



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:10 PM GMT

PDB ID : 4KRA
Title : Salmonella typhi OmpF complex with Ciprofloxacin
Authors : Madhuranayaki, T.; Balasubramaniam, D.; Krishnaswamy, S.
Deposited on : 2013-05-16
Resolution : 3.32 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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

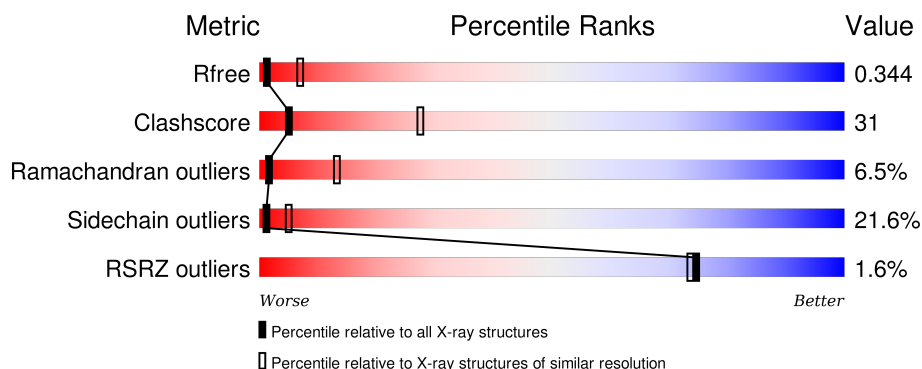
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.32 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}	91344	1198 (3.40-3.24)
Clashscore	102246	1280 (3.40-3.24)
Ramachandran outliers	100387	1260 (3.40-3.24)
Sidechain outliers	100360	1259 (3.40-3.24)
RSRZ outliers	91569	1203 (3.40-3.24)

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	341	<div> <div>45%</div> <div>43%</div> <div>12%</div> <div>.</div> </div>
1	B	341	<div> <div>2%</div> <div>47%</div> <div>40%</div> <div>12%</div> <div>.</div> </div>
1	C	341	<div> <div>2%</div> <div>46%</div> <div>41%</div> <div>11%</div> <div>..</div> </div>

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
2	CPF	C	401	-	-	X	-

2 Entry composition [i](#)

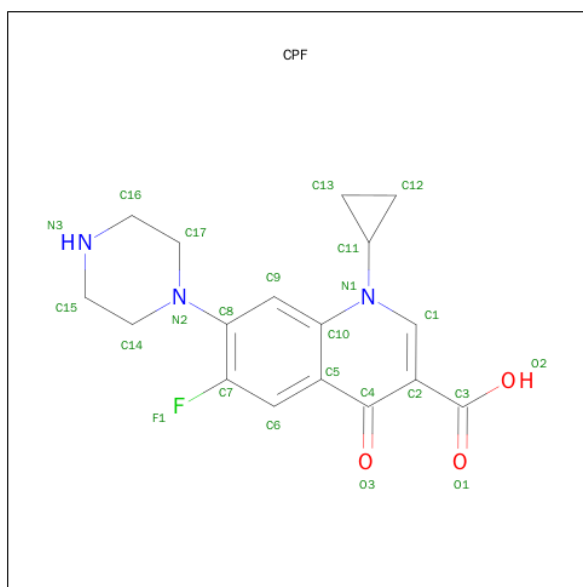
There are 2 unique types of molecules in this entry. The entry contains 7690 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Outer membrane protein F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	341	Total	C	N	O	S	0	0	0
			2537	1571	430	530	6			
1	B	340	Total	C	N	O	S	0	0	0
			2557	1592	430	529	6			
1	C	337	Total	C	N	O	S	0	0	0
			2572	1601	427	537	7			

- Molecule 2 is 1-CYCLOPROPYL-6-FLUORO-4-OXO-7-PIPERAZIN-1-YL-1,4-DIHYDRO QUINOLINE-3-CARBOXYLIC ACID (three-letter code: CPF) (formula: C₁₇H₁₈FN₃O₃).

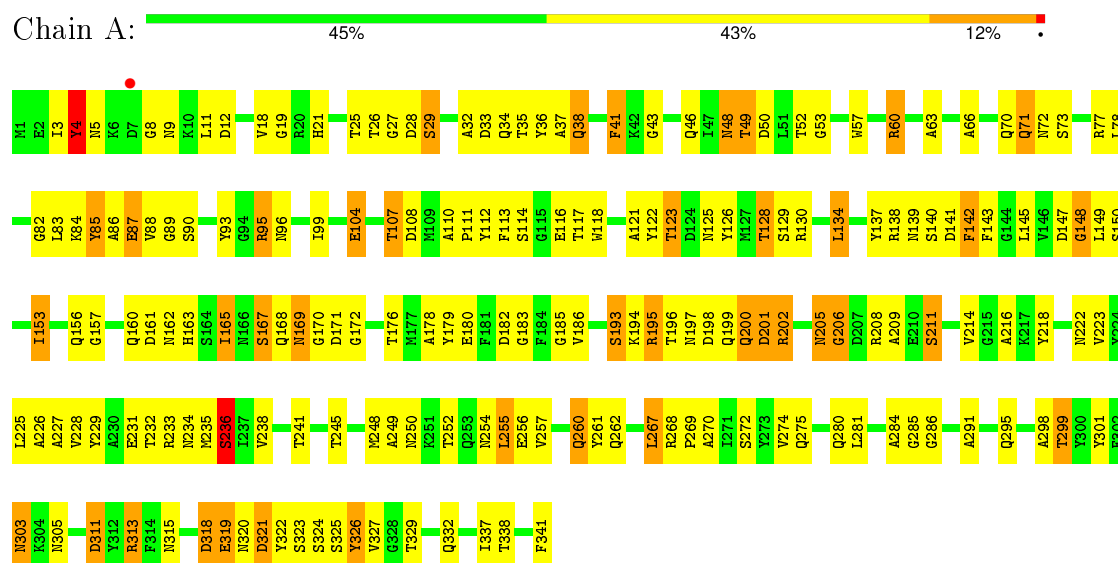


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	F	N	O	0	0
			24	17	1	3	3		

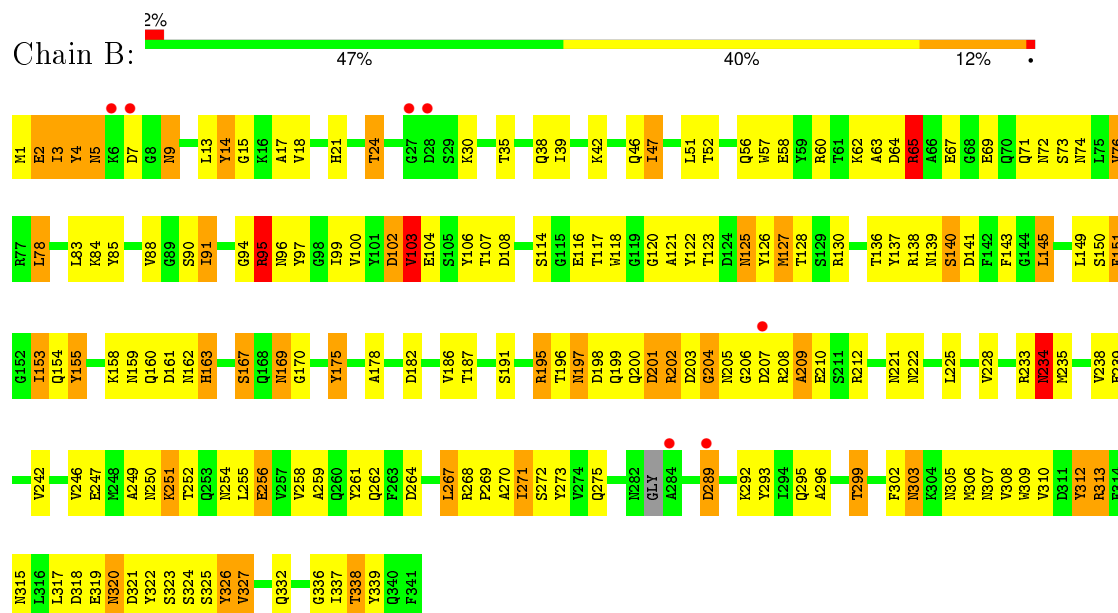
3 Residue-property plots

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.

