LEU:HD22	1.95	0.48
1:A:354:TRP:CZ3	1:A:499:PRO:HD3	2.48	0.48
1:A:65:LYS:HB3	2:C:117:TRP:CD2	2.49	0.48
2:D:146:ASN:HD21	2:D:197:ARG:HH21	1.60	0.48
1:B:189:SER:O	1:B:193:ILE:HG12	2.14	0.48
1:B:65:LYS:HB3	2:D:117:TRP:CD2	2.48	0.48
2:C:319:ASN:OD1	3:E:78:ARG:HD3	2.13	0.48
1:B:186:ARG:HA	2:D:73:THR:OG1	2.13	0.48
1:B:213:THR:O	1:B:216:LEU:HB3	2.12	0.48
2:D:388:LEU:CD2	2:D:389:LYS:HG3	2.42	0.48
1:B:65:LYS:HB3	2:D:117:TRP:CG	2.48	0.48
2:D:339:PHE:HB2	2:D:389:LYS:HG2	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:GLY:CA	1:B:188:PHE:HB3	2.44	0.48
2:D:213:VAL:HB	2:D:214:PRO:CD	2.44	0.48
2:C:275:ASN:C	2:C:278:PRO:HD2	2.34	0.47
1:A:65:LYS:HB3	2:C:117:TRP:CG	2.49	0.47
1:A:113:GLY:HA3	1:A:188:PHE:CD2	2.50	0.47
1:A:521:ASN:OD1	1:A:523:VAL:HG12	2.15	0.47
1:B:495:LEU:HD11	1:B:512:ILE:CG1	2.45	0.47
3:F:146:ASN:HB3	3:F:149:ASP:OD2	2.15	0.47
1:A:113:GLY:HA3	1:A:188:PHE:HD2	1.79	0.47
1:A:189:SER:O	1:A:193:ILE:HG12	2.14	0.47
1:A:192:PHE:CE2	1:A:204:LEU:HA	2.50	0.47
1:B:216:LEU:HD13	1:B:286:LEU:HD13	1.96	0.47
1:A:184:MET:CE	1:A:188:PHE:HB2	2.45	0.47
3:E:165:HIS:HE1	3:E:167:GLN:HE21	1.63	0.47
1:B:155:ASN:HD22	1:B:168:HIS:HD2	1.61	0.46
1:B:419:ARG:HA	6:B:5157:HOH:O	2.14	0.46
2:D:144:PHE:CZ	2:D:342:LEU:HD23	2.50	0.46
1:A:104:LYS:HG2	1:A:168:HIS:CD2	2.50	0.46
1:B:124:LEU:HD21	1:B:201:SER:HB2	1.96	0.46
2:C:310:SER:O	2:C:314:ARG:HG3	2.15	0.46
1:B:164:ASP:OD1	1:B:489:ARG:NH2	2.49	0.46
1:B:470:PHE:O	1:B:474:GLU:HB2	2.16	0.46
2:C:364:ILE:HA	2:C:368:ALA:HB3	1.96	0.46
1:B:185:LYS:HA	1:B:189:SER:HB2	1.98	0.46
1:B:43:ARG:HD2	1:B:43:ARG:C	2.36	0.46
2:C:118:ARG:NH2	2:D:112:ASP:OD1	2.48	0.46
3:F:44:ARG:HD3	3:F:47:TYR:CZ	2.50	0.46
2:D:381:VAL:O	2:D:385:LEU:HB2	2.16	0.46
3:E:44:ARG:HD3	3:E:47:TYR:CZ	2.51	0.46
1:A:185:LYS:HA	1:A:189:SER:HB2	1.98	0.46
1:B:123:MET:HE2	1:B:197:ALA:HB2	1.97	0.46
2:C:112:ASP:OD1	2:D:118:ARG:NH2	2.49	0.46
