WORLDWIDE
wwPDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

May 21, 2014 – 03:48 AM EDT

PDB ID	:	4KR8
Title	:	Salmonella typhi OmpF complex with Daunomycin
Authors	:	Madhuranayaki, T.; Balasubramaniam, D.; Krishnaswamy, S.
Deposited on	:	2013-05-16
Resolution	:	3.10 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html
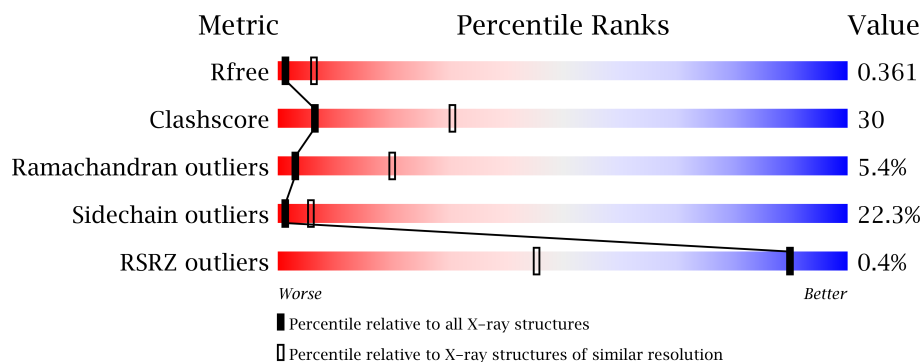

The following versions of software and data (see references) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.16 November 2013
Xtriage (Phenix)	:	dev-1439
EDS	:	stable22978
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22978

1 Overall quality at a glance ⓘ

The reported resolution of this entry is 3.10 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	Percentile Ranks	Value
Rfree		0.361
Clashscore		30
Ramachandran outliers		5.4%
Sidechain outliers		22.3%
RSRZ outliers		0.4%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1007 (3.18-3.02)
Clashscore	79885	1078 (3.16-3.04)
Ramachandran outliers	78287	1044 (3.16-3.04)
Sidechain outliers	78261	1044 (3.16-3.04)
RSRZ outliers	66119	1008 (3.18-3.02)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	341	
1	B	341	
1	C	341	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

| Mol	Type	Chain	Res	Geometry	Electron density
2	DM1	C	401[A]	-	X
2	DM1	C	401[B]	-	X

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 7769 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Outer membrane protein F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	0	0	0
			2540	1584	430	519	7			
1	B	340	Total	C	N	O	S	0	0	0
			2610	1628	440	535	7			
1	C	340	Total	C	N	O	S	0	0	0
			2571	1601	433	531	6			

- Molecule 2 is DAUNOMYCIN (three-letter code: DM1) (formula: $C_{27}H_{29}NO_{10}$).
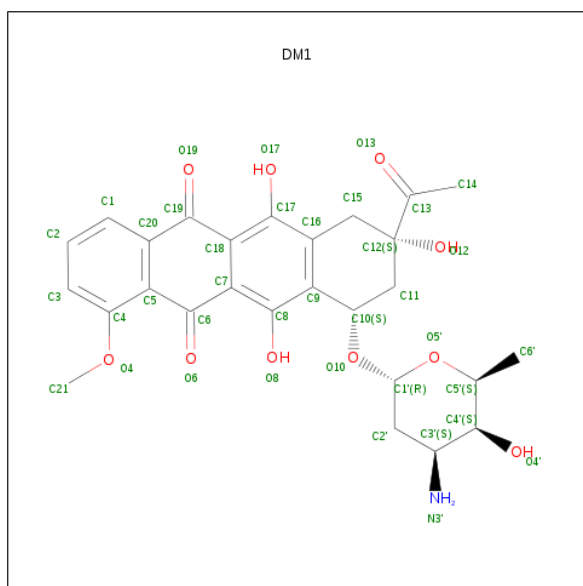
| Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	1
			48	33	2	13		

3   Residue-property plots ⓘ

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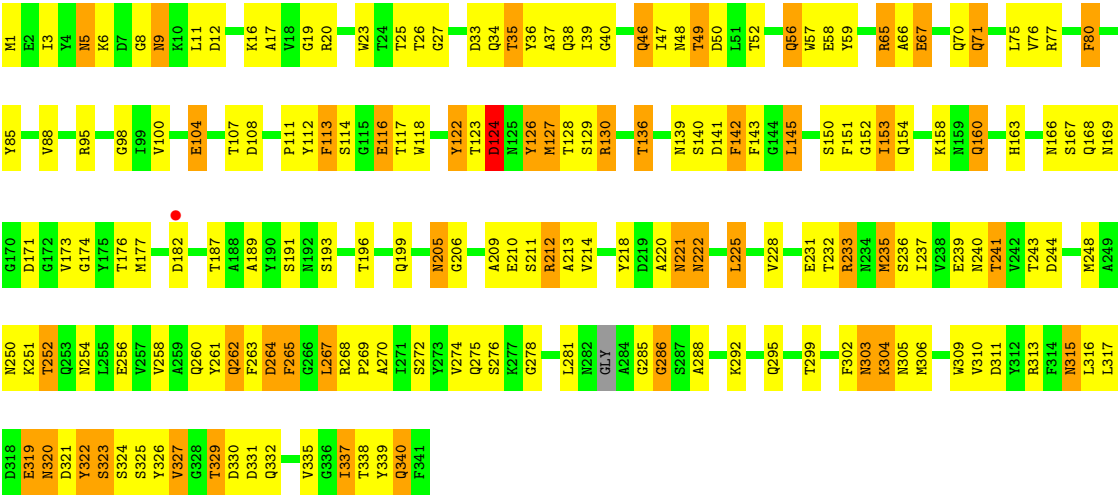
- Molecule 1: Outer membrane protein F

Chain A:

- Molecule 1: Outer membrane protein F

Chain B:

- Molecule 1: Outer membrane protein F

Chain C:
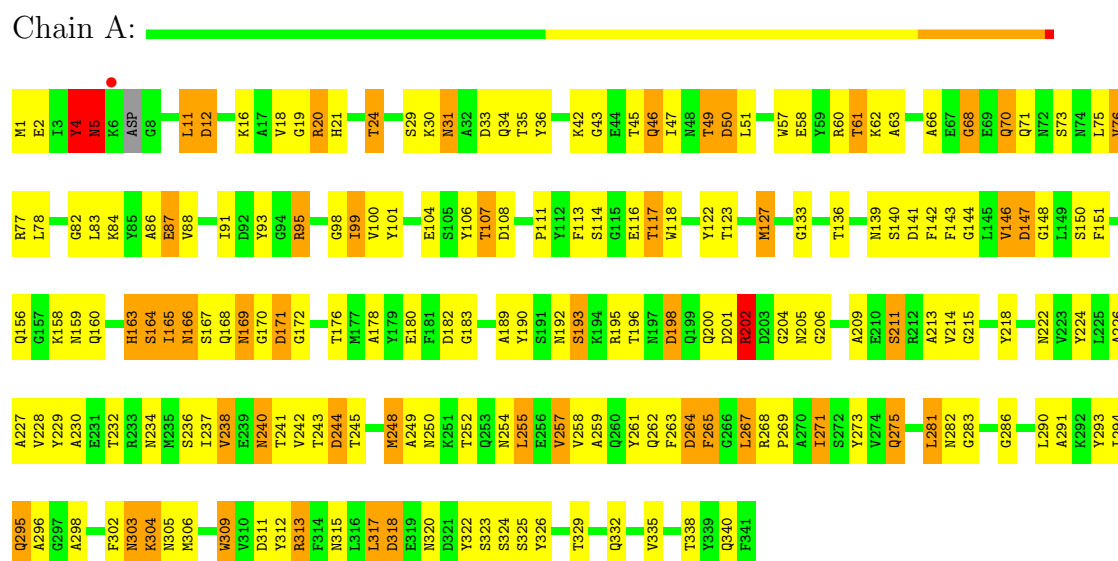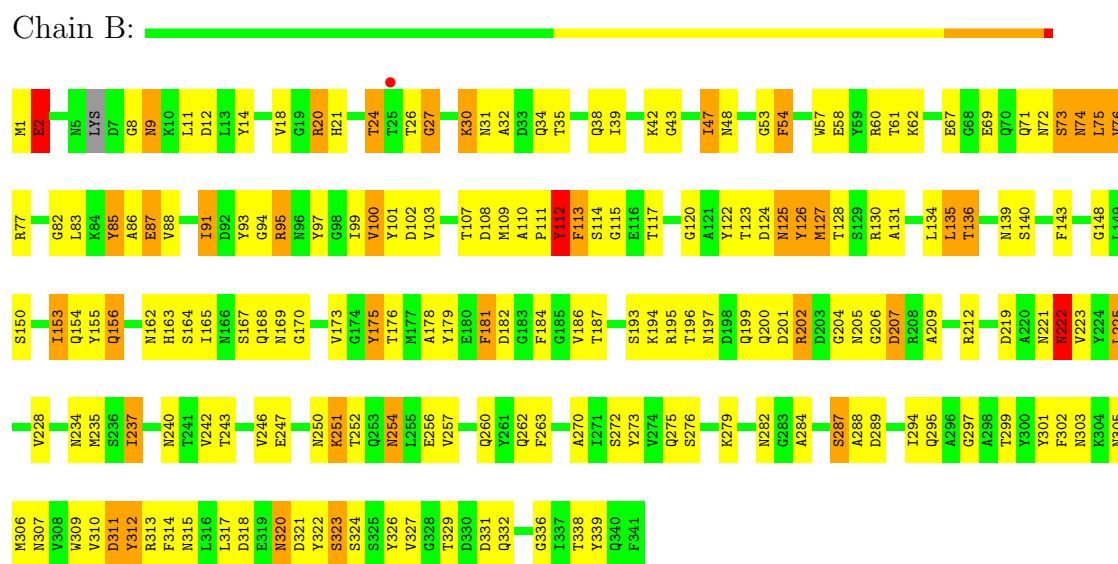
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	84.71Å 132.39Å 150.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.10 49.63 – 3.10	Depositor EDS
% Data completeness (in resolution range)	98.3 (50.00-3.10) 98.3 (49.63-3.10)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$<I/\sigma(I)>$ [1]	2.42 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.293 , 0.366 0.294 , 0.361	Depositor DCC
R_{free} test set	1559 reflections (5.31%)	DCC
Wilson B-factor (Å^2)	75.6	Xtriage
Anisotropy	0.837	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 35.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$<|L|> = 0.46, <L^2> = 0.29$	Xtriage
Outliers	0 of 30931 reflections	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	7769	wwPDB-VP
Average B, all atoms (Å^2)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1]Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: DM1

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	0.57	0/2590	0.72	1/3519 (0.0%)
1	B	0.62	0/2662	0.73	0/3609
1	C	0.59	0/2623	0.72	0/3566
All	All	0.59	0/7875	0.73	1/10694 (0.0%)

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	A	281	LEU	CA-CB-CG	5.05	126.92	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2540	0	2237	156	0
1	B	2610	0	2352	156	0
1	C	2571	0	2246	157	0
2	C	48	0	26	3	0
All	All	7769	0	6861	436	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 30.