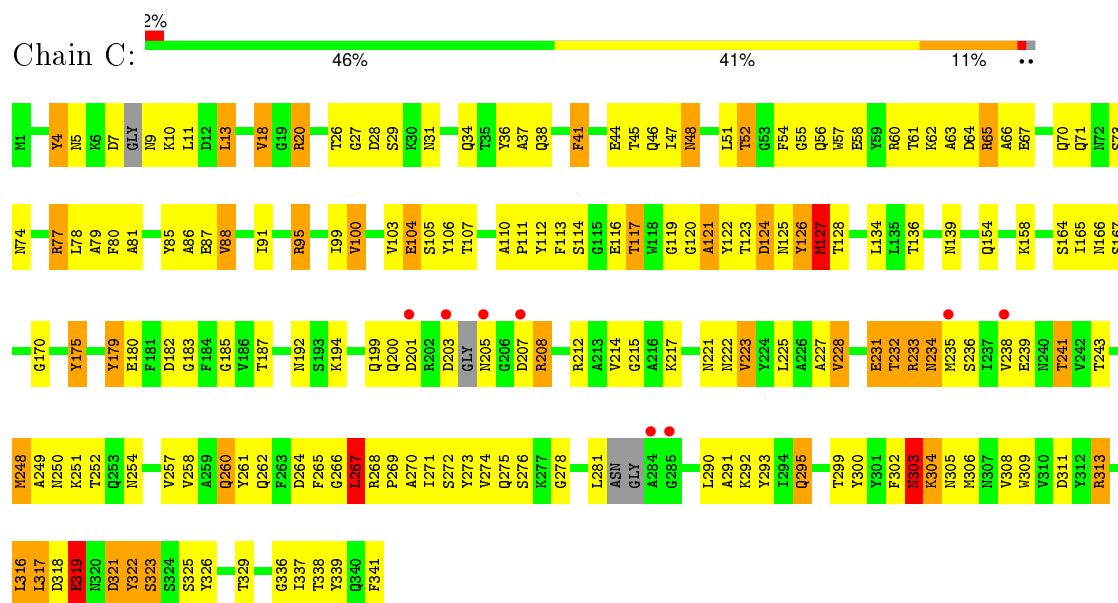
• Molecule 1: Outer membrane protein F



• Molecule 1: Outer membrane protein F



● Molecule 1: Outer membrane protein F



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	85.16Å 139.11Å 151.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.32 43.36 – 3.32	Depositor EDS
% Data completeness (in resolution range)	99.7 (50.00-3.32) 99.7 (43.36-3.32)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.33 (at 3.32Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.272 , 0.339 0.276 , 0.344	Depositor DCC
R_{free} test set	1365 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	89.8	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 44.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 27136 reflections	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	7690	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0/2588	0.70	0/3519
1	B	0.59	0/2609	0.73	0/3549
1	C	0.59	0/2623	0.72	1/3560 (0.0%)
All	All	0.58	0/7820	0.72	1/10628 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	267	LEU	CA-CB-CG	5.24	127.35	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2537	0	2170	139	0
1	B	2557	0	2223	173	0
1	C	2572	0	2250	151	0
2	C	24	0	17	13	0
All	All	7690	0	6660	444	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 31.

