Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:26 AM GMT

PDB ID	:	2X2Z
Title	:	Crystal structure AMA1 from Toxoplasma gondii
Authors	:	Crawford, J.; Tonkin, M.L.; Grujic, O.; Boulanger, M.J.
Deposited on	:	2010-01-18
Resolution	:	2.00 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 ①) were used in the production of this report:

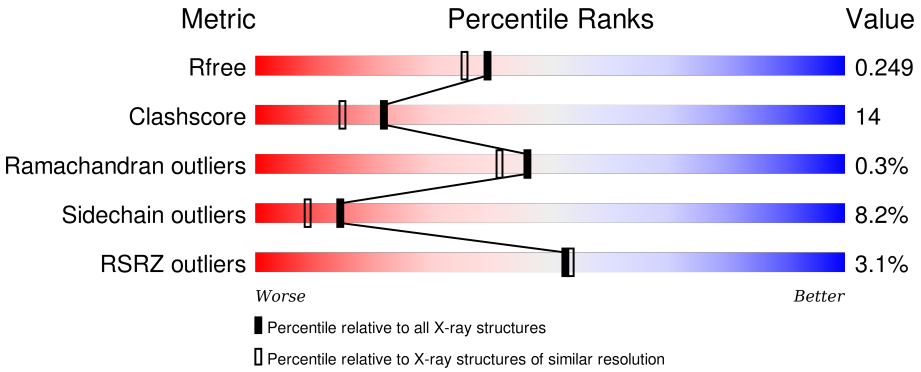
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.00 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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 <=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	456	2% 68% 18% • 11%
1	B	456	% 66% 17% • • 12%
1	D	456	5% 58% 18% • • 20%
1	E	456	2% 60% 22% • 13%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	E	1001	-	-	-	X

2 Entry composition

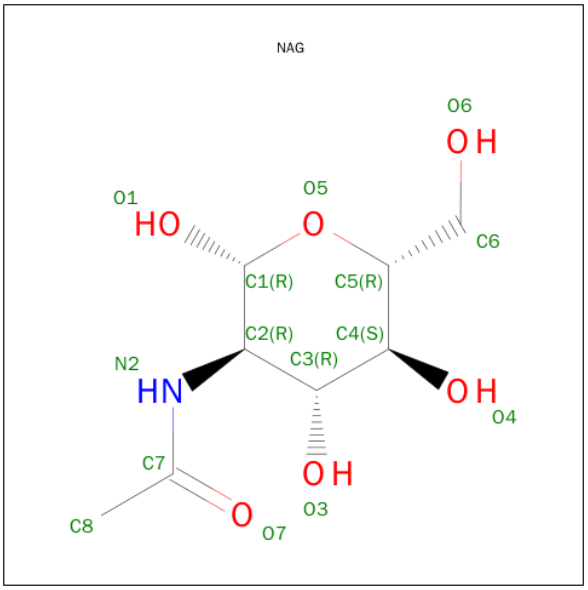
There are 4 unique types of molecules in this entry. The entry contains 13675 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 APICAL MEMBRANE ANTIGEN 1, PUTATIVE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	407	Total	C	N	O	S	0	1	0
			3218	2022	550	624	22			
1	B	401	Total	C	N	O	S	0	0	0
			3173	1999	540	612	22			
1	D	367	Total	C	N	O	S	0	0	0
			2909	1836	497	556	20			
1	E	396	Total	C	N	O	S	0	1	0
			3143	1978	537	606	22			

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



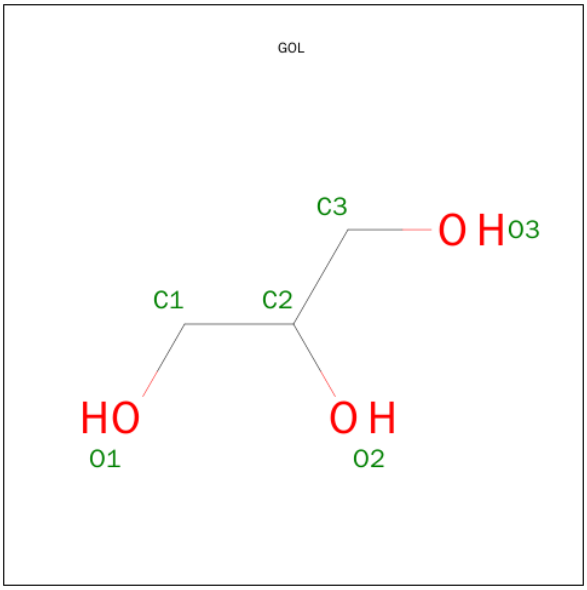
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total C N O 14 8 1 5	0	0
2	E	1	Total C N O 14 8 1 5	0	0