2:C:213:VAL:HB	2:C:214:PRO:CD	2.46	0.46
2:C:339:PHE:CZ	2:C:352:ILE:HD12	2.51	0.46
1:B:23:VAL:HB	2:D:195:LEU:HD11	1.98	0.46
2:D:235:TRP:CD1	2:D:235:TRP:C	2.89	0.46
1:A:525:ALA:HA	6:A:5199:HOH:O	2.16	0.46
1:A:162:GLY:HA3	6:A:5007:HOH:O	2.15	0.46
1:B:192:PHE:CE2	1:B:204:LEU:HA	2.51	0.46
2:D:145:ILE:O	2:D:149:TRP:HB3	2.16	0.46
2:D:146:ASN:ND2	2:D:197:ARG:HH21	2.13	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:484:GLU:OE1	3:F:6:ILE:N	2.49	0.46
1:A:188:PHE:CE1	1:A:282:PHE:CE2	3.05	0.45
1:A:227:ASN:HD21	1:A:296:PHE:H	1.63	0.45
1:B:281:TYR:CZ	1:B:285:VAL:HG21	2.50	0.45
2:D:240:ASP:OD1	3:F:125:VAL:HG21	2.17	0.45
3:F:153:GLU:CD	3:F:153:GLU:H	2.19	0.45
1:B:138:LEU:HD22	2:D:160:PHE:CZ	2.52	0.45
2:D:255:LEU:HD21	2:D:363:TRP:CG	2.50	0.45
1:A:43:ARG:C	1:A:43:ARG:HD2	2.36	0.45
1:A:469:ILE:HG13	1:A:470:PHE:N	2.32	0.45
1:B:50:TYR:CD1	1:B:198:VAL:HG21	2.51	0.45
2:C:336:MET:HE1	2:C:356:LEU:HD21	1.98	0.45
1:A:302:VAL:CG1	1:A:376:TYR:HE2	2.29	0.45
1:A:461:PRO:HG2	3:E:159:ARG:CZ	2.47	0.45
2:D:77:HIS:CD2	3:F:140:MET:HG2	2.50	0.45
1:A:316:ILE:HG12	1:A:316:ILE:O	2.16	0.45
1:A:365:ASP:OD2	1:A:365:ASP:C	2.55	0.45
1:A:360:ARG:HG2	1:A:498:GLN:HB2	1.99	0.45
1:B:490:SER:OG	2:D:32:ASN:HB2	2.16	0.45
1:A:186:ARG:HB3	6:A:5035:HOH:O	2.16	0.45
1:A:187:VAL:HG12	1:A:277:THR:HG22	1.98	0.45
1:B:65:LYS:HD2	2:D:117:TRP:HB2	1.99	0.45
3:F:120:PRO:HD3	3:F:128:PHE:CG	2.52	0.45
1:B:108:ASN:HD21	1:B:175:ARG:NE	2.09	0.45
1:B:354:TRP:CG	1:B:355:PRO:HD3	2.52	0.45
2:D:89:GLU:OE2	3:F:125:VAL:HG22	2.17	0.45
2:D:326:GLU:CB	2:D:327:PRO:HD3	2.47	0.45
1:A:32:LEU:HD12	1:A:35:PHE:CD2	2.53	0.44
2:C:102:LEU:HD13	6:C:5267:HOH:O	2.17	0.44
1:A:119:ALA:O	2:C:168:ARG:HD2	2.17	0.44
1:B:78:GLN:HE21	1:B:235:VAL:HA	1.82	0.44
2:D:161:ASN:HB3	2:D:235:TRP:CE2	2.52	0.44
1:A:397:ASP:HA	1:A:398:PRO:HD3	1.83	0.44
1:B:460:GLU:HB3	1:B:463:ARG:HG3	1.99	0.44
1:B:489:ARG:HH11	1:B:496:ILE:HA	1.81	0.44
