



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 07:14 am BST

PDB ID : 5HY7  
Title : SF3B10-SF3B130 from Chaetomium thermophilum  
Authors : Ponce-Salvatierra, A.; Schmitzova, J.; Pena, V.  
Deposited on : 2016-02-01  
Resolution : 2.90 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Xtrriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

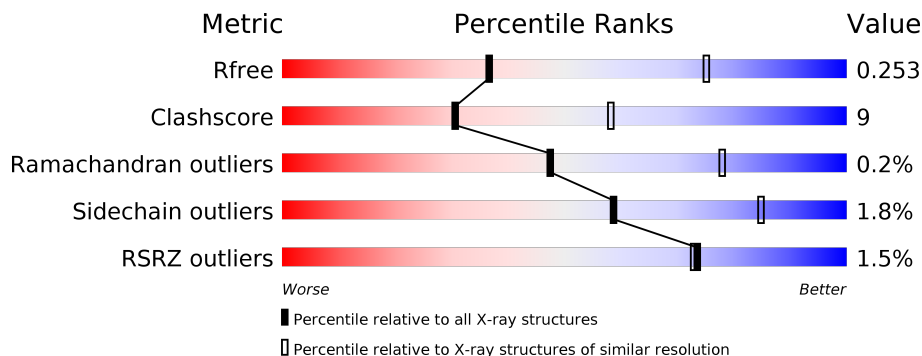
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	1213	 2% 74% 22%
1	B	1213	 1% 76% 19%
2	C	95	 47% 9% 42%
2	D	95	 45% 13% 42%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CA	A	1303	-	-	-	X
3	CA	B	1304	-	-	-	X

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 19210 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 Putative pre-mRNA splicing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1173	9164	5827	1556	1742	39	0	0	0
1	B	1170	9149	5815	1555	1741	38	0	0	0

- Molecule 2 is a protein called YSF3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	55	444	288	78	75	3	0	0	0
2	C	55	444	288	78	75	3	0	0	0

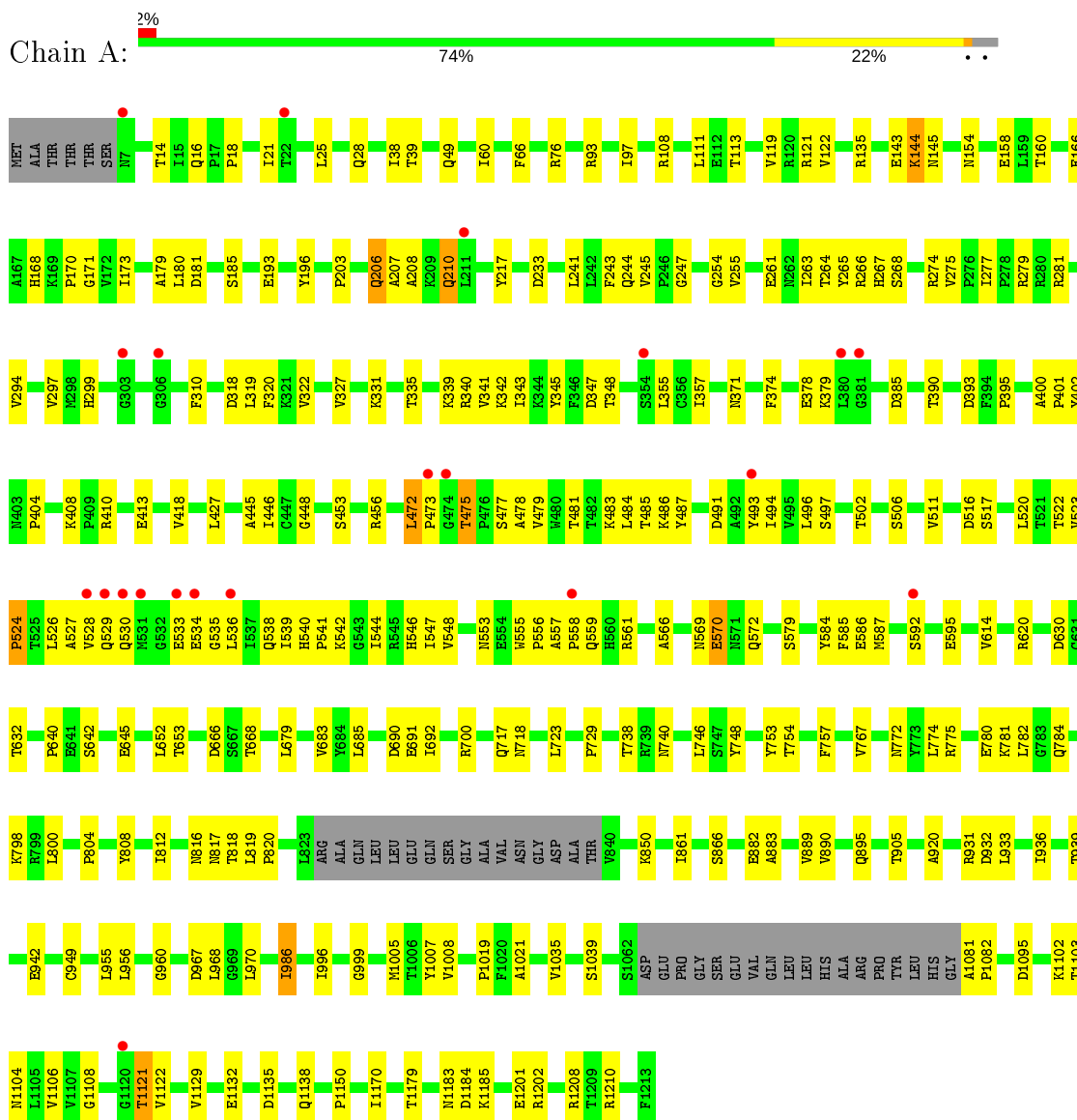
- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	5	Total	Ca	0	0
			5	5		
3	A	4	Total	Ca	0	0
			4	4		