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



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

- Molecule 4 is water.

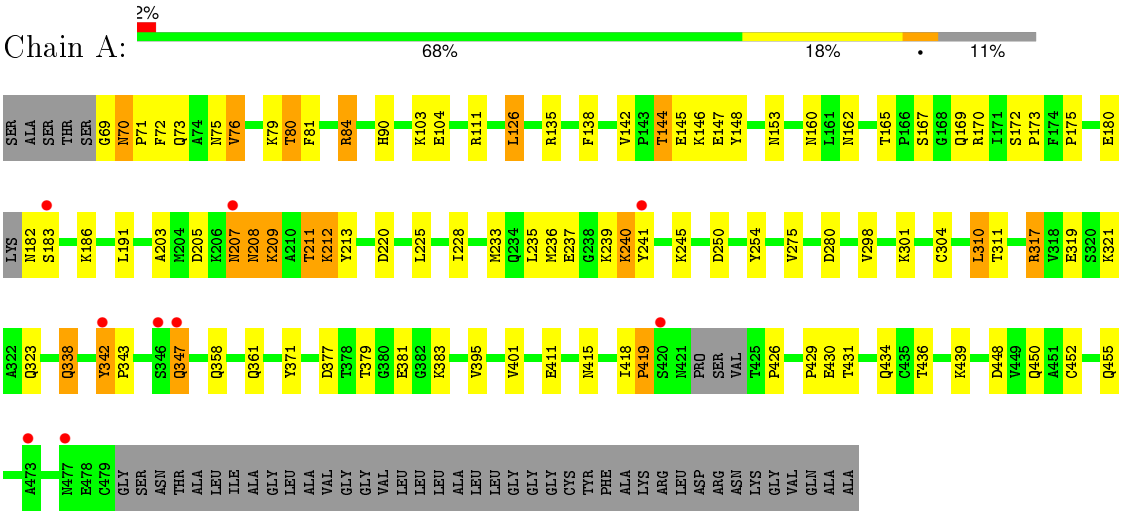
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	316	Total O 316 316	0	0
4	B	294	Total O 294 294	0	0
4	D	276	Total O 276 276	0	0
4	E	284	Total O 284 284	0	0

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

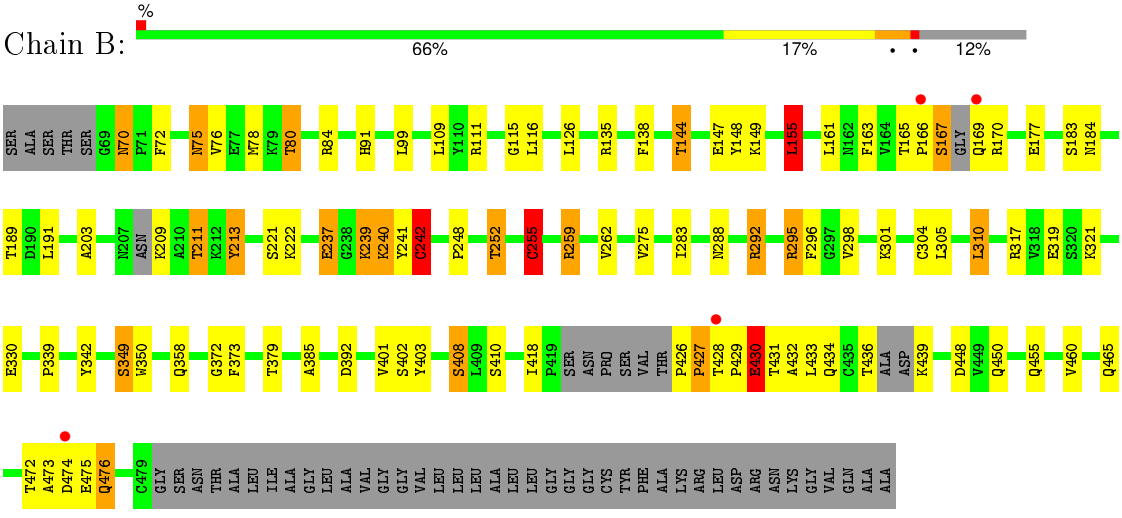
- Molecule 1: APICAL MEMBRANE ANTIGEN 1, PUTATIVE