1:B:31:TRP:CZ2	2:D:210:SER:HA	2.52	0.44
2:D:325:LEU:O	2:D:329:ILE:HG13	2.18	0.44
1:B:182:LYS:O	2:D:73:THR:HG21	2.17	0.44
3:F:19:ILE:HG12	3:F:60:LEU:CD1	2.47	0.44
1:A:230:GLU:C	1:A:233:PRO:HD2	2.38	0.44
1:A:249:ASN:HA	1:A:252:GLN:HG2	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:VAL:HB	2:D:195:LEU:CD1	2.47	0.44
1:A:230:GLU:OE2	2:C:9:ARG:NH1	2.50	0.44
1:A:354:TRP:CG	1:A:355:PRO:HD3	2.53	0.44
2:C:275:ASN:HD21	2:D:270:PRO:HG2	1.82	0.44
1:B:119:ALA:O	2:D:168:ARG:HD2	2.17	0.44
1:A:20:PRO:HG3	2:C:129:ALA:HB2	2.00	0.44
1:B:104:LYS:HG2	1:B:168:HIS:CD2	2.53	0.44
2:C:318:ARG:NH2	6:C:5045:HOH:O	2.51	0.44
2:D:80:ARG:HB2	6:D:390:HOH:O	2.17	0.44
3:F:44:ARG:HG3	3:F:46:SER:O	2.18	0.44
1:A:292:TYR:CD2	1:A:347:TYR:CD2	3.06	0.44
3:E:120:PRO:HD3	3:E:128:PHE:CG	2.53	0.44
1:B:487:GLY:C	1:B:488:LEU:HD12	2.38	0.44
2:C:77:HIS:CD2	3:E:140:MET:HG2	2.52	0.44
1:A:343:HIS:CD2	1:A:343:HIS:H	2.36	0.43
2:C:146:ASN:HD21	2:C:197:ARG:NH2	2.16	0.43
1:A:262:ALA:HA	1:A:265:LYS:HZ3	1.82	0.43
1:B:184:MET:CE	1:B:188:PHE:HB2	2.47	0.43
1:B:444:GLU:HA	1:B:444:GLU:OE2	2.18	0.43
2:D:189:ILE:HD12	2:D:284:ALA:HB2	2.00	0.43
1:A:116:ASN:ND2	1:A:189:SER:HA	2.33	0.43
1:A:263:SER:O	1:A:267:LEU:HB2	2.18	0.43
1:A:283:THR:HB	1:A:284:PRO:CD	2.47	0.43
1:B:185:LYS:CA	1:B:189:SER:HB2	2.49	0.43
1:B:373:GLU:OE2	1:B:377:PRO:HA	2.18	0.43
2:C:235:TRP:CD1	2:C:235:TRP:C	2.90	0.43
1:A:114:GLU:CD	1:A:147:HIS:HB3	2.38	0.43
1:A:58:GLU:OE2	1:A:135:ASN:HB3	2.19	0.43
1:B:249:ASN:HA	1:B:252:GLN:HG2	2.00	0.43
1:B:207:VAL:HG22	1:B:313:TRP:HZ2	1.81	0.43
1:B:106:VAL:O	1:B:110:LEU:HG	2.19	0.43
1:B:516:ASN:ND2	6:B:5139:HOH:O	2.51	0.43
2:D:147:ARG:HD2	2:D:148:TYR:CE1	2.53	0.43
2:D:319:ASN:OD1	3:F:78:ARG:HD3	2.19	0.43
1:B:49:LYS:HD3	3:F:140:MET:HB3	2.01	0.43
3:F:15:TRP:O	3:F:19:ILE:HG13	2.19	0.43
3:F:41:THR:O	3:F:44:ARG:CD	2.64	0.43
3:F:73:ASN:OD1	3:F:75:VAL:HG13	2.18	0.43