All (444) 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:B:3:ILE:HG22	1:B:4:TYR:H	1.02	1.11
1:A:168:GLN:HB3	1:A:196:THR:HG21	1.37	1.07
1:C:77:ARG:HG2	1:C:77:ARG:HH11	0.90	1.07
1:B:178:ALA:HA	1:B:187:THR:HG22	1.33	1.07
1:B:233:ARG:O	1:B:234:ASN:HB2	1.47	1.06
1:B:139:ASN:HB3	1:B:151:PHE:CE2	1.93	1.03
1:B:139:ASN:HB3	1:B:151:PHE:HE2	1.24	1.02
1:C:77:ARG:NH1	1:C:77:ARG:HG2	1.66	1.01
1:B:320:ASN:OD1	1:B:321:ASP:N	1.96	0.98
1:B:140:SER:O	1:B:150:SER:HB3	1.63	0.97
1:B:3:ILE:HG22	1:B:4:TYR:N	1.82	0.93
1:A:107:THR:HG21	1:A:228:VAL:HG12	1.51	0.91
1:C:41:PHE:O	1:C:41:PHE:HD1	1.52	0.91
1:B:126:TYR:CE1	1:B:169:ASN:HB2	2.05	0.91
1:A:140:SER:HA	1:A:150:SER:HB3	1.50	0.90
1:A:60:ARG:HE	1:A:77:ARG:HH11	1.18	0.89
1:C:103:VAL:HG12	1:C:228:VAL:HG21	1.52	0.89
1:C:100:VAL:HG23	1:C:127:MET:O	1.73	0.89
1:B:159:ASN:HB2	1:B:169:ASN:ND2	1.90	0.87
1:B:160:GLN:HG2	1:B:161:ASP:H	1.37	0.87
1:B:158:LYS:HG3	1:B:170:GLY:HA2	1.56	0.86
2:C:401:CPF:C13	2:C:401:CPF:H9	2.01	0.86
1:B:42:LYS:HG3	1:B:56:GLN:HG3	1.58	0.86
1:B:15:GLY:HA3	1:B:39:ILE:HD12	1.58	0.85
1:B:234:ASN:HA	1:B:249:ALA:O	1.77	0.85
1:A:89:GLY:HA3	1:A:137:TYR:HE1	1.38	0.84
1:C:208:ARG:HH21	1:C:208:ARG:HG3	1.42	0.84
1:A:170:GLY:HA3	1:A:194:LYS:O	1.78	0.84
1:A:325:SER:O	1:A:326:TYR:HB2	1.78	0.82
1:B:18:VAL:HG13	1:B:338:THR:HB	1.60	0.82
1:A:60:ARG:NE	1:A:77:ARG:NH1	2.28	0.81
1:A:267:LEU:HD11	1:A:298:ALA:HB1	1.61	0.81
1:A:66:ALA:HB1	1:C:124:ASP:OD1	1.79	0.81
1:B:303:ASN:HB3	1:B:305:ASN:H	1.47	0.80
1:B:139:ASN:CB	1:B:151:PHE:HE2	1.95	0.80
1:B:210:GLU:HG2	1:B:233:ARG:HB2	1.63	0.80
1:A:60:ARG:HE	1:A:77:ARG:NH1	1.80	0.79
1:B:313:ARG:NH2	1:B:327:VAL:HG21	1.99	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:ILE:CG2	1:B:4:TYR:H	1.86	0.78
1:B:272:SER:OG	1:B:295:GLN:HG3	1.84	0.77
1:B:195:ARG:NH2	1:B:199:GLN:HA	1.99	0.77
1:B:258:VAL:HG13	1:B:272:SER:HB3	1.64	0.77
1:A:183:GLY:HA3	1:A:218:TYR:CE1	2.19	0.77
1:A:313:ARG:O	1:A:313:ARG:HG3	1.84	0.76
1:C:116:GLU:HA	2:C:401:CPF:C16	2.16	0.76
1:C:36:TYR:HB2	1:C:61:THR:O	1.85	0.76
1:A:60:ARG:NE	1:A:77:ARG:HH11	1.82	0.76
1:C:77:ARG:HH11	1:C:77:ARG:CG	1.83	0.76
1:A:3:ILE:O	1:A:4:TYR:HB2	1.83	0.76
1:A:89:GLY:HA3	1:A:137:TYR:CE1	2.20	0.76
1:B:289:ASP:O	1:B:320:ASN:ND2	2.19	0.75
1:C:57:TRP:HA	1:C:78:LEU:O	1.87	0.74
1:A:165:ILE:H	1:A:165:ILE:HD12	1.52	0.74
1:B:1:MET:H1	1:B:14:TYR:HB3	1.53	0.74
1:C:192:ASN:HD21	1:C:208:ARG:HD3	1.51	0.74
1:B:307:ASN:OD1	1:B:338:THR:HG23	1.87	0.73
1:C:233:ARG:O	1:C:234:ASN:HB2	1.89	0.73
1:C:262:GLN:HB2	1:C:268:ARG:NH1	2.05	0.72
1:C:264:ASP:OD2	1:C:265:PHE:HD2	1.72	0.72
1:B:88:VAL:HG12	1:B:88:VAL:O	1.88	0.72
1:B:267:LEU:HD12	1:B:268:ARG:H	1.56	0.71
1:B:326:TYR:O	1:B:327:VAL:CG2	2.38	0.71
1:B:76:VAL:H	1:C:70:GLN:HE22	1.36	0.71
1:B:326:TYR:O	1:B:327:VAL:HG22	1.91	0.71
1:A:142:PHE:CD1	1:A:149:LEU:HD23	2.26	0.70
1:A:33:ASP:OD1	1:A:34:GLN:N	2.24	0.70
1:A:195:ARG:HH21	1:A:248:MET:HG3	1.56	0.70
1:A:18:VAL:HG22	1:A:338:THR:HG23	1.73	0.70
1:C:95:ARG:NH2	1:C:124:ASP:OD2	2.24	0.70
1:C:322:TYR:O	1:C:323:SER:O	2.10	0.70
2:C:401:CPF:C13	2:C:401:CPF:C9	2.70	0.70
1:C:127:MET:CE	1:C:154:GLN:HG3	2.22	0.69
1:A:232:THR:OG1	1:A:252:THR:HB	1.91	0.69
1:C:46:GLN:NE2	1:C:52:THR:HG23	2.07	0.69
1:A:19:GLY:HA2	1:A:35:THR:HG23	1.75	0.69
1:A:222:ASN:HB3	1:A:262:GLN:O	1.92	0.69
1:C:116:GLU:OE1	1:C:313:ARG:NH1	2.26	0.69
1:B:239:GLU:HG2	1:B:325:SER:OG	1.92	0.69
1:B:24:THR:HG22	1:B:30:LYS:H	1.58	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:116:GLU:HA	2:C:401:CPF:C17	2.23	0.69
1:A:107:THR:HG21	1:A:228:VAL:CG1	2.22	0.69
1:C:60:ARG:NH2	2:C:401:CPF:O1	2.26	0.68
1:B:139:ASN:HD21	1:B:143:PHE:N	1.91	0.68
1:C:208:ARG:HH21	1:C:208:ARG:CG	2.06	0.68
1:B:313:ARG:HG2	1:B:332:GLN:H	1.58	0.68
1:B:199:GLN:O	1:B:203:ASP:HB3	1.94	0.68
1:A:195:ARG:HD2	1:A:209:ALA:HB2	1.74	0.68
1:B:273:TYR:CE2	1:B:275:GLN:HB2	2.30	0.67
1:C:46:GLN:HE22	1:C:52:THR:HG23	1.60	0.67
1:A:108:ASP:HA	1:A:114:SER:OG	1.95	0.67
1:B:62:LYS:HB3	1:B:64:ASP:OD1	1.94	0.67
1:C:41:PHE:O	1:C:41:PHE:CD1	2.42	0.67
1:B:273:TYR:HE2	1:B:275:GLN:HB2	1.59	0.67
1:A:257:VAL:O	1:A:272:SER:HB2	1.95	0.66
1:C:38:GLN:HG3	1:C:60:ARG:HB2	1.77	0.66
1:C:319:GLU:HG2	1:C:329:THR:HG21	1.78	0.66
1:B:233:ARG:O	1:B:234:ASN:CB	2.34	0.66
1:B:83:LEU:O	1:B:90:SER:HB2	1.95	0.66
1:C:103:VAL:CG1	1:C:228:VAL:HG21	2.25	0.66
1:C:104:GLU:HG3	1:C:119:GLY:HA3	1.78	0.65
1:C:36:TYR:CD1	1:C:60:ARG:HG3	2.32	0.65
1:C:13:LEU:O	1:C:13:LEU:HG	1.95	0.65
1:C:77:ARG:NH1	1:C:77:ARG:CG	2.49	0.65
1:B:58:GLU:HB2	1:B:78:LEU:HD12	1.77	0.65
1:C:121:ALA:H	2:C:401:CPF:H171	1.60	0.65
1:C:20:ARG:NH2	1:C:112:TYR:HE1	1.94	0.65
1:B:76:VAL:N	1:C:70:GLN:HE22	1.94	0.65
1:C:241:THR:OG1	1:C:323:SER:HB2	1.97	0.64
1:B:116:GLU:O	1:B:121:ALA:HB2	1.97	0.63
1:C:227:ALA:HB2	1:C:257:VAL:HG23	1.79	0.63
1:B:100:VAL:HG23	1:B:127:MET:HB2	1.81	0.63
1:A:303:ASN:ND2	1:A:305:ASN:H	1.96	0.63
1:A:87:GLU:O	1:A:143:PHE:HA	1.99	0.62
1:B:309:TRP:CH2	1:B:336:GLY:HA3	2.33	0.62
1:B:178:ALA:CA	1:B:187:THR:HG22	2.21	0.62
1:B:15:GLY:HA3	1:B:39:ILE:CD1	2.29	0.62
1:A:267:LEU:HG	1:A:268:ARG:N	2.14	0.62
1:A:43:GLY:HA3	1:B:339:TYR:CE2	2.34	0.62
1:B:267:LEU:HD12	1:B:268:ARG:N	2.14	0.62
1:B:322:TYR:O	1:B:324:SER:N	2.31	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:252:THR:HG22	1:C:278:GLY:HA2	1.81	0.62
1:C:179:TYR:O	1:C:185:GLY:HA2	1.99	0.62
1:B:14:TYR:C	1:B:14:TYR:CD1	2.73	0.62
1:A:211:SER:OG	1:A:232:THR:HG22	2.00	0.62
1:A:162:ASN:HB2	1:B:65:ARG:HD2	1.81	0.61
1:A:60:ARG:NH2	1:A:77:ARG:HH12	1.98	0.61
1:C:106:TYR:CD2	1:C:217:LYS:HB3	2.35	0.61
1:B:107:THR:HG21	1:B:256:GLU:HB3	1.82	0.61
1:C:321:ASP:O	1:C:322:TYR:HB2	2.01	0.61
1:B:160:GLN:HG2	1:B:161:ASP:N	2.14	0.60
1:C:305:ASN:O	1:C:339:TYR:HD1	1.85	0.60
1:B:205:ASN:HB2	1:B:234:ASN:ND2	2.17	0.60
1:A:241:THR:HG22	1:A:321:ASP:O	2.01	0.60
1:B:108:ASP:HA	1:B:114:SER:HB2	1.83	0.60
1:B:117:THR:HG21	1:B:256:GLU:OE2	2.01	0.60
1:C:127:MET:HE3	1:C:154:GLN:HG3	1.84	0.60
1:A:26:THR:HG22	1:A:27:GLY:H	1.65	0.60
1:C:116:GLU:HA	2:C:401:CPF:H161	1.84	0.60
1:A:41:PHE:HZ	1:B:17:ALA:HB2	1.66	0.60
1:B:57:TRP:CD1	1:C:37:ALA:HB3	2.37	0.60
1:B:272:SER:OG	1:B:295:GLN:CG	2.49	0.59
1:C:9:ASN:HB3	1:C:45:THR:HA	1.84	0.59
1:A:96:ASN:HB3	1:A:134:LEU:HD12	1.82	0.59
1:C:215:GLY:HA3	1:C:228:VAL:HG23	1.85	0.59
1:B:1:MET:N	1:B:14:TYR:HB3	2.18	0.59
1:C:113:PHE:CE2	1:C:313:ARG:HB3	2.37	0.58
1:B:76:VAL:H	1:C:70:GLN:NE2	2.00	0.58
1:B:196:THR:O	1:B:198:ASP:N	2.37	0.58