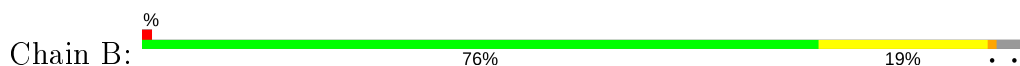
### 3 Residue-property plots [i](#)

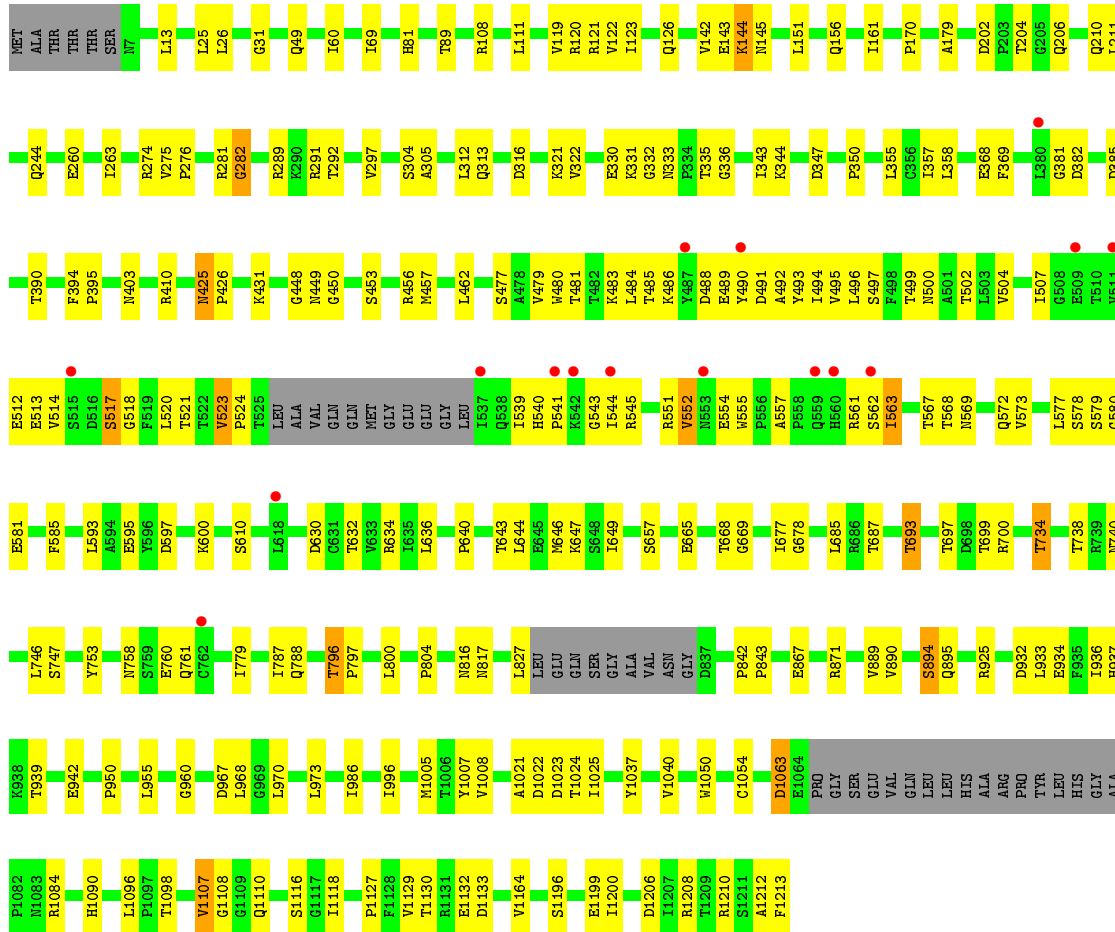
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

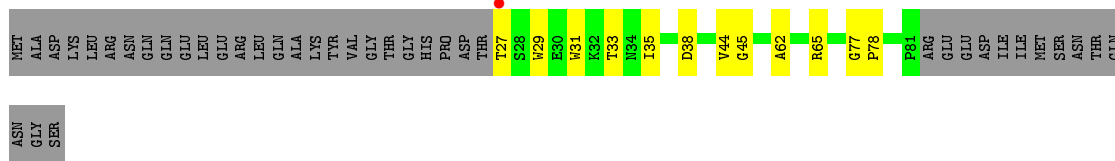


- Molecule 1: Putative pre-mRNA splicing protein





• Molecule 2: YSF3



• Molecule 2: YSF3



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	197.08Å 197.08Å 446.45Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.27 – 2.90 49.27 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.27-2.90) 99.7 (49.27-2.70)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.96 (at 2.69Å)	Xtrriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, $R_{free}$	0.214 , 0.253 0.214 , 0.253	Depositor DCC
$R_{free}$ test set	7005 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	97.7	Xtrriage
Anisotropy	0.037	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 48.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	19210	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	91.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.62% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.32	0/9363	0.50	0/12721
1	B	0.35	1/9347 (0.0%)	0.51	0/12698
2	C	0.34	0/460	0.42	0/629
2	D	0.30	0/460	0.39	0/629
All	All	0.33	1/19630 (0.0%)	0.50	0/26677

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	425	ASN	C-N	-5.55	1.23	1.34

There are no bond angle outliers.

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	9164	0	9131	180	0
1	B	9149	0	9110	170	0
2	C	444	0	448	7	0
2	D	444	0	448	8	0
3	A	4	0	0	0	0
3	B	5	0	0	0	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	19210	0	19137	353	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 9.