1:A:45:LYS:HA	3:E:133:ARG:HD2	2.00	0.43
1:B:116:ASN:CB	1:B:189:SER:HA	2.49	0.43
1:B:341:TRP:CE2	1:B:431:LYS:HD3	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:145:ILE:O	2:C:149:TRP:HB3	2.19	0.43
3:F:36:ARG:CZ	3:F:119:LYS:HB3	2.49	0.43
1:A:185:LYS:CA	1:A:189:SER:HB2	2.48	0.43
2:C:277:THR:HB	2:C:278:PRO:HD3	1.99	0.43
2:C:353:THR:HG21	6:C:5233:HOH:O	2.17	0.43
2:D:152:PHE:O	2:D:155:ASN:HB3	2.19	0.43
1:B:230:GLU:C	1:B:233:PRO:HD2	2.39	0.43
2:C:314:ARG:O	2:C:318:ARG:HB2	2.19	0.43
2:C:333:ARG:NH1	6:C:5040:HOH:O	2.41	0.43
3:E:153:GLU:H	3:E:153:GLU:CD	2.22	0.43
1:A:321:LEU:O	1:A:326:VAL:HB	2.19	0.42
1:A:334:ASP:HB3	6:A:5181:HOH:O	2.19	0.42
1:B:212:PHE:O	1:B:215:PRO:HD2	2.19	0.42
2:C:42:ARG:HB2	2:C:99:ARG:HG3	2.01	0.42
2:D:377:ARG:O	2:D:381:VAL:HG23	2.19	0.42
1:A:362:ALA:HB2	1:A:501:VAL:HG13	2.00	0.42
1:B:121:THR:HG21	1:B:140:GLN:CG	2.48	0.42
2:C:189:ILE:HD11	2:C:287:TYR:CD1	2.54	0.42
1:B:489:ARG:HB3	2:D:30:ASP:OD2	2.19	0.42
2:C:291:ALA:O	2:C:295:VAL:HG23	2.19	0.42
3:E:41:THR:O	3:E:44:ARG:CD	2.64	0.42
1:A:315:GLY:N	1:A:318:ILE:HG22	2.35	0.42
1:B:207:VAL:O	1:B:211:CYS:HB3	2.19	0.42
1:B:292:TYR:OH	1:B:344:HIS:CD2	2.69	0.42
1:B:365:ASP:C	1:B:365:ASP:OD2	2.57	0.42
1:B:461:PRO:HG2	3:F:159:ARG:CZ	2.50	0.42
2:C:263:GLU:OE2	2:C:263:GLU:HA	2.19	0.42
2:C:102:LEU:HD11	2:C:290:ILE:HG12	2.02	0.42
1:A:363:LEU:HD11	1:A:395:CYS:SG	2.59	0.42
1:A:71:GLU:OE2	1:A:242:ASP:OD2	2.38	0.42
1:B:313:TRP:HA	1:B:317:TRP:HB3	2.01	0.42
1:B:44:THR:HG21	6:B:5175:HOH:O	2.19	0.42
2:C:240:ASP:OD1	3:E:125:VAL:HG21	2.19	0.42
1:B:403:ILE:O	1:B:403:ILE:HG13	2.18	0.42
2:C:261:ARG:NE	2:C:285:GLN:HE22	2.05	0.42
2:D:155:ASN:ND2	2:D:252:TYR:OH	2.52	0.42
3:E:44:ARG:HG3	3:E:46:SER:O	2.20	0.42
1:B:249:ASN:HA	1:B:252:GLN:CG	2.49	0.42
1:B:323:LYS:HG3	1:B:324:TYR:CE1	2.55	0.42
3:F:69:ALA:HA	6:F:225:HOH:O	2.20	0.42