1:B:103:VAL:O	1:B:106:TYR:HB2	2.04	0.58
1:B:1:MET:O	1:B:2:GLU:HB2	2.03	0.58
1:A:275:GLN:HA	1:A:291:ALA:O	2.04	0.58
1:C:121:ALA:H	2:C:401:CPF:C17	2.16	0.58
1:B:143:PHE:HB2	1:B:145:LEU:HD22	1.86	0.58
1:B:103:VAL:HG12	1:B:104:GLU:N	2.19	0.58
1:B:38:GLN:OE1	1:B:60:ARG:NE	2.36	0.58
1:C:110:ALA:HB3	1:C:114:SER:OG	2.04	0.58
1:C:302:PHE:O	1:C:303:ASN:HB3	2.03	0.58
1:A:60:ARG:CZ	1:A:77:ARG:HH12	2.17	0.57
1:A:156:GLN:HG2	1:A:157:GLY:N	2.18	0.57
1:B:175:TYR:N	1:B:175:TYR:CD2	2.72	0.57
1:C:260:GLN:HE21	1:C:270:ALA:HB1	1.68	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:TYR:O	1:A:269:PRO:HD2	2.05	0.57
1:B:155:TYR:HD2	1:B:155:TYR:N	2.03	0.57
1:B:196:THR:HG22	1:B:197:ASN:N	2.20	0.57
1:A:21:HIS:HD2	1:A:32:ALA:O	1.87	0.57
1:A:303:ASN:C	1:A:303:ASN:HD22	2.08	0.56
1:B:3:ILE:CG2	1:B:4:TYR:N	2.56	0.56
1:C:299:THR:HG23	1:C:309:TRP:HB3	1.88	0.56
1:B:200:GLN:OE1	1:B:200:GLN:N	2.38	0.56
1:C:20:ARG:NH1	1:C:34:GLN:HB3	2.20	0.56
1:A:71:GLN:O	1:A:72:ASN:HB2	2.04	0.56
2:C:401:CPF:C9	2:C:401:CPF:H132	2.36	0.56
1:B:103:VAL:CG1	1:B:104:GLU:N	2.69	0.56
1:B:139:ASN:HB3	1:B:151:PHE:CD2	2.41	0.56
1:C:264:ASP:OD2	1:C:265:PHE:CD2	2.57	0.56
1:B:155:TYR:N	1:B:155:TYR:CD2	2.73	0.56
1:B:99:ILE:N	1:B:154:GLN:OE1	2.39	0.56
1:A:325:SER:O	1:A:326:TYR:CB	2.54	0.55
1:B:137:TYR:HB3	1:B:153:ILE:HD13	1.88	0.55
1:C:4:TYR:HB2	1:C:11:LEU:H	1.71	0.55
1:B:275:GLN:HG3	1:B:292:LYS:HE2	1.88	0.55
1:B:259:ALA:O	1:B:271:ILE:HD12	2.06	0.55
1:C:121:ALA:N	2:C:401:CPF:H171	2.22	0.55
1:B:107:THR:HG23	1:B:228:VAL:HG13	1.87	0.55
1:A:200:GLN:C	1:A:202:ARG:H	2.09	0.55
1:A:113:PHE:HD1	1:A:116:GLU:OE1	1.90	0.55
1:A:113:PHE:HZ	1:A:332:GLN:HB3	1.72	0.54
1:A:172:GLY:HA2	1:A:193:SER:HA	1.89	0.54
1:A:165:ILE:H	1:A:165:ILE:CD1	2.15	0.54
1:C:103:VAL:CG1	1:C:228:VAL:CG2	2.85	0.54
1:A:121:ALA:O	1:A:122:TYR:HD2	1.89	0.54
1:A:57:TRP:HA	1:A:78:LEU:O	2.08	0.54
1:A:60:ARG:CZ	1:A:77:ARG:NH1	2.71	0.54
1:A:303:ASN:HD22	1:A:305:ASN:H	1.55	0.54
1:B:57:TRP:CD1	1:C:37:ALA:CB	2.91	0.54
1:B:136:THR:OG1	1:B:154:GLN:HG3	2.08	0.54
1:B:313:ARG:O	1:B:313:ARG:HG3	2.08	0.54
1:C:26:THR:HG22	1:C:27:GLY:H	1.73	0.54
1:A:85:TYR:HB3	1:A:88:VAL:HB	1.87	0.54
1:C:274:VAL:CG2	1:C:293:TYR:CZ	2.90	0.54
1:B:102:ASP:O	1:B:103:VAL:HB	2.07	0.53
1:A:48:ASN:HD22	1:A:49:THR:H	1.56	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:VAL:HG12	1:B:104:GLU:H	1.73	0.53
1:C:127:MET:HE2	1:C:154:GLN:HG3	1.91	0.53
1:B:57:TRP:NE1	1:C:37:ALA:HB3	2.23	0.53
1:B:14:TYR:C	1:B:14:TYR:HD1	2.10	0.53
1:A:169:ASN:O	1:A:196:THR:HG22	2.09	0.53
1:A:110:ALA:HB3	1:A:114:SER:HB2	1.90	0.53
1:C:273:TYR:CE2	1:C:275:GLN:HB2	2.43	0.53
1:B:18:VAL:O	1:B:35:THR:HG23	2.09	0.52
1:A:148:GLY:O	1:A:179:TYR:HA	2.10	0.52
1:C:55:GLY:HA2	1:C:80:PHE:O	2.08	0.52
1:C:231:GLU:HA	1:C:252:THR:O	2.09	0.52
1:C:275:GLN:HG3	1:C:292:LYS:HG3	1.90	0.52
1:B:325:SER:O	1:B:326:TYR:CG	2.62	0.52
1:A:121:ALA:C	1:A:122:TYR:HD2	2.12	0.52
1:B:9:ASN:ND2	1:B:46:GLN:HG3	2.24	0.52
1:A:323:SER:O	1:A:325:SER:N	2.42	0.52
1:A:235:MET:O	1:A:236:SER:HB2	2.09	0.52
1:C:304:LYS:HG3	1:C:305:ASN:HD22	1.73	0.52
1:C:113:PHE:CD2	1:C:311:ASP:OD2	2.62	0.52
1:C:56:GLN:O	1:C:79:ALA:HA	2.10	0.52
1:A:170:GLY:CA	1:A:194:LYS:O	2.56	0.52
1:A:26:THR:HG22	1:A:27:GLY:N	2.24	0.52
1:B:95:ARG:HB3	1:C:63:ALA:HB1	1.92	0.52
1:C:170:GLY:HA3	1:C:194:LYS:O	2.10	0.52
1:B:222:ASN:HB3	1:B:262:GLN:O	2.09	0.52
1:B:313:ARG:CG	1:B:332:GLN:H	2.21	0.51
1:B:140:SER:O	1:B:150:SER:CB	2.48	0.51
1:A:86:ALA:O	1:A:88:VAL:N	2.41	0.51
1:C:232:THR:HG21	1:C:236:SER:OG	2.10	0.51
1:C:260:GLN:HE21	1:C:270:ALA:CB	2.24	0.51
1:C:199:GLN:O	1:C:201:ASP:N	2.44	0.50
1:A:11:LEU:C	1:A:11:LEU:HD23	2.32	0.50
1:C:36:TYR:CD1	1:C:60:ARG:CG	2.95	0.50
1:C:238:VAL:HG23	1:C:325:SER:CB	2.42	0.50
1:A:216:ALA:O	1:A:226:ALA:HB1	2.10	0.50
1:A:126:TYR:OH	1:A:195:ARG:HA	2.12	0.50
1:A:337:ILE:HG23	1:C:81:ALA:HB3	1.93	0.50
1:B:308:VAL:HB	1:B:337:ILE:CD1	2.42	0.50
1:A:168:GLN:CB	1:A:196:THR:HG21	2.27	0.50
1:B:88:VAL:O	1:B:88:VAL:CG1	2.58	0.50
1:A:113:PHE:HZ	1:A:332:GLN:CB	2.24	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:ASP:OD2	1:B:246:VAL:HG23	2.12	0.50
1:B:120:GLY:C	1:B:122:TYR:H	2.15	0.49
1:B:318:ASP:O	1:B:320:ASN:N	2.46	0.49
1:B:312:TYR:HD1	1:B:313:ARG:N	2.11	0.49
1:C:48:ASN:C	1:C:48:ASN:HD22	2.15	0.49
1:A:111:PRO:HG2	1:A:311:ASP:OD2	2.11	0.49
1:A:160:GLN:HA	1:A:168:GLN:HG2	1.93	0.49
1:C:236:SER:HB2	1:C:249:ALA:HB3	1.93	0.49
1:A:41:PHE:CD1	1:A:41:PHE:O	2.65	0.49
1:B:313:ARG:CZ	1:B:327:VAL:HG21	2.41	0.49
1:A:93:TYR:OH	1:B:21:HIS:HD2	1.96	0.49
1:A:284:ALA:O	1:A:286:GLY:N	2.46	0.49
1:C:36:TYR:HD1	1:C:60:ARG:HG3	1.75	0.49
1:B:158:LYS:NZ	1:B:160:GLN:OE1	2.46	0.49
1:A:163:HIS:HB3	1:A:167:SER:OG	2.13	0.49
1:A:149:LEU:HA	1:A:178:ALA:O	2.13	0.49
1:A:231:GLU:HA	1:A:252:THR:O	2.12	0.49
1:A:37:ALA:O	1:A:38:GLN:HB2	2.13	0.49
1:A:70:GLN:O	1:A:73:SER:HB2	2.13	0.49
1:C:126:TYR:O	1:C:128:THR:HG23	2.13	0.49
1:B:242:VAL:HG23	1:B:321:ASP:OD2	2.13	0.49
1:C:223:VAL:HG23	1:C:261:TYR:HB2	1.95	0.49
1:A:209:ALA:HB2	1:A:234:ASN:HB2	1.95	0.49
1:A:77:ARG:HG2	1:A:130:ARG:NH2	2.27	0.48
1:B:163:HIS:ND1	1:B:163:HIS:N	2.61	0.48
1:C:238:VAL:HG23	1:C:325:SER:HB3	1.95	0.48
2:C:401:CPF:H9	2:C:401:CPF:H132	1.87	0.48
1:B:200:GLN:O	1:B:202:ARG:N	2.45	0.48
1:C:235:MET:HA	1:C:248:MET:HE3	1.94	0.48
1:C:179:TYR:HD1	1:C:180:GLU:N	2.11	0.48
1:C:9:ASN:O	1:C:44:GLU:O	2.31	0.48
1:A:260:GLN:HB3	1:A:270:ALA:CB	2.43	0.48
1:B:18:VAL:HG13	1:B:338:THR:CB	2.39	0.48
1:C:233:ARG:NH1	1:C:251:LYS:HG2	2.28	0.48
1:C:302:PHE:HE2	1:C:308:VAL:HG12	1.79	0.48
1:B:252:THR:O	1:B:254:ASN:ND2	2.46	0.48
1:B:97:TYR:CZ	1:B:130:ARG:HD3	2.48	0.48
1:C:274:VAL:HG21	1:C:293:TYR:CZ	2.49	0.48
1:C:292:LYS:HG2	1:C:316:LEU:CD1	2.44	0.48
1:A:8:GLY:H	1:A:9:ASN:HD22	1.62	0.48
1:A:41:PHE:C	1:A:41:PHE:CD1	2.87	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:275:GLN:HG2	1:C:276:SER:N	2.29	0.48
1:B:167:SER:HB3	1:C:66:ALA:CB	2.44	0.48
1:B:270:ALA:O	1:B:296:ALA:HA	2.14	0.47
1:B:292:LYS:O	1:B:293:TYR:HB3	2.14	0.47
1:A:256:GLU:HG2	1:A:274:VAL:HG13	1.96	0.47
1:B:72:ASN:ND2	1:C:71:GLN:HB3	2.29	0.47
1:A:86:ALA:O	1:A:87:GLU:HG2	2.14	0.47
1:B:47:ILE:HB	1:B:51:LEU:HB3	1.96	0.47
1:B:96:ASN:OD1	1:B:97:TYR:N	2.40	0.47
1:B:205:ASN:HB2	1:B:234:ASN:HD21	1.77	0.47
1:B:169:ASN:OD1	1:B:170:GLY:O	2.32	0.47
1:A:33:ASP:OD1	1:A:33:ASP:C	2.53	0.47
1:C:182:ASP:OD1	1:C:183:GLY:N	2.48	0.47
1:B:1:MET:O	1:B:2:GLU:CB	2.63	0.47