All (353) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:535:GLY:HA2	1:A:547:ILE:O	1.67	0.93
1:A:319:LEU:HB2	1:A:347:ASP:O	1.69	0.92
1:A:527:ALA:HB2	1:A:536:LEU:HD23	1.53	0.90
1:A:506:SER:H	1:A:511:VAL:HG21	1.38	0.87
1:B:1007:TYR:HB2	1:B:1021:ALA:HB3	1.61	0.81
1:B:122:VAL:O	1:B:145:ASN:ND2	2.14	0.80
1:B:939:THR:HG21	1:B:973:LEU:H	1.48	0.78
1:B:108:ARG:HD2	1:B:111:LEU:HB2	1.66	0.78
1:A:1007:TYR:HB2	1:A:1021:ALA:HB3	1.65	0.77
1:B:448:GLY:HA3	1:B:453:SER:HA	1.66	0.76
1:A:233:ASP:OD2	1:A:266:ARG:NH2	2.13	0.75
1:A:717:GLN:NE2	1:A:780:GLU:O	2.20	0.75
1:B:554:GLU:HB3	1:B:555:TRP:HB2	1.67	0.74
1:B:551:ARG:HB3	1:B:552:VAL:HA	1.67	0.74
1:B:687:THR:HG22	1:B:699:THR:HG22	1.70	0.74
1:A:1106:VAL:HG12	1:A:1108:GLY:H	1.54	0.72
1:B:479:VAL:HG22	1:B:496:LEU:HG	1.71	0.71
1:B:1037:TYR:OH	1:B:1063:ASP:OD2	2.07	0.71
1:A:486:LYS:HG3	1:A:530:GLN:HA	1.73	0.71
1:B:368:GLU:O	1:B:425:ASN:ND2	2.24	0.70
1:A:206:GLN:HA	1:A:207:ALA:HB3	1.73	0.69
1:A:448:GLY:HA3	1:A:453:SER:HA	1.75	0.69
1:B:481:THR:HG22	1:B:494:ILE:HG13	1.74	0.69
1:B:291:ARG:NH1	1:B:316:ASP:OD2	2.23	0.69
1:A:206:GLN:HB2	1:A:208:ALA:N	2.08	0.68
1:A:572:GLN:NE2	1:A:584:TYR:OH	2.25	0.68
1:A:530:GLN:NE2	1:A:570:GLU:OE1	2.26	0.68
1:A:1129:VAL:HG21	1:A:1210:ARG:HH22	1.57	0.67
1:B:563:ILE:HA	1:B:577:LEU:HA	1.77	0.67
1:A:729:PRO:HG2	1:A:746:LEU:HB2	1.78	0.66
1:A:808:TYR:OH	1:A:931:ARG:NH1	2.27	0.66
1:A:524:PRO:HD2	1:A:539:ILE:HB	1.76	0.65
1:A:371:ASN:OD1	1:A:456:ARG:NH2	2.28	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:PHE:O	1:A:255:VAL:HA	1.96	0.65
1:A:1035:VAL:O	1:A:1102:LYS:NZ	2.28	0.65
1:B:761:GLN:OE1	1:B:761:GLN:N	2.29	0.65
1:B:490:TYR:HB2	1:B:758:ASN:HB3	1.79	0.64
1:A:49:GLN:HB2	1:A:60:ILE:HD11	1.79	0.64
1:B:554:GLU:N	1:B:554:GLU:OE1	2.30	0.64
1:B:322:VAL:HG22	1:B:343:ILE:HG12	1.79	0.64
1:B:636:LEU:HD13	1:B:646:MET:HA	1.78	0.64
1:B:544:ILE:O	1:B:555:TRP:N	2.31	0.63
1:A:122:VAL:O	1:A:145:ASN:ND2	2.31	0.63
1:A:586:GLU:OE2	1:A:620:ARG:NE	2.26	0.63
1:A:506:SER:N	1:A:511:VAL:HG21	2.12	0.63
1:B:119:VAL:HG11	2:C:44:GLY:HA3	1.81	0.63
1:A:18:PRO:HG3	1:A:1121:THR:HG23	1.81	0.63
1:A:385:ASP:OD2	1:A:410:ARG:NH1	2.29	0.63
1:B:513:GLU:HG3	1:B:514:VAL:H	1.64	0.63
1:B:1110:GLN:HG2	1:B:1127:PRO:HG2	1.81	0.62
1:B:996:ILE:HB	1:B:1008:VAL:HG22	1.79	0.62
1:A:378:GLU:HB2	1:A:379:LYS:HA	1.81	0.62
1:B:942:GLU:N	1:B:942:GLU:OE1	2.31	0.62
1:B:517:SER:OG	1:B:545:ARG:NE	2.31	0.62
1:A:717:GLN:HE21	1:A:781:LYS:HA	1.64	0.62
1:B:804:PRO:HD3	1:B:889:VAL:HG11	1.81	0.62
1:B:49:GLN:HB2	1:B:60:ILE:HD11	1.82	0.62
1:A:410:ARG:NH1	1:A:413:GLU:OE2	2.28	0.62
1:B:1206:ASP:OD2	1:B:1210:ARG:NH1	2.33	0.61
1:B:456:ARG:NH1	1:B:788:GLN:OE1	2.33	0.61
1:A:890:VAL:HG21	1:A:955:LEU:HD13	1.82	0.61
1:A:97:ILE:HA	1:A:108:ARG:HA	1.82	0.61
1:B:1096:LEU:HB3	1:B:1118:ILE:HG13	1.82	0.61
1:A:942:GLU:OE1	1:A:942:GLU:N	2.30	0.61
1:B:523:VAL:HG12	1:B:524:PRO:HD3	1.83	0.61
1:B:263:ILE:HD12	1:B:343:ILE:HD11	1.82	0.61
1:A:556:PRO:HB2	1:A:558:PRO:HB3	1.83	0.60
1:B:202:ASP:OD1	1:B:204:THR:HG22	2.00	0.60
1:B:431:LYS:NZ	1:B:800:LEU:O	2.35	0.60
1:A:310:PHE:HB2	1:A:322:VAL:HB	1.84	0.60
1:B:450:GLY:H	1:B:796:THR:HG22	1.66	0.60
1:A:524:PRO:CD	1:A:539:ILE:HB	2.32	0.60
1:B:121:ARG:NH1	2:C:37:ASP:OD1	2.31	0.60
1:A:569:ASN:HD21	1:A:614:VAL:HG22	1.67	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1022:ASP:HB3	1:B:1084:ARG:HH11	1.67	0.59
1:B:1129:VAL:HG13	1:B:1130:THR:HG23	1.84	0.59
1:B:204:THR:HG23	1:B:206:GLN:H	1.67	0.59
1:B:894:SER:HB2	1:B:895:GLN:HE21	1.67	0.59