Chain A:



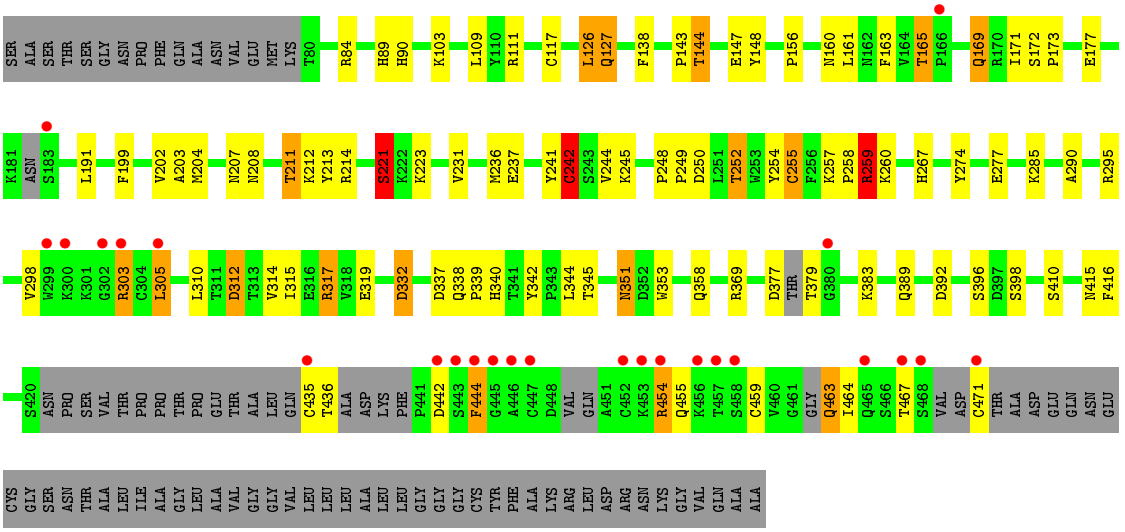
- Molecule 1: APICAL MEMBRANE ANTIGEN 1, PUTATIVE

Chain B:



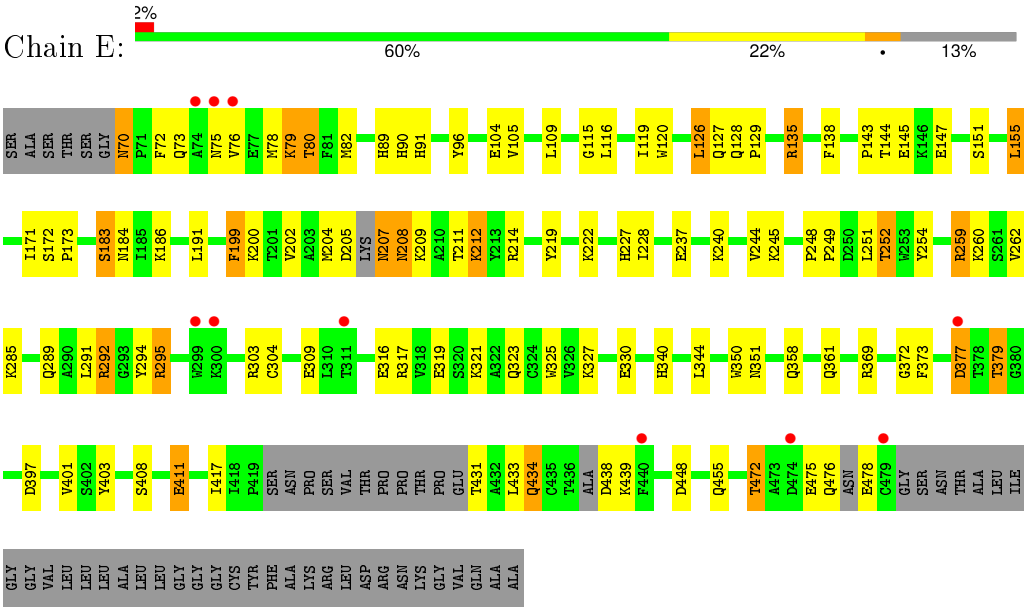
- Molecule 1: APICAL MEMBRANE ANTIGEN 1, PUTATIVE

Chain D:



• Molecule 1: APICAL MEMBRANE ANTIGEN 1, PUTATIVE

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	66.15Å 76.07Å 88.25Å 72.19° 71.44° 72.90°	Depositor
Resolution (Å)	43.90 – 2.00 43.90 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.4 (43.90-2.00) 88.4 (43.90-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.00 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.180 , 0.248 0.179 , 0.249	Depositor DCC
R_{free} test set	4915 reflections (5.24%)	DCC
Wilson B-factor (Å^2)	23.1	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 56.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 98628 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13675	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.37% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: GOL, NAG

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	1.05	4/3308 (0.1%)	0.93	5/4491 (0.1%)
1	B	1.13	8/3258 (0.2%)	0.98	11/4418 (0.2%)
1	D	1.22	12/2985 (0.4%)	0.97	8/4039 (0.2%)
1	E	1.04	3/3228 (0.1%)	0.94	2/4375 (0.0%)
All	All	1.11	27/12779 (0.2%)	0.95	26/17323 (0.2%)

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	1
1	B	0	2
1	D	0	2
1	E	0	1
All	All	0	6

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	255	CYS	CB-SG	-17.41	1.52	1.82
1	B	255	CYS	CB-SG	-16.93	1.53	1.82
1	D	242	CYS	CB-SG	13.20	2.04	1.82
1	B	242	CYS	CB-SG	11.61	2.02	1.82
1	D	177	GLU	CD-OE2	10.00	1.36	1.25
1	D	242	CYS	CA-CB	7.07	1.69	1.53
1	D	290	ALA	CA-CB	6.83	1.66	1.52
1	B	242	CYS	CA-CB	6.51	1.68	1.53
1	D	221	SER	CB-OG	-6.45	1.33	1.42
1	B	408	SER	CB-OG	-6.11	1.34	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	274	TYR	CE2-CZ	5.84	1.46	1.38
1	E	96	TYR	CD1-CE1	5.83	1.48	1.39
1	D	260	LYS	CB-CG	5.75	1.68	1.52
1	A	371	TYR	CE2-CZ	5.59	1.45	1.38
1	E	275	VAL	CB-CG2	5.46	1.64	1.52
1	B	237	GLU	CB-CG	5.42	1.62	1.52
1	A	170	ARG	CB-CG	-5.41	1.38	1.52
1	E	219	TYR	CD2-CE2	5.28	1.47	1.39
1	D	231	VAL	CB-CG1	5.28	1.64	1.52
1	B	213	TYR	CD2-CE2	5.27	1.47	1.39
1	A	395	VAL	CB-CG2	5.14	1.63	1.52
1	D	117	CYS	CB-SG	5.12	1.91	1.82
1	B	221	SER	CB-OG	-5.06	1.35	1.42
1	D	177	GLU	CG-CD	5.06	1.59	1.51
1	A	275	VAL	CB-CG2	5.05	1.63	1.52
1	B	275	VAL	CB-CG2	5.05	1.63	1.52
1	D	255	CYS	CA-CB	-5.01	1.43	1.53

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	295	ARG	NE-CZ-NH1	9.70	125.15	120.30
1	B	295	ARG	NE-CZ-NH2	-8.84	115.88	120.30
1	A	170	ARG	CG-CD-NE	-8.68	93.58	111.80
1	A	135	ARG	NE-CