



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:02 PM GMT

PDB ID : 4QQ1  
Title : Crystal structure of the isotype 1 Transferrin binding protein B (TbpB) from serogroup B *Neisseria meningitidis*  
Authors : Calmettes, C.; Moraes, T.F.  
Deposited on : 2014-06-26  
Resolution : 3.33 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  
<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

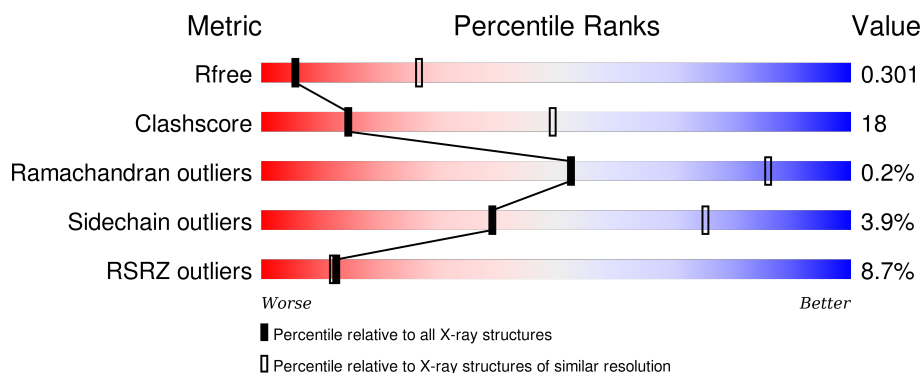
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.33 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	1004 (3.40-3.28)
Clashscore	102246	1072 (3.40-3.28)
Ramachandran outliers	100387	1055 (3.40-3.28)
Sidechain outliers	100360	1054 (3.40-3.28)
RSRZ outliers	91569	1009 (3.40-3.28)

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. 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	543	<div> <div>5%</div> <div>66%</div> <div>27%</div> <div>• •</div> </div>
1	B	543	<div> <div>10%</div> <div>66%</div> <div>21%</div> <div>• 11%</div> </div>
1	C	543	<div> <div>9%</div> <div>71%</div> <div>22%</div> <div>• 5%</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
3	GOL	B	603	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11828 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 Transferrin-binding protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	521	Total	C	N	O	S	129	0	0
			4023	2514	700	800	9			
1	B	485	Total	C	N	O	S	145	0	0
			3768	2368	651	740	9			
1	C	515	Total	C	N	O	S	109	0	0
			3982	2494	689	790	9			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	37	SER	-	EXPRESSION TAG	UNP Q06988
B	37	SER	-	EXPRESSION TAG	UNP Q06988
C	37	SER	-	EXPRESSION TAG	UNP Q06988

- Molecule 2 is CESIUM ION (three-letter code: CS) (formula: Cs).

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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).

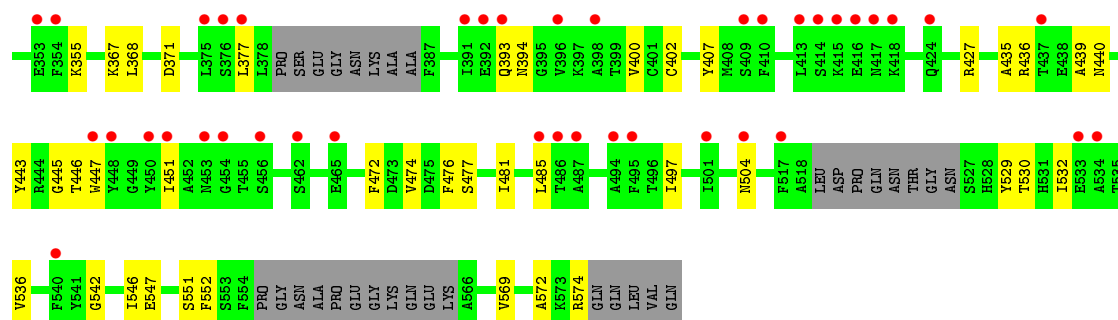


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	O	S	0	0
			5	4	1		

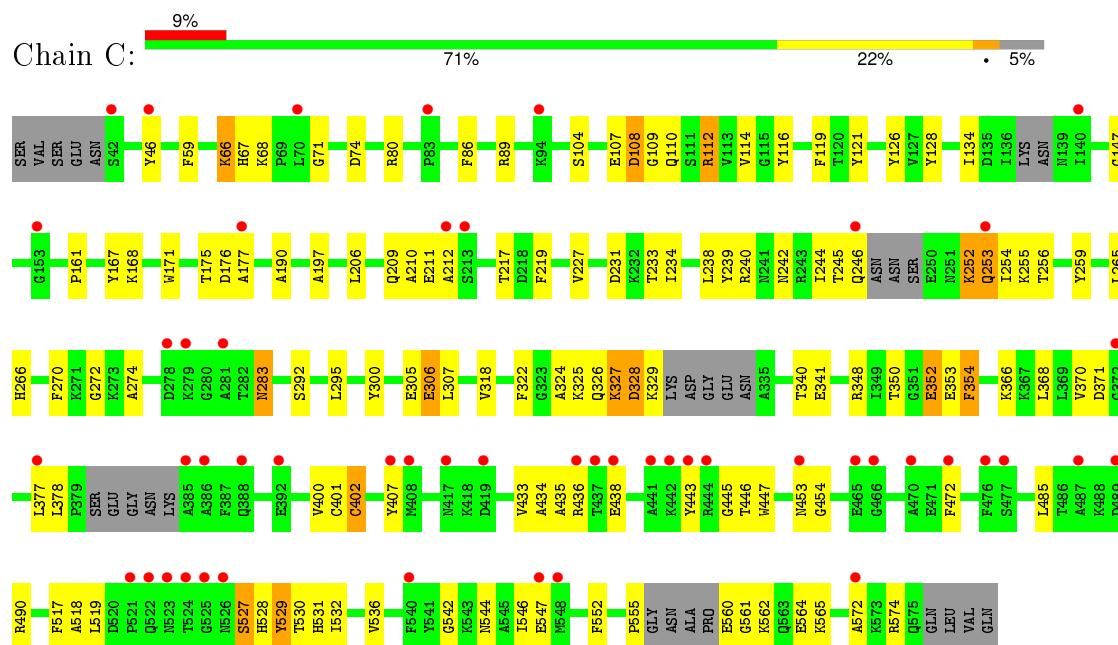
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	15	Total 15	O 15	0	0
5	B	5	Total 5	O 5	0	0
5	C	10	Total 10	O 10	0	0