1:A:523:VAL:HB	1:A:524:PRO:HD3	1.85	0.59
1:B:211:LEU:HD23	2:C:72:LEU:HD22	1.85	0.59
1:B:1130:THR:OG1	1:B:1133:ASP:OD2	2.20	0.58
1:A:485:THR:HG22	1:A:487:TYR:H	1.68	0.58
1:A:331:LYS:HD2	1:A:331:LYS:H	1.68	0.57
1:B:313:GLN:NE2	1:B:350:PRO:O	2.36	0.57
1:B:665:GLU:HG3	1:B:734:THR:HG21	1.86	0.57
1:B:274:ARG:HD3	1:B:395:PRO:O	2.05	0.57
1:A:804:PRO:HD3	1:A:889:VAL:HG11	1.86	0.57
1:B:1096:LEU:HD22	1:B:1118:ILE:HD11	1.86	0.57
1:B:449:ASN:HA	1:B:796:THR:HB	1.86	0.57
1:A:540:HIS:ND1	1:A:541:PRO:O	2.38	0.57
1:B:126:GLN:HG2	1:B:142:VAL:HG22	1.86	0.57
1:A:738:THR:OG1	1:A:740:ASN:OD1	2.21	0.57
1:A:524:PRO:HG3	1:A:566:ALA:HB3	1.87	0.56
1:A:544:ILE:HB	1:A:555:TRP:HB3	1.86	0.56
1:A:816:ASN:OD1	1:A:817:ASN:ND2	2.37	0.56
1:B:179:ALA:O	1:B:244:GLN:NE2	2.29	0.56
1:B:569:ASN:OD1	1:B:572:GLN:N	2.37	0.56
1:A:119:VAL:HG11	2:D:45:GLY:HA3	1.87	0.56
1:A:281:ARG:HB3	1:A:408:LYS:HD2	1.87	0.55
1:B:562:SER:O	1:B:578:SER:N	2.38	0.55
1:B:491:ASP:OD1	1:B:758:ASN:HB2	2.06	0.55
1:B:925:ARG:HB3	1:B:936:ILE:HD11	1.87	0.55
1:A:143:GLU:HB2	1:A:173:ILE:HD13	1.87	0.55
1:A:1095:ASP:OD2	1:A:1121:THR:OG1	2.18	0.55
1:B:867:GLU:OE2	1:B:871:ARG:NH1	2.39	0.55
1:B:512:GLU:N	1:B:512:GLU:OE1	2.39	0.55
1:B:561:ARG:HH11	1:B:579:SER:HB3	1.70	0.55
1:B:144:LYS:HG3	1:B:170:PRO:HA	1.88	0.55
1:A:493:TYR:HA	1:A:506:SER:HA	1.88	0.55
1:A:483:LYS:HE2	1:A:491:ASP:HB3	1.88	0.54
1:A:816:ASN:OD1	1:A:817:ASN:N	2.40	0.54
1:A:528:VAL:HG13	1:A:570:GLU:O	2.08	0.54
1:B:297:VAL:HG11	1:B:357:ILE:HG13	1.90	0.54
1:B:289:ARG:NH2	1:B:316:ASP:OD1	2.39	0.54
1:B:483:LYS:HG3	1:B:492:ALA:HB2	1.90	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:545:ARG:HG2	1:B:554:GLU:O	2.08	0.54
1:A:542:LYS:HA	1:A:557:ALA:HB2	1.90	0.54
1:B:746:LEU:HD21	1:B:779:ILE:HD11	1.89	0.54
1:A:486:LYS:NZ	1:A:527:ALA:HB3	2.22	0.53
1:A:534:GLU:HB3	1:A:548:VAL:HG13	1.89	0.53
1:A:122:VAL:HA	1:A:143:GLU:O	2.09	0.53
1:B:483:LYS:HD2	1:B:490:TYR:C	2.29	0.53
1:A:539:ILE:HG23	1:A:544:ILE:HG12	1.91	0.53
1:B:457:MET:O	1:B:788:GLN:HA	2.09	0.52
1:A:522:THR:HB	1:A:538:GLN:HE21	1.74	0.52
1:B:816:ASN:OD1	1:B:817:ASN:N	2.43	0.52
1:B:643:THR:HG22	1:B:644:LEU:HD12	1.91	0.52
1:A:427:LEU:HD11	1:A:445:ALA:HB1	1.91	0.52
1:A:108:ARG:HD2	1:A:111:LEU:HB2	1.92	0.51
1:A:166:GLU:OE1	1:A:168:HIS:NE2	2.43	0.51
1:B:297:VAL:CG2	1:B:355:LEU:HB2	2.41	0.51
1:B:483:LYS:HB2	1:B:491:ASP:HA	1.92	0.51
2:D:29:TRP:NE1	2:D:77:GLY:O	2.41	0.51
1:A:524:PRO:HG2	1:A:539:ILE:HD12	1.92	0.51
1:A:685:LEU:HA	1:A:700:ARG:O	2.10	0.51
1:B:481:THR:HA	1:B:493:TYR:O	2.11	0.51
1:A:294:VAL:HG13	2:D:62:ALA:HB3	1.92	0.51
1:B:523:VAL:N	1:B:539:ILE:O	2.42	0.51
1:B:573:VAL:HB	1:B:585:PHE:HB2	1.91	0.51
1:B:120:ARG:HD2	1:B:123:ILE:HD12	1.93	0.51
1:A:569:ASN:OD1	1:A:570:GLU:N	2.43	0.51
1:B:69:ILE:HA	1:B:89:THR:HG22	1.92	0.51
1:A:1129:VAL:HG21	1:A:1210:ARG:NH2	2.25	0.50
1:A:668:THR:HB	1:A:1183:ASN:HD21	1.75	0.50
1:B:1024:THR:OG1	1:B:1025:ILE:N	2.44	0.50
1:B:552:VAL:HB	1:B:554:GLU:OE1	2.12	0.50
1:B:581:GLU:HA	1:B:600:LYS:O	2.11	0.50
1:A:486:LYS:CG	1:A:530:GLN:HA	2.41	0.50
1:A:481:THR:HG22	1:A:494:ILE:HG13	1.94	0.50
1:A:754:THR:HA	1:A:767:VAL:O	2.11	0.50
1:A:254:GLY:HA2	1:A:267:HIS:HD2	1.77	0.50
1:A:516:ASP:OD1	1:A:517:SER:N	2.45	0.50
1:A:895:GLN:NE2	1:B:970:LEU:HB2	2.27	0.49
1:B:344:LYS:NZ	1:B:382:ASP:O	2.31	0.49
1:B:156:GLN:OE1	1:B:156:GLN:N	2.45	0.49
1:B:121:ARG:NE	1:B:143:GLU:OE2	2.45	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:ARG:NH2	1:A:185:SER:O	2.38	0.49
1:B:932:ASP:OD1	1:B:933:LEU:N	2.41	0.49