1:A:282:PHE:O	1:A:283:THR:C	2.58	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:137:ASN:HA	2:C:138:PRO:HD3	1.91	0.42
2:D:146:ASN:HD21	2:D:197:ARG:NH2	2.17	0.42
1:A:118:ILE:HD13	1:A:145:ILE:HG12	2.01	0.42
1:A:223:TRP:CZ3	1:A:297:LYS:HA	2.55	0.42
1:A:249:ASN:HA	1:A:252:GLN:CG	2.49	0.42
1:A:91:ALA:HB1	6:A:5010:HOH:O	2.19	0.42
2:C:136:MET:HE2	2:C:141:ARG:HB2	2.02	0.42
2:D:228:ARG:HH11	2:D:228:ARG:HG2	1.85	0.42
1:A:302:VAL:HG12	1:A:340:TYR:HA	2.02	0.41
2:C:98:HIS:HE1	2:C:178:SER:OG	2.04	0.41
2:D:156:GLU:HA	2:D:156:GLU:OE2	2.19	0.41
2:D:277:THR:HB	2:D:278:PRO:HD3	2.01	0.41
1:A:116:ASN:HB2	1:A:188:PHE:O	2.20	0.41
2:D:184:PHE:O	2:D:187:ILE:HG22	2.20	0.41
1:A:123:MET:HB2	2:C:168:ARG:HD3	2.01	0.41
1:A:460:GLU:N	1:A:461:PRO:HD3	2.36	0.41
2:C:324:TRP:O	2:C:327:PRO:HD2	2.20	0.41
1:B:193:ILE:HB	2:D:168:ARG:NH2	2.35	0.41
3:E:15:TRP:O	3:E:19:ILE:HG13	2.21	0.41
3:E:75:VAL:HG12	6:E:190:HOH:O	2.19	0.41
1:A:306:ASP:OD2	1:A:336:LYS:NZ	2.50	0.41
1:A:459:ALA:C	1:A:461:PRO:HD3	2.41	0.41
1:A:50:TYR:CD1	1:A:198:VAL:HG21	2.56	0.41
1:B:109:PHE:O	1:B:112:VAL:HG12	2.19	0.41
2:C:377:ARG:O	2:C:381:VAL:HG23	2.21	0.41
3:F:40:THR:C	3:F:41:THR:HG23	2.41	0.41
1:A:402:PHE:O	1:A:403:ILE:HD12	2.19	0.41
1:A:201:SER:OG	1:A:253:THR:HG21	2.20	0.41
1:A:338:ASP:O	1:A:342:ALA:CB	2.69	0.41
1:A:90:ASN:HD22	1:A:90:ASN:HA	1.59	0.41
1:B:125:TRP:C	1:B:125:TRP:CD1	2.94	0.41
1:B:439:HIS:HB3	3:F:161:VAL:HG22	2.01	0.41
2:C:223:VAL:HG23	6:C:5021:HOH:O	2.19	0.41
2:C:155:ASN:ND2	2:C:252:TYR:OH	2.52	0.41
1:A:167:GLY:O	1:A:171:ALA:HB2	2.21	0.41
1:A:23:VAL:HB	2:C:195:LEU:HD12	2.03	0.41
1:B:113:GLY:HA3	1:B:188:PHE:HD2	1.86	0.41
1:B:460:GLU:OE1	1:B:463:ARG:HD3	2.20	0.41
1:B:90:ASN:HD22	1:B:90:ASN:HA	1.59	0.41
2:D:314:ARG:O	2:D:318:ARG:HB2	2.21	0.41
2:D:42:ARG:HB2	2:D:99:ARG:HG3	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:MET:HE3	1:A:188:PHE:HB2	2.02	0.41
1:A:283:THR:HB	1:A:284:PRO:HD3	2.03	0.41