1:B:69:GLU:HA	1:B:71:GLN:HE22	1.78	0.47
1:B:308:VAL:HG23	1:B:336:GLY:O	2.15	0.47
1:C:64:ASP:OD1	1:C:64:ASP:N	2.48	0.47
1:A:139:ASN:OD1	1:A:142:PHE:HA	2.15	0.47
1:C:302:PHE:CE2	1:C:308:VAL:HG12	2.50	0.46
1:C:48:ASN:ND2	1:C:51:LEU:H	2.12	0.46
1:A:123:THR:O	1:A:129:SER:HB3	2.15	0.46
1:B:91:ILE:O	1:B:91:ILE:HG13	2.10	0.46
1:C:262:GLN:HB2	1:C:268:ARG:HH11	1.79	0.46
1:B:94:GLY:O	1:B:95:ARG:C	2.54	0.46
1:A:140:SER:HA	1:A:150:SER:CB	2.35	0.46
1:B:303:ASN:HB3	1:B:305:ASN:N	2.23	0.46
1:A:41:PHE:HD1	1:A:41:PHE:O	1.98	0.46
1:A:113:PHE:CZ	1:A:332:GLN:HB2	2.51	0.46
1:B:1:MET:N	1:B:13:LEU:O	2.48	0.46
1:A:320:ASN:HD22	1:A:322:TYR:H	1.64	0.46
1:C:18:VAL:HG21	1:C:36:TYR:CZ	2.50	0.46
1:C:120:GLY:O	1:C:122:TYR:N	2.49	0.46
1:A:229:TYR:HD1	1:A:255:LEU:HD12	1.81	0.46
1:B:125:ASN:ND2	1:B:235:MET:O	2.49	0.45
1:C:112:TYR:O	1:C:113:PHE:HB2	2.16	0.45
1:C:273:TYR:HE2	1:C:275:GLN:HB2	1.80	0.45
1:B:141:ASP:HA	1:B:149:LEU:O	2.15	0.45
1:A:260:GLN:HB3	1:A:270:ALA:HB2	1.98	0.45
1:A:227:ALA:HA	1:A:256:GLU:O	2.16	0.45
1:A:28:ASP:O	1:A:29:SER:HB2	2.16	0.45
1:B:39:ILE:HA	1:B:39:ILE:HD12	1.66	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:HIS:CD2	1:A:32:ALA:O	2.68	0.45
1:C:322:TYR:O	1:C:323:SER:C	2.54	0.45
1:C:262:GLN:HB2	1:C:268:ARG:HH12	1.78	0.45
1:B:62:LYS:HB2	1:B:73:SER:O	2.17	0.45
1:C:116:GLU:OE1	1:C:313:ARG:NH2	2.49	0.45
1:C:85:TYR:HB3	1:C:88:VAL:HG13	1.99	0.45
1:B:205:ASN:O	1:B:207:ASP:N	2.50	0.44
1:C:222:ASN:O	1:C:262:GLN:N	2.48	0.44
1:A:149:LEU:HD12	1:A:179:TYR:HB2	1.99	0.44
1:B:196:THR:C	1:B:198:ASP:N	2.70	0.44
1:B:261:TYR:O	1:B:269:PRO:HD2	2.17	0.44
1:C:117:THR:HA	1:C:326:TYR:CD2	2.52	0.44
1:B:326:TYR:O	1:B:327:VAL:HG23	2.15	0.44
1:C:272:SER:OG	1:C:295:GLN:HG3	2.16	0.44
1:C:121:ALA:HA	2:C:401:CPF:H142	1.98	0.44
1:A:140:SER:CA	1:A:150:SER:HB3	2.36	0.44
1:B:222:ASN:O	1:B:261:TYR:CD1	2.70	0.44
1:A:104:GLU:HG2	1:A:118:TRP:CZ2	2.52	0.44
1:B:255:LEU:HG	1:B:256:GLU:N	2.32	0.44
1:B:167:SER:HB3	1:C:66:ALA:HB2	2.00	0.44
1:A:233:ARG:HA	1:A:250:ASN:O	2.18	0.44
1:C:123:THR:O	1:C:125:ASN:N	2.48	0.44
1:B:204:GLY:O	1:B:234:ASN:ND2	2.49	0.44
1:B:315:ASN:HD21	1:B:317:LEU:HB3	1.83	0.44
1:C:222:ASN:O	1:C:261:TYR:HA	2.18	0.44
1:B:117:THR:OG1	1:B:118:TRP:HD1	2.01	0.44
1:C:317:LEU:HD22	1:C:318:ASP:O	2.18	0.44
1:C:304:LYS:HG3	1:C:305:ASN:ND2	2.33	0.43
1:A:43:GLY:HA3	1:B:339:TYR:CZ	2.53	0.43
1:C:249:ALA:HB1	1:C:252:THR:CG2	2.48	0.43
1:C:51:LEU:HA	1:C:51:LEU:HD12	1.89	0.43
1:A:199:GLN:C	1:A:201:ASP:H	2.20	0.43
1:C:267:LEU:HD12	1:C:269:PRO:HD3	2.00	0.43
1:C:175:TYR:N	1:C:175:TYR:CD2	2.87	0.43
1:A:90:SER:OG	1:A:138:ARG:HB2	2.17	0.43
1:A:53:GLY:HA3	1:B:306:MET:HG3	2.00	0.43
1:A:137:TYR:HB3	1:A:153:ILE:HG23	1.99	0.43
1:A:196:THR:C	1:A:198:ASP:N	2.72	0.43
1:C:309:TRP:CD1	1:C:309:TRP:C	2.91	0.43
1:C:26:THR:HG22	1:C:27:GLY:N	2.33	0.43
1:B:250:ASN:O	1:B:251:LYS:C	2.57	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:38:GLN:NE2	1:C:58:GLU:OE2	2.51	0.43
1:A:113:PHE:CZ	1:A:332:GLN:CB	3.02	0.43
1:C:215:GLY:CA	1:C:228:VAL:HG23	2.48	0.43
1:B:293:TYR:HB3	1:B:315:ASN:HA	2.01	0.43
1:C:260:GLN:HB3	1:C:270:ALA:HA	2.00	0.43
1:A:36:TYR:HD1	1:A:37:ALA:O	2.02	0.43
1:B:117:THR:OG1	1:B:118:TRP:N	2.51	0.43
1:A:11:LEU:HD23	1:A:12:ASP:N	2.34	0.43
1:C:111:PRO:HG2	1:C:311:ASP:OD1	2.19	0.42
1:B:42:LYS:HE3	1:B:56:GLN:NE2	2.34	0.42
1:A:108:ASP:HA	1:A:114:SER:HG	1.83	0.42
1:A:82:GLY:C	1:A:83:LEU:HD22	2.40	0.42
1:B:210:GLU:CG	1:B:233:ARG:HB2	2.43	0.42
1:C:208:ARG:NH2	1:C:208:ARG:CG	2.74	0.42
1:C:308:VAL:HA	1:C:337:ILE:HA	2.01	0.42
1:C:341:PHE:CD2	1:C:341:PHE:O	2.73	0.42
1:B:308:VAL:HB	1:B:337:ILE:HD13	2.02	0.42
1:B:130:ARG:HH21	1:C:67:GLU:CD	2.22	0.42
1:C:113:PHE:CD2	1:C:313:ARG:HB3	2.54	0.42
1:B:139:ASN:HD21	1:B:143:PHE:H	1.62	0.42
1:C:203:ASP:C	1:C:250:ASN:HD21	2.23	0.42
1:A:180:GLU:HA	1:A:185:GLY:HA2	2.01	0.42
1:B:5:ASN:ND2	1:B:5:ASN:O	2.46	0.42
1:B:35:THR:O	1:B:63:ALA:HB3	2.20	0.42
1:A:139:ASN:ND2	1:A:141:ASP:OD2	2.53	0.42
1:B:302:PHE:HD2	1:B:306:MET:HB3	1.83	0.42
1:C:86:ALA:O	1:C:87:GLU:HB2	2.20	0.42
1:A:196:THR:C	1:A:198:ASP:H	2.21	0.42
1:C:62:LYS:N	1:C:73:SER:O	2.52	0.42
1:A:165:ILE:C	1:A:167:SER:H	2.23	0.42
1:A:95:ARG:HH12	1:B:67:GLU:HG3	1.85	0.42
1:C:262:GLN:OE1	1:C:268:ARG:HB2	2.19	0.42
1:B:196:THR:C	1:B:198:ASP:H	2.23	0.42
1:C:275:GLN:HA	1:C:291:ALA:O	2.20	0.42
1:B:102:ASP:O	1:B:103:VAL:CB	2.68	0.42
1:A:48:ASN:O	1:A:50:ASP:N	2.53	0.42
1:B:95:ARG:HG2	1:C:63:ALA:HB1	2.01	0.42
1:B:126:TYR:HE1	1:B:169:ASN:HB2	1.72	0.41
1:A:99:ILE:HG23	1:A:176:THR:HB	2.02	0.41
1:C:4:TYR:HB3	1:C:10:LYS:H	1.84	0.41
1:A:8:GLY:HA3	1:A:46:GLN:CG	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:LEU:O	1:A:90:SER:HA	2.20	0.41
1:C:107:THR:HG22	1:C:258:VAL:HG23	2.01	0.41
1:B:195:ARG:HH21	1:B:199:GLN:HA	1.80	0.41
1:A:107:THR:CG2	1:A:228:VAL:CG1	2.95	0.41
1:A:170:GLY:O	1:A:172:GLY:N	2.53	0.41
1:A:117:THR:O	1:A:121:ALA:CB	2.68	0.41
1:C:38:GLN:HG3	1:C:60:ARG:CB	2.49	0.41
1:B:299:THR:HG23	1:B:309:TRP:HB3	2.01	0.41
1:B:196:THR:CG2	1:B:197:ASN:N	2.84	0.41
1:C:110:ALA:CB	1:C:114:SER:OG	2.69	0.41
1:A:229:TYR:HA	1:A:254:ASN:O	2.20	0.41
1:C:65:ARG:HD3	1:C:65:ARG:HA	1.88	0.41
1:A:125:ASN:O	1:A:128:THR:HG23	2.21	0.41
1:C:233:ARG:HA	1:C:250:ASN:O	2.20	0.41
1:C:77:ARG:NH2	2:C:401:CPF:O1	2.48	0.41
1:A:299:THR:OG1	1:A:301:TYR:HE2	2.03	0.41
1:A:272:SER:OG	1:A:295:GLN:HG3	2.21	0.41
1:B:195:ARG:HG3	1:B:209:ALA:HB2	2.03	0.41
1:B:141:ASP:O	1:B:141:ASP:OD1	2.39	0.41
1:B:18:VAL:HA	1:B:338:THR:HB	2.02	0.41
1:B:326:TYR:C	1:B:327:VAL:HG22	2.41	0.41
1:C:236:SER:O	1:C:248:MET:HA	2.21	0.41
1:A:205:ASN:O	1:A:206:GLY:C	2.59	0.41
1:B:238:VAL:HG22	1:B:247:GLU:O	2.21	0.41
1:C:266:GLY:O	1:C:300:TYR:CD1	2.74	0.41
1:B:2:GLU:C	1:B:3:ILE:HD12	2.42	0.41
1:B:141:ASP:O	1:B:143:PHE:N	2.49	0.41
1:A:63:ALA:HB1	1:C:95:ARG:HB2	2.02	0.41
1:C:47:ILE:HB	1:C:51:LEU:HB3	2.03	0.40
1:A:301:TYR:CD2	1:A:301:TYR:N	2.89	0.40
1:A:60:ARG:NH2	1:A:77:ARG:NH1	2.66	0.40
1:B:84:LYS:HA	1:B:90:SER:HB2	2.04	0.40
1:B:69:GLU:HA	1:B:71:GLN:NE2	2.36	0.40
1:A:318:ASP:O	1:A:319:GLU:C	2.58	0.40
1:B:195:ARG:HD2	1:B:234:ASN:OD1	2.21	0.40
1:B:162:ASN:HB3	1:C:65:ARG:NH1	2.37	0.40
1:A:41:PHE:C	1:A:41:PHE:HD1	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	339/341 (99%)	263 (78%)	51 (15%)	25 (7%)	1	10
1	B	336/341 (98%)	269 (80%)	44 (13%)	23 (7%)	1	12
1	C	329/341 (96%)	276 (84%)	36 (11%)	17 (5%)	2	19
All	All	1004/1023 (98%)	808 (80%)	131 (13%)	65 (6%)	1	13