1:A:932:ASP:OD1	1:A:933:LEU:N	2.41	0.49
1:B:369:PHE:HA	1:B:425:ASN:HD22	1.78	0.49
1:A:700:ARG:HG2	1:A:1202:ARG:HG3	1.94	0.49
1:A:999:GLY:HA2	1:A:1005:MET:HE1	1.94	0.49
1:A:483:LYS:HG2	1:A:491:ASP:HB3	1.93	0.49
1:A:154:ASN:OD1	1:A:158:GLU:N	2.41	0.49
1:B:144:LYS:HD3	1:B:145:ASN:OD1	2.12	0.49
1:B:543:GLY:HA2	1:B:557:ALA:HB2	1.95	0.49
1:B:738:THR:OG1	1:B:740:ASN:OD1	2.26	0.49
1:A:472:LEU:H	1:A:473:PRO:HA	1.77	0.48
1:A:819:LEU:HD12	1:A:820:PRO:HD2	1.94	0.48
1:A:956:LEU:HD11	1:A:996:ILE:HD13	1.95	0.48
1:B:544:ILE:H	1:B:555:TRP:HE3	1.59	0.48
1:B:925:ARG:HG2	1:B:934:GLU:HB3	1.94	0.48
1:A:1008:VAL:HA	1:A:1019:PRO:HA	1.95	0.48
1:A:14:THR:O	1:A:1208:ARG:NH2	2.46	0.48
1:A:261:GLU:OE1	1:A:402:TYR:OH	2.19	0.48
1:A:487:TYR:HE2	1:A:533:GLU:HG2	1.77	0.48
1:A:883:ALA:O	1:A:905:THR:HA	2.13	0.48
1:B:634:ARG:HG2	1:B:649:ILE:HG13	1.94	0.48
1:A:559:GLN:CD	1:A:559:GLN:H	2.15	0.48
1:B:330:GLU:N	1:B:330:GLU:OE1	2.41	0.48
1:A:936:ILE:HG21	1:B:970:LEU:HD21	1.95	0.48
1:A:207:ALA:N	1:A:210:GLN:OE1	2.47	0.48
1:A:208:ALA:C	1:A:210:GLN:H	2.16	0.48
1:A:475:THR:HG22	1:A:772:ASN:OD1	2.14	0.48
1:B:630:ASP:OD1	1:B:632:THR:OG1	2.21	0.48
1:B:281:ARG:HA	1:B:282:GLY:HA2	1.71	0.47
1:B:967:ASP:OD1	1:B:968:LEU:N	2.47	0.47
2:D:29:TRP:O	2:D:33:THR:OG1	2.26	0.47
1:B:502:THR:HB	1:B:518:GLY:O	2.14	0.47
1:B:499:THR:HA	1:B:500:ASN:HA	1.40	0.47
1:A:245:VAL:HG21	1:A:265:TYR:HE1	1.78	0.47
1:B:1063:ASP:N	1:B:1063:ASP:OD1	2.46	0.47
1:B:210:GLN:N	1:B:210:GLN:OE1	2.48	0.47
1:B:263:ILE:HD13	1:B:312:LEU:HD12	1.96	0.47
1:A:267:HIS:CG	1:A:268:SER:H	2.33	0.47
1:B:520:LEU:HG	1:B:521:THR:H	1.79	0.47
1:A:318:ASP:OD1	1:A:348:THR:OG1	2.29	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:LYS:HG2	1:A:390:THR:HG22	1.96	0.46
1:A:478:ALA:HB3	1:A:497:SER:HB3	1.97	0.46
1:A:630:ASP:OD1	1:A:632:THR:OG1	2.24	0.46
1:A:494:ILE:HD11	1:A:757:PHE:HE2	1.80	0.46
1:A:28:GLN:NE2	1:A:76:ARG:HH12	2.13	0.46
2:D:31:TRP:O	2:D:35:ILE:HG12	2.15	0.46
1:A:66:PHE:HB2	1:A:1150:PRO:HB3	1.98	0.46
1:B:489:GLU:HA	1:B:490:TYR:HA	1.59	0.46
1:B:520:LEU:HG	1:B:521:THR:N	2.30	0.46
1:B:490:TYR:CB	1:B:758:ASN:HB3	2.45	0.46
1:A:180:LEU:HD11	1:A:217:TYR:CZ	2.50	0.46
1:A:477:SER:N	1:A:497:SER:O	2.35	0.46
1:A:496:LEU:HD21	1:A:774:LEU:HD12	1.98	0.46
1:A:339:LYS:HG3	1:A:340:ARG:HG3	1.98	0.46
1:B:331:LYS:O	1:B:333:ASN:N	2.44	0.46
1:B:685:LEU:HA	1:B:700:ARG:O	2.15	0.46
1:A:320:PHE:CD1	1:A:345:TYR:HA	2.51	0.46
1:A:666:ASP:OD2	1:A:668:THR:OG1	2.34	0.45
1:B:1212:ALA:O	1:B:1213:PHE:HB2	2.15	0.45
1:B:585:PHE:HD2	1:B:593:LEU:HB3	1.80	0.45
1:A:297:VAL:CG2	1:A:355:LEU:HB2	2.46	0.45
1:A:486:LYS:HZ1	1:A:527:ALA:HB3	1.79	0.45
1:A:502:THR:OG1	1:A:520:LEU:O	2.23	0.45
1:A:264:THR:HG22	1:A:266:ARG:HB2	1.97	0.45
1:B:567:THR:HG21	1:B:610:SER:HA	1.99	0.45
1:A:181:ASP:O	1:A:247:GLY:HA3	2.16	0.45
1:A:487:TYR:CE2	1:A:533:GLU:HG2	2.52	0.45
1:A:905:THR:OG1	1:A:920:ALA:HB3	2.16	0.45
1:B:1090:HIS:CD2	1:B:1164:VAL:HB	2.52	0.45
1:A:967:ASP:OD1	1:A:968:LEU:N	2.50	0.45
1:A:592:SER:OG	1:A:592:SER:O	2.32	0.45
1:B:960:GLY:O	1:B:986:ILE:HG12	2.17	0.45
1:A:723:LEU:HD23	1:A:754:THR:HG21	1.98	0.44
1:B:747:SER:HB2	1:B:787:ILE:HD12	1.98	0.44
1:B:477:SER:OG	1:B:497:SER:O	2.25	0.44
1:B:890:VAL:HG22	1:B:950:PRO:HG3	1.99	0.44
1:A:527:ALA:HA	1:A:536:LEU:HA	1.99	0.44
1:A:748:TYR:OH	1:A:775:ARG:HD3	2.18	0.44
1:B:385:ASP:OD2	1:B:410:ARG:NH2	2.50	0.44
1:A:16:GLN:HB2	1:A:1122:VAL:HB	1.98	0.44
1:B:1107:VAL:HG23	1:B:1108:GLY:H	1.83	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:551:ARG:HD2	1:B:551:ARG:HA	1.89	0.44