1:B:354:TRP:CH2	1:B:499:PRO:HD3	2.55	0.41
2:D:102:LEU:CD1	2:D:290:ILE:HG12	2.51	0.41
2:D:98:HIS:HE1	2:D:178:SER:OG	2.04	0.41
3:F:165:HIS:HE1	3:F:167:GLN:NE2	2.19	0.41
1:B:268:ASN:HA	1:B:268:ASN:HD22	1.69	0.41
1:B:446:HIS:HB3	1:B:448:PHE:CZ	2.56	0.41
1:A:193:ILE:HB	2:C:168:ARG:NH2	2.36	0.41
1:B:128:ALA:O	1:B:134:LYS:HE2	2.21	0.41
1:B:216:LEU:HA	1:B:308:TRP:CH2	2.55	0.41
3:E:130:ASP:OD1	3:E:133:ARG:NH1	2.54	0.41
1:A:260:ASP:HA	1:A:261:PRO:HD3	1.96	0.40
1:A:365:ASP:OD2	1:A:368:GLU:HG3	2.20	0.40
1:B:195:GLY:HA2	6:D:516:HOH:O	2.21	0.40
1:B:227:ASN:HD21	1:B:296:PHE:H	1.68	0.40
1:B:313:TRP:CZ2	1:B:318:ILE:HD11	2.56	0.40
1:A:125:TRP:C	1:A:125:TRP:CD1	2.95	0.40
1:A:212:PHE:O	1:A:216:LEU:CB	2.68	0.40
1:B:83:GLN:HG2	6:B:5128:HOH:O	2.20	0.40
1:B:39:PHE:CD2	2:D:232:GLU:HG2	2.56	0.40
2:D:336:MET:HE3	2:D:352:ILE:HG21	2.03	0.40
1:A:254:VAL:O	1:A:254:VAL:HG12	2.20	0.40
1:A:179:PRO:HB3	1:A:469:ILE:HD13	2.02	0.40
1:B:185:LYS:C	1:B:189:SER:HB2	2.42	0.40
2:C:147:ARG:HD2	2:C:148:TYR:CE1	2.57	0.40
2:C:156:GLU:OE2	2:C:156:GLU:HA	2.21	0.40
2:C:203:ILE:HG13	2:C:204:VAL:HG23	2.03	0.40
2:D:357:TYR:CE2	2:D:381:VAL:HG21	2.57	0.40
1:A:310:TYR:C	1:A:312:ASP:H	2.25	0.40
1:A:460:GLU:HB3	1:A:463:ARG:CG	2.50	0.40
1:B:110:LEU:O	1:B:114:GLU:HG2	2.21	0.40
1:B:254:VAL:HG12	1:B:254:VAL:O	2.22	0.40
1:B:366:GLN:HG3	6:B:5123:HOH:O	2.22	0.40
2:C:132:GLN:HB3	6:C:5188:HOH:O	2.21	0.40
2:D:203:ILE:HG13	2:D:204:VAL:HG23	2.03	0.40
1:B:50:TYR:HB2	1:B:198:VAL:HG21	2.02	0.40
6:A:5161:HOH:O	1:B:76:GLU:HB3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	466 (92%)	40 (8%)	2 (0%)	38	46
1	B	508/527 (96%)	470 (92%)	35 (7%)	3 (1%)	28	34
2	C	386/388 (100%)	369 (96%)	16 (4%)	1 (0%)	44	54
2	D	386/388 (100%)	372 (96%)	12 (3%)	2 (0%)	32	39
3	E	164/169 (97%)	161 (98%)	3 (2%)	0	100	100
3	F	164/169 (97%)	161 (98%)	3 (2%)	0	100	100
All	All	2116/2168 (98%)	1999 (94%)	109 (5%)	8 (0%)	38	46