All (65) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	TYR
1	A	87	GLU
1	A	285	GLY
1	A	324	SER
1	A	326	TYR
1	B	2	GLU
1	B	9	ASN
1	B	182	ASP
1	B	201	ASP
1	B	202	ARG
1	B	319	GLU
1	B	326	TYR
1	C	117	THR
1	C	127	MET
1	C	165	ILE
1	C	200	GLN
1	C	207	ASP
1	C	221	ASN
1	C	234	ASN
1	C	322	TYR
1	C	323	SER
1	A	29	SER
1	A	161	ASP
1	A	171	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	202	ARG
1	A	205	ASN
1	A	206	GLY
1	A	249	ALA
1	A	280	GLN
1	B	125	ASN
1	B	197	ASN
1	B	206	GLY
1	B	234	ASN
1	B	251	LYS
1	B	327	VAL
1	C	303	ASN
1	C	304	LYS
1	A	38	GLN
1	A	148	GLY
1	A	197	ASN
1	A	200	GLN
1	A	208	ARG
1	A	236	SER
1	A	267	LEU
1	A	319	GLU
1	B	3	ILE
1	B	7	ASP
1	B	209	ALA
1	C	121	ALA
1	C	126	TYR
1	C	321	ASP
1	A	201	ASP
1	B	95	ARG
1	B	195	ARG
1	B	204	GLY
1	B	323	SER
1	C	167	SER
1	C	319	GLU
1	A	112	TYR
1	A	142	PHE
1	B	65	ARG
1	B	103	VAL
1	B	221	ASN
1	A	327	VAL
1	C	336	GLY