• Molecule 1: Transferrin-binding protein 2





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	135.33Å 99.97Å 160.16Å 90.00° 93.47° 90.00°	Depositor
Resolution (Å)	45.17 – 3.33 43.69 – 3.33	Depositor EDS
% Data completeness (in resolution range)	98.5 (45.17-3.33) 91.1 (43.69-3.33)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.80 (at 3.32Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.249 , 0.301 0.249 , 0.301	Depositor DCC
$R_{free}$ test set	2984 reflections (4.94%)	DCC
Wilson B-factor (Å <sup>2</sup> )	96.8	Xtriage
Anisotropy	0.684	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 119.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 30866 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	11828	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	125.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% 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, 0.375 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: CS, GOL, SO4

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	0.28	0/4101	0.50	1/5510 (0.0%)
1	B	0.28	0/3840	0.48	2/5149 (0.0%)
1	C	0.27	0/4058	0.56	4/5448 (0.1%)
All	All	0.28	0/11999	0.52	7/16107 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	3
All	All	0	6

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	352	GLU	CB-CA-C	-12.73	84.94	110.40
1	C	353	GLU	N-CA-C	-8.78	87.31	111.00
1	C	352	GLU	N-CA-C	-7.54	90.63	111.00
1	A	249	SER	N-CA-C	5.91	126.96	111.00
1	C	327	LYS	N-CA-CB	-5.33	101.01	110.60
1	B	111	SER	N-CA-C	5.09	124.75	111.00
1	B	283	ASN	N-CA-C	5.07	124.70	111.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	105	LYS	Peptide
1	A	106	TRP	Peptide
1	A	251	ASN	Peptide
1	B	106	TRP	Peptide
1	B	281	ALA	Mainchain
1	B	282	THR	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4023	0	3879	156	0
1	B	3768	0	3647	114	0
1	C	3982	0	3846	126	0
2	A	4	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
3	A	6	0	8	1	0
3	B	6	0	8	1	0
4	C	5	0	0	0	0
5	A	15	0	0	5	0
5	B	5	0	0	0	0
5	C	10	0	0	0	0
All	All	11828	0	11388	394	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 18.

All (394) 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:C:325:LYS:CE	1:C:328:ASP:HB2	1.77	1.13
1:B:281:ALA:CB	1:B:282:THR:HA	1.79	1.12
1:A:107:GLU:HG2	1:A:110:GLN:H	1.11	1.10
1:B:135:ASP:CB	1:B:140:ILE:HG22	1.81	1.09
1:B:107:GLU:HG2	1:B:110:GLN:H	1.14	1.08
1:A:546:ILE:HG22	1:A:574:ARG:HH11	1.13	1.07

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:ASP:HB3	1:B:140:ILE:HG22	1.12	1.07
1:A:110:GLN:HG2	1:A:207:ARG:HD3	1.35	1.06
1:B:112:ARG:NH2	1:B:219:PHE:CD1	2.25	1.04
1:C:325:LYS:HE2	1:C:328:ASP:HB2	1.40	1.03
1:A:251:ASN:HB2	1:A:252:LYS:HB2	1.39	1.03
1:B:281:ALA:HB1	1:B:282:THR:HA	1.45	0.97
1:A:546:ILE:HG22	1:A:574:ARG:NH1	1.78	0.96
1:C:325:LYS:NZ	1:C:328:ASP:HB2	1.81	0.95
1:A:110:GLN:CG	1:A:207:ARG:HD3	1.95	0.95
1:A:281:ALA:HB3	1:A:289:ILE:HG12	1.51	0.92
1:B:135:ASP:HB3	1:B:140:ILE:CG2	2.00	0.92
1:B:107:GLU:HB3	1:B:109:GLY:H	1.36	0.89
1:A:453:ASN:HB2	1:A:454:GLY:C	1.92	0.89
1:B:190:ALA:O	1:B:197:ALA:HA	1.72	0.89
1:C:325:LYS:NZ	1:C:328:ASP:CB	2.37	0.88
1:B:107:GLU:HG2	1:B:110:GLN:N	1.88	0.88
1:A:107:GLU:CG	1:A:110:GLN:H	1.87	0.88
1:A:107:GLU:HG2	1:A:110:GLN:N	1.87	0.87
1:A:432:ASP:O	1:A:436:ARG:HG3	1.74	0.86
1:A:370:VAL:O	1:A:370:VAL:HG12	1.73	0.86
1:B:107:GLU:CG	1:B:110:GLN:H	1.90	0.84
1:C:350:THR:O	1:C:352:GLU:HA	1.75	0.84
1:B:107:GLU:HB3	1:B:108:ASP:HA	1.60	0.83
1:C:252:LYS:O	1:C:253:GLN:HB2	1.77	0.83
1:C:119:PHE:CE1	1:C:325:LYS:HB2	2.13	0.82
1:B:193:ASP:O	1:B:194:LYS:HB2	1.79	0.82
1:C:453:ASN:H	1:C:454:GLY:HA2	1.44	0.82
1:B:107:GLU:HB3	1:B:109:GLY:N	1.93	0.82
1:C:530:THR:HG22	1:C:532:ILE:HG13	1.60	0.81
1:C:254:ILE:HG23	1:C:255:LYS:H	1.44	0.81
1:C:206:LEU:HD11	1:C:211:GLU:HG2	1.63	0.81
1:A:139:ASN:O	1:A:140:ILE:HG13	1.81	0.81
1:B:110:GLN:HB3	1:B:207:ARG:HG2	1.62	0.80
1:A:453:ASN:H	1:A:454:GLY:HA2	1.46	0.80
1:B:281:ALA:HB3	1:B:282:THR:HA	1.62	0.80
1:C:239:TYR:CG	1:C:255:LYS:HD2	2.17	0.79
1:A:107:GLU:HB3	1:A:109:GLY:H	1.46	0.79
1:B:107:GLU:CB	1:B:109:GLY:H	1.96	0.79
1:A:88:GLU:O	1:A:92:LEU:HD23	1.83	0.79
1:B:281:ALA:CB	1:B:282:THR:CA	2.62	0.78
1:C:350:THR:O	1:C:352:GLU:CA	2.33	0.76

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:SER:O	1:B:170:THR:HG21	1.85	0.76
1:A:80:ARG:HD3	1:A:371:ASP:O	1.86	0.76
1:B:281:ALA:HB1	1:B:282:THR:CA	2.17	0.75
1:B:107:GLU:HB3	1:B:108:ASP:CA	2.16	0.75
1:A:107:GLU:HB3	1:A:109:GLY:N	2.01	0.75
1:B:530:THR:HG22	1:B:532:ILE:HG13	1.70	0.74
1:A:107:GLU:CB	1:A:109:GLY:H	2.00	0.74
1:B:110:GLN:CB	1:B:207:ARG:HG2	2.18	0.73
1:B:135:ASP:CB	1:B:140:ILE:CG2	2.62	0.73
1:C:119:PHE:CZ	1:C:325:LYS:HB2	2.23	0.73
1:A:453:ASN:HB2	1:A:454:GLY:O	1.88	0.73
1:B:112:ARG:NH2	1:B:219:PHE:HD1	1.86	0.72
1:C:239:TYR:CG	1:C:255:LYS:CD	2.72	0.72
1:B:56:ASN:OD1	1:B:140:ILE:HD12	1.89	0.72
1:B:56:ASN:CG	1:B:140:ILE:HD12	2.10	0.72
1:B:530:THR:CG2	1:B:532:ILE:HG13	2.19	0.72
1:A:194:LYS:N	5:A:702:HOH:O	2.21	0.72
1:C:490:ARG:NH1	1:C:518:ALA:O	2.23	0.72
1:C:352:GLU:HG2	1:C:565:LYS:HD2	1.70	0.72
1:C:108:ASP:OD2	1:C:108:ASP:N	2.22	0.71
1:A:107:GLU:HB3	1:A:108:ASP:HA	1.70	0.71
1:A:101:LEU:CD2	1:A:129:LEU:HD11	2.20	0.71
1:B:232:LYS:HG3	1:B:265:LEU:HB2	1.71	0.71
1:A:251:ASN:HB2	1:A:252:LYS:CB	2.18	0.70
1:C:254:ILE:HG23	1:C:255:LYS:N	2.06	0.70
1:B:393:GLN:HG3	1:B:394:ASN:H	1.55	0.69
1:A:92:LEU:HD21	1:A:148:TYR:HE2	1.56	0.69
1:A:110:GLN:CB	1:A:207:ARG:HD3	2.22	0.69
1:A:107:GLU:HB3	1:A:108:ASP:CA	2.22	0.69
1:C:119:PHE:CZ	1:C:325:LYS:CB	2.76	0.69
1:C:530:THR:CG2	1:C:532:ILE:HG13	2.22	0.69
1:B:68:LYS:HB3	1:B:177:ALA:HB3	1.74	0.68
1:A:110:GLN:HG2	1:A:207:ARG:CD	2.21	0.68
1:A:112:ARG:NH1	1:A:207:ARG:O	2.26	0.68
1:C:255:LYS:HZ3	1:C:255:LYS:HB2	1.59	0.68
1:A:354:PHE:HB3	1:A:555:PRO:HG3	1.76	0.67
1:B:107:GLU:HA	1:B:107:GLU:OE2	1.94	0.67
1:B:546:ILE:HG13	1:B:547:GLU:HG3	1.77	0.67
1:C:68:LYS:HB3	1:C:177:ALA:HB3	1.76	0.67
1:B:436:ARG:HG2	1:B:477:SER:H	1.60	0.66
1:A:128:TYR:O	1:A:129:LEU:HD12	1.94	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:209:GLN:HG3	1:C:210:ALA:H	1.60	0.66
1:C:325:LYS:HZ1	1:C:328:ASP:CB	2.08	0.66
1:A:110:GLN:HB3	1:A:207:ARG:HD3	1.77	0.65
1:A:546:ILE:CG2	1:A:574:ARG:HH11	2.00	0.65
1:A:325:LYS:NZ	5:A:701:HOH:O	2.29	0.65
1:B:254:ILE:HG22	1:B:255:LYS:HG3	1.78	0.65
1:A:546:ILE:HG13	1:A:547:GLU:HG3	1.78	0.65
1:A:101:LEU:HD23	1:A:129:LEU:HD11	1.77	0.65
1:A:128:TYR:C	1:A:129:LEU:HD12	2.18	0.65
1:A:193:ASP:HA	5:A:702:HOH:O	1.96	0.65
1:A:180:LYS:N	1:A:193:ASP:OD2	2.30	0.65
1:C:227:VAL:HG22	1:C:234:ILE:HG23	1.79	0.65
1:C:546:ILE:HG13	1:C:547:GLU:HG3	1.78	0.65
1:A:179:GLU:HA	1:A:193:ASP:OD2	1.97	0.64
1:A:88:GLU:O	1:A:92:LEU:CD2	2.45	0.64
1:C:244:ILE:HG22	1:C:245:THR:H	1.62	0.64
1:B:107:GLU:CB	1:B:108:ASP:HA	2.22	0.64
1:B:106:TRP:HD1	1:B:112:ARG:CB	2.11	0.64
1:A:92:LEU:HD21	1:A:148:TYR:CE2	2.33	0.64
1:A:107:GLU:CG	1:A:109:GLY:H	2.11	0.63
1:C:121:TYR:HD2	1:C:306:GLU:OE1	1.82	0.63
1:A:111:SER:O	1:A:170:THR:HG21	2.00	0.62
1:C:246:GLN:HG3	1:C:246:GLN:O	1.99	0.62
1:A:78:LEU:HD23	1:A:152:LYS:HD2	1.81	0.62
1:C:307:LEU:CD1	1:C:324:ALA:HB3	2.29	0.62
1:B:242:ASN:HD21	1:B:256:THR:HG23	1.65	0.61
1:C:239:TYR:CD1	1:C:255:LYS:CD	2.83	0.61
1:A:455:THR:O	1:A:519:LEU:HD13	2.00	0.61
1:C:560:GLU:HB3	1:C:562:LYS:HG2	1.83	0.61
1:A:252:LYS:HD3	1:A:253:GLN:H	1.65	0.61
1:B:107:GLU:CG	1:B:109:GLY:H	2.14	0.61
1:A:446:THR:OG1	1:A:447:TRP:N	2.34	0.61
1:B:240:ARG:NH1	1:B:242:ASN:OD1	2.29	0.60
1:A:140:ILE:HD11	1:B:93:GLU:HG2	1.82	0.60
1:C:530:THR:HG22	1:C:531:HIS:N	2.16	0.60
1:A:110:GLN:HB3	1:A:207:ARG:CD	2.31	0.60
1:C:80:ARG:HD3	1:C:371:ASP:O	2.01	0.60
1:A:530:THR:HG23	1:A:530:THR:O	2.02	0.60
1:B:274:ALA:HB3	1:B:292:SER:HB3	1.83	0.60
1:A:248:ASN:O	1:A:248:ASN:ND2	2.26	0.60
1:C:325:LYS:HZ1	1:C:328:ASP:CG	2.06	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:ASN:OD1	1:A:519:LEU:HD11	2.02	0.59
1:C:209:GLN:HG3	1:C:210:ALA:N	2.17	0.59
1:A:368:LEU:HD23	1:A:377:LEU:HD11	1.83	0.59
1:A:92:LEU:HD12	1:A:129:LEU:HD13	1.83	0.59
1:A:384:LYS:HB2	1:A:385:ALA:HB2	1.85	0.59
1:C:116:TYR:CE1	1:C:327:LYS:HG2	2.37	0.59
1:B:265:LEU:HD21	1:B:299:PHE:HE2	1.67	0.59
1:C:274:ALA:HB3	1:C:292:SER:HB3	1.83	0.59
1:A:546:ILE:HA	1:A:574:ARG:HE	1.68	0.59
1:A:125:GLY:O	1:A:149:LEU:HD12	2.03	0.59
1:C:305:GLU:OE1	1:C:306:GLU:OE1	2.21	0.58
1:C:527:SER:OG	1:C:528:HIS:N	2.36	0.58
1:C:119:PHE:CE1	1:C:325:LYS:CB	2.85	0.58
1:A:227:VAL:HG22	1:A:234:ILE:HG23	1.85	0.58
1:B:109:GLY:O	1:B:207:ARG:HB3	2.03	0.58
1:A:102:ILE:N	1:A:102:ILE:HD12	2.19	0.58
1:B:350:THR:OG1	1:B:355:LYS:O	2.21	0.58
1:C:368:LEU:HD23	1:C:377:LEU:HD11	1.86	0.58
1:B:536:VAL:HA	1:B:552:PHE:HB3	1.86	0.58
1:C:544:ASN:O	1:C:574:ARG:NH2	2.36	0.57
1:B:112:ARG:H	1:B:112:ARG:HD3	1.69	0.57
1:C:239:TYR:CD1	1:C:255:LYS:HD2	2.38	0.57
1:A:106:TRP:N	1:A:106:TRP:CE3	2.73	0.57
1:B:407:TYR:CG	1:B:542:GLY:HA2	2.40	0.57
1:C:407:TYR:CG	1:C:542:GLY:HA2	2.40	0.57
1:C:322:PHE:CD2	1:C:322:PHE:N	2.73	0.57
1:C:443:TYR:HB2	1:C:472:PHE:HB2	1.86	0.57
1:B:377:LEU:HB3	1:B:400:VAL:HG11	1.87	0.56
1:C:112:ARG:HD3	1:C:219:PHE:HB2	1.87	0.56
1:A:107:GLU:CB	1:A:108:ASP:HA	2.33	0.56
1:B:161:PRO:HA	1:B:340:THR:HA	1.87	0.56
1:C:245:THR:OG1	1:C:246:GLN:N	2.38	0.56
1:C:254:ILE:CG2	1:C:255:LYS:H	2.18	0.56
1:B:106:TRP:HD1	1:B:112:ARG:HB3	1.71	0.56
1:C:119:PHE:CE1	1:C:325:LYS:N	2.74	0.56
1:C:119:PHE:HA	1:C:306:GLU:OE2	2.06	0.55
1:C:305:GLU:OE2	1:C:326:GLN:HG2	2.05	0.55
1:C:107:GLU:HB2	1:C:109:GLY:N	2.21	0.55
1:A:407:TYR:CG	1:A:542:GLY:HA2	2.41	0.55
1:B:80:ARG:HD3	1:B:371:ASP:O	2.06	0.55
1:A:265:LEU:HD13	1:A:270:PHE:HB3	1.87	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:307:LEU:HD11	1:C:324:ALA:HB3	1.89	0.55
1:A:80:ARG:NH1	1:A:371:ASP:O	2.39	0.55
1:A:460:GLU:O	1:A:468:ASN:ND2	2.29	0.55
1:A:93:GLU:OE2	1:A:96:ARG:NH2	2.40	0.55
1:B:342:THR:O	1:B:504:ASN:ND2	2.40	0.55
1:C:161:PRO:HA	1:C:340:THR:HA	1.88	0.55
1:C:354:PHE:HB3	1:C:555:PRO:HB3	1.88	0.55
1:B:111:SER:HA	1:B:219:PHE:O	2.07	0.54
1:A:60:ASN:HB2	1:A:64:LYS:HE3	1.90	0.54
1:A:511:LYS:NZ	5:A:715:HOH:O	2.39	0.54
1:C:325:LYS:HG2	1:C:326:GLN:O	2.06	0.54
1:C:211:GLU:HG3	1:C:212:ALA:H	1.73	0.54
1:C:325:LYS:HZ3	1:C:328:ASP:CB	2.18	0.54
1:A:104:SER:HB3	1:A:126:TYR:CZ	2.41	0.54
1:A:370:VAL:O	1:A:371:ASP:HB2	2.08	0.53
1:A:445:GLY:HA3	1:A:572:ALA:HA	1.91	0.53
1:B:135:ASP:HB2	1:B:140:ILE:HG22	1.82	0.53
1:A:370:VAL:CG1	1:A:370:VAL:O	2.47	0.53
1:A:68:LYS:HB3	1:A:177:ALA:HB3	1.91	0.53
1:C:239:TYR:CG	1:C:255:LYS:HD3	2.43	0.53
1:A:139:ASN:C	1:A:140:ILE:HG13	2.28	0.53
1:B:446:THR:OG1	1:B:447:TRP:N	2.41	0.53
1:C:168:LYS:O	1:C:325:LYS:O	2.27	0.53
1:C:252:LYS:O	1:C:253:GLN:CB	2.51	0.53
1:C:377:LEU:HB3	1:C:400:VAL:HG11	1.91	0.53
1:A:193:ASP:O	1:A:194:LYS:HB2	2.09	0.52
1:C:80:ARG:CD	1:C:371:ASP:O	2.57	0.52
1:C:265:LEU:HD13	1:C:270:PHE:HB3	1.90	0.52
1:A:436:ARG:NH2	1:A:438:GLU:OE2	2.42	0.52
1:C:305:GLU:OE1	1:C:306:GLU:CD	2.48	0.52
1:A:139:ASN:O	1:A:140:ILE:CG1	2.56	0.52
1:C:239:TYR:CD1	1:C:255:LYS:HD3	2.44	0.51
1:C:445:GLY:HA3	1:C:572:ALA:HA	1.92	0.51
1:A:536:VAL:HA	1:A:552:PHE:HB3	1.92	0.51
1:C:255:LYS:NZ	1:C:255:LYS:HB2	2.24	0.51
1:B:135:ASP:HB2	1:B:140:ILE:CG2	2.39	0.51
1:A:251:ASN:N	1:A:251:ASN:OD1	2.43	0.51
1:A:238:LEU:HB2	1:A:259:TYR:HB2	1.92	0.51
1:C:446:THR:OG1	1:C:447:TRP:N	2.44	0.51
1:B:257:THR:HB	3:B:603:GOL:H2	1.93	0.51
1:B:108:ASP:N	1:B:108:ASP:OD2	2.30	0.50

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:530:THR:CG2	1:C:531:HIS:N	2.74	0.50
1:B:269:ARG:NH1	1:B:296:GLU:OE2	2.44	0.50
1:B:46:TYR:O	1:B:300:TYR:OH	2.24	0.50
1:B:110:GLN:CA	1:B:207:ARG:HG2	2.41	0.50
1:A:453:ASN:O	1:A:563:GLN:O	2.29	0.50
1:B:80:ARG:NH1	1:B:371:ASP:O	2.44	0.50
1:A:437:THR:HG23	1:A:477:SER:HB3	1.93	0.50
1:C:167:TYR:CD1	1:C:326:GLN:HB3	2.47	0.50
1:B:443:TYR:CE1	1:B:574:ARG:HB2	2.47	0.50
1:A:112:ARG:O	1:A:219:PHE:HB2	2.12	0.50
1:C:254:ILE:CG2	1:C:255:LYS:N	2.75	0.50
1:C:244:ILE:HD13	1:C:244:ILE:N	2.27	0.50
1:C:517:PHE:O	1:C:529:TYR:HB2	2.11	0.50
1:A:125:GLY:O	1:A:149:LEU:CD1	2.59	0.49
1:A:105:LYS:C	1:A:106:TRP:CE3	2.85	0.49
1:B:83:PRO:HD3	1:B:154:LYS:HD3	1.93	0.49
1:B:107:GLU:H	1:B:108:ASP:HA	1.77	0.49
1:A:107:GLU:HG2	1:A:110:GLN:O	2.12	0.49
1:B:110:GLN:HA	1:B:207:ARG:HG2	1.94	0.49
1:A:44:ALA:HB1	1:A:269:ARG:HH11	1.77	0.49
1:A:193:ASP:CA	5:A:702:HOH:O	2.58	0.49
1:C:536:VAL:HA	1:C:552:PHE:HB3	1.95	0.49
1:C:107:GLU:N	1:C:108:ASP:HA	2.28	0.49
1:A:179:GLU:HG2	1:A:180:LYS:HG3	1.93	0.49
1:C:434:ALA:N	1:C:435:ALA:HA	2.27	0.49
1:A:396:VAL:HG12	1:A:415:LYS:HB3	1.95	0.49
1:B:238:LEU:HB2	1:B:259:TYR:HB2	1.95	0.49
1:B:497:ILE:HG23	1:B:536:VAL:HG11	1.95	0.48
1:A:104:SER:HB3	1:A:126:TYR:CE2	2.47	0.48
1:B:443:TYR:HB2	1:B:472:PHE:HB2	1.95	0.48
1:A:173:TYR:H	1:A:199:SER:HB3	1.78	0.48
1:A:104:SER:OG	1:A:126:TYR:N	2.43	0.48
1:C:107:GLU:HG3	1:C:110:GLN:HB2	1.95	0.48
1:C:366:LYS:HD2	1:C:378:LEU:HD11	1.96	0.48
1:B:436:ARG:HA	1:B:476:PHE:HB3	1.96	0.48
1:C:175:THR:HG22	1:C:318:VAL:HG22	1.96	0.48
1:B:116:TYR:CE2	1:B:168:LYS:HD2	2.48	0.48
1:A:110:GLN:HG2	1:A:207:ARG:HB3	1.95	0.48
1:A:443:TYR:HB2	1:A:472:PHE:HB2	1.96	0.48
1:A:531:HIS:CD2	1:A:531:HIS:H	2.31	0.48
1:A:85:SER:HA	1:A:89:ARG:HD3	1.95	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:ASN:C	1:A:248:ASN:HD22	2.14	0.47
1:C:530:THR:HG21	1:C:532:ILE:HD11	1.95	0.47
1:B:133:ASN:HB3	1:B:142:LEU:HB2	1.96	0.47
1:A:104:SER:HB3	1:A:126:TYR:CE1	2.49	0.47
1:C:239:TYR:CB	1:C:255:LYS:HD3	2.43	0.47
1:C:377:LEU:HD13	1:C:400:VAL:HG21	1.97	0.47
1:A:281:ALA:CB	1:A:289:ILE:HG12	2.36	0.47
1:B:104:SER:OG	1:B:126:TYR:N	2.48	0.47
1:A:453:ASN:N	1:A:454:GLY:HA2	2.20	0.47
1:A:453:ASN:HB2	1:A:454:GLY:CA	2.44	0.47
1:A:116:TYR:CE2	1:A:168:LYS:HD2	2.49	0.47
1:C:242:ASN:HD21	1:C:256:THR:HG23	1.80	0.47
1:C:119:PHE:CD1	1:C:325:LYS:HB2	2.50	0.47
1:A:198:LEU:HG	1:A:200:ALA:H	1.80	0.47
1:C:564:GLU:N	1:C:564:GLU:OE2	2.48	0.47
1:A:214:SER:OG	1:A:215:GLY:N	2.46	0.47
1:B:193:ASP:OD2	1:B:194:LYS:N	2.47	0.47
1:A:161:PRO:HA	1:A:340:THR:HA	1.96	0.47
1:B:474:VAL:HG13	1:B:481:ILE:HG12	1.96	0.46
1:C:370:VAL:O	1:C:371:ASP:HB2	2.15	0.46
1:C:114:VAL:HB	1:C:217:THR:HA	1.98	0.46
1:C:239:TYR:HB3	1:C:255:LYS:CD	2.45	0.46
1:A:190:ALA:O	1:A:197:ALA:HA	2.16	0.46
1:C:560:GLU:OE2	1:C:561:GLY:N	2.49	0.46
1:B:345:ASP:OD2	1:B:427:ARG:NE	2.35	0.46
1:C:447:TRP:CD2	1:C:485:LEU:HD13	2.50	0.46
1:B:367:LYS:HA	1:B:377:LEU:HG	1.98	0.45
1:C:283:ASN:N	1:C:283:ASN:OD1	2.42	0.45
1:B:135:ASP:OD1	1:B:137:LYS:HB2	2.17	0.45
1:B:118:ASN:HD21	1:B:329:LYS:HG2	1.81	0.45
1:A:342:THR:O	1:A:504:ASN:ND2	2.41	0.45
1:A:450:TYR:HD1	1:A:458:SER:HB3	1.81	0.45
1:A:195:SER:OG	1:A:196:GLY:N	2.50	0.45
1:C:190:ALA:O	1:C:197:ALA:HA	2.16	0.45
1:A:245:THR:HB	1:A:248:ASN:HA	1.98	0.45
1:B:97:GLY:HA3	1:B:99:SER:N	2.31	0.45
1:A:240:ARG:HB3	1:A:256:THR:HB	1.98	0.45
1:C:307:LEU:HD11	1:C:324:ALA:CB	2.47	0.45
1:A:149:LEU:HD11	1:A:321:VAL:HG22	1.98	0.45
1:A:475:ASP:OD1	1:A:478:THR:OG1	2.25	0.45
1:A:107:GLU:H	1:A:108:ASP:HA	1.82	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:368:LEU:HD23	1:B:377:LEU:HD11	1.99	0.45
1:C:104:SER:OG	1:C:126:TYR:N	2.50	0.45
1:B:111:SER:OG	1:B:220:GLY:HA3	2.17	0.45
1:A:211:GLU:OE1	1:A:211:GLU:N	2.50	0.45
1:A:530:THR:OG1	1:A:564:GLU:OE1	2.34	0.44
1:A:105:LYS:O	1:A:106:TRP:CD2	2.70	0.44
1:C:66:LYS:HD2	1:C:67:HIS:H	1.82	0.44
1:A:175:THR:HG22	1:A:318:VAL:HG22	2.00	0.44
1:A:497:ILE:HG23	1:A:536:VAL:HG11	1.99	0.44
1:A:67:HIS:NE2	1:A:176:ASP:OD2	2.42	0.44
1:B:236:GLY:O	1:B:261:ILE:N	2.40	0.44
1:B:105:LYS:C	1:B:106:TRP:CE3	2.91	0.44
1:A:101:LEU:CD2	1:A:129:LEU:CD1	2.94	0.44
1:A:269:ARG:HA	1:A:298:GLY:HA2	2.00	0.44
1:B:89:ARG:HH21	1:B:103:GLU:CD	2.21	0.44
1:A:107:GLU:HG3	1:A:109:GLY:H	1.83	0.43
1:C:436:ARG:O	1:C:438:GLU:HG3	2.18	0.43
1:B:183:PHE:HD2	1:B:284:GLY:O	2.00	0.43
1:A:107:GLU:H	1:A:108:ASP:CA	2.32	0.43
1:C:433:VAL:HG21	1:C:544:ASN:HA	2.01	0.43
1:B:439:ALA:O	1:B:440:ASN:CG	2.56	0.43
1:A:443:TYR:CE1	1:A:574:ARG:HB2	2.53	0.43
1:A:530:THR:CG2	1:A:530:THR:O	2.65	0.43
1:C:528:HIS:HB3	1:C:529:TYR:H	1.61	0.43
1:B:173:TYR:H	1:B:199:SER:HB3	1.83	0.43
1:A:272:GLY:O	1:A:295:LEU:HB3	2.18	0.43
1:A:67:HIS:CE1	1:A:69:PRO:HB3	2.54	0.43
1:C:401:CYS:HA	1:C:402:CYS:HA	1.75	0.43
1:A:252:LYS:HD3	1:A:253:GLN:N	2.32	0.43
1:C:239:TYR:HB3	1:C:255:LYS:HG2	2.01	0.43
1:B:451:ILE:HG23	1:B:532:ILE:HD11	2.01	0.43
1:A:123:ARG:NE	3:A:605:GOL:O2	2.52	0.43
1:C:329:LYS:O	1:C:329:LYS:HG2	2.18	0.43
1:B:435:ALA:HA	1:B:436:ARG:HB2	2.00	0.43
1:A:49:ALA:O	1:A:76:LYS:HG2	2.18	0.43
1:A:254:ILE:HG13	1:A:255:LYS:HG3	2.01	0.43
1:A:107:GLU:N	1:A:108:ASP:HA	2.33	0.43
1:A:353:GLU:HG3	1:A:354:PHE:CD1	2.54	0.43
1:A:367:LYS:HA	1:A:377:LEU:HG	2.01	0.43
1:C:231:ASP:HB3	1:C:233:THR:HG22	2.01	0.43
1:A:138:ASN:HA	1:A:139:ASN:HA	1.65	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:238:LEU:HB2	1:C:259:TYR:HB2	2.01	0.42
1:C:86:PHE:CZ	1:C:89:ARG:HB2	2.54	0.42
1:A:128:TYR:CD1	1:A:145:PRO:HB3	2.54	0.42
1:C:244:ILE:HG22	1:C:245:THR:N	2.30	0.42
1:B:107:GLU:N	1:B:108:ASP:HA	2.31	0.42
1:B:107:GLU:HB3	1:B:108:ASP:C	2.36	0.42
1:C:340:THR:OG1	1:C:341:GLU:N	2.52	0.42
1:B:447:TRP:CE2	1:B:485:LEU:HD13	2.54	0.42
1:B:445:GLY:HA3	1:B:572:ALA:HA	2.01	0.42
1:A:384:LYS:HA	1:A:385:ALA:HA	1.83	0.42
1:C:272:GLY:O	1:C:295:LEU:HB3	2.20	0.42
1:B:227:VAL:HG22	1:B:234:ILE:HG23	2.01	0.42
1:A:52:LEU:HA	1:A:53:PRO:HD3	1.83	0.42
1:A:401:CYS:HA	1:A:402:CYS:HA	1.78	0.42
1:A:343:VAL:HG23	1:A:344:ILE:HG13	2.01	0.42
1:A:260:THR:OG1	1:A:275:LEU:HB2	2.20	0.42
1:B:435:ALA:CA	1:B:436:ARG:HB2	2.50	0.42
1:B:66:LYS:HD3	1:B:67:HIS:H	1.84	0.42
1:B:106:TRP:HD1	1:B:112:ARG:HB2	1.85	0.42
1:A:113:VAL:HG13	1:A:217:THR:HG22	2.02	0.42
1:B:216:HIS:NE2	1:B:218:ASP:O	2.53	0.42
1:B:163:GLU:HG3	1:B:165:ILE:HD11	2.00	0.42
1:B:504:ASN:OD1	1:B:504:ASN:N	2.50	0.41
1:C:46:TYR:O	1:C:300:TYR:OH	2.25	0.41
1:B:472:PHE:HZ	1:B:497:ILE:HD12	1.84	0.41
1:B:377:LEU:HD13	1:B:400:VAL:HG21	2.02	0.41
1:B:440:ASN:C	1:B:440:ASN:OD1	2.59	0.41
1:C:176:ASP:N	1:C:176:ASP:OD1	2.52	0.41
1:C:325:LYS:HG2	1:C:326:GLN:N	2.34	0.41
1:B:546:ILE:HA	1:B:574:ARG:HB3	2.02	0.41
1:B:109:GLY:O	1:B:207:ARG:O	2.36	0.41
1:B:60:ASN:HB2	1:B:64:LYS:HE3	2.02	0.41
1:C:328:ASP:O	1:C:329:LYS:HB3	2.20	0.41
1:C:239:TYR:CB	1:C:255:LYS:CD	2.98	0.41
1:C:239:TYR:CD2	1:C:255:LYS:HD2	2.55	0.41
1:A:248:ASN:C	1:A:248:ASN:ND2	2.72	0.41
1:B:551:SER:HB3	1:B:569:VAL:HG12	2.01	0.41
1:B:111:SER:O	1:B:170:THR:CG2	2.65	0.41
1:B:128:TYR:HA	1:B:147:GLY:HA3	2.02	0.41
1:C:239:TYR:HB3	1:C:255:LYS:CG	2.51	0.41
1:A:106:TRP:HE3	1:A:106:TRP:N	2.18	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:ILE:HG21	1:A:567:SER:HB2	2.03	0.41
1:C:116:TYR:CZ	1:C:168:LYS:HD2	2.56	0.41
1:C:71:GLY:N	1:C:74:ASP:OD2	2.53	0.41
1:A:109:GLY:C	1:A:110:GLN:HG3	2.40	0.41
1:C:240:ARG:HD3	1:C:242:ASN:OD1	2.21	0.41
1:A:351:GLY:HA2	1:A:352:GLU:HA	1.57	0.41
1:A:107:GLU:HB3	1:A:108:ASP:C	2.41	0.40
1:B:138:ASN:HA	1:B:139:ASN:HA	1.74	0.40
1:A:244:ILE:HG23	1:A:248:ASN:OD1	2.22	0.40
1:C:519:LEU:HG	1:C:529:TYR:HA	2.02	0.40
1:A:232:LYS:HA	1:A:265:LEU:HD23	2.03	0.40
1:A:532:ILE:HG23	1:A:554:PHE:HD2	1.86	0.40
1:C:307:LEU:HG	1:C:324:ALA:HB3	2.03	0.40
1:A:447:TRP:CD2	1:A:485:LEU:HD13	2.57	0.40
1:C:171:TRP:CE2	1:C:238:LEU:HB3	2.57	0.40
1:C:116:TYR:CD1	1:C:168:LYS:HB2	2.56	0.40
1:B:137:LYS:O	1:B:138:ASN:HB2	2.21	0.40
1:A:140:ILE:CD1	1:B:93:GLU:CG	2.99	0.40
1:C:128:TYR:HA	1:C:147:GLY:HA3	2.04	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	513/543 (94%)	432 (84%)	80 (16%)	1 (0%)	52	86
1	B	471/543 (87%)	414 (88%)	57 (12%)	0	100	100
1	C	503/543 (93%)	435 (86%)	66 (13%)	2 (0%)	39	77
All	All	1487/1629 (91%)	1281 (86%)	203 (14%)	3 (0%)	52	86

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	253	GLN
1	C	527	SER
1	A	138	ASN

### 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	420/439 (96%)	397 (94%)	23 (6%)	27	65
1	B	393/439 (90%)	382 (97%)	11 (3%)	51	82
1	C	415/439 (94%)	401 (97%)	14 (3%)	44	78
All	All	1228/1317 (93%)	1180 (96%)	48 (4%)	39	75

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	PHE
1	A	66	LYS
1	A	106	TRP
1	A	108	ASP
1	A	111	SER
1	A	112	ARG
1	A	149	LEU
1	A	209	GLN
1	A	211	GLU
1	A	240	ARG
1	A	243	ARG
1	A	248	ASN
1	A	249	SER
1	A	251	ASN
1	A	252	LYS
1	A	266	HIS
1	A	348	ARG
1	A	354	PHE
1	A	402	CYS
1	A	531	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	533	GLU
1	A	554	PHE
1	A	565	LYS
1	B	59	PHE
1	B	66	LYS
1	B	96	ARG
1	B	108	ASP
1	B	110	GLN
1	B	111	SER
1	B	112	ARG
1	B	283	ASN
1	B	350	THR
1	B	402	CYS
1	B	529	TYR
1	C	59	PHE
1	C	66	LYS
1	C	108	ASP
1	C	112	ARG
1	C	134	ILE
1	C	252	LYS
1	C	266	HIS
1	C	283	ASN
1	C	306	GLU
1	C	328	ASP
1	C	348	ARG
1	C	354	PHE
1	C	402	CYS
1	C	529	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	118	ASN
1	A	181	GLN
1	A	424	GLN
1	A	531	HIS
1	B	424	GLN
1	C	424	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 11 ligands modelled in this entry, 8 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	GOL	A	605	-	5,5,5	0.35	0	5,5,5	0.20	0
3	GOL	B	603	-	5,5,5	0.35	0	5,5,5	0.24	0
4	SO4	C	603	-	4,4,4	0.23	0	6,6,6	0.08	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	605	-	-	0/4/4/4	0/0/0/0
3	GOL	B	603	-	-	0/4/4/4	0/0/0/0
4	SO4	C	603	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.



There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	605	GOL	1	0
3	B	603	GOL	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	521/543 (95%)	0.46	29 (5%) 28 27	46, 97, 184, 282	35 (6%)
1	B	485/543 (89%)	0.73	52 (10%) 8 7	53, 121, 247, 487	39 (8%)
1	C	515/543 (94%)	0.60	51 (9%) 9 10	66, 123, 220, 312	29 (5%)
All	All	1521/1629 (93%)	0.59	132 (8%) 13 12	46, 116, 221, 487	103 (6%)

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	557	ASN	12.1
1	B	456	SER	11.3
1	C	437	THR	6.9
1	B	114	VAL	6.5
1	B	414	SER	6.1
1	B	450	TYR	6.0
1	B	377	LEU	5.9
1	C	523	ASN	5.8
1	B	99	SER	5.7
1	B	392	GLU	5.6
1	A	556	GLY	5.3
1	C	522	GLN	5.1
1	B	391	ILE	4.9
1	C	436	ARG	4.5
1	B	100	GLU	4.5
1	B	487	ALA	4.5
1	A	523	ASN	4.3
1	C	487	ALA	4.3
1	C	465	GLU	4.2
1	C	392	GLU	4.2
1	B	413	LEU	4.0
1	C	42	SER	3.9
1	C	278	ASP	3.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	494	ALA	3.8
1	A	441	ALA	3.8
1	B	465	GLU	3.7
1	A	563	GLN	3.7
1	C	212	ALA	3.6
1	C	489	ASP	3.6
1	B	448	TYR	3.5
1	B	451	ILE	3.5
1	B	396	VAL	3.4
1	C	443	TYR	3.4
1	C	372	GLY	3.4
1	B	504	ASN	3.4
1	C	521	PRO	3.4
1	B	540	PHE	3.4
1	B	485	LEU	3.3
1	A	371	ASP	3.3
1	A	474	VAL	3.3
1	C	419	ASP	3.3
1	C	213	SER	3.3
1	B	415	LYS	3.3
1	B	486	THR	3.2
1	A	518	ALA	3.2
1	C	470	ALA	3.2
1	C	540	PHE	3.2
1	C	83	PRO	3.2
1	A	484	THR	3.2
1	B	375	LEU	3.1
1	C	526	ASN	3.0
1	A	405	LEU	3.0
1	B	495	PHE	3.0
1	C	548	MET	3.0
1	B	533	GLU	3.0
1	B	376	SER	3.0
1	B	98	SER	3.0
1	B	517	PHE	3.0
1	B	417	ASN	2.9
1	C	386	ALA	2.9
1	A	395	GLY	2.9
1	C	525	GLY	2.9
1	C	177	ALA	2.9
1	C	477	SER	2.9
1	B	447	TRP	2.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	548	MET	2.9
1	B	350	THR	2.8
1	C	417	ASN	2.8
1	C	442	LYS	2.8
1	B	501	ILE	2.8
1	B	454	GLY	2.8
1	C	279	LYS	2.7
1	C	572	ALA	2.7
1	A	451	ILE	2.7
1	C	441	ALA	2.7
1	B	534	ALA	2.7
1	A	487	ALA	2.7
1	C	407	TYR	2.6
1	C	408	MET	2.6
1	C	70	LEU	2.6
1	C	547	GLU	2.6
1	A	521	PRO	2.6
1	B	83	PRO	2.6
1	B	42	SER	2.6
1	B	354	PHE	2.6
1	A	517	PHE	2.6
1	C	444	ARG	2.6
1	A	108	ASP	2.5
1	C	253	GLN	2.5
1	C	94	LYS	2.5
1	A	493	PRO	2.5
1	A	43	GLY	2.5
1	B	393	GLN	2.5
1	B	136	ILE	2.5
1	C	388	GLN	2.5
1	B	409	SER	2.5
1	A	107	GLU	2.4
1	B	115	GLY	2.4
1	B	353	GLU	2.4
1	C	524	THR	2.3
1	B	424	GLN	2.3
1	C	246	GLN	2.3
1	C	476	PHE	2.3
1	C	385	ALA	2.3
1	B	418	LYS	2.2
1	C	377	LEU	2.2
1	B	453	ASN	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	289	ILE	2.2
1	B	216	HIS	2.2
1	B	494	ALA	2.2
1	B	462	SER	2.2
1	A	540	PHE	2.2
1	B	410	PHE	2.2
1	C	153	GLY	2.2
1	A	574	ARG	2.2
1	B	416	GLU	2.2
1	C	281	ALA	2.2
1	B	97	GLY	2.2
1	A	318	VAL	2.1
1	B	437	THR	2.1
1	A	486	THR	2.1
1	C	140	ILE	2.1
1	C	466	GLY	2.1
1	C	46	TYR	2.1
1	A	370	VAL	2.1
1	B	398	ALA	2.1
1	C	438	GLU	2.0
1	C	453	ASN	2.0
1	A	433	VAL	2.0
1	B	304	GLY	2.0
1	A	529	TYR	2.0
1	C	472	PHE	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, 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GOL	B	603	6/6	0.90	0.49	2.19	62,94,110,122	0
3	GOL	A	605	6/6	0.62	0.39	0.91	81,85,103,119	0
2	CS	B	601	1/1	0.95	0.12	-2.34	177,177,177,177	0
4	SO4	C	603	5/5	0.83	0.65	-	226,227,227,227	5
2	CS	A	601	1/1	0.97	0.22	-	179,179,179,179	0
2	CS	A	602	1/1	0.99	0.07	-	190,190,190,190	0
2	CS	A	603	1/1	0.95	0.12	-	200,200,200,200	0
2	CS	C	601	1/1	0.93	0.21	-	196,196,196,196	0
2	CS	A	604	1/1	0.73	0.18	-	231,231,231,231	0
2	CS	B	602	1/1	0.97	0.15	-	192,192,192,192	0
2	CS	C	602	1/1	0.87	0.09	-	262,262,262,262	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.