2:C:26:THR:HG22	2:C:27:SER:H	1.82	0.44
1:B:275:VAL:HG11	1:B:343:ILE:HG13	2.00	0.44
2:D:44:VAL:HG13	2:D:65:ARG:HG3	1.98	0.44
1:A:484:LEU:HD11	1:A:493:TYR:HE1	1.83	0.44
1:B:1196:SER:OG	1:B:1199:GLU:HB2	2.18	0.44
1:B:500:ASN:O	1:B:521:THR:N	2.51	0.44
1:B:541:PRO:HD2	1:B:543:GLY:O	2.18	0.43
1:A:25:LEU:HB3	1:A:38:ILE:HG22	2.00	0.43
1:A:483:LYS:HG2	1:A:491:ASP:CB	2.48	0.43
1:A:652:LEU:HD13	1:A:679:LEU:HD21	2.00	0.43
1:B:151:LEU:HD23	1:B:161:ILE:CD1	2.48	0.43
1:B:321:LYS:HZ1	1:B:381:GLY:H	1.64	0.43
1:B:585:PHE:HB3	1:B:593:LEU:HG	2.00	0.43
1:B:936:ILE:HG22	1:B:937:HIS:ND1	2.33	0.43
1:A:690:ASP:O	1:A:691:GLU:HB2	2.18	0.43
1:A:1103:THR:OG1	1:A:1104:ASN:N	2.52	0.43
1:A:327:VAL:O	1:A:335:THR:HG22	2.19	0.43
1:A:475:THR:OG1	1:A:475:THR:O	2.32	0.43
1:A:798:LYS:HB2	1:A:812:ILE:HG13	2.01	0.43
1:A:882:GLU:HG2	1:A:905:THR:HB	2.01	0.43
1:B:577:LEU:HD11	1:B:581:GLU:N	2.34	0.43
1:A:546:HIS:HB3	1:A:553:ASN:O	2.19	0.43
1:A:558:PRO:HD2	1:A:559:GLN:NE2	2.33	0.43
1:A:572:GLN:NE2	1:A:620:ARG:HB2	2.33	0.43
1:B:540:HIS:ND1	1:B:543:GLY:O	2.51	0.43
1:A:1179:THR:HG22	1:A:1201:GLU:OE1	2.19	0.43
1:A:171:GLY:HA2	1:A:196:TYR:CE2	2.53	0.43
1:B:894:SER:OG	1:B:967:ASP:OD1	2.27	0.43
1:A:642:SER:HB2	1:A:645:GLU:OE1	2.19	0.43
1:A:960:GLY:O	1:A:986:ILE:HG12	2.19	0.43
1:B:304:SER:HA	1:B:305:ALA:HA	1.84	0.43
1:B:1005:MET:HE3	1:B:1050:TRP:HH2	1.83	0.43
1:B:13:LEU:HD22	1:B:1208:ARG:NH1	2.33	0.43
1:B:26:LEU:HD11	1:B:358:LEU:HD12	2.00	0.43
1:B:485:THR:HG22	1:B:486:LYS:HG3	2.00	0.43
1:B:677:ILE:HB	1:B:685:LEU:HB2	2.00	0.43
1:A:203:PRO:O	2:D:78:PRO:HB2	2.19	0.42
1:A:949:CYS:O	1:A:956:LEU:HB2	2.19	0.42
1:A:206:GLN:HB2	1:A:207:ALA:C	2.40	0.42
1:A:491:ASP:N	1:A:491:ASP:OD1	2.51	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:ILE:HD11	1:A:277:ILE:HD11	2.02	0.42
1:B:1132:GLU:N	1:B:1132:GLU:OE1	2.39	0.42
1:B:369:PHE:HB3	1:B:426:PRO:HG3	2.02	0.42
1:B:595:GLU:HB3	1:B:597:ASP:OD1	2.20	0.42
1:A:1184:ASP:OD1	1:A:1185:LYS:N	2.52	0.42
1:A:144:LYS:HG2	1:A:170:PRO:HA	2.01	0.42
1:A:241:LEU:HA	1:A:241:LEU:HD23	1.87	0.42
1:B:480:TRP:HE3	1:B:495:VAL:HG23	1.85	0.42
1:A:1132:GLU:N	1:A:1132:GLU:OE1	2.47	0.42
1:A:93:ARG:HG2	1:A:113:THR:HA	2.01	0.42
1:A:322:VAL:HA	1:A:342:LYS:O	2.20	0.42
1:B:480:TRP:HB2	1:B:495:VAL:HG22	2.01	0.42
1:B:462:LEU:N	1:B:787:ILE:HD11	2.35	0.42
1:B:453:SER:HB3	1:B:797:PRO:HD3	2.02	0.42
1:B:335:THR:OG1	1:B:336:GLY:N	2.52	0.42
1:A:275:VAL:HG11	1:A:343:ILE:HG13	2.02	0.42
1:A:279:ARG:HE	1:A:404:PRO:HB3	1.84	0.42
1:A:341:VAL:O	1:A:390:THR:HA	2.18	0.42
1:B:260:GLU:HA	1:B:292:THR:HG22	2.02	0.42
1:A:970:LEU:HB2	1:B:895:GLN:OE1	2.19	0.42
1:B:126:GLN:NE2	2:C:43:VAL:HG12	2.34	0.42
1:A:861:ILE:HD11	1:A:933:LEU:HG	2.01	0.42
1:B:31:GLY:O	1:B:81:HIS:ND1	2.46	0.42
1:B:483:LYS:HG2	1:B:484:LEU:H	1.85	0.42
1:B:539:ILE:HG22	1:B:540:HIS:HB2	2.02	0.42
1:B:541:PRO:HG3	1:B:545:ARG:HG3	2.01	0.42
1:B:640:PRO:O	1:B:643:THR:OG1	2.38	0.42
1:A:179:ALA:O	1:A:244:GLN:NE2	2.49	0.41
1:B:657:SER:N	1:B:678:GLY:O	2.49	0.41
1:B:842:PRO:HA	1:B:843:PRO:HD3	1.91	0.41
1:A:446:ILE:HD13	1:A:800:LEU:HB2	2.01	0.41
1:A:818:THR:HG22	1:A:850:LYS:HD3	2.02	0.41
2:C:28:TRP:O	2:C:32:THR:OG1	2.27	0.41
1:A:585:PHE:CE2	1:A:595:GLU:HB2	2.55	0.41
1:A:378:GLU:CB	1:A:379:LYS:HA	2.49	0.41
1:B:1098:THR:HG1	1:B:1116:SER:HG	1.68	0.41
1:B:25:LEU:HD12	1:B:25:LEU:HA	1.91	0.41
1:A:254:GLY:HA2	1:A:267:HIS:CD2	2.54	0.41
1:A:297:VAL:HG11	1:A:357:ILE:HG13	2.03	0.41
1:A:374:PHE:O	1:A:418:VAL:HG22	2.20	0.41
1:B:577:LEU:HD12	1:B:580:GLY:H	1.86	0.41