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	40	LYS
1	A	311	GLU
2	C	64	ALA
2	D	64	ALA
1	B	213	THR
1	A	316	ILE
1	B	284	PRO
2	D	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.

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	423/442 (96%)	406 (96%)	17 (4%)	36	49
1	B	422/442 (96%)	411 (97%)	11 (3%)	51	68
2	C	316/323 (98%)	309 (98%)	7 (2%)	57	74
2	D	312/323 (97%)	305 (98%)	7 (2%)	57	74
3	E	143/146 (98%)	142 (99%)	1 (1%)	87	94
3	F	142/146 (97%)	141 (99%)	1 (1%)	87	94
All	All	1758/1822 (96%)	1714 (98%)	44 (2%)	53	70

All (44) 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	71	GLU
1	A	90	ASN
1	A	125	TRP
1	A	175	ARG
1	A	186	ARG
1	A	279	GLN
1	A	302	VAL
1	A	334	ASP
1	A	348	LEU
1	A	403	ILE
1	A	437	ARG
1	A	467	GLN
1	A	479	SER
1	A	520	LYS
1	B	43	ARG
1	B	71	GLU
1	B	90	ASN
1	B	125	TRP
1	B	175	ARG
1	B	186	ARG
1	B	279	GLN
1	B	334	ASP
1	B	440	GLU
1	B	451	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	516	ASN
2	C	35	MET
2	C	80	ARG
2	C	153	LEU
2	C	168	ARG
2	C	173	ASP
2	C	356	LEU
2	C	382	LYS
2	D	35	MET
2	D	80	ARG
2	D	153	LEU
2	D	168	ARG
2	D	173	ASP
2	D	356	LEU
2	D	389	LYS
3	E	44	ARG
3	F	44	ARG

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	59	GLN
1	A	78	GLN
1	A	90	ASN
1	A	100	ASN
1	A	108	ASN
1	A	140	GLN
1	A	155	ASN
1	A	168	HIS
1	A	205	GLN
1	A	227	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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	472	GLN
1	B	42	ASN
1	B	59	GLN
1	B	78	GLN
1	B	90	ASN
1	B	100	ASN
1	B	108	ASN
1	B	116	ASN
1	B	140	GLN
1	B	155	ASN
1	B	168	HIS
1	B	205	GLN
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	382	HIS
1	B	413	HIS
1	B	439	HIS
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	275	ASN
2	C	285	GLN
2	C	301	ASN
2	D	98	HIS
2	D	146	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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	F	45	ASN
3	F	144	ASN
3	F	165	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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%)	0.18	39 (7%)	15 20	23, 41, 98, 114	0
1	B	510/527 (96%)	0.03	34 (6%)	19 25	23, 39, 82, 104	0
2	C	388/388 (100%)	-0.20	5 (1%)	77 81	22, 33, 52, 61	0
2	D	388/388 (100%)	0.22	35 (9%)	10 14	26, 41, 60, 98	0
3	E	166/169 (98%)	-0.14	1 (0%)	89 92	26, 40, 57, 65	0
3	F	166/169 (98%)	0.49	12 (7%)	16 22	32, 47, 60, 68	0
All	All	2128/2168 (98%)	0.08	126 (5%)	23 30	22, 40, 78, 114	0

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	375	ALA	6.5
2	D	389	LYS	6.3
1	A	324	TYR	5.5
1	B	320	ARG	5.5
1	A	252	GLN	5.0
3	F	69	ALA	4.9
1	A	322	GLY	4.9
1	A	257	ILE	4.9
2	D	203	ILE	4.9
1	A	316	ILE	4.8
1	B	259	ASN	4.7
2	D	220	ASN	4.7
2	D	205	PRO	4.7
1	B	53	ALA	4.7
2	D	136	MET	4.6
1	A	317	TRP	4.6
1	B	323	LYS	4.4
1	A	262	ALA	4.3
1	A	214	ASN	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	325	GLY	3.9
1	A	434	SER	3.9
1	A	315	GLY	3.8
1	A	314	GLY	3.8
1	B	21	THR	3.7
1	B	39	PHE	3.7
1	B	258	ALA	3.7
1	A	264	ALA	3.6
1	B	324	TYR	3.5
2	D	206	GLY	3.5
1	A	323	LYS	3.5
1	A	325	GLY	3.5
1	A	212	PHE	3.4
1	B	20	PRO	3.3
3	F	23	ASN	3.3
1	A	210	ALA	3.3
1	B	57	LYS	3.3
2	D	139	THR	3.3
1	A	213	THR	3.2
2	D	344	ALA	3.2
2	D	270	PRO	3.2
1	A	251	TYR	3.2
2	D	339	PHE	3.2
1	A	258	ALA	3.2
3	F	101	ALA	3.1
2	D	380	ILE	3.1
1	B	261	PRO	3.1
1	A	318	ILE	3.1
1	A	321	LEU	3.0
1	B	19	ALA	3.0
2	D	354	ALA	3.0
1	A	265	LYS	3.0
1	A	194	SER	2.9
2	D	343	PRO	2.9
1	A	206	LEU	2.9
1	B	206	LEU	2.9
3	F	21	GLN	2.9
1	A	261	PRO	2.9
1	A	198	VAL	2.9
3	F	70	ARG	2.9
1	A	326	VAL	2.8
2	D	377	ARG	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	342	LEU	2.7
3	E	23	ASN	2.7
3	F	22	LEU	2.7
1	B	263	SER	2.7
1	A	259	ASN	2.7
1	B	44	THR	2.7
2	D	381	VAL	2.7
3	F	72	PHE	2.7
1	A	201	SER	2.6
2	C	2	SER	2.6
2	D	140	TRP	2.6
1	A	310	TYR	2.6
2	D	352	ILE	2.6
1	B	22	SER	2.6
2	D	349	LYS	2.6
1	B	311	GLU	2.5
3	F	89	SER	2.5
2	C	281	ILE	2.5
1	B	333	LYS	2.5
1	A	263	SER	2.4
2	D	207	PHE	2.4
1	A	195	GLY	2.4
2	D	388	LEU	2.4
2	D	227	ALA	2.4
1	A	308	TRP	2.4
1	A	319	GLY	2.4
1	B	23	VAL	2.4
1	B	54	ASN	2.4
1	B	310	TYR	2.4
2	D	347	THR	2.4
1	A	255	VAL	2.4
1	B	255	VAL	2.4
1	A	199	GLU	2.3
1	B	204	LEU	2.3
2	D	138	PRO	2.3
3	F	96	ALA	2.3
2	C	189	ILE	2.3
2	D	219	THR	2.3
2	D	357	TYR	2.3
1	A	260	ASP	2.3
1	B	248	ALA	2.3
3	F	26	GLU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	374	LYS	2.3
3	F	102	LYS	2.3
1	A	211	CYS	2.2
1	B	52	MET	2.2
3	F	100	ALA	2.2
1	A	202	LEU	2.2
2	D	141	ARG	2.2
2	D	350	GLU	2.2
1	B	260	ASP	2.2
2	D	373	PHE	2.2
1	B	59	GLN	2.1
1	B	253	THR	2.1
1	B	38	ASP	2.1
2	C	389	LYS	2.1
1	B	257	ILE	2.1
2	D	379	GLN	2.1
1	B	41	ASN	2.1
1	B	42	ASN	2.1
2	D	148	TYR	2.1
2	C	149	TRP	2.1
2	D	348	ASP	2.0
2	D	346	THR	2.0
1	B	40	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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(\AA^2)	Q<0.9
4	MN	A	5001	1/1	0.99	0.06	-1.94	32,32,32,32	0
4	MN	A	5002	1/1	0.98	0.03	-2.53	39,39,39,39	0
4	MN	B	5004	1/1	0.99	0.06	-2.62	48,48,48,48	0
4	MN	B	5003	1/1	0.94	0.06	-3.06	35,35,35,35	0
5	CA	A	5006	1/1	0.95	0.04	-5.36	47,47,47,47	0
5	CA	C	5008	1/1	0.96	0.08	-	56,56,56,56	0
5	CA	C	5005	1/1	0.99	0.05	-	37,37,37,37	0
5	CA	C	5007	1/1	0.94	0.04	-	57,57,57,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.