All (436) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:293:TYR:HB3	1:A:315:ASN:HD22	1.21	1.06
1:C:65:ARG:HH11	1:C:65:ARG:HG2	1.18	1.05
1:A:295:GLN:HB2	1:A:312:TYR:O	1.62	0.98
1:C:123:THR:O	1:C:124:ASP:HB2	1.66	0.95
1:A:211:SER:OG	1:A:232:THR:HA	1.67	0.94
1:B:299:THR:HG23	1:B:309:TRP:HB3	1.54	0.90
1:C:168:GLN:HB3	1:C:196:THR:HG21	1.53	0.88
1:C:16:LYS:HB3	1:C:340:GLN:HB2	1.53	0.88
1:A:57:TRP:HA	1:A:78:LEU:O	1.74	0.88
1:B:320:ASN:HD22	1:B:322:TYR:H	1.22	0.86
1:C:210:GLU:HB2	1:C:233:ARG:HB2	1.54	0.86
1:B:85:TYR:HB3	1:B:88:VAL:HB	1.58	0.85
1:B:82:GLY:HA2	1:C:337:ILE:HD11	1.57	0.85
1:B:153:ILE:HD11	1:B:155:TYR:CE2	2.11	0.85
1:A:20:ARG:HG3	1:A:34:GLN:O	1.78	0.84
1:C:8:GLY:O	1:C:9:ASN:HB2	1.78	0.83
1:A:163:HIS:HB3	1:A:167:SER:OG	1.79	0.82
1:A:165:ILE:O	1:A:166:ASN:HB2	1.77	0.82
1:C:272:SER:OG	1:C:295:GLN:CG	2.29	0.80
1:B:279:LYS:HA	1:B:287:SER:HB3	1.64	0.79
1:A:293:TYR:HB3	1:A:315:ASN:ND2	1.98	0.78
1:A:302:PHE:HB3	1:C:47:ILE:HD12	1.67	0.77
1:B:95:ARG:O	1:B:95:ARG:HG3	1.83	0.77
1:B:1:MET:O	1:B:2:GLU:HB3	1.85	0.76
1:A:76:VAL:HG11	1:B:61:THR:HB	1.66	0.76
1:A:91:ILE:HA	1:A:136:THR:O	1.86	0.76
1:B:26:THR:HG22	1:B:27:GLY:N	2.00	0.75
1:C:113:PHE:H	2:C:401[B]:DM1:H4'	1.49	0.75
1:B:76:VAL:H	1:C:70:GLN:HE22	1.35	0.74
1:A:291:ALA:HA	1:A:317:LEU:HD12	1.70	0.74
1:A:76:VAL:CG1	1:B:61:THR:HB	2.18	0.74
1:C:272:SER:OG	1:C:295:GLN:HG2	1.88	0.73
1:B:112:TYR:O	1:B:113:PHE:CG	2.41	0.73
1:C:65:ARG:CG	1:C:65:ARG:HH11	1.98	0.73
1:B:242:VAL:HG21	1:B:321:ASP:OD2	1.89	0.72
1:C:166:ASN:HD22	1:C:237:ILE:HG21	1.54	0.72
1:A:62:LYS:HB2	1:A:73:SER:HB3	1.70	0.72
1:B:320:ASN:HB3	1:B:323:SER:OG	1.89	0.72
1:A:93:TYR:OH	1:B:21:HIS:HD2	1.72	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:272:SER:OG	1:C:295:GLN:HG3	1.90	0.71
1:C:65:ARG:HG2	1:C:65:ARG:NH1	1.93	0.71
1:C:136:THR:HB	1:C:154:GLN:HB3	1.73	0.71
1:B:26:THR:CG2	1:B:27:GLY:N	2.54	0.70
1:B:26:THR:CG2	1:B:27:GLY:H	2.04	0.70
1:C:210:GLU:HB2	1:C:233:ARG:CB	2.21	0.70
1:C:85:TYR:HB3	1:C:88:VAL:HG13	1.74	0.69
1:C:56:GLN:HB3	1:C:80:PHE:HE1	1.58	0.69
1:B:30:LYS:HD3	1:B:31:ASN:H	1.56	0.69
1:A:33:ASP:OD1	1:A:34:GLN:N	2.26	0.68
1:C:153:ILE:HA	1:C:174:GLY:O	1.92	0.68
1:C:116:GLU:OE1	2:C:401[B]:DM1:N3'	2.27	0.68
1:C:288:ALA:HB1	1:C:320:ASN:ND2	2.09	0.67
1:A:117:THR:HG22	1:A:118:TRP:N	2.08	0.67
1:A:45:THR:OG1	1:B:303:ASN:ND2	2.27	0.67
1:A:117:THR:HG22	1:A:118:TRP:HD1	1.59	0.67
1:A:158:LYS:HA	1:A:170:GLY:HA2	1.76	0.67
1:C:123:THR:O	1:C:124:ASP:CB	2.43	0.67
1:B:53:GLY:HA3	1:C:306:MET:HG3	1.77	0.66
1:A:222:ASN:HB3	1:A:261:TYR:CE1	2.32	0.65
1:A:82:GLY:HA3	1:A:91:ILE:O	1.95	0.65
1:B:195:ARG:CZ	1:B:199:GLN:HB2	2.26	0.65
1:C:252:THR:HG22	1:C:278:GLY:HA2	1.78	0.65
1:C:33:ASP:OD2	1:C:34:GLN:N	2.30	0.65
1:A:2:GLU:HA	1:A:12:ASP:HB3	1.77	0.64
1:A:165:ILE:O	1:A:166:ASN:CB	2.46	0.64
1:A:303:ASN:O	1:A:306:MET:N	2.30	0.64
1:C:262:GLN:HE21	1:C:268:ARG:HH11	1.43	0.64
1:B:111:PRO:O	1:B:112:TYR:HB2	1.96	0.64
1:B:221:ASN:O	1:B:223:VAL:HG23	1.96	0.64
1:B:76:VAL:N	1:C:70:GLN:HE22	1.95	0.64
1:B:99:ILE:H	1:B:154:GLN:HE22	1.45	0.64
1:B:322:TYR:O	1:B:324:SER:N	2.31	0.64
1:B:62:LYS:HB2	1:B:73:SER:CB	2.28	0.63
1:A:11:LEU:HA	1:A:42:LYS:O	1.99	0.63
1:B:309:TRP:CE2	1:B:336:GLY:HA3	2.34	0.63
1:A:19:GLY:HA2	1:A:35:THR:HG23	1.81	0.63
1:B:257:VAL:HG12	1:B:273:TYR:HB3	1.80	0.63
1:A:150:SER:OG	1:A:178:ALA:HB3	1.99	0.63
1:B:115:GLY:O	1:B:120:GLY:HA3	1.98	0.63
1:A:281:LEU:O	1:A:286:GLY:HA2	1.99	0.63
1:A:95:ARG:HH22	1:B:67:GLU:HG3	1.63	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:259:ALA:O	1:A:271:ILE:HD12	1.99	0.62
1:B:125:ASN:O	1:B:126:TYR:CD2	2.52	0.62
1:B:272:SER:OG	1:B:295:GLN:HG3	1.99	0.62
1:C:193:SER:HB2	1:C:209:ALA:HB3	1.81	0.62
1:A:61:THR:OG1	1:C:76:VAL:HG11	1.99	0.62
1:A:47:ILE:HD12	1:A:51:LEU:HG	1.82	0.62
1:B:91:ILE:HA	1:B:136:THR:O	1.99	0.62
1:B:26:THR:HB	1:B:331:ASP:H	1.65	0.62
1:B:120:GLY:C	1:B:122:TYR:H	2.03	0.61
1:C:56:GLN:HB3	1:C:80:PHE:CE1	2.34	0.61
1:B:82:GLY:HA2	1:C:337:ILE:CD1	2.30	0.61
1:C:126:TYR:HD1	1:C:235:MET:HB3	1.65	0.61
1:C:48:ASN:O	1:C:50:ASP:N	2.34	0.61
1:A:113:PHE:HD2	1:A:311:ASP:OD1	1.84	0.61
1:C:218:TYR:HB3	1:C:225:LEU:HD12	1.83	0.60
1:B:11:LEU:HA	1:B:43:GLY:HA2	1.83	0.60
1:A:236:SER:HB2	1:A:249:ALA:HB3	1.83	0.60
1:A:295:GLN:HB2	1:A:313:ARG:HA	1.83	0.60
1:B:178:ALA:HA	1:B:187:THR:HG22	1.84	0.60
1:A:111:PRO:HG2	1:A:311:ASP:OD2	2.01	0.59
1:A:18:VAL:HG22	1:A:338:THR:HG23	1.83	0.59
1:A:257:VAL:HG12	1:A:273:TYR:HB3	1.85	0.59
1:B:181:PHE:N	1:B:181:PHE:CD2	2.70	0.59
1:C:126:TYR:O	1:C:128:THR:HG23	2.02	0.59
1:B:196:THR:HG22	1:B:197:ASN:N	2.17	0.59
1:A:165:ILE:O	1:A:165:ILE:HG13	2.02	0.58
1:A:293:TYR:CB	1:A:315:ASN:HD22	2.08	0.58
1:C:20:ARG:NH1	1:C:34:GLN:HB3	2.18	0.58
1:A:117:THR:HG22	1:A:118:TRP:CD1	2.38	0.58
1:A:160:GLN:NE2	1:A:196:THR:HB	2.18	0.58
1:C:117:THR:O	1:C:326:TYR:CE1	2.57	0.58
1:C:107:THR:HG21	1:C:228:VAL:HG12	1.86	0.58
1:B:165:ILE:HA	1:B:168:GLN:HE21	1.68	0.58
1:B:38:GLN:HG3	1:B:60:ARG:HB2	1.85	0.58
1:A:93:TYR:OH	1:B:21:HIS:CD2	2.57	0.57
1:C:288:ALA:HB1	1:C:320:ASN:HD21	1.67	0.57
1:A:159:ASN:N	1:A:169:ASN:O	2.37	0.57
1:B:21:HIS:HE1	1:B:31:ASN:ND2	2.02	0.57
1:C:143:PHE:HB2	1:C:145:LEU:HD22	1.87	0.57
1:C:16:LYS:CB	1:C:340:GLN:HB2	2.30	0.57
1:A:222:ASN:O	1:A:261:TYR:HD1	1.87	0.57
1:B:313:ARG:NH2	1:B:332:GLN:OE1	2.34	0.56

