



Full wwPDB X-ray Structure Validation Report ⓘ

May 4, 2016 – 08:06 PM EDT

PDB ID : 5E70
Title : Crystal structure of Ecoli Branching Enzyme with gamma cyclodextrin
Authors : Feng, L.; Nosrati, M.; Geiger, J.H.
Deposited on : 2015-10-11
Resolution : 2.33 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
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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027457
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) : rb-20027457

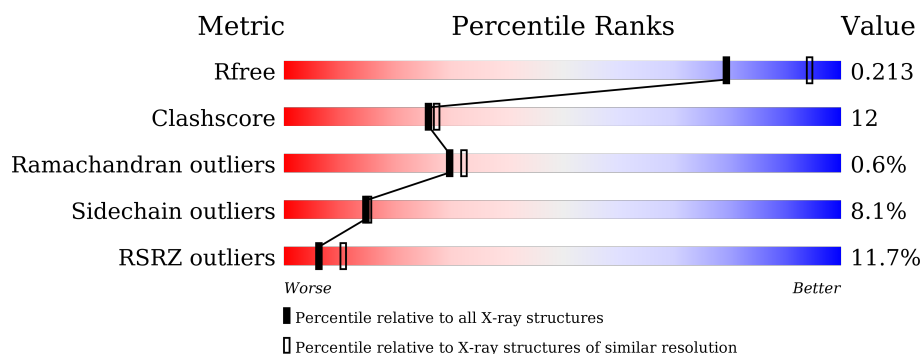
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.33 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	1406 (2.36-2.32)
Clashscore	102246	1509 (2.36-2.32)
Ramachandran outliers	100387	1490 (2.36-2.32)
Sidechain outliers	100360	1491 (2.36-2.32)
RSRZ outliers	91569	1412 (2.36-2.32)

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	612	<div> <div>11%</div> <div> <div></div> <div>72%</div> <div>20%</div> <div>• •</div> </div> </div>
1	B	612	<div> <div>%</div> <div> <div></div> <div>77%</div> <div>17%</div> <div>• •</div> </div> </div>
1	C	612	<div> <div>32%</div> <div> <div></div> <div>70%</div> <div>21%</div> <div>• 6%</div> </div> </div>
1	D	612	<div> <div>2%</div> <div> <div></div> <div>73%</div> <div>19%</div> <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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	RCD	B	801	-	-	-	X
2	RCD	C	801	-	-	-	X
2	RCD	D	801	-	-	-	X
3	GOL	A	802	-	-	-	X
3	GOL	A	803	-	-	-	X
3	GOL	B	803	-	-	-	X

2 Entry composition [i](#)

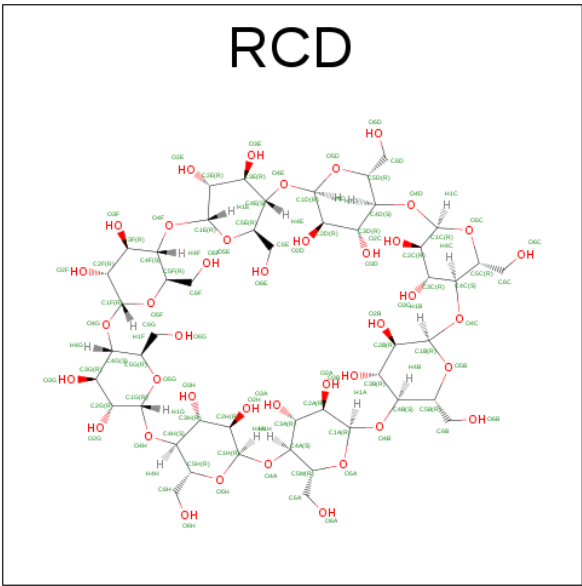
There are 4 unique types of molecules in this entry. The entry contains 21132 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 1,4-alpha-glucan branching enzyme GlgB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	586	Total	C	N	O	S	0	6	0
			4871	3110	868	877	16			
1	B	600	Total	C	N	O	S	0	2	0
			4960	3170	880	894	16			
1	C	578	Total	C	N	O	S	0	2	0
			4768	3052	845	855	16			
1	D	588	Total	C	N	O	S	0	2	0
			4852	3103	862	871	16			

- Molecule 2 is gamma-cyclodextrin (three-letter code: RCD) (formula: C₄₈H₈₀O₄₀).



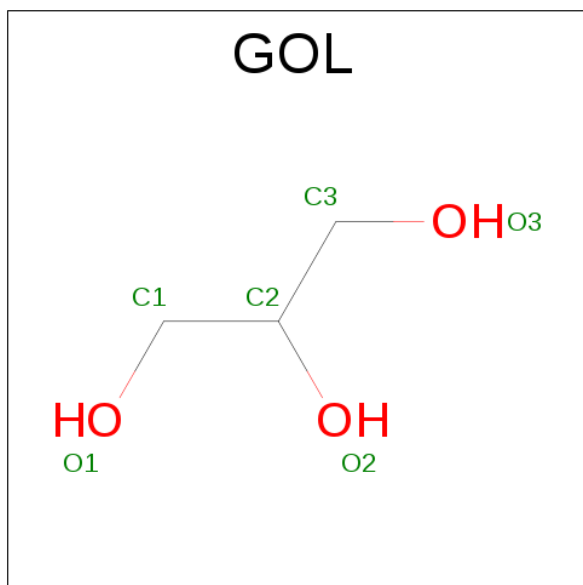
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			88	48	40		
2	B	1	Total	C	O	0	0
			88	48	40		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			88	48	40		
2	D	1	Total	C	O	0	0
			88	48	40		
2	D	1	Total	C	O	0	0
			88	48	40		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

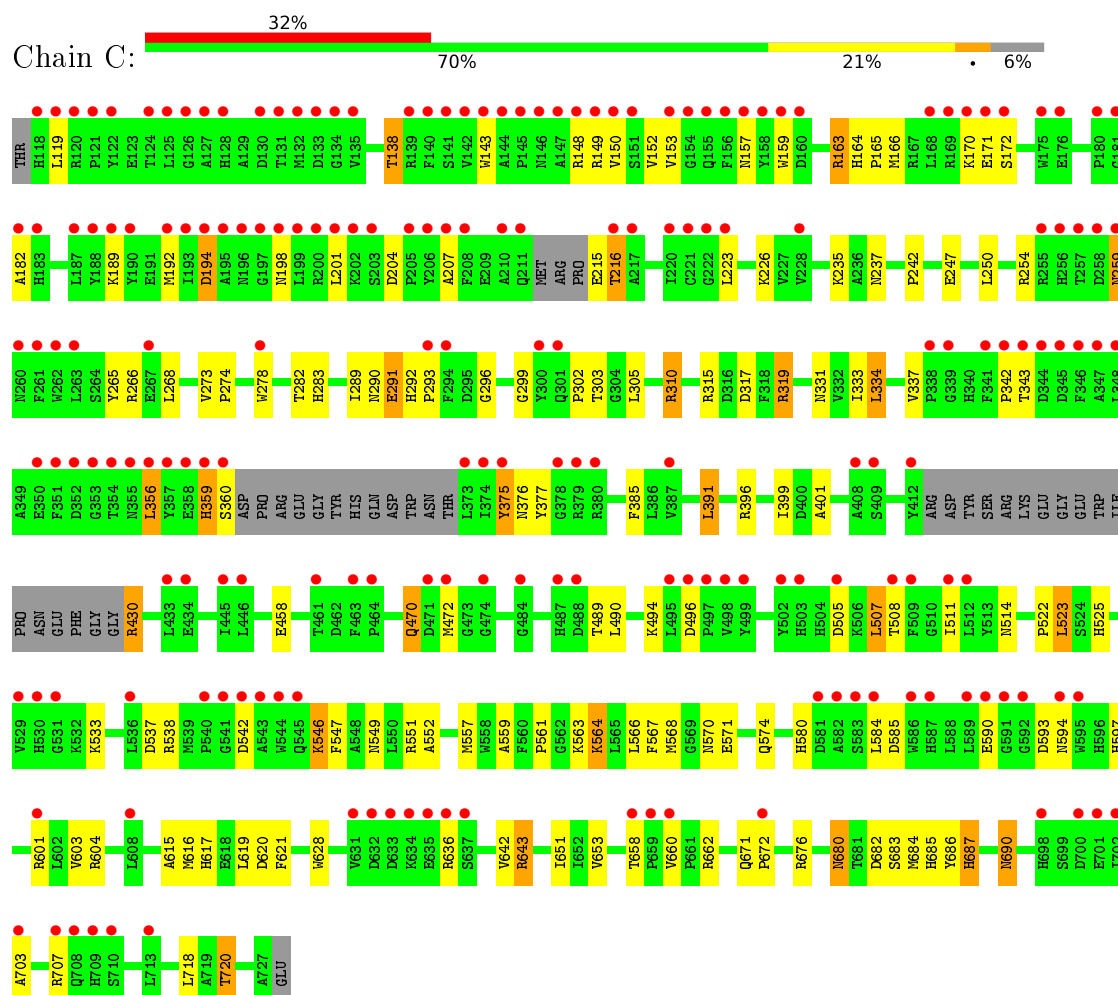


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		

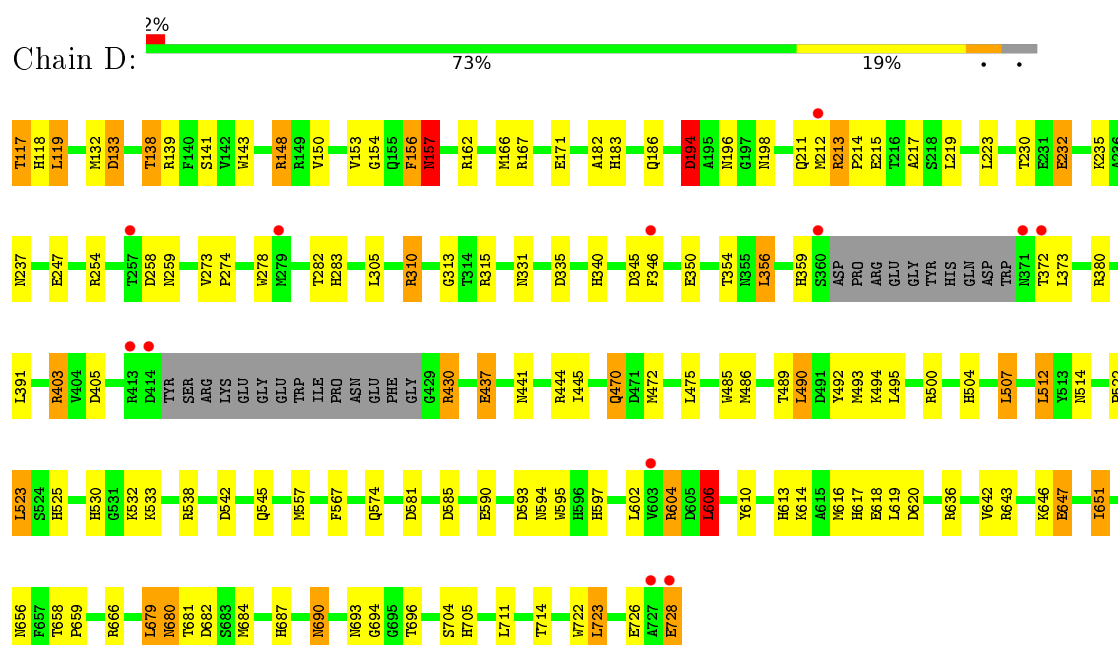
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	310	Total 310	O 310	0	0
4	B	480	Total 480	O 480	0	0
4	C	75	Total 75	O 75	0	0
4	D	340	Total 340	O 340	0	0

• Molecule 1: 1,4-alpha-glucan branching enzyme GlgB



• Molecule 1: 1,4-alpha-glucan branching enzyme GlgB



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	92.10 Å 103.22 Å 186.69 Å 90.00° 91.73° 90.00°	Depositor
Resolution (Å)	50.00 – 2.33 45.60 – 2.33	Depositor EDS
% Data completeness (in resolution range)	94.6 (50.00-2.33) 94.6 (45.60-2.33)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.10 (at 2.34 Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.170 , 0.217 0.167 , 0.213	Depositor DCC
R_{free} test set	14049 reflections (11.11%)	DCC
Wilson B-factor (Å ²)	38.6	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 53.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	21132	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% 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

5.1 Standard geometry

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

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	0.65	0/5028	0.68	5/6827 (0.1%)
1	B	0.77	0/5120	0.77	7/6953 (0.1%)
1	C	0.40	0/4918	0.51	0/6677
1	D	0.65	0/5006	0.73	8/6796 (0.1%)
All	All	0.64	0/20072	0.68	20/27253 (0.1%)

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	D	0	1

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	538	ARG	NE-CZ-NH2	-8.43	116.09	120.30
1	B	723	LEU	CA-CB-CG	7.54	132.64	115.30
1	A	723	LEU	CA-CB-CG	6.89	131.15	115.30
1	D	723	LEU	CA-CB-CG	6.65	130.59	115.30
1	D	403	ARG	NE-CZ-NH1	-6.46	117.07	120.30
1	D	636	ARG	NE-CZ-NH2	-6.45	117.08	120.30
1	A	606	LEU	CA-CB-CG	6.00	129.11	115.30
1	B	403	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	D	604	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	B	355	ASN	CB-CA-C	-5.96	98.48	110.40
1	D	194	ASP	CB-CG-OD1	-5.93	112.97	118.30
1	A	606	LEU	CB-CG-CD1	5.90	121.03	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	606	LEU	CA-CB-CG	5.62	128.21	115.30
1	A	311	ARG	NE-CZ-NH1	-5.57	117.52	120.30
1	D	157	ASN	N-CA-CB	-5.39	100.89	110.60
1	B	622	ASP	CB-CG-OD1	5.33	123.10	118.30
1	D	604	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	D	606	LEU	CA-CB-CG	5.26	127.40	115.30
1	A	403	ARG	NE-CZ-NH1	-5.22	117.69	120.30
1	B	604	ARG	NE-CZ-NH2	-5.07	117.77	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	156	PHE	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	4871	0	4596	131	0
1	B	4960	0	4666	109	0
1	C	4768	0	4505	111	0
1	D	4852	0	4584	119	1
2	A	88	0	80	15	0
2	B	88	0	80	1	0
2	C	88	0	80	2	0
2	D	176	0	160	4	1
3	A	12	0	16	3	0
3	B	12	0	16	2	0
3	D	12	0	16	1	0
4	A	310	0	0	17	0
4	B	480	0	0	17	0
4	C	75	0	0	8	0
4	D	340	0	0	19	0
All	All	21132	0	18799	479	1

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 12.

All (479) 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:211:GLN:NE2	1:A:217:ALA:HB3	1.54	1.21
1:D:117:THR:N	1:D:118:HIS:HB2	1.56	1.21
1:D:470:GLN:H	1:D:470:GLN:NE2	1.45	1.13
1:D:470:GLN:N	1:D:470:GLN:HE21	1.48	1.12
1:D:213:ARG:H	1:D:213:ARG:HD3	1.16	1.03
1:A:666:ARG:H	3:A:802:GOL:H31	1.27	0.97
1:D:437:GLU:HG3	4:D:924:HOH:O	1.65	0.96
1:B:444:ARG:HD3	4:B:927:HOH:O	1.64	0.96
1:C:470:GLN:H	1:C:470:GLN:HE21	0.96	0.95
1:A:213:ARG:HA	1:A:214:PRO:O	1.65	0.94
1:B:470:GLN:NE2	1:B:470:GLN:H	1.66	0.92
1:C:319:ARG:NH2	1:C:396:ARG:O	2.02	0.92
1:A:157:ASN:HB3	4:A:1053:HOH:O	1.70	0.92
1:B:157:ASN:HD22	1:B:164:HIS:HD2	1.17	0.91
1:A:211:GLN:OE1	1:A:215:GLU:HB3	1.70	0.91
1:B:138:THR:HG22	1:B:182:ALA:O	1.70	0.91
1:C:470:GLN:N	1:C:470:GLN:HE21	1.70	0.90
1:B:470:GLN:HE21	1:B:470:GLN:N	1.69	0.89
1:D:278:TRP:O	1:D:604:ARG:HD2	1.73	0.89
1:B:666:ARG:O	3:B:803:GOL:H32	1.73	0.88
1:C:594:ASN:H	1:C:597:HIS:HD2	1.19	0.88
1:A:262:TRP:CZ3	1:A:311:ARG:HG2	2.11	0.86
1:B:164:HIS:HE1	4:B:1282:HOH:O	1.57	0.85
1:D:138:THR:HG22	1:D:182:ALA:O	1.77	0.85
1:C:684[A]:MET:CE	1:D:684:MET:SD	2.66	0.84
1:A:211:GLN:HE21	1:A:217:ALA:HB3	1.42	0.83
1:A:512:LEU:HD21	2:A:801:RCD:H6E	1.61	0.83
1:D:154:GLY:O	1:D:157:ASN:HB3	1.79	0.82
1:D:213:ARG:H	1:D:213:ARG:CD	1.92	0.82
1:C:658:THR:HG22	1:C:660:VAL:H	1.42	0.82
1:B:415:TYR:CD1	1:B:430:ARG:HD3	2.14	0.82
1:C:163:ARG:HH11	1:C:163:ARG:CG	1.91	0.81
1:A:594:ASN:H	1:A:597:HIS:HD2	1.25	0.81
1:D:117:THR:CA	1:D:118:HIS:HB2	2.10	0.81
1:B:157:ASN:HD22	1:B:164:HIS:CD2	1.99	0.80
1:C:684[A]:MET:HE1	1:D:684:MET:SD	2.21	0.80
1:C:430:ARG:HA	1:C:430:ARG:HE	1.46	0.79
1:D:213:ARG:N	1:D:213:ARG:HD3	1.96	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:574:GLN:NE2	1:A:585:ASP:H	1.81	0.79
1:A:676[B]:ARG:HH11	1:A:676[B]:ARG:HG3	1.48	0.78
4:C:961:HOH:O	1:D:590:GLU:HG2	1.84	0.78
1:A:157:ASN:CB	4:A:1053:HOH:O	2.30	0.77
1:C:470:GLN:H	1:C:470:GLN:NE2	1.80	0.77
1:A:262:TRP:CH2	1:A:311:ARG:HG2	2.19	0.77
1:C:237:ASN:ND2	1:C:283:HIS:HE1	1.82	0.77
1:C:334:LEU:HD23	1:C:399:ILE:HG21	1.65	0.76
2:A:801:RCD:H5B	2:A:801:RCD:H6C	1.67	0.76
1:B:247:GLU:OE1	1:B:525:HIS:HD2	1.69	0.76
1:B:594:ASN:H	1:B:597:HIS:HD2	1.33	0.76
1:A:533:LYS:O	1:A:538:ARG:NH2	2.19	0.75
1:D:156:PHE:HD1	1:D:186:GLN:OE1	1.68	0.75
1:C:250:LEU:HD22	1:C:268:LEU:HD13	1.68	0.75
1:A:676[B]:ARG:HH11	1:A:676[B]:ARG:CG	1.99	0.75
1:D:282:THR:OG1	1:D:283:HIS:HD2	1.68	0.74
1:B:211:GLN:HG2	1:B:212:MET:SD	2.28	0.74
1:A:148:ARG:O	1:A:149:ARG:HB3	1.88	0.74
1:A:676[B]:ARG:NH1	1:A:676[B]:ARG:HG3	1.98	0.74
1:D:684:MET:H	1:D:690:ASN:ND2	1.86	0.74
1:C:163:ARG:HH11	1:C:163:ARG:HG2	1.52	0.73
1:C:594:ASN:H	1:C:597:HIS:CD2	2.06	0.73
1:B:658:THR:HG22	1:B:660:VAL:H	1.54	0.73
1:A:709:HIS:HD2	4:A:1059:HOH:O	1.71	0.73
1:A:282:THR:OG1	1:A:283:HIS:HD2	1.71	0.73
1:A:666:ARG:H	3:A:802:GOL:C3	2.02	0.72
1:C:170:LYS:HA	1:C:170:LYS:HE2	1.71	0.72
1:C:542:ASP:O	1:C:546:LYS:HG3	1.89	0.72
1:C:686:TYR:O	1:C:687:HIS:HB2	1.89	0.72
1:C:302:PRO:O	1:C:342:PRO:HB3	1.89	0.72
1:D:504:HIS:HD2	4:D:982:HOH:O	1.72	0.71
1:B:470:GLN:HE21	1:B:470:GLN:H	0.83	0.71
1:A:693:ASN:HD21	1:A:714:THR:H	1.39	0.71
1:B:415:TYR:CD1	1:B:415:TYR:C	2.64	0.70
1:D:117:THR:HA	1:D:119:LEU:H	1.56	0.70
1:D:693:ASN:HD21	1:D:714:THR:H	1.38	0.70
1:D:138:THR:CG2	1:D:182:ALA:O	2.39	0.70
1:A:153:VAL:HA	4:A:1053:HOH:O	1.92	0.70
1:A:120:ARG:NH1	4:A:902:HOH:O	2.24	0.70
1:A:161:GLY:HA3	1:A:191:GLU:OE2	1.92	0.70
1:B:143:TRP:CH2	1:B:356:LEU:HD22	2.27	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:415:TYR:HD1	1:B:415:TYR:C	1.95	0.69
1:B:425:ASN:HD22	1:B:427:PHE:H	1.41	0.69
1:A:211:GLN:NE2	1:A:217:ALA:CB	2.45	0.69
1:C:601[B]:ARG:HG2	1:C:601[B]:ARG:HH11	1.57	0.69
1:D:340:HIS:HE1	1:D:405:ASP:OD2	1.76	0.69
1:B:289:ILE:HG13	1:B:334:LEU:HD11	1.75	0.69
1:B:413:ARG:O	1:B:414:ASP:HB2	1.93	0.68
1:B:282:THR:OG1	1:B:283:HIS:HD2	1.75	0.68
1:D:247:GLU:OE1	1:D:525:HIS:HD2	1.76	0.68
1:A:594:ASN:H	1:A:597:HIS:CD2	2.11	0.68
1:D:696:THR:OG1	1:D:726:GLU:OE1	2.11	0.68
1:D:574:GLN:NE2	1:D:585:ASP:H	1.93	0.67
1:B:237:ASN:ND2	1:B:283:HIS:HE1	1.93	0.67
1:A:214:PRO:O	1:A:215:GLU:O	2.13	0.66
1:B:684:MET:H	1:B:690:ASN:HD22	1.43	0.66
1:A:340:HIS:HE1	1:A:405:ASP:OD2	1.78	0.66
1:A:508:THR:OG1	2:A:801:RCD:H6D	1.95	0.66
1:D:194:ASP:HB3	1:D:196:ASN:H	1.60	0.66
1:D:684:MET:H	1:D:690:ASN:HD22	1.41	0.66
1:A:237:ASN:ND2	1:A:283:HIS:HE1	1.94	0.66
1:A:157:ASN:HD21	1:A:164:HIS:HB2	1.61	0.65
2:A:801:RCD:H3H	2:A:801:RCD:O5G	1.96	0.65
1:D:441:ASN:O	4:D:901:HOH:O	2.13	0.65
1:B:414:ASP:O	1:B:422:TRP:CD1	2.49	0.65
1:D:213:ARG:HB3	1:D:214:PRO:HA	1.78	0.65
1:D:156:PHE:CD2	1:D:157:ASN:HB2	2.32	0.65
1:B:480:LYS:HE3	4:B:910:HOH:O	1.96	0.65
1:B:594:ASN:H	1:B:597:HIS:CD2	2.16	0.64
1:D:494[A]:LYS:HG2	1:D:538:ARG:HB3	1.80	0.64
1:D:530:HIS:HE1	4:D:1208:HOH:O	1.81	0.64
1:B:149:ARG:HD2	1:B:150:VAL:N	2.12	0.63
1:A:209:GLU:HG2	1:A:219:LEU:CD2	2.29	0.63
1:D:183:HIS:CE1	1:D:186:GLN:HE21	2.16	0.63
1:A:148:ARG:O	1:A:193:ILE:HB	1.98	0.63
1:A:704:SER:OG	1:A:705:HIS:HD2	1.82	0.62
1:B:492:TYR:CZ	1:B:500:ARG:HG2	2.34	0.62
2:B:801:RCD:H6EA	4:B:1329:HOH:O	1.99	0.62
1:D:117:THR:HA	1:D:119:LEU:N	2.15	0.62
1:D:616:MET:SD	1:D:651:ILE:HG12	2.40	0.62
1:B:602:LEU:HG	1:B:606:LEU:HD22	1.81	0.62
1:C:685:HIS:HD2	4:D:1217:HOH:O	1.83	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:GLU:HA	1:A:354:THR:O	2.00	0.61
1:B:340:HIS:HE1	1:B:405:ASP:OD2	1.82	0.61
1:D:235:LYS:HG3	4:D:1030:HOH:O	2.01	0.61
1:A:213:ARG:CG	1:A:214:PRO:HA	2.31	0.61
1:A:666:ARG:N	3:A:802:GOL:H31	2.09	0.61
1:D:237:ASN:HD22	1:D:283:HIS:HE1	1.47	0.61
1:D:680:ASN:ND2	1:D:682:ASP:H	1.98	0.61
1:A:157:ASN:C	1:A:159:TRP:N	2.54	0.61
1:D:237:ASN:ND2	1:D:283:HIS:HE1	1.98	0.61
1:A:157:ASN:C	1:A:159:TRP:H	2.04	0.60
1:A:704:SER:OG	1:A:705:HIS:CD2	2.53	0.60
1:B:117:THR:HB	1:B:118:HIS:HD2	1.66	0.60
1:C:684[A]:MET:H	1:C:690:ASN:ND2	1.98	0.60
1:B:259:ASN:HD22	1:B:261:PHE:H	1.48	0.60
1:A:512:LEU:CD2	2:A:801:RCD:H6E	2.30	0.60
1:D:167:ARG:NH2	4:D:905:HOH:O	2.35	0.60
2:C:801:RCD:H1A	2:C:801:RCD:H6BA	1.82	0.60
2:C:801:RCD:C1A	2:C:801:RCD:H6BA	2.31	0.60
1:B:644:ARG:CG	1:B:650:GLU:HG2	2.33	0.59
1:B:138:THR:HG23	1:B:182:ALA:HB3	1.84	0.59
1:B:680:ASN:HD22	1:B:680:ASN:C	2.05	0.59
1:B:259:ASN:HB2	1:B:261:PHE:CE2	2.37	0.59
1:B:335:ASP:OD1	1:B:403:ARG:HD3	2.02	0.59
1:B:593:ASP:OD2	1:B:687:HIS:CE1	2.55	0.59
1:D:156:PHE:CD1	1:D:186:GLN:OE1	2.53	0.59
1:C:296:GLY:HA2	1:C:580:HIS:CE1	2.38	0.59
1:C:138:THR:HG22	1:C:182:ALA:O	2.03	0.59
1:A:504:HIS:HD2	4:A:1010:HOH:O	1.85	0.58
1:A:680:ASN:HD22	1:A:682:ASP:H	1.50	0.58
1:B:579:ASN:ND2	1:B:581:ASP:H	2.00	0.58
1:D:651:ILE:CD1	1:D:722:TRP:HB3	2.32	0.58
1:D:680:ASN:C	1:D:680:ASN:HD22	2.07	0.58
1:B:237:ASN:HD22	1:B:283:HIS:HE1	1.51	0.58
1:C:163:ARG:NH1	1:C:163:ARG:CG	2.56	0.58
1:C:157:ASN:HD22	1:C:164:HIS:HD2	1.50	0.58
1:B:213:ARG:HE	1:B:213:ARG:H	1.52	0.58
1:B:574:GLN:NE2	1:B:585:ASP:H	2.01	0.58
1:C:684[B]:MET:H	1:C:690:ASN:ND2	2.01	0.58
1:A:209:GLU:HG2	1:A:219:LEU:HD23	1.85	0.58
1:D:232:GLU:N	1:D:232:GLU:OE1	2.37	0.58
1:B:441:ASN:OD1	1:B:444:ARG:NH1	2.38	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:594:ASN:H	1:D:597:HIS:HD2	1.53	0.57
1:B:671:GLN:OE1	1:B:725:ARG:NH1	2.38	0.57
1:C:680:ASN:C	1:C:680:ASN:HD22	2.09	0.57
1:A:512:LEU:HD22	1:A:512:LEU:N	2.20	0.57
1:B:425:ASN:ND2	1:B:427:PHE:H	2.02	0.56
1:D:273:VAL:HB	1:D:274:PRO:HD3	1.87	0.56
1:D:593:ASP:OD2	1:D:687:HIS:HE1	1.87	0.56
1:B:658:THR:CG2	1:B:660:VAL:H	2.19	0.56
1:B:213:ARG:NE	1:B:213:ARG:H	2.04	0.56
1:A:247:GLU:OE1	1:A:525:HIS:HD2	1.89	0.56
1:D:148:ARG:HG3	1:D:194:ASP:O	2.06	0.56
1:B:674:LYS:NZ	4:B:904:HOH:O	2.30	0.56
1:A:579:ASN:ND2	1:A:581:ASP:H	2.04	0.55
1:B:684:MET:H	1:B:690:ASN:ND2	2.03	0.55
1:B:593:ASP:OD2	1:B:687:HIS:HE1	1.90	0.55
1:B:247:GLU:OE1	1:B:525:HIS:CD2	2.57	0.55
1:C:237:ASN:HD21	1:C:283:HIS:HE1	1.52	0.55
1:C:430:ARG:HA	1:C:430:ARG:NE	2.12	0.55
1:C:552:ALA:O	1:C:720:THR:HG21	2.07	0.55
1:A:247:GLU:OE1	1:A:525:HIS:CD2	2.60	0.55
1:A:709:HIS:CD2	4:A:1059:HOH:O	2.51	0.55
1:D:132:MET:CE	1:D:139:ARG:NH1	2.70	0.55
1:D:514:ASN:ND2	4:D:915:HOH:O	2.40	0.55
1:B:606:LEU:HD13	1:B:679:LEU:HD11	1.88	0.55
1:C:310:ARG:HD3	1:C:310:ARG:O	2.06	0.55
1:C:564:LYS:N	1:C:564:LYS:HD3	2.22	0.55
1:C:568:MET:HG3	1:C:584:LEU:HD11	1.89	0.55
1:A:580:HIS:HD2	4:A:1116:HOH:O	1.89	0.54
1:C:604:ARG:NH2	4:C:903:HOH:O	2.39	0.54
1:C:703:ALA:HA	1:C:707:ARG:O	2.06	0.54
1:A:151:SER:HB2	1:A:164:HIS:O	2.06	0.54
1:D:694:GLY:N	4:D:906:HOH:O	2.35	0.54
1:D:444:ARG:NE	4:D:901:HOH:O	2.39	0.54
1:D:492:TYR:CZ	1:D:500:ARG:HG2	2.42	0.54
1:C:337:VAL:HG23	1:C:337:VAL:O	2.08	0.54
1:C:508:THR:O	1:C:511:ILE:HG22	2.07	0.54
1:C:574:GLN:NE2	1:C:585:ASP:H	2.06	0.54
1:D:211:GLN:HE22	1:D:215:GLU:HG3	1.72	0.54
2:D:802:RCD:O2D	2:D:802:RCD:O3E	2.25	0.54
1:A:148:ARG:O	1:A:148:ARG:HG2	2.08	0.54
1:A:430:ARG:NH1	4:A:910:HOH:O	2.39	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:GLN:O	1:A:472:MET:O	2.26	0.54
1:B:199:LEU:HD13	1:B:199:LEU:C	2.29	0.54
1:A:337:VAL:HG23	1:A:337:VAL:O	2.07	0.53
1:A:635:GLU:H	1:A:635:GLU:CD	2.10	0.53
1:C:684[A]:MET:SD	1:C:685:HIS:ND1	2.80	0.53
1:A:213:ARG:HG3	1:A:214:PRO:HA	1.91	0.53
1:B:259:ASN:HB2	1:B:261:PHE:CD2	2.43	0.53
1:D:613:HIS:HB3	3:D:803:GOL:H12	1.89	0.53
1:A:187:LEU:HD22	1:A:211:GLN:HE21	1.73	0.53
1:C:150:VAL:HG13	1:C:192:MET:HB2	1.91	0.53
1:C:601[B]:ARG:CG	1:C:601[B]:ARG:HH11	2.22	0.53
1:A:593:ASP:OD2	1:A:687:HIS:HE1	1.91	0.53
1:B:270:ASP:OD2	4:B:901:HOH:O	2.19	0.53
1:C:289:ILE:HG13	1:C:334:LEU:HD11	1.90	0.53
1:A:606:LEU:HD13	1:A:679:LEU:HD11	1.91	0.53
1:B:403:ARG:NH2	4:B:913:HOH:O	2.41	0.53
1:C:265:TYR:HB2	1:C:317:ASP:HB3	1.91	0.52
1:A:295:ASP:OD2	1:A:311:ARG:NH2	2.38	0.52
1:A:532:LYS:O	1:A:533:LYS:HB2	2.09	0.52
1:B:579:ASN:HD22	1:B:581:ASP:H	1.58	0.52
1:D:490:LEU:O	1:D:494[A]:LYS:HG3	2.10	0.52
1:A:403:ARG:NH1	4:A:913:HOH:O	2.40	0.52
1:B:594:ASN:N	1:B:597:HIS:HD2	2.03	0.52
1:D:680:ASN:HD22	1:D:682:ASP:H	1.57	0.52
1:B:161:GLY:HA3	1:B:191:GLU:OE2	2.10	0.52
1:B:504:HIS:HD2	4:B:1005:HOH:O	1.92	0.52
1:C:194:ASP:HB2	1:C:198:ASN:O	2.09	0.52
1:A:680:ASN:ND2	1:A:682:ASP:H	2.07	0.52
1:D:148:ARG:CG	1:D:194:ASP:O	2.57	0.52
1:D:532:LYS:O	1:D:533:LYS:HB2	2.09	0.52
1:D:523:LEU:HD22	1:D:557:MET:SD	2.50	0.52
1:A:494:LYS:HD3	1:A:538:ARG:HG2	1.92	0.52
1:C:163:ARG:HG3	1:C:163:ARG:NH1	2.25	0.51
1:D:542:ASP:H	1:D:545:GLN:HE21	1.59	0.51
1:A:157:ASN:O	1:A:159:TRP:N	2.44	0.51
1:A:259:ASN:HD22	1:A:260:ASN:N	2.09	0.51
1:D:444:ARG:HB3	4:D:901:HOH:O	2.10	0.51
1:C:305:LEU:HD12	1:C:385:PHE:CE2	2.45	0.51
1:C:375:TYR:HB2	1:C:377:TYR:CZ	2.46	0.51
1:C:658:THR:HB	4:C:913:HOH:O	2.11	0.51
1:D:658:THR:HB	1:D:659:PRO:HD2	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:437:GLU:CG	4:D:924:HOH:O	2.39	0.51
1:A:256:HIS:HB2	1:A:259:ASN:HD21	1.75	0.51
1:A:335:ASP:OD1	1:A:403:ARG:HD3	2.09	0.51
1:A:552:ALA:O	1:A:720:THR:CG2	2.58	0.51
1:A:680:ASN:C	1:A:680:ASN:HD22	2.14	0.51
1:B:580:HIS:HD2	4:B:1294:HOH:O	1.93	0.51
2:A:801:RCD:O2H	2:A:801:RCD:C3A	2.58	0.51
1:B:118:HIS:CD2	1:B:118:HIS:H	2.29	0.51
1:C:552:ALA:O	1:C:720:THR:CG2	2.59	0.51
1:D:651:ILE:HD11	1:D:722:TRP:HB3	1.92	0.51
1:D:258:ASP:O	1:D:259:ASN:CG	2.50	0.51
1:A:213:ARG:HA	1:A:214:PRO:C	2.29	0.51
1:B:130:ASP:OD1	1:B:139:ARG:NH1	2.30	0.50
1:C:273:VAL:HB	1:C:274:PRO:HD3	1.93	0.50
1:D:215:GLU:HG2	2:D:802:RCD:O2G	2.11	0.50
1:B:674:LYS:CE	4:B:904:HOH:O	2.60	0.50
1:B:350:GLU:HA	1:B:354:THR:O	2.11	0.50
1:A:256:HIS:HD2	1:B:728:GLU:O	1.93	0.50
1:C:189:LYS:HD2	1:C:201:LEU:HD12	1.94	0.50
1:C:523:LEU:HD22	1:C:557:MET:SD	2.52	0.50
1:A:213:ARG:HG2	1:A:214:PRO:HA	1.94	0.50
1:A:617:HIS:HE1	4:A:1129:HOH:O	1.93	0.50
1:A:647:GLU:HG2	4:A:1102:HOH:O	2.12	0.50
1:B:337:VAL:HG22	4:B:955:HOH:O	2.12	0.49
1:C:170:LYS:CA	1:C:170:LYS:HE2	2.41	0.49
1:C:684[A]:MET:HE2	1:D:684:MET:SD	2.51	0.49
2:A:801:RCD:C3H	2:A:801:RCD:O5G	2.55	0.49
1:C:291:GLU:OE1	1:C:291:GLU:HA	2.11	0.49
1:A:577:GLU:OE2	4:A:901:HOH:O	2.20	0.49
1:B:680:ASN:HD22	1:B:682:ASP:H	1.59	0.49
1:A:593:ASP:OD2	1:A:687:HIS:CE1	2.66	0.49
1:B:680:ASN:ND2	1:B:682:ASP:H	2.11	0.49
1:A:181:GLY:N	4:A:917:HOH:O	2.44	0.49
1:A:198:ASN:ND2	1:A:200:ARG:HH21	2.10	0.49
1:A:254:ARG:NE	4:A:922:HOH:O	2.46	0.49
2:A:801:RCD:C5F	2:A:801:RCD:H6G	2.43	0.49
1:A:685[A]:HIS:CE1	1:B:685[A]:HIS:CE1	3.00	0.49
1:C:563:LYS:C	1:C:564:LYS:HD3	2.33	0.49
1:D:445:ILE:HG13	4:D:901:HOH:O	2.11	0.49
1:C:559:ALA:HB1	1:C:653:VAL:HG21	1.94	0.48
2:A:801:RCD:H5F	2:A:801:RCD:H6G	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:606:LEU:HD13	1:D:679:LEU:HD11	1.95	0.48
1:B:117:THR:HB	1:B:118:HIS:CD2	2.48	0.48
1:D:594:ASN:H	1:D:597:HIS:CD2	2.30	0.48
1:D:728:GLU:HG2	1:D:728:GLU:OXT	2.13	0.48
1:B:294:PHE:HB3	4:B:1353:HOH:O	2.13	0.48
1:C:680:ASN:HD22	1:C:682:ASP:H	1.61	0.48
1:B:425:ASN:C	1:B:425:ASN:HD22	2.17	0.48
1:C:636:ARG:HG2	1:C:662:ARG:CZ	2.44	0.48
1:A:681:THR:HG23	1:A:720:THR:O	2.14	0.48
2:A:801:RCD:O2H	2:A:801:RCD:O3A	2.28	0.48
1:B:256:HIS:HE1	1:B:267:GLU:OE2	1.97	0.48
1:C:533:LYS:HE2	1:C:537:ASP:HB3	1.96	0.48
1:C:680:ASN:ND2	1:C:682:ASP:H	2.12	0.48
1:A:594:ASN:N	1:A:597:HIS:HD2	2.02	0.48
4:A:1092:HOH:O	1:B:685[B]:HIS:HE1	1.96	0.48
1:D:486:MET:O	1:D:490:LEU:HB2	2.13	0.48
1:B:415:TYR:C	1:B:430:ARG:HB3	2.34	0.47
1:D:211:GLN:NE2	1:D:217:ALA:H	2.12	0.47
1:B:644:ARG:HG2	1:B:650:GLU:HG2	1.96	0.47
1:D:614:LYS:O	1:D:618:GLU:HB2	2.14	0.47
1:B:559:ALA:HB1	1:B:653:VAL:HG21	1.95	0.47
1:D:162:ARG:HH21	1:D:162:ARG:HG2	1.78	0.47
1:D:350:GLU:HA	1:D:354:THR:O	2.14	0.47
1:A:290[B]:ASN:HD21	1:A:337:VAL:HG21	1.78	0.47
1:B:138:THR:CG2	1:B:182:ALA:O	2.55	0.47
1:D:680:ASN:HD22	1:D:681:THR:N	2.13	0.47
1:A:512:LEU:CD2	2:A:801:RCD:C6E	2.93	0.47
1:C:333:ILE:HG12	1:C:401:ALA:HB3	1.95	0.47
1:A:693:ASN:ND2	1:A:714:THR:H	2.08	0.46
1:D:684:MET:N	1:D:690:ASN:HD22	2.12	0.46
1:B:542:ASP:OD2	1:B:545:GLN:HG3	2.14	0.46
1:A:209:GLU:HG2	1:A:219:LEU:HD22	1.98	0.46
1:A:684:MET:H	1:A:690:ASN:HD22	1.62	0.46
1:C:282:THR:OG1	1:C:283:HIS:HD2	1.98	0.46
1:D:602:LEU:HG	1:D:606:LEU:HD22	1.97	0.46
1:B:635:GLU:HA	1:B:635:GLU:OE2	2.15	0.46
2:A:801:RCD:H6G	2:A:801:RCD:H6FA	1.97	0.46
1:C:684[A]:MET:H	1:C:690:ASN:HD22	1.64	0.46
1:D:211:GLN:HE21	1:D:217:ALA:HB3	1.81	0.45
1:A:154:GLY:HA2	1:A:188:TYR:HA	1.98	0.45
2:A:801:RCD:H6G	2:A:801:RCD:C6F	2.46	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:170:LYS:HA	1:C:170:LYS:CE	2.41	0.45
1:C:356:LEU:HD23	1:C:356:LEU:HA	1.85	0.45
1:A:285:GLU:OE1	1:A:403:ARG:HD2	2.17	0.45
1:B:660:VAL:HA	1:B:661:PRO:HD3	1.86	0.45
1:A:259:ASN:ND2	1:A:261:PHE:H	2.15	0.45
1:A:559:ALA:HB1	1:A:653:VAL:HG21	1.99	0.45
1:C:215:GLU:CG	4:C:968:HOH:O	2.64	0.45
1:B:212:MET:HG2	4:B:1291:HOH:O	2.16	0.45
1:A:523:LEU:HD22	1:A:557:MET:SD	2.56	0.45
1:B:422:TRP:HZ2	1:B:430:ARG:HH21	1.65	0.45
1:C:171:GLU:CG	1:C:172:SER:N	2.80	0.45
1:C:620:ASP:OD2	1:C:643:ARG:NH2	2.31	0.45
1:C:247:GLU:OE1	1:C:525:HIS:CD2	2.70	0.45
1:D:150:VAL:HG12	1:D:166:MET:SD	2.57	0.45
1:D:138:THR:HG23	1:D:182:ALA:HB3	1.99	0.45
1:D:310:ARG:NE	4:D:904:HOH:O	2.34	0.45
1:D:620:ASP:OD2	1:D:643:ARG:NH2	2.43	0.45
1:B:644:ARG:HG3	1:B:650:GLU:HG2	1.98	0.45
1:B:658:THR:HG23	1:B:659:PRO:HD2	1.99	0.45
1:C:375:TYR:O	1:C:376:ASN:HB3	2.17	0.44
1:A:512:LEU:HD22	1:A:512:LEU:H	1.82	0.44
1:C:559:ALA:HA	1:C:616:MET:HE3	1.99	0.44
1:A:349:ALA:O	1:A:350:GLU:C	2.56	0.44
1:A:676[B]:ARG:NE	1:A:726:GLU:OE1	2.51	0.44
1:C:490:LEU:HD12	1:C:490:LEU:HA	1.90	0.44
1:C:547:PHE:O	1:C:551:ARG:HG3	2.18	0.44
1:A:154:GLY:HA3	1:A:156:PHE:CZ	2.52	0.44
1:C:615:ALA:HB3	1:C:651:ILE:HD13	1.99	0.44
1:D:693:ASN:ND2	1:D:714:THR:H	2.10	0.44
1:B:164:HIS:CE1	4:B:1282:HOH:O	2.45	0.44
1:B:439:LEU:HA	1:B:439:LEU:HD23	1.82	0.44
1:C:247:GLU:OE1	1:C:525:HIS:HD2	2.00	0.44
1:A:684:MET:HG3	1:A:685[B]:HIS:N	2.32	0.44
1:B:533:LYS:O	1:B:538:ARG:NH2	2.51	0.44
1:C:237:ASN:ND2	1:C:283:HIS:CE1	2.74	0.44
1:B:215:GLU:HG2	1:B:215:GLU:H	1.59	0.43
1:D:335:ASP:OD1	1:D:403:ARG:HD3	2.18	0.43
1:A:237:ASN:HD22	1:A:283:HIS:HE1	1.62	0.43
1:A:289:ILE:HG13	1:A:334:LEU:HD11	1.99	0.43
1:C:511:ILE:HG21	1:C:628:TRP:HE1	1.83	0.43
1:C:571:GLU:HA	1:C:603:VAL:HG21	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:647:GLU:CD	4:D:947:HOH:O	2.56	0.43
1:B:289:ILE:HG13	1:B:334:LEU:CD1	2.46	0.43
1:B:425:ASN:HD22	1:B:427:PHE:N	2.13	0.43
1:D:247:GLU:OE1	1:D:525:HIS:CD2	2.64	0.43
1:D:646:LYS:HE3	1:D:646:LYS:HB2	1.75	0.43
1:A:138:THR:HG21	1:A:220:ILE:HG21	1.99	0.43
1:A:292:HIS:O	1:A:311:ARG:NH1	2.39	0.43
1:A:199:LEU:HD23	1:A:199:LEU:HA	1.80	0.43
1:B:256:HIS:CE1	1:B:267:GLU:OE2	2.72	0.43
1:C:621:PHE:N	4:C:905:HOH:O	2.46	0.43
1:C:684[A]:MET:CE	1:D:684:MET:CG	2.97	0.43
1:B:414:ASP:O	1:B:422:TRP:CG	2.72	0.43
1:D:380:ARG:HD2	1:D:380:ARG:HA	1.82	0.43
1:B:601:ARG:HD2	1:B:685[A]:HIS:CE1	2.53	0.43
1:D:430:ARG:HA	1:D:430:ARG:HD2	1.63	0.43
1:B:709:HIS:HE1	4:D:902:HOH:O	2.01	0.43
1:C:359:HIS:HB3	1:C:360:SER:H	1.42	0.43
1:A:512:LEU:HD13	1:A:512:LEU:HA	1.80	0.43
1:B:117:THR:HB	1:B:118:HIS:H	1.25	0.43
1:B:226:LYS:NZ	4:B:905:HOH:O	2.33	0.43
1:A:168:LEU:HB2	1:A:175:TRP:CD2	2.53	0.42
1:C:293:PRO:HD3	1:C:303:THR:HG23	2.02	0.42
1:C:594:ASN:N	1:C:597:HIS:HD2	2.01	0.42
1:C:593:ASP:OD2	1:C:687:HIS:HE1	2.02	0.42
1:D:143:TRP:CH2	1:D:356:LEU:HD22	2.54	0.42
1:D:525:HIS:HB3	1:D:567:PHE:CE1	2.54	0.42
1:A:410:MET:HE1	1:A:439:LEU:HD21	2.01	0.42
1:C:204:ASP:HB3	1:C:207:ALA:HB2	2.01	0.42
1:C:489:THR:HG22	1:C:507:LEU:HD12	2.01	0.42
1:C:514:ASN:ND2	4:C:907:HOH:O	2.52	0.42
1:A:376:ASN:C	1:A:376:ASN:HD22	2.21	0.42
1:B:138:THR:HG23	1:B:182:ALA:CB	2.49	0.42
1:A:684:MET:HG3	1:A:685[A]:HIS:N	2.33	0.42
1:C:242:PRO:HD3	1:C:617:HIS:CE1	2.54	0.42
1:C:143:TRP:CH2	1:C:356:LEU:HD22	2.54	0.42
1:C:254:ARG:HG3	4:C:960:HOH:O	2.19	0.42
1:A:187:LEU:HD13	1:A:211:GLN:NE2	2.34	0.42
1:A:356:LEU:HD23	1:A:356:LEU:HA	1.74	0.42
1:B:666:ARG:O	3:B:803:GOL:C3	2.56	0.42
1:C:601[B]:ARG:CG	1:C:601[B]:ARG:NH1	2.81	0.42
1:A:290[B]:ASN:HD21	1:A:337:VAL:CG2	2.33	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290[B]:ASN:ND2	1:A:337:VAL:CG2	2.83	0.42
1:C:671:GLN:HA	1:C:672:PRO:HD2	1.87	0.42
1:A:407:VAL:HA	1:A:410:MET:HE2	2.01	0.42
1:D:211:GLN:NE2	1:D:217:ALA:HB3	2.35	0.42
1:C:215:GLU:HG2	4:C:968:HOH:O	2.20	0.42
1:D:132:MET:HE3	1:D:139:ARG:NH1	2.34	0.42
1:D:194:ASP:HB2	1:D:198:ASN:H	1.85	0.42
1:A:525:HIS:HB3	1:A:567:PHE:CE1	2.55	0.41
1:B:511:ILE:HG23	1:B:511:ILE:HD12	1.81	0.41
1:C:153:VAL:HB	1:C:159:TRP:HA	2.02	0.41
1:D:143:TRP:CZ3	1:D:356:LEU:HD13	2.55	0.41
1:C:152:VAL:HG23	1:C:166:MET:SD	2.61	0.41
1:C:259:ASN:HD22	1:C:259:ASN:H	1.67	0.41
1:C:525:HIS:HB3	1:C:567:PHE:CE1	2.55	0.41
1:A:256:HIS:HE1	1:A:267:GLU:OE2	2.03	0.41
1:A:552:ALA:O	1:A:720:THR:HG23	2.20	0.41
2:A:801:RCD:H1C	2:A:801:RCD:H6DA	2.01	0.41
1:A:290[B]:ASN:O	1:A:290[B]:ASN:OD1	2.38	0.41
1:B:656:ASN:C	1:B:656:ASN:HD22	2.24	0.41
1:C:566:LEU:HG	1:C:570:ASN:HB2	2.01	0.41
1:B:606:LEU:HD13	1:B:679:LEU:CD1	2.50	0.41
1:D:704:SER:OG	1:D:705:HIS:HD2	2.04	0.41
1:D:215:GLU:CG	2:D:802:RCD:O2G	2.69	0.41
1:A:144:ALA:HA	1:A:145:PRO:HD2	1.89	0.41
1:A:163:ARG:HB2	1:A:163:ARG:HE	1.77	0.41
1:A:179:ILE:HA	1:A:180:PRO:HD2	1.88	0.41
1:A:656:ASN:HD22	1:A:656:ASN:C	2.22	0.41
1:B:376:ASN:ND2	4:B:935:HOH:O	2.53	0.41
1:C:215:GLU:O	1:C:216:THR:CB	2.68	0.41
1:C:494:LYS:HD3	1:C:538:ARG:HG2	2.03	0.41
1:D:153:VAL:HA	1:D:157:ASN:ND2	2.35	0.41
1:D:230:THR:OG1	1:D:232:GLU:HG2	2.20	0.41
1:D:254:ARG:NE	4:D:941:HOH:O	2.53	0.41
1:D:489:THR:O	1:D:493:MET:HG2	2.21	0.41
1:D:610:TYR:O	1:D:617:HIS:HD2	2.03	0.41
1:A:120:ARG:HG2	1:A:122:TYR:OH	2.21	0.41
1:D:305:LEU:HA	1:D:305:LEU:HD13	1.78	0.41
1:D:345:ASP:O	1:D:346:PHE:C	2.58	0.41
1:C:684[A]:MET:HE1	1:D:684:MET:CG	2.50	0.41
1:C:549:ASN:OD1	1:C:718:LEU:HD22	2.21	0.41
1:D:138:THR:CG2	1:D:182:ALA:C	2.89	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:666:ARG:HA	1:D:711:LEU:O	2.21	0.41
1:A:118:HIS:O	1:A:384:ASN:ND2	2.53	0.41
1:A:574:GLN:HE21	1:A:585:ASP:H	1.60	0.41
1:C:523:LEU:HA	1:C:523:LEU:HD12	1.90	0.41
1:C:684[B]:MET:H	1:C:690:ASN:HD22	1.68	0.41
1:D:213:ARG:HB3	4:D:1225:HOH:O	2.21	0.41
1:D:485:TRP:CE2	1:D:489:THR:HG21	2.56	0.41
1:B:211:GLN:CD	1:B:215:GLU:HB2	2.42	0.41
1:C:237:ASN:HD22	1:C:283:HIS:HE1	1.65	0.41
1:C:292:HIS:CG	1:C:299:GLY:HA2	2.56	0.41
1:D:492:TYR:CZ	1:D:507:LEU:HD22	2.56	0.41
2:D:801:RCD:H3H	4:D:1187:HOH:O	2.21	0.41
1:A:444:ARG:O	1:A:448:GLU:HG3	2.21	0.41
1:D:542:ASP:H	1:D:545:GLN:NE2	2.19	0.41
1:B:259:ASN:ND2	1:B:259:ASN:H	2.18	0.40
1:C:561:PRO:HA	1:C:643:ARG:NH2	2.35	0.40
1:D:310:ARG:HD2	1:D:313:GLY:O	2.20	0.40
1:A:198:ASN:HD22	1:A:200:ARG:HH21	1.69	0.40
1:A:492:TYR:CZ	1:A:507:LEU:HD22	2.57	0.40
1:A:610:TYR:O	1:A:617:HIS:HD2	2.04	0.40
1:D:133:ASP:OD2	1:D:133:ASP:N	2.54	0.40
1:A:181:GLY:HA2	4:A:917:HOH:O	2.20	0.40
1:A:674:LYS:HB3	1:A:696:THR:HG23	2.03	0.40
1:B:264:SER:HB2	4:B:1214:HOH:O	2.20	0.40
1:B:341:PHE:HA	1:B:342:PRO:HD3	1.91	0.40
1:B:442:THR:HG22	1:B:446:LEU:HD22	2.03	0.40
1:C:149:ARG:NH1	1:C:165:PRO:HB3	2.36	0.40
1:D:211:GLN:NE2	1:D:215:GLU:HG3	2.36	0.40
1:D:512:LEU:HD23	1:D:512:LEU:HA	1.80	0.40
2:A:801:RCD:HO2H	2:A:801:RCD:C3A	2.31	0.40
1:C:391:LEU:HA	1:C:391:LEU:HD12	1.80	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:133:ASP:OD1	2:D:801:RCD:O6D[2_655]	2.18	0.02

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	586/612 (96%)	557 (95%)	25 (4%)	4 (1%)	26	28
1	B	596/612 (97%)	580 (97%)	13 (2%)	3 (0%)	34	37
1	C	572/612 (94%)	538 (94%)	30 (5%)	4 (1%)	26	28
1	D	584/612 (95%)	558 (96%)	22 (4%)	4 (1%)	26	28
All	All	2338/2448 (96%)	2233 (96%)	90 (4%)	15 (1%)	30	32

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	214	PRO
1	A	215	GLU
1	C	216	THR
1	D	194	ASP
1	B	355	ASN
1	B	414	ASP
1	B	522	PRO
1	C	194	ASP
1	D	157	ASN
1	D	372	THR
1	A	522	PRO
1	C	687	HIS
1	D	522	PRO
1	A	158	TYR
1	C	522	PRO

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	504/521 (97%)	467 (93%)	37 (7%)	17	18
1	B	512/521 (98%)	470 (92%)	42 (8%)	14	14
1	C	492/521 (94%)	451 (92%)	41 (8%)	14	14
1	D	501/521 (96%)	459 (92%)	42 (8%)	14	14
All	All	2009/2084 (96%)	1847 (92%)	162 (8%)	15	15

All (162) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	131	THR
1	A	132	MET
1	A	142	VAL
1	A	146	ASN
1	A	148	ARG
1	A	199	LEU
1	A	216	THR
1	A	223	LEU
1	A	231	GLU
1	A	259	ASN
1	A	305	LEU
1	A	315	ARG
1	A	331	ASN
1	A	356	LEU
1	A	359	HIS
1	A	376	ASN
1	A	391	LEU
1	A	462	ASP
1	A	475	LEU
1	A	490	LEU
1	A	498	VAL
1	A	504	HIS
1	A	505[A]	ASP
1	A	505[B]	ASP
1	A	507	LEU
1	A	523	LEU
1	A	579	ASN
1	A	606	LEU
1	A	619	LEU
1	A	642	VAL
1	A	647	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	656	ASN
1	A	679	LEU
1	A	680	ASN
1	A	684	MET
1	A	720	THR
1	A	723	LEU
1	B	117	THR
1	B	133	ASP
1	B	138	THR
1	B	151	SER
1	B	163	ARG
1	B	168	LEU
1	B	212	MET
1	B	213	ARG
1	B	215	GLU
1	B	218	SER
1	B	223	LEU
1	B	259	ASN
1	B	290	ASN
1	B	305	LEU
1	B	315	ARG
1	B	331	ASN
1	B	334	LEU
1	B	356	LEU
1	B	363	ARG
1	B	364	GLU
1	B	372	THR
1	B	376	ASN
1	B	391	LEU
1	B	415	TYR
1	B	425	ASN
1	B	446	LEU
1	B	470	GLN
1	B	475	LEU
1	B	490	LEU
1	B	507	LEU
1	B	512	LEU
1	B	523	LEU
1	B	546	LYS
1	B	579	ASN
1	B	581	ASP
1	B	606	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	619	LEU
1	B	642	VAL
1	B	656	ASN
1	B	658	THR
1	B	680	ASN
1	B	723	LEU
1	C	119	LEU
1	C	138	THR
1	C	148	ARG
1	C	163	ARG
1	C	223	LEU
1	C	226	LYS
1	C	235	LYS
1	C	259	ASN
1	C	266	ARG
1	C	278	TRP
1	C	290	ASN
1	C	291	GLU
1	C	310	ARG
1	C	315	ARG
1	C	319	ARG
1	C	331	ASN
1	C	334	LEU
1	C	343	THR
1	C	356	LEU
1	C	359	HIS
1	C	375	TYR
1	C	391	LEU
1	C	430	ARG
1	C	458	GLU
1	C	470	GLN
1	C	472	MET
1	C	496	ASP
1	C	505	ASP
1	C	507	LEU
1	C	523	LEU
1	C	546	LYS
1	C	564	LYS
1	C	590	GLU
1	C	619	LEU
1	C	642	VAL
1	C	643	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	676	ARG
1	C	680	ASN
1	C	683	SER
1	C	690	ASN
1	C	720	THR
1	D	117	THR
1	D	119	LEU
1	D	133	ASP
1	D	138	THR
1	D	141	SER
1	D	148	ARG
1	D	171	GLU
1	D	212	MET
1	D	213	ARG
1	D	219	LEU
1	D	223	LEU
1	D	232	GLU
1	D	310	ARG
1	D	315	ARG
1	D	331	ASN
1	D	356	LEU
1	D	359	HIS
1	D	373	LEU
1	D	391	LEU
1	D	430	ARG
1	D	437	GLU
1	D	470	GLN
1	D	472	MET
1	D	475	LEU
1	D	490	LEU
1	D	495	LEU
1	D	507	LEU
1	D	512	LEU
1	D	523	LEU
1	D	581	ASP
1	D	595	TRP
1	D	606	LEU
1	D	619	LEU
1	D	642	VAL
1	D	647	GLU
1	D	651	ILE
1	D	656	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	679	LEU
1	D	680	ASN
1	D	690	ASN
1	D	723	LEU
1	D	728	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (109) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	146	ASN
1	A	157	ASN
1	A	198	ASN
1	A	237	ASN
1	A	256	HIS
1	A	259	ASN
1	A	283	HIS
1	A	331	ASN
1	A	340	HIS
1	A	359	HIS
1	A	376	ASN
1	A	504	HIS
1	A	514	ASN
1	A	525	HIS
1	A	530	HIS
1	A	570	ASN
1	A	574	GLN
1	A	579	ASN
1	A	597	HIS
1	A	617	HIS
1	A	656	ASN
1	A	680	ASN
1	A	687	HIS
1	A	690	ASN
1	A	693	ASN
1	A	705	HIS
1	A	709	HIS
1	B	118	HIS
1	B	164	HIS
1	B	183	HIS
1	B	198	ASN
1	B	237	ASN
1	B	256	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	259	ASN
1	B	283	HIS
1	B	331	ASN
1	B	340	HIS
1	B	359	HIS
1	B	376	ASN
1	B	425	ASN
1	B	470	GLN
1	B	504	HIS
1	B	514	ASN
1	B	525	HIS
1	B	545	GLN
1	B	570	ASN
1	B	574	GLN
1	B	579	ASN
1	B	597	HIS
1	B	617	HIS
1	B	656	ASN
1	B	680	ASN
1	B	687	HIS
1	B	690	ASN
1	B	705	HIS
1	B	709	HIS
1	C	164	HIS
1	C	237	ASN
1	C	259	ASN
1	C	283	HIS
1	C	290	ASN
1	C	301	GLN
1	C	331	ASN
1	C	355	ASN
1	C	470	GLN
1	C	501	GLN
1	C	525	HIS
1	C	530	HIS
1	C	545	GLN
1	C	570	ASN
1	C	574	GLN
1	C	580	HIS
1	C	597	HIS
1	C	617	HIS
1	C	656	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	680	ASN
1	C	687	HIS
1	C	690	ASN
1	C	693	ASN
1	C	708	GLN
1	D	157	ASN
1	D	164	HIS
1	D	186	GLN
1	D	211	GLN
1	D	237	ASN
1	D	238	GLN
1	D	283	HIS
1	D	290	ASN
1	D	331	ASN
1	D	340	HIS
1	D	441	ASN
1	D	443	ASN
1	D	470	GLN
1	D	504	HIS
1	D	514	ASN
1	D	525	HIS
1	D	545	GLN
1	D	570	ASN
1	D	574	GLN
1	D	597	HIS
1	D	617	HIS
1	D	656	ASN
1	D	680	ASN
1	D	685	HIS
1	D	687	HIS
1	D	690	ASN
1	D	693	ASN
1	D	705	HIS
1	D	708	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

11 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	RCD	A	801	-	96,96,96	0.55	0	144,144,144	1.17	10 (6%)
3	GOL	A	802	-	5,5,5	0.34	0	5,5,5	1.13	1 (20%)
3	GOL	A	803	-	5,5,5	0.45	0	5,5,5	0.69	0
2	RCD	B	801	-	96,96,96	0.52	0	144,144,144	1.04	8 (5%)
3	GOL	B	802	-	5,5,5	0.38	0	5,5,5	0.71	0
3	GOL	B	803	-	5,5,5	0.50	0	5,5,5	0.44	0
2	RCD	C	801	-	96,96,96	0.40	0	144,144,144	0.89	3 (2%)
2	RCD	D	801	-	96,96,96	0.49	0	144,144,144	1.04	11 (7%)
2	RCD	D	802	-	96,96,96	0.45	0	144,144,144	0.94	5 (3%)
3	GOL	D	803	-	5,5,5	0.34	0	5,5,5	0.56	0
3	GOL	D	804	-	5,5,5	0.44	0	5,5,5	0.25	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
2	RCD	A	801	-	-	0/48/208/208	0/0/9/9
3	GOL	A	802	-	-	0/4/4/4	0/0/0/0
3	GOL	A	803	-	-	0/4/4/4	0/0/0/0
2	RCD	B	801	-	-	0/48/208/208	0/0/9/9
3	GOL	B	802	-	-	0/4/4/4	0/0/0/0
3	GOL	B	803	-	-	0/4/4/4	0/0/0/0
2	RCD	C	801	-	-	0/48/208/208	0/0/9/9

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	RCD	D	801	-	-	0/48/208/208	0/0/9/9
2	RCD	D	802	-	-	0/48/208/208	0/0/9/9
3	GOL	D	803	-	-	0/4/4/4	0/0/0/0
3	GOL	D	804	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	RCD	C1E-O4F-C4F	-2.87	110.37	118.00
2	D	801	RCD	C1H-O4A-C4A	-2.65	110.95	118.00
2	D	801	RCD	O5B-C1B-C2B	-2.49	105.11	110.28
2	A	801	RCD	C1F-O4G-C4G	-2.47	111.43	118.00
2	B	801	RCD	C1D-O5D-C5D	-2.43	108.98	113.74
2	D	801	RCD	C1A-O4B-C4B	-2.33	111.82	118.00
2	C	801	RCD	C1D-O4E-C4E	-2.30	111.89	118.00
2	B	801	RCD	C1F-O4G-C4G	-2.27	111.96	118.00
2	B	801	RCD	C1H-O4A-C4A	-2.23	112.07	118.00
2	D	802	RCD	C1C-O4D-C4D	-2.16	112.25	118.00
2	D	801	RCD	C1D-O4E-C4E	-2.13	112.33	118.00
2	B	801	RCD	C1B-O4C-C4C	-2.09	112.44	118.00
2	C	801	RCD	C1B-O4C-C4C	-2.07	112.51	118.00
2	D	801	RCD	C6C-C5C-C4C	-2.02	107.31	113.25
3	A	802	GOL	C3-C2-C1	-2.02	102.57	111.06
2	A	801	RCD	O5C-C5C-C4C	2.07	114.18	109.78
2	D	801	RCD	O5H-C5H-C4H	2.10	114.25	109.78
2	D	801	RCD	O5C-C5C-C4C	2.10	114.26	109.78
2	C	801	RCD	C2H-C3H-C4H	2.14	114.35	109.63
2	D	801	RCD	O4F-C4F-C3F	2.15	112.79	107.18
2	B	801	RCD	C2D-C3D-C4D	2.22	114.54	109.63
2	D	801	RCD	O4A-C4A-C3A	2.24	113.04	107.18
2	A	801	RCD	O5H-C5H-C6H	2.28	112.28	106.38
2	D	802	RCD	C2C-C3C-C4C	2.28	114.66	109.63
2	B	801	RCD	C1D-C2D-C3D	2.41	114.77	109.98
2	D	802	RCD	O5D-C5D-C4D	2.43	114.97	109.78
2	A	801	RCD	O4H-C4H-C3H	2.47	113.63	107.18
2	D	801	RCD	C1C-O5C-C5C	2.79	119.23	113.74
2	D	802	RCD	O4A-C1H-C2H	2.80	115.06	108.12
2	D	801	RCD	O5F-C5F-C6F	2.80	113.65	106.38
2	B	801	RCD	O5F-C5F-C4F	2.85	115.86	109.78
2	A	801	RCD	C1A-O5A-C5M	2.89	119.42	113.74
2	A	801	RCD	C1F-C2F-C3F	2.95	115.83	109.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	RCD	C2F-C3F-C4F	2.97	116.18	109.63
2	D	802	RCD	C1D-O5D-C5D	2.98	119.58	113.74
2	A	801	RCD	O5D-C5D-C4D	3.14	116.48	109.78
2	A	801	RCD	C1D-O5D-C5D	3.17	119.96	113.74
2	A	801	RCD	C1H-O5H-C5H	3.87	121.33	113.74

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	RCD	15	0
3	A	802	GOL	3	0
2	B	801	RCD	1	0
3	B	803	GOL	2	0
2	C	801	RCD	2	0
2	D	801	RCD	1	1
2	D	802	RCD	3	0
3	D	803	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, 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	586/612 (95%)	0.38	66 (11%) 7 12	19, 38, 105, 134	7 (1%)
1	B	600/612 (98%)	-0.01	4 (0%) 89 93	16, 31, 56, 75	6 (1%)
1	C	578/612 (94%)	1.59	193 (33%) 0 0	49, 79, 117, 140	2 (0%)
1	D	588/612 (96%)	-0.07	12 (2%) 68 79	24, 38, 60, 84	4 (0%)
All	All	2352/2448 (96%)	0.46	275 (11%) 6 10	16, 41, 102, 140	19 (0%)

All (275) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	360	SER	9.5
1	C	133	ASP	9.0
1	C	132	MET	8.2
1	C	343	THR	7.7
1	C	499	TYR	7.5
1	A	429	GLY	6.8
1	C	200	ARG	6.7
1	C	150	VAL	6.7
1	C	159	TRP	6.5
1	C	199	LEU	6.4
1	C	258	ASP	6.2
1	C	261	PHE	6.1
1	C	190	TYR	6.0
1	C	216	THR	6.0
1	C	257	THR	5.9
1	C	502	TYR	5.7
1	C	660	VAL	5.7
1	A	149	ARG	5.6
1	C	464	PRO	5.5
1	C	201	LEU	5.4
1	A	195	ALA	5.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	131	THR	5.2
1	B	415	TYR	5.1
1	C	294	PHE	5.1
1	C	341	PHE	5.1
1	A	380	ARG	5.1
1	A	158	TYR	5.0
1	C	357	TYR	5.0
1	C	350	GLU	5.0
1	C	210	ALA	4.9
1	C	509	PHE	4.9
1	C	134	GLY	4.9
1	C	543	ALA	4.9
1	C	127	ALA	4.7
1	C	355	ASN	4.7
1	C	595	TRP	4.7
1	C	512	LEU	4.7
1	C	144	ALA	4.7
1	A	144	ALA	4.7
1	C	196	ASN	4.6
1	A	131	THR	4.6
1	C	708	GLN	4.6
1	A	162	ARG	4.5
1	C	170	LYS	4.5
1	C	155	GLN	4.5
1	C	702	ILE	4.5
1	C	207	ALA	4.4
1	C	208	PHE	4.4
1	A	147	ALA	4.4
1	B	133	ASP	4.4
1	C	168	LEU	4.4
1	C	222	GLY	4.3
1	C	511	ILE	4.3
1	C	211	GLN	4.3
1	C	124	THR	4.3
1	C	259	ASN	4.3
1	C	496	ASP	4.3
1	C	587	HIS	4.3
1	C	147	ALA	4.3
1	C	189	LYS	4.3
1	A	199	LEU	4.2
1	C	260	ASN	4.2
1	A	472	MET	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	175	TRP	4.2
1	C	194	ASP	4.2
1	A	153	VAL	4.2
1	C	148	ARG	4.2
1	C	498	VAL	4.1
1	C	263	LEU	4.1
1	A	168	LEU	4.1
1	C	433	LEU	4.1
1	C	709	HIS	4.1
1	C	631	VAL	4.0
1	C	156	PHE	4.0
1	C	175	TRP	4.0
1	C	203	SER	4.0
1	A	196	ASN	4.0
1	A	145	PRO	4.0
1	C	378	GLY	4.0
1	C	145	PRO	4.0
1	C	463	PHE	4.0
1	C	217	ALA	3.9
1	C	172	SER	3.9
1	C	187	LEU	3.9
1	C	374	ILE	3.9
1	C	379	ARG	3.9
1	A	201	LEU	3.9
1	C	188	TYR	3.8
1	C	192	MET	3.8
1	A	354	THR	3.8
1	C	375	TYR	3.8
1	C	121	PRO	3.8
1	C	698	HIS	3.8
1	A	166	MET	3.8
1	C	346	PHE	3.8
1	C	181	GLY	3.8
1	C	223	LEU	3.8
1	C	495	LEU	3.8
1	A	146	ASN	3.8
1	C	154	GLY	3.7
1	C	344	ASP	3.7
1	C	262	TRP	3.7
1	A	150	VAL	3.7
1	C	356	LEU	3.7
1	C	373	LEU	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	584	LEU	3.6
1	C	503	HIS	3.6
1	A	159	TRP	3.6
1	C	544	TRP	3.6
1	C	126	GLY	3.6
1	C	592	GLY	3.6
1	C	347	ALA	3.6
1	C	380	ARG	3.5
1	C	497	PRO	3.5
1	C	345	ASP	3.5
1	A	193	ILE	3.5
1	D	413	ARG	3.5
1	C	206	TYR	3.5
1	C	118	HIS	3.5
1	C	484	GLY	3.5
1	C	601[A]	ARG	3.5
1	C	149	ARG	3.5
1	C	171	GLU	3.4
1	A	148	ARG	3.4
1	C	348	LEU	3.4
1	C	408	ALA	3.4
1	A	212	MET	3.4
1	C	353	GLY	3.4
1	D	728	GLU	3.4
1	A	152	VAL	3.4
1	C	202	LYS	3.4
1	C	658	THR	3.4
1	C	536	LEU	3.3
1	C	359	HIS	3.3
1	C	505	ASP	3.3
1	C	540	PRO	3.3
1	C	352	ASP	3.3
1	D	371	ASN	3.2
1	A	167	ARG	3.2
1	C	122	TYR	3.2
1	C	445	ILE	3.2
1	A	192	MET	3.2
1	C	635	GLU	3.2
1	C	256	HIS	3.2
1	A	165	PRO	3.2
1	C	542	ASP	3.2
1	C	228	VAL	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	193	ILE	3.1
1	A	471	ASP	3.1
1	A	130	ASP	3.0
1	C	412	TYR	3.0
1	C	710	SER	3.0
1	C	354	THR	3.0
1	C	590	GLU	3.0
1	C	672	PRO	3.0
1	A	194	ASP	3.0
1	C	581	ASP	3.0
1	A	374	ILE	3.0
1	C	582	ALA	3.0
1	C	541	GLY	3.0
1	A	160	ASP	3.0
1	C	278	TRP	3.0
1	C	158	TYR	2.9
1	C	300	TYR	2.9
1	D	372	THR	2.9
1	A	200	ARG	2.9
1	C	529	VAL	2.9
1	C	135	VAL	2.9
1	C	143	TRP	2.9
1	C	140	PHE	2.9
1	C	142	VAL	2.9
1	A	190	TYR	2.9
1	C	169	ARG	2.9
1	C	221	CYS	2.8
1	C	387	VAL	2.8
1	A	171	GLU	2.8
1	C	703	ALA	2.8
1	A	161	GLY	2.8
1	C	342	PRO	2.8
1	C	157	ASN	2.8
1	C	141	SER	2.8
1	C	487	HIS	2.8
1	C	119	LEU	2.8
1	C	545	GLN	2.7
1	A	164	HIS	2.7
1	A	170	LYS	2.7
1	A	154	GLY	2.7
1	C	198	ASN	2.7
1	D	414	ASP	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	636	ARG	2.7
1	A	133	ASP	2.7
1	A	129	ALA	2.7
1	C	351	PHE	2.7
1	D	346	PHE	2.7
1	C	139	ARG	2.7
1	C	183	HIS	2.7
1	D	257	THR	2.7
1	C	339	GLY	2.7
1	C	205	PRO	2.6
1	C	338	PRO	2.6
1	A	117	THR	2.6
1	B	132	MET	2.6
1	A	360	SER	2.6
1	A	169	ARG	2.6
1	A	346	PHE	2.6
1	C	586	TRP	2.6
1	C	632	ASP	2.6
1	A	163	ARG	2.5
1	C	255	ARG	2.5
1	C	472	MET	2.5
1	C	120	ARG	2.5
1	C	659	PRO	2.4
1	A	142	VAL	2.4
1	C	197	GLY	2.4
1	C	713	LEU	2.4
1	C	267	GLU	2.4
1	C	471	ASP	2.4
1	C	637	SER	2.4
1	C	128	HIS	2.4
1	C	176	GLU	2.4
1	C	130	ASP	2.4
1	C	182	ALA	2.4
1	C	195	ALA	2.4
1	A	352	ASP	2.4
1	C	530	HIS	2.4
1	C	151	SER	2.4
1	A	177	LEU	2.3
1	D	212	MET	2.3
1	C	634	LYS	2.3
1	A	156	PHE	2.3
1	A	151	SER	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	125	LEU	2.3
1	C	358	GLU	2.2
1	C	220	ILE	2.2
1	A	197	GLY	2.2
1	C	508	THR	2.2
1	A	475	LEU	2.2
1	D	279	MET	2.2
1	A	172	SER	2.2
1	B	276	ALA	2.2
1	A	176	GLU	2.2
1	C	583	SER	2.2
1	C	591	GLY	2.2
1	C	700	ASP	2.2
1	C	707	ARG	2.2
1	C	180	PRO	2.2
1	C	146	ASN	2.2
1	C	589	LEU	2.2
1	C	474	GLY	2.2
1	C	531	GLY	2.2
1	A	359	HIS	2.1
1	A	135	VAL	2.1
1	C	160	ASP	2.1
1	A	355	ASN	2.1
1	C	633	ASP	2.1
1	A	373	LEU	2.1
1	C	301	GLN	2.1
1	A	372	THR	2.1
1	A	134	GLY	2.1
1	C	293	PRO	2.1
1	C	608	LEU	2.1
1	A	174	ILE	2.1
1	C	446	LEU	2.1
1	C	434	GLU	2.1
1	C	488	ASP	2.1
1	C	701	GLU	2.1
1	D	360	SER	2.0
1	A	143	TRP	2.0
1	D	603	VAL	2.0
1	A	353	GLY	2.0
1	C	461	THR	2.0
1	C	409	SER	2.0
1	C	153	VAL	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	594	ASN	2.0
1	D	727	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(Å ²)	Q<0.9
3	GOL	A	802	6/6	0.92	0.20	8.12	42,44,44,46	0
2	RCD	B	801	88/88	0.88	0.20	4.10	32,60,72,73	20
2	RCD	C	801	88/88	0.59	0.51	2.55	96,100,104,104	77
3	GOL	A	803	6/6	0.96	0.19	2.43	27,31,32,34	0
3	GOL	B	803	6/6	0.94	0.14	2.09	45,45,45,46	0
2	RCD	D	801	88/88	0.87	0.20	2.07	42,63,69,70	0
2	RCD	D	802	88/88	0.76	0.30	1.44	75,87,92,92	35
2	RCD	A	801	88/88	0.80	0.23	1.32	45,71,79,79	34
3	GOL	D	804	6/6	0.96	0.13	0.40	45,45,46,48	0
3	GOL	B	802	6/6	0.95	0.17	0.13	30,34,35,36	0
3	GOL	D	803	6/6	0.94	0.16	0.11	50,53,53,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.