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:668:THR:OG1	1:B:669:GLY:N	2.53	0.41
1:A:21:ILE:HG23	1:A:39:THR:HB	2.02	0.41
1:A:970:LEU:HD21	1:B:936:ILE:HG21	2.01	0.41
1:B:276:PRO:HG3	1:B:394:PHE:CE1	2.56	0.41
1:B:483:LYS:NZ	1:B:491:ASP:O	2.53	0.41
1:A:1081:ALA:N	1:A:1082:PRO:HD3	2.35	0.41
1:A:486:LYS:HG3	1:A:529:GLN:O	2.21	0.41
1:B:1196:SER:O	1:B:1200:ILE:HG12	2.20	0.41
1:A:143:GLU:HA	1:A:144:LYS:HA	1.83	0.41
1:A:173:ILE:O	1:A:193:GLU:HA	2.21	0.41
1:A:526:LEU:HD23	1:A:527:ALA:N	2.36	0.41
1:B:1022:ASP:OD1	1:B:1023:ASP:N	2.51	0.41
1:B:492:ALA:HA	1:B:507:ILE:HG13	2.02	0.41
1:A:1138:GLN:HA	1:A:1170:ILE:HD12	2.03	0.41
1:A:154:ASN:HB3	1:A:160:THR:CG2	2.51	0.41
1:A:274:ARG:HG2	1:A:395:PRO:O	2.21	0.41
1:A:299:HIS:HB2	1:A:357:ILE:HD12	2.03	0.41
1:B:540:HIS:CE1	1:B:563:ILE:HG12	2.55	0.41
1:B:939:THR:HG21	1:B:973:LEU:N	2.26	0.41
1:A:121:ARG:HD3	2:D:38:ASP:OD1	2.22	0.40
1:A:679:LEU:HD12	1:A:683:VAL:HB	2.04	0.40
1:B:1007:TYR:CE2	1:B:1054:CYS:HB2	2.56	0.40
1:A:400:ALA:HA	1:A:401:PRO:HD3	1.98	0.40
1:A:620:ARG:NH1	1:A:640:PRO:HD3	2.37	0.40
1:B:1007:TYR:OH	1:B:1040:VAL:HG12	2.21	0.40
1:B:647:LYS:HE3	1:B:693:THR:O	2.21	0.40
1:B:760:GLU:O	1:B:760:GLU:HG3	2.21	0.40
1:A:539:ILE:HG12	1:A:544:ILE:HG12	2.01	0.40
1:B:504:VAL:O	1:B:512:GLU:HB3	2.22	0.40
1:B:540:HIS:CG	1:B:563:ILE:HG12	2.56	0.40
1:A:561:ARG:HG2	1:A:579:SER:HB3	2.04	0.40
1:B:890:VAL:HG21	1:B:955:LEU:HD13	2.03	0.40
2:C:79:PRO:HA	2:C:80:PRO:HD3	1.93	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1167/1213 (96%)	1101 (94%)	63 (5%)	3 (0%)	41	71
1	B	1162/1213 (96%)	1082 (93%)	77 (7%)	3 (0%)	41	71
2	C	53/95 (56%)	53 (100%)	0	0	100	100
2	D	53/95 (56%)	52 (98%)	1 (2%)	0	100	100
All	All	2435/2616 (93%)	2288 (94%)	141 (6%)	6 (0%)	47	78

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	524	PRO
1	A	570	GLU
1	B	332	GLY
1	B	144	LYS
1	A	472	LEU
1	B	282	GLY

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1010/1041 (97%)	991 (98%)	19 (2%)	57	84
1	B	1009/1041 (97%)	991 (98%)	18 (2%)	59	85
2	C	50/85 (59%)	49 (98%)	1 (2%)	55	82
2	D	50/85 (59%)	49 (98%)	1 (2%)	55	82

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2119/2252 (94%)	2080 (98%)	39 (2%)	59 85

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	144	LYS
1	A	206	GLN
1	A	210	GLN
1	A	393	ASP
1	A	475	THR
1	A	479	VAL
1	A	587	MET
1	A	653	THR
1	A	692	ILE
1	A	718	ASN
1	A	753	TYR
1	A	782	LEU
1	A	784	GLN
1	A	866	SER
1	A	939	THR
1	A	986	ILE
1	A	1039	SER
1	A	1121	THR
1	A	1135	ASP
2	D	27	THR
1	B	347	ASP
1	B	390	THR
1	B	403	ASN
1	B	488	ASP
1	B	517	SER
1	B	523	VAL
1	B	552	VAL
1	B	563	ILE
1	B	568	THR
1	B	693	THR
1	B	697	THR
1	B	734	THR
1	B	753	TYR
1	B	796	THR
1	B	827	LEU
1	B	894	SER
1	B	1063	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	1107	VAL
2	C	26	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	530	GLN
1	A	572	GLN
1	A	717	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 9 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 [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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1173/1213 (96%)	-0.15	21 (1%) 68 67	50, 88, 145, 190	0
1	B	1170/1213 (96%)	-0.18	16 (1%) 75 75	48, 82, 155, 207	0
2	C	55/95 (57%)	-0.02	0 100 100	53, 68, 99, 124	0
2	D	55/95 (57%)	-0.09	1 (1%) 68 67	63, 85, 111, 125	0
All	All	2453/2616 (93%)	-0.16	38 (1%) 73 73	48, 84, 150, 207	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	531	MET	6.8
1	B	487	TYR	6.8
1	B	762	CYS	6.5
1	A	473	PRO	5.8
1	A	530	GLN	5.4
1	A	493	TYR	4.6
1	A	381	GLY	4.3
1	A	529	GLN	4.2
1	B	541	PRO	3.9
1	A	558	PRO	3.8
1	A	380	LEU	3.7
1	B	511	VAL	3.6
1	B	542	LYS	3.4
1	B	490	TYR	3.3
1	B	380	LEU	3.3
1	B	544	ILE	3.1
1	A	533	GLU	3.0
1	B	553	ASN	2.9
1	B	537	ILE	2.9
1	B	560	HIS	2.8
1	A	474	GLY	2.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	211	LEU	2.7
1	A	536	LEU	2.7
1	A	534	GLU	2.5
1	A	303	GLY	2.5
2	D	27	THR	2.4
1	B	515	SER	2.4
1	B	559	GLN	2.4
1	A	306	GLY	2.3
1	A	528	VAL	2.3
1	B	562	SER	2.3
1	A	7	ASN	2.2
1	B	509	GLU	2.2
1	B	618	LEU	2.2
1	A	592	SER	2.1
1	A	22	THR	2.1
1	A	1120	GLY	2.0
1	A	354	SER	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. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	CA	B	1304	1/1	0.25	0.99	313,313,313,313	0
3	CA	A	1303	1/1	0.70	0.49	191,191,191,191	0
3	CA	B	1302	1/1	0.77	0.34	124,124,124,124	0
3	CA	B	1305	1/1	0.92	0.55	140,140,140,140	0
3	CA	A	1304	1/1	0.92	0.51	138,138,138,138	0
3	CA	B	1303	1/1	0.94	0.15	123,123,123,123	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CA	A	1301	1/1	0.95	0.12	88,88,88,88	0
3	CA	A	1302	1/1	0.95	0.10	134,134,134,134	0
3	CA	B	1301	1/1	0.97	0.13	76,76,76,76	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.