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:202:ARG:HB3	1:B:282:ASN:OD1	2.05	0.56
1:C:166:ASN:ND2	1:C:237:ILE:HG21	2.19	0.56
1:C:123:THR:HG23	1:C:123:THR:O	2.06	0.56
1:A:24:THR:HB	1:A:30:LYS:H	1.70	0.56
1:C:140:SER:O	1:C:150:SER:HB3	2.05	0.56
1:C:59:TYR:HD2	1:C:76:VAL:CG1	2.19	0.56
1:C:129:SER:O	1:C:130:ARG:C	2.43	0.56
1:B:150:SER:OG	1:B:178:ALA:HB3	2.06	0.56
1:B:270:ALA:N	1:B:297:GLY:O	2.38	0.56
1:A:222:ASN:HB3	1:A:261:TYR:HE1	1.70	0.56
1:C:323:SER:O	1:C:324:SER:C	2.44	0.56
1:B:20:ARG:HD3	1:B:34:GLN:HB3	1.87	0.56
1:C:59:TYR:HD2	1:C:76:VAL:HG12	1.69	0.56
1:A:195:ARG:HH21	1:A:248:MET:HB2	1.70	0.56
1:B:117:THR:O	1:B:326:TYR:CE1	2.59	0.55
1:C:141:ASP:O	1:C:143:PHE:N	2.40	0.55
1:C:220:ALA:O	1:C:221:ASN:C	2.44	0.55
1:C:126:TYR:CD1	1:C:235:MET:HB3	2.41	0.55
1:A:183:GLY:HA3	1:A:218:TYR:CE1	2.41	0.55
1:B:148:GLY:O	1:B:179:TYR:HA	2.06	0.55
1:B:99:ILE:HD11	1:B:176:THR:HG22	1.89	0.55
1:C:56:GLN:HG3	1:C:57:TRP:N	2.21	0.55
1:B:240:ASN:HB3	1:B:243:THR:HG22	1.88	0.55
1:C:260:GLN:HB3	1:C:270:ALA:HA	1.89	0.55
1:C:11:LEU:HG	1:C:12:ASP:N	2.22	0.55
1:A:33:ASP:O	1:A:34:GLN:HG2	2.06	0.54
1:A:142:PHE:HB3	1:A:146:VAL:HG23	1.89	0.54
1:A:47:ILE:HG23	1:B:302:PHE:HB3	1.90	0.54
1:A:238:VAL:HB	1:A:322:TYR:HD1	1.71	0.54
1:B:93:TYR:HA	1:B:134:LEU:O	2.07	0.54
1:C:111:PRO:HG2	1:C:311:ASP:OD1	2.07	0.54
1:C:264:ASP:O	1:C:265:PHE:HB3	2.06	0.54
1:A:43:GLY:HA3	1:B:339:TYR:CE2	2.43	0.54
1:B:306:MET:HE1	1:B:339:TYR:HB2	1.90	0.54
1:A:263:PHE:O	1:A:265:PHE:N	2.41	0.54
1:C:299:THR:HG23	1:C:309:TRP:HB3	1.89	0.54
1:C:315:ASN:N	1:C:331:ASP:OD1	2.29	0.54
1:C:107:THR:CG2	1:C:228:VAL:HG12	2.38	0.53
1:B:250:ASN:O	1:B:251:LYS:O	2.25	0.53
1:C:122:TYR:CZ	1:C:237:ILE:HB	2.43	0.53
1:C:160:GLN:HA	1:C:168:GLN:HG2	1.89	0.53
1:C:59:TYR:CD2	1:C:76:VAL:HG12	2.42	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:107:THR:OG1	1:A:228:VAL:HG22	2.08	0.53
1:B:107:THR:HG23	1:B:228:VAL:HG13	1.89	0.53
1:B:75:LEU:HD22	1:C:67:GLU:HG3	1.90	0.53
1:B:126:TYR:CE1	1:B:169:ASN:HB2	2.44	0.53
1:B:222:ASN:HB2	1:B:262:GLN:O	2.09	0.53
1:A:204:GLY:HA2	1:A:250:ASN:ND2	2.24	0.53
1:B:202:ARG:HH21	1:B:282:ASN:HB2	1.74	0.53
1:C:232:THR:HG23	1:C:235:MET:HG3	1.91	0.53
1:C:261:TYR:CE2	1:C:263:PHE:HA	2.43	0.53
1:A:313:ARG:O	1:A:313:ARG:HG3	2.08	0.53
1:C:122:TYR:CE1	1:C:237:ILE:HB	2.44	0.53
1:A:141:ASP:OD2	1:A:144:GLY:HA2	2.09	0.53
1:B:97:TYR:HA	1:B:130:ARG:HA	1.90	0.53
1:C:187:THR:O	1:C:214:VAL:HA	2.09	0.53
1:C:95:ARG:NH2	1:C:124:ASP:OD2	2.41	0.53
1:B:140:SER:O	1:B:150:SER:HB3	2.09	0.52
1:C:315:ASN:HD22	1:C:315:ASN:C	2.13	0.52
1:C:158:LYS:HA	1:C:169:ASN:O	2.09	0.52
1:A:209:ALA:HA	1:A:234:ASN:HB2	1.90	0.52
1:A:151:PHE:HB2	1:A:176:THR:O	2.09	0.52
1:A:227:ALA:HB2	1:A:257:VAL:HG23	1.92	0.52
1:B:101:TYR:HB2	1:B:128:THR:O	2.10	0.52
1:B:26:THR:HG22	1:B:27:GLY:H	1.69	0.52
1:B:91:ILE:O	1:B:91:ILE:HG13	2.07	0.52
1:A:303:ASN:O	1:A:305:ASN:N	2.43	0.52
1:B:181:PHE:O	1:B:184:PHE:HB2	2.10	0.52
1:C:163:HIS:HB3	1:C:167:SER:HB2	1.92	0.52
1:A:230:ALA:N	1:A:254:ASN:O	2.42	0.52
1:B:117:THR:O	1:B:326:TYR:CZ	2.62	0.52
1:B:62:LYS:HB2	1:B:73:SER:HB2	1.90	0.52
1:C:27:GLY:HA3	1:C:330:ASP:OD1	2.10	0.52
1:B:14:TYR:HE2	1:B:42:LYS:HG3	1.75	0.52
1:A:117:THR:CG2	1:A:118:TRP:N	2.73	0.51
1:A:205:ASN:HB3	1:A:234:ASN:HD21	1.75	0.51
1:B:303:ASN:HB3	1:B:305:ASN:H	1.76	0.51
1:C:117:THR:HG23	1:C:118:TRP:H	1.75	0.51
1:B:54:PHE:HD1	1:B:54:PHE:O	1.92	0.51
1:B:252:THR:O	1:B:254:ASN:ND2	2.43	0.51
1:B:8:GLY:O	1:B:9:ASN:HB2	2.10	0.51
1:C:222:ASN:HB3	1:C:262:GLN:O	2.11	0.51
1:B:168:GLN:OE1	1:B:196:THR:HG21	2.11	0.51
1:A:46:GLN:HE21	1:A:46:GLN:CA	2.24	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:16:LYS:HB3	1:C:340:GLN:CB	2.33	0.51
1:A:195:ARG:HD3	1:A:206:GLY:O	2.11	0.51
1:B:312:TYR:HD1	1:B:313:ARG:N	2.08	0.51
1:A:213:ALA:HB1	1:A:229:TYR:O	2.10	0.50
1:B:163:HIS:HB3	1:B:167:SER:HB2	1.93	0.50
1:C:59:TYR:CD2	1:C:76:VAL:CG1	2.94	0.50
1:C:116:GLU:HG2	2:C:401[A]:DM1:H4'	1.92	0.50
1:A:11:LEU:HG	1:A:12:ASP:N	2.27	0.50
1:A:60:ARG:NH1	1:A:77:ARG:NH1	2.59	0.50
1:A:215:GLY:HA3	1:A:228:VAL:HG12	1.94	0.50
1:C:23:TRP:O	1:C:332:GLN:HG3	2.12	0.50
1:A:267:LEU:HD11	1:A:298:ALA:HB1	1.94	0.50
1:A:47:ILE:CG2	1:B:302:PHE:HB3	2.42	0.50
1:B:60:ARG:O	1:B:74:ASN:HA	2.11	0.50
1:B:76:VAL:H	1:C:70:GLN:NE2	2.05	0.50
1:A:242:VAL:C	1:A:244:ASP:H	2.15	0.50
1:C:1:MET:C	1:C:12:ASP:OD2	2.51	0.50
1:C:127:MET:CE	1:C:154:GLN:HG3	2.42	0.49
1:C:205:ASN:HB2	1:C:250:ASN:HD21	1.76	0.49
1:A:228:VAL:O	1:A:255:LEU:HD12	2.12	0.49
1:C:313:ARG:NH1	1:C:327:VAL:HG22	2.26	0.49
1:A:101:TYR:O	1:A:104:GLU:N	2.45	0.49
1:A:273:TYR:HA	1:A:294:ILE:HG23	1.93	0.49
1:B:21:HIS:HE1	1:B:31:ASN:HD21	1.60	0.49
1:C:127:MET:HE3	1:C:154:GLN:HG3	1.95	0.49
1:A:267:LEU:HD12	1:A:269:PRO:HG3	1.95	0.49
1:B:205:ASN:O	1:B:207:ASP:N	2.46	0.49
1:A:106:TYR:H	1:A:106:TYR:HD1	1.61	0.49
1:B:140:SER:HA	1:B:150:SER:HB2	1.95	0.49
1:A:16:LYS:HE3	1:A:36:TYR:CE1	2.48	0.49
1:B:108:ASP:OD1	1:B:114:SER:OG	2.24	0.49
1:A:50:ASP:HB3	1:A:86:ALA:HB3	1.94	0.49
1:C:16:LYS:HG2	1:C:38:GLN:HB3	1.95	0.49
1:C:262:GLN:NE2	1:C:268:ARG:HH11	2.10	0.49
1:A:164:SER:O	1:A:165:ILE:C	2.51	0.49
1:B:168:GLN:O	1:B:169:ASN:HB3	2.13	0.49
1:C:136:THR:HB	1:C:154:GLN:CB	2.42	0.49
1:B:54:PHE:CD1	1:B:54:PHE:C	2.85	0.48
1:A:172:GLY:HA3	1:A:193:SER:OG	2.13	0.48
1:B:196:THR:CG2	1:B:197:ASN:N	2.76	0.48
1:A:4:TYR:O	1:A:5:ASN:CB	2.61	0.48
1:B:204:GLY:O	1:B:205:ASN:HB2	2.12	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:160:GLN:HE21	1:A:196:THR:HB	1.76	0.48
1:B:26:THR:HG23	1:B:27:GLY:H	1.79	0.48
1:C:232:THR:HG21	1:C:236:SER:OG	2.14	0.48
1:A:140:SER:O	1:A:150:SER:HB3	2.12	0.48
1:C:319:GLU:HA	1:C:329:THR:HG21	1.96	0.48
1:B:87:GLU:O	1:B:143:PHE:HA	2.12	0.48
1:B:2:GLU:HA	1:B:12:ASP:OD1	2.14	0.48
1:B:320:ASN:HD22	1:B:322:TYR:N	2.01	0.48
1:B:20:ARG:NH1	1:B:34:GLN:HG3	2.29	0.47
1:C:322:TYR:O	1:C:323:SER:C	2.51	0.47
1:A:262:GLN:OE1	1:A:268:ARG:NH1	2.46	0.47
1:A:142:PHE:CD2	1:A:142:PHE:O	2.67	0.47
1:B:54:PHE:HD1	1:B:54:PHE:C	2.16	0.47
1:C:104:GLU:HG2	1:C:118:TRP:CZ2	2.48	0.47
1:C:233:ARG:O	1:C:250:ASN:HA	2.14	0.47
1:C:19:GLY:HA2	1:C:35:THR:OG1	2.14	0.47
1:A:99:ILE:H	1:A:127:MET:HE3	1.78	0.47
1:B:24:THR:OG1	1:B:30:LYS:O	2.32	0.47
1:C:152:GLY:N	1:C:176:THR:O	2.47	0.47
1:C:323:SER:O	1:C:325:SER:N	2.47	0.47
1:A:163:HIS:N	1:A:163:HIS:ND1	2.63	0.47
1:B:93:TYR:HB2	1:B:135:LEU:HD22	1.96	0.47
1:C:127:MET:HE3	1:C:154:GLN:CG	2.44	0.47
1:C:256:GLU:HG2	1:C:274:VAL:HB	1.95	0.47
1:A:295:GLN:CB	1:A:313:ARG:HA	2.44	0.47
1:C:58:GLU:HG2	1:C:77:ARG:HB2	1.97	0.47
1:B:57:TRP:CZ3	1:C:39:ILE:HD12	2.50	0.47
1:A:16:LYS:HE3	1:A:36:TYR:HE1	1.80	0.47
1:A:82:GLY:O	1:A:83:LEU:HD23	2.15	0.47
1:B:235:MET:O	1:B:237:ILE:HD13	2.14	0.47
1:A:127:MET:HE3	1:A:127:MET:HB3	1.78	0.47
1:B:320:ASN:CB	1:B:323:SER:OG	2.60	0.47
1:A:95:ARG:NH2	1:B:67:GLU:HG3	2.29	0.46
1:C:321:ASP:O	1:C:323:SER:N	2.48	0.46
1:A:93:TYR:CE1	1:A:133:GLY:HA2	2.50	0.46
1:B:100:VAL:HB	1:B:127:MET:O	2.15	0.46
1:A:76:VAL:HG12	1:B:61:THR:HB	1.94	0.46
1:C:240:ASN:HB3	1:C:243:THR:O	2.15	0.46
1:B:99:ILE:O	1:B:100:VAL:C	2.53	0.46
1:A:165:ILE:N	1:A:168:GLN:HE21	2.14	0.46
1:C:241:THR:OG1	1:C:323:SER:CB	2.63	0.46
1:C:88:VAL:HG22	1:C:88:VAL:O	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:320:ASN:ND2	1:B:322:TYR:H	2.02	0.46
1:C:40:GLY:HA3	1:C:57:TRP:O	2.16	0.46
1:B:75:LEU:HA	1:C:70:GLN:NE2	2.31	0.46
1:C:88:VAL:O	1:C:88:VAL:CG2	2.64	0.46
1:A:147:ASP:N	1:A:147:ASP:OD1	2.49	0.46
1:A:70:GLN:NE2	1:C:76:VAL:H	2.14	0.46
1:A:226:ALA:HB3	1:A:258:VAL:HG13	1.98	0.46
1:B:201:ASP:O	1:B:202:ARG:C	2.53	0.46
1:C:252:THR:CG2	1:C:278:GLY:HA2	2.46	0.46
1:A:232:THR:HG21	1:A:236:SER:OG	2.16	0.46
1:C:71:GLN:HE21	1:C:71:GLN:HB3	1.62	0.46
1:C:151:PHE:HA	1:C:177:MET:HA	1.98	0.45
1:B:108:ASP:HA	1:B:114:SER:HB2	1.98	0.45
1:C:17:ALA:N	1:C:339:TYR:O	2.45	0.45
1:A:35:THR:HB	1:A:63:ALA:HB3	1.99	0.45
1:A:108:ASP:HA	1:A:114:SER:HB2	1.98	0.45
1:C:16:LYS:CB	1:C:340:GLN:CB	2.94	0.45
1:C:46:GLN:HA	1:C:52:THR:HG22	1.98	0.45
1:A:309:TRP:C	1:A:309:TRP:CD1	2.90	0.45
1:A:320:ASN:HB2	1:A:323:SER:OG	2.16	0.45
1:A:290:LEU:C	1:A:317:LEU:HD11	2.37	0.45
1:C:189:ALA:N	1:C:213:ALA:O	2.50	0.45
1:A:113:PHE:CD2	1:A:311:ASP:OD1	2.69	0.45
1:C:262:GLN:NE2	1:C:268:ARG:HD2	2.31	0.45
1:A:295:GLN:HG2	1:A:296:ALA:O	2.16	0.45
1:B:125:ASN:O	1:B:126:TYR:HD2	1.97	0.44
1:B:164:SER:O	1:B:168:GLN:HG3	2.18	0.44
1:B:99:ILE:H	1:B:154:GLN:NE2	2.14	0.44
1:C:23:TRP:HZ3	1:C:335:VAL:HG12	1.81	0.44
1:A:51:LEU:HD12	1:A:84:LYS:O	2.16	0.44
1:B:110:ALA:C	1:B:112:TYR:N	2.71	0.44
1:C:112:TYR:O	1:C:113:PHE:HB2	2.18	0.44
1:A:98:GLY:HA3	1:A:127:MET:O	2.17	0.44
1:B:153:ILE:C	1:B:153:ILE:HD13	2.37	0.44
1:C:142:PHE:O	1:C:145:LEU:HB2	2.18	0.44
1:A:100:VAL:HG12	1:A:100:VAL:O	2.17	0.44
1:B:57:TRP:CD1	1:C:37:ALA:HB3	2.52	0.44
1:A:291:ALA:HA	1:A:317:LEU:CD1	2.43	0.44
1:A:238:VAL:HG13	1:A:325:SER:HB3	2.00	0.44
1:B:170:GLY:HA3	1:B:194:LYS:O	2.17	0.43
1:B:301:TYR:HD1	1:B:307:ASN:HB2	1.83	0.43
1:B:18:VAL:O	1:B:35:THR:HG23	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:139:ASN:O	1:C:150:SER:HB2	2.18	0.43
1:A:117:THR:HG22	1:A:118:TRP:H	1.81	0.43
1:A:263:PHE:HB2	1:A:265:PHE:CD2	2.53	0.43
1:A:275:GLN:HA	1:A:291:ALA:O	2.17	0.43
1:B:225:LEU:N	1:B:225:LEU:HD23	2.32	0.43
1:C:313:ARG:HH12	1:C:327:VAL:HG22	1.84	0.43
1:B:320:ASN:HD22	1:B:321:ASP:N	2.17	0.43
1:B:47:ILE:H	1:B:47:ILE:HG13	1.54	0.43
1:C:129:SER:O	1:C:130:ARG:O	2.37	0.43
1:A:295:GLN:CD	1:A:295:GLN:C	2.77	0.43
1:B:93:TYR:CG	1:B:94:GLY:N	2.85	0.43
1:C:100:VAL:CG2	1:C:191:SER:HB3	2.49	0.43
1:A:146:VAL:C	1:A:148:GLY:H	2.22	0.43
1:A:305:ASN:O	1:A:306:MET:HG2	2.17	0.43
1:C:212:ARG:HE	1:C:233:ARG:HH11	1.66	0.43
1:B:110:ALA:C	1:B:112:TYR:H	2.21	0.43
1:C:113:PHE:HZ	1:C:332:GLN:HG2	1.82	0.43
1:A:21:HIS:CE1	1:A:31:ASN:HD21	2.37	0.43
1:C:218:TYR:CZ	1:C:220:ALA:HB3	2.54	0.43
1:C:33:ASP:OD2	1:C:35:THR:N	2.51	0.43
1:B:113:PHE:CD2	1:B:311:ASP:OD1	2.71	0.43
1:A:163:HIS:HB3	1:A:167:SER:HG	1.80	0.43
1:C:304:LYS:O	1:C:340:GLN:NE2	2.52	0.43
1:B:139:ASN:HD21	1:B:143:PHE:N	2.16	0.42
1:A:139:ASN:O	1:A:150:SER:HA	2.19	0.42
1:B:204:GLY:CA	1:B:250:ASN:HD21	2.32	0.42
1:B:86:ALA:C	1:B:88:VAL:H	2.22	0.42
1:C:292:LYS:HG2	1:C:316:LEU:HB2	2.01	0.42
1:A:70:GLN:HE21	1:C:76:VAL:H	1.66	0.42
1:B:131:ALA:HB3	1:B:134:LEU:HD11	2.02	0.42
1:B:262:GLN:HG3	1:B:263:PHE:N	2.34	0.42
1:C:281:LEU:HD22	1:C:286:GLY:HA2	2.01	0.42
1:B:250:ASN:O	1:B:251:LYS:C	2.58	0.42
1:A:100:VAL:HA	1:A:189:ALA:HB1	2.00	0.42
1:A:318:ASP:O	1:A:329:THR:HG23	2.20	0.42
1:B:62:LYS:HB2	1:B:73:SER:HB3	2.00	0.42
1:C:98:GLY:HA3	1:C:127:MET:C	2.39	0.42
1:A:229:TYR:HD1	1:A:255:LEU:HB2	1.85	0.42
1:B:112:TYR:O	1:B:113:PHE:CD2	2.71	0.42
1:B:109:MET:HB2	1:B:260:GLN:NE2	2.35	0.42
1:C:151:PHE:HA	1:C:176:THR:O	2.19	0.42
1:A:295:GLN:O	1:A:295:GLN:CD	2.58	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:199:GLN:C	1:B:201:ASP:N	2.73	0.42
1:B:219:ASP:OD1	1:B:219:ASP:O	2.38	0.42
1:B:83:LEU:HD21	1:C:302:PHE:CE2	2.54	0.42
1:A:141:ASP:CG	1:A:144:GLY:HA2	2.40	0.41
1:A:242:VAL:HG23	1:A:243:THR:H	1.85	0.41
1:A:303:ASN:O	1:A:304:LYS:C	2.59	0.41
1:A:232:THR:HB	1:A:252:THR:HB	2.03	0.41
1:B:156:GLN:HE21	1:B:156:GLN:HB3	1.61	0.41
1:B:205:ASN:HA	1:B:205:ASN:HD22	1.69	0.41
1:A:117:THR:O	1:A:326:TYR:CZ	2.73	0.41
1:B:209:ALA:CB	1:B:234:ASN:HB3	2.51	0.41
1:B:257:VAL:CG1	1:B:273:TYR:HB3	2.49	0.41
1:A:45:THR:HG21	1:B:306:MET:HB2	2.03	0.41
1:B:18:VAL:HG13	1:B:338:THR:HB	2.01	0.41
1:C:211:SER:HB3	1:C:235:MET:SD	2.61	0.41
1:C:303:ASN:O	1:C:305:ASN:N	2.53	0.41
1:C:23:TRP:CZ3	1:C:335:VAL:HG12	2.55	0.41
1:A:240:ASN:HD22	1:A:241:THR:N	2.18	0.41
1:B:175:TYR:CD2	1:B:175:TYR:N	2.88	0.41
1:C:254:ASN:ND2	1:C:276:SER:OG	2.53	0.41
1:C:20:ARG:NH1	1:C:36:TYR:CD2	2.89	0.41
1:B:75:LEU:CB	1:C:70:GLN:NE2	2.83	0.41
1:A:150:SER:O	1:A:178:ALA:N	2.53	0.41
1:A:313:ARG:HD2	1:A:315:ASN:HB2	2.02	0.41
1:B:75:LEU:CA	1:C:70:GLN:NE2	2.84	0.41
1:C:5:ASN:C	1:C:5:ASN:HD22	2.23	0.41
1:A:87:GLU:HB3	1:A:143:PHE:C	2.41	0.41
1:A:66:ALA:HB2	1:C:163:HIS:HD2	1.85	0.41
1:B:61:THR:HG22	1:B:74:ASN:HB3	2.02	0.41
1:B:86:ALA:O	1:B:88:VAL:N	2.51	0.41
1:A:68:GLY:HA2	1:C:75:LEU:HD21	2.02	0.41
1:A:139:ASN:OD1	1:A:142:PHE:HA	2.21	0.41
1:A:204:GLY:HA2	1:A:250:ASN:CG	2.41	0.41
1:A:281:LEU:N	1:A:286:GLY:O	2.47	0.41
1:C:261:TYR:HE2	1:C:263:PHE:CD2	2.39	0.41
1:B:124:ASP:HB2	1:C:66:ALA:HB1	2.03	0.41
1:A:195:ARG:HH21	1:A:248:MET:CB	2.33	0.41
1:A:302:PHE:HB3	1:C:47:ILE:HG23	2.02	0.41
1:A:313:ARG:NH2	1:A:332:GLN:OE1	2.53	0.41
1:A:77:ARG:O	1:A:95:ARG:HG2	2.20	0.41
1:B:237:ILE:HG22	1:B:246:VAL:HG12	2.02	0.41
1:B:47:ILE:O	1:B:48:ASN:HB3	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:261:TYR:O	1:A:269:PRO:HD2	2.21	0.41
1:C:107:THR:O	1:C:258:VAL:HG21	2.21	0.41
1:B:301:TYR:HD1	1:B:307:ASN:CB	2.34	0.40
1:C:267:LEU:HD12	1:C:269:PRO:HD3	2.04	0.40
1:A:170:GLY:O	1:A:171:ASP:C	2.60	0.40
1:A:46:GLN:NE2	1:A:46:GLN:HA	2.36	0.40
1:B:294:ILE:HB	1:B:314:PHE:HB2	2.04	0.40
1:B:58:GLU:HB3	1:B:77:ARG:HB2	2.04	0.40
1:A:122:TYR:CE2	1:A:237:ILE:HB	2.56	0.40
1:A:165:ILE:H	1:A:168:GLN:HE21	1.68	0.40
1:B:288:ALA:HB1	1:B:320:ASN:HD21	1.86	0.40
1:C:108:ASP:HA	1:C:114:SER:HB2	2.03	0.40
1:C:231:GLU:OE2	1:C:233:ARG:NH1	2.54	0.40
1:A:202:ARG:HD3	1:A:202:ARG:HA	1.93	0.40
1:A:224:TYR:O	1:A:259:ALA:HA	2.22	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	336/341 (98%)	266 (79%)	52 (16%)	18 (5%)	3	20
1	B	336/341 (98%)	271 (81%)	49 (15%)	16 (5%)	4	23
1	C	336/341 (98%)	271 (81%)	45 (13%)	20 (6%)	2	17
All	All	1008/1023 (98%)	808 (80%)	146 (14%)	54 (5%)	3	20

All (54) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	SER
1	A	165	ILE
1	A	202	ARG
1	B	9	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	112	TYR
1	B	113	PHE
1	B	126	TYR
1	B	251	LYS
1	B	323	SER
1	C	9	ASN
1	C	49	THR
1	C	113	PHE
1	C	124	ASP
1	C	142	PHE
1	C	251	LYS
1	C	265	PHE
1	C	304	LYS
1	A	5	ASN
1	A	166	ASN
1	A	182	ASP
1	A	264	ASP
1	A	304	LYS
1	A	318	ASP
1	B	2	GLU
1	B	27	GLY
1	B	202	ARG
1	B	206	GLY
1	B	284	ALA
1	C	6	LYS
1	C	35	THR
1	C	122	TYR
1	C	285	GLY
1	A	4	TYR
1	A	171	ASP
1	A	303	ASN
1	B	32	ALA
1	B	87	GLU
1	B	207	ASP
1	C	126	TYR
1	C	130	ARG
1	C	221	ASN
1	A	49	THR
1	A	68	GLY
1	B	222	ASN
1	C	182	ASP
1	C	323	SER

Continued from previous page...

Mol	Chain	Res	Type
1	A	283	GLY
1	C	244	ASP
1	A	198	ASP
1	A	244	ASP
1	C	206	GLY
1	C	286	GLY
1	A	88	VAL
1	B	100	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	237/272 (87%)	177 (75%)	60 (25%)	1	3
1	B	254/272 (93%)	199 (78%)	55 (22%)	1	6
1	C	239/272 (88%)	191 (80%)	48 (20%)	2	8
All	All	730/816 (90%)	567 (78%)	163 (22%)	1	6

All (163) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	4	TYR
1	A	5	ASN
1	A	11	LEU
1	A	12	ASP
1	A	20	ARG
1	A	24	THR
1	A	31	ASN
1	A	46	GLN
1	A	49	THR
1	A	50	ASP
1	A	58	GLU
1	A	61	THR
1	A	70	GLN
1	A	71	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	75	LEU
1	A	76	VAL
1	A	87	GLU
1	A	95	ARG
1	A	99	ILE
1	A	107	THR
1	A	116	GLU
1	A	117	THR
1	A	123	THR
1	A	127	MET
1	A	146	VAL
1	A	147	ASP
1	A	156	GLN
1	A	163	HIS
1	A	164	SER
1	A	169	ASN
1	A	180	GLU
1	A	190	TYR
1	A	192	ASN
1	A	193	SER
1	A	198	ASP
1	A	200	GLN
1	A	201	ASP
1	A	202	ARG
1	A	211	SER
1	A	214	VAL
1	A	238	VAL
1	A	240	ASN
1	A	245	THR
1	A	248	MET
1	A	255	LEU
1	A	257	VAL
1	A	264	ASP
1	A	265	PHE
1	A	267	LEU
1	A	271	ILE
1	A	275	GLN
1	A	282	ASN
1	A	295	GLN
1	A	309	TRP
1	A	313	ARG
1	A	317	LEU

Continued from previous page...

Mol	Chain	Res	Type
1	A	324	SER
1	A	335	VAL
1	A	340	GLN
1	B	2	GLU
1	B	20	ARG
1	B	24	THR
1	B	30	LYS
1	B	39	ILE
1	B	47	ILE
1	B	54	PHE
1	B	69	GLU
1	B	71	GLN
1	B	72	ASN
1	B	73	SER
1	B	74	ASN
1	B	75	LEU
1	B	76	VAL
1	B	85	TYR
1	B	91	ILE
1	B	95	ARG
1	B	102	ASP
1	B	103	VAL
1	B	112	TYR
1	B	123	THR
1	B	125	ASN
1	B	127	MET
1	B	135	LEU
1	B	136	THR
1	B	153	ILE
1	B	156	GLN
1	B	162	ASN
1	B	173	VAL
1	B	175	TYR
1	B	181	PHE
1	B	182	ASP
1	B	186	VAL
1	B	193	SER
1	B	200	GLN
1	B	212	ARG
1	B	222	ASN
1	B	225	LEU
1	B	237	ILE

Continued from previous page...

Mol	Chain	Res	Type
1	B	247	GLU
1	B	254	ASN
1	B	256	GLU
1	B	275	GLN
1	B	276	SER
1	B	287	SER
1	B	289	ASP
1	B	310	VAL
1	B	311	ASP
1	B	312	TYR
1	B	315	ASN
1	B	317	LEU
1	B	318	ASP
1	B	320	ASN
1	B	327	VAL
1	B	329	THR
1	C	3	ILE
1	C	5	ASN
1	C	25	THR
1	C	26	THR
1	C	46	GLN
1	C	49	THR
1	C	56	GLN
1	C	65	ARG
1	C	67	GLU
1	C	71	GLN
1	C	80	PHE
1	C	104	GLU
1	C	116	GLU
1	C	124	ASP
1	C	127	MET
1	C	136	THR
1	C	145	LEU
1	C	153	ILE
1	C	160	GLN
1	C	171	ASP
1	C	173	VAL
1	C	199	GLN
1	C	205	ASN
1	C	212	ARG
1	C	222	ASN
1	C	225	LEU

Continued from previous page...

Mol	Chain	Res	Type
1	C	233	ARG
1	C	235	MET
1	C	239	GLU
1	C	241	THR
1	C	248	MET
1	C	252	THR
1	C	262	GLN
1	C	264	ASP
1	C	267	LEU
1	C	275	GLN
1	C	303	ASN
1	C	310	VAL
1	C	315	ASN
1	C	317	LEU
1	C	319	GLU
1	C	320	ASN
1	C	322	TYR
1	C	327	VAL
1	C	329	THR
1	C	337	ILE
1	C	338	THR
1	C	340	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	HIS
1	A	46	GLN
1	A	70	GLN
1	A	71	GLN
1	A	159	ASN
1	A	160	GLN
1	A	168	GLN
1	A	192	ASN
1	A	197	ASN
1	A	240	ASN
1	A	305	ASN
1	A	315	ASN
1	B	21	HIS
1	B	31	ASN
1	B	71	GLN
1	B	72	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	74	ASN
1	B	139	ASN
1	B	156	GLN
1	B	162	ASN
1	B	166	ASN
1	B	168	GLN
1	B	205	ASN
1	B	222	ASN
1	B	254	ASN
1	B	260	GLN
1	B	275	GLN
1	B	295	GLN
1	B	303	ASN
1	B	320	ASN
1	C	5	ASN
1	C	46	GLN
1	C	48	ASN
1	C	56	GLN
1	C	70	GLN
1	C	71	GLN
1	C	72	ASN
1	C	74	ASN
1	C	156	GLN
1	C	159	ASN
1	C	163	HIS
1	C	166	ASN
1	C	169	ASN
1	C	254	ASN
1	C	262	GLN
1	C	315	ASN
1	C	340	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

2 ligands are modelled in this entry.

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	#$|Z| > 2$
2	DM1	C	401[A]	-	10,10,42	1.37	1 (10%)	12,14,66	0.81	0
2	DM1	C	401[B]	-	10,10,42	1.44	1 (10%)	12,14,66	2.01	3 (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
2	DM1	C	401[A]	-	-	0/0/16/58	0/1/1/5
2	DM1	C	401[B]	-	-	0/0/16/58	0/1/1/5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401[A]	DM1	O10-C1'	4.01	1.43	1.23
2	C	401[B]	DM1	O10-C1'	3.86	1.42	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	401[B]	DM1	C2'-C3'-C4'	-4.87	102.74	110.13
2	C	401[B]	DM1	C1'-C2'-C3'	-2.48	106.75	111.89
2	C	401[B]	DM1	C5'-C4'-C3'	-2.02	106.14	110.07

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers (i)

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(Å²)	Q<0.9
1	A	340/341 (99%)	-0.07	1 (0%)	91	53	56, 88, 104, 112	0
1	B	340/341 (99%)	-0.08	1 (0%)	91	53	56, 81, 96, 106	0
1	C	340/341 (99%)	-0.05	1 (0%)	91	53	54, 84, 101, 111	0
All	All	1020/1023 (99%)	-0.07	3 (0%)	90	53	54, 84, 103, 112	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	6	LYS	2.4
1	C	182	ASP	2.1
1	B	25	THR	2.0

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

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

6.3　Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4　Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors($Å^2$)	Q<0.9
2	DM1	C	401[B]	10/38	0.35	1.30	121,122,122,122	10
2	DM1	C	401[A]	10/38	0.35	1.30	122,122,123,123	10

6.5　Other polymers　ⓘ

There are no such residues in this entry.