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	230/272 (85%)	184 (80%)	46 (20%)	1	6
1	B	239/272 (88%)	193 (81%)	46 (19%)	2	7
1	C	244/272 (90%)	182 (75%)	62 (25%)	1	2
All	All	713/816 (87%)	559 (78%)	154 (22%)	1	5

All (154) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	TYR
1	A	5	ASN
1	A	25	THR
1	A	41	PHE
1	A	48	ASN
1	A	49	THR
1	A	52	THR
1	A	60	ARG
1	A	71	GLN
1	A	84	LYS
1	A	85	TYR
1	A	95	ARG
1	A	104	GLU
1	A	107	THR
1	A	123	THR
1	A	128	THR
1	A	134	LEU
1	A	145	LEU
1	A	147	ASP
1	A	153	ILE
1	A	165	ILE
1	A	167	SER
1	A	169	ASN
1	A	182	ASP
1	A	186	VAL
1	A	193	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	195	ARG
1	A	211	SER
1	A	214	VAL
1	A	223	VAL
1	A	225	LEU
1	A	236	SER
1	A	238	VAL
1	A	245	THR
1	A	255	LEU
1	A	260	GLN
1	A	281	LEU
1	A	299	THR
1	A	303	ASN
1	A	311	ASP
1	A	313	ARG
1	A	315	ASN
1	A	318	ASP
1	A	321	ASP
1	A	329	THR
1	A	341	PHE
1	B	4	TYR
1	B	5	ASN
1	B	14	TYR
1	B	24	THR
1	B	47	ILE
1	B	52	THR
1	B	65	ARG
1	B	74	ASN
1	B	76	VAL
1	B	78	LEU
1	B	85	TYR
1	B	91	ILE
1	B	95	ARG
1	B	102	ASP
1	B	103	VAL
1	B	123	THR
1	B	127	MET
1	B	128	THR
1	B	138	ARG
1	B	140	SER
1	B	145	LEU
1	B	151	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	153	ILE
1	B	155	TYR
1	B	163	HIS
1	B	167	SER
1	B	169	ASN
1	B	175	TYR
1	B	186	VAL
1	B	191	SER
1	B	208	ARG
1	B	212	ARG
1	B	225	LEU
1	B	234	ASN
1	B	256	GLU
1	B	264	ASP
1	B	267	LEU
1	B	271	ILE
1	B	289	ASP
1	B	299	THR
1	B	303	ASN
1	B	310	VAL
1	B	312	TYR
1	B	313	ARG
1	B	320	ASN
1	B	338	THR
1	C	4	TYR
1	C	5	ASN
1	C	7	ASP
1	C	13	LEU
1	C	18	VAL
1	C	20	ARG
1	C	28	ASP
1	C	29	SER
1	C	31	ASN
1	C	41	PHE
1	C	48	ASN
1	C	52	THR
1	C	54	PHE
1	C	65	ARG
1	C	74	ASN
1	C	77	ARG
1	C	88	VAL
1	C	91	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	95	ARG
1	C	99	ILE
1	C	100	VAL
1	C	104	GLU
1	C	105	SER
1	C	124	ASP
1	C	127	MET
1	C	134	LEU
1	C	136	THR
1	C	139	ASN
1	C	158	LYS
1	C	164	SER
1	C	166	ASN
1	C	175	TYR
1	C	179	TYR
1	C	187	THR
1	C	205	ASN
1	C	208	ARG
1	C	212	ARG
1	C	214	VAL
1	C	223	VAL
1	C	225	LEU
1	C	228	VAL
1	C	231	GLU
1	C	232	THR
1	C	233	ARG
1	C	239	GLU
1	C	241	THR
1	C	243	THR
1	C	248	MET
1	C	254	ASN
1	C	260	GLN
1	C	267	LEU
1	C	271	ILE
1	C	281	LEU
1	C	290	LEU
1	C	295	GLN
1	C	303	ASN
1	C	306	MET
1	C	313	ARG
1	C	316	LEU
1	C	317	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	319	GLU
1	C	338	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	9	ASN
1	A	21	HIS
1	A	34	GLN
1	A	46	GLN
1	A	48	ASN
1	A	71	GLN
1	A	160	GLN
1	A	166	ASN
1	A	168	GLN
1	A	197	ASN
1	A	200	GLN
1	A	303	ASN
1	A	305	ASN
1	A	315	ASN
1	A	320	ASN
1	B	21	HIS
1	B	34	GLN
1	B	56	GLN
1	B	72	ASN
1	B	139	ASN
1	B	156	GLN
1	B	159	ASN
1	B	169	ASN
1	B	254	ASN
1	B	315	ASN
1	C	5	ASN
1	C	46	GLN
1	C	48	ASN
1	C	70	GLN
1	C	163	HIS
1	C	250	ASN
1	C	254	ASN
1	C	260	GLN
1	C	305	ASN

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 ⓘ

1 ligand is 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	CPF	C	401	-	21,27,27	1.92	5 (23%)	28,40,40	4.32	15 (53%)

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	CPF	C	401	-	-	0/4/22/22	0/3/4/4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	CPF	C10-N1	2.47	1.43	1.40
2	C	401	CPF	C12-C11	2.65	1.53	1.48
2	C	401	CPF	C13-C11	2.83	1.54	1.48
2	C	401	CPF	C4-C5	3.69	1.46	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	CPF	C6-C7	5.07	1.40	1.35

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	CPF	C9-C8-N2	-9.52	109.99	122.71
2	C	401	CPF	C6-C7-C8	-8.32	116.69	123.41
2	C	401	CPF	C2-C4-C5	-3.68	115.62	121.87
2	C	401	CPF	C1-N1-C10	-3.27	118.06	121.39
2	C	401	CPF	C11-N1-C10	-2.87	117.49	120.87
2	C	401	CPF	C16-C17-N2	-2.41	104.78	110.70
2	C	401	CPF	C15-C14-N2	-2.40	104.81	110.70
2	C	401	CPF	C6-C5-C10	2.66	122.70	118.49
2	C	401	CPF	C15-N3-C16	4.01	123.62	110.33
2	C	401	CPF	C1-N1-C11	4.57	124.43	119.25
2	C	401	CPF	F1-C7-C8	4.64	122.83	118.45
2	C	401	CPF	C7-C8-N2	5.00	126.28	120.48
2	C	401	CPF	C14-N2-C17	6.84	125.95	111.59
2	C	401	CPF	C9-C8-C7	7.83	123.73	116.40
2	C	401	CPF	C5-C10-N1	10.35	125.67	118.92

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	401	CPF	13	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	341/341 (100%)	-0.26	1 (0%) 94 95	66, 99, 120, 126	0
1	B	340/341 (99%)	-0.12	7 (2%) 67 66	62, 97, 112, 125	0
1	C	337/341 (98%)	-0.09	8 (2%) 62 61	50, 97, 128, 144	0
All	All	1018/1023 (99%)	-0.16	16 (1%) 74 73	50, 98, 121, 144	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	6	LYS	3.7
1	C	285	GLY	3.7
1	C	284	ALA	3.6
1	B	7	ASP	3.5
1	B	27	GLY	3.3
1	C	207	ASP	3.2
1	C	238	VAL	3.2
1	C	205	ASN	3.1
1	A	7	ASP	3.0
1	B	289	ASP	2.5
1	C	201	ASP	2.4
1	C	203	ASP	2.4
1	B	207	ASP	2.3
1	C	235	MET	2.2
1	B	28	ASP	2.0
1	B	284	ALA	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
2	CPF	C	401	24/24	0.82	0.27	1.38	83,90,92,92	0

6.5 Other polymers [i](#)

There are no such residues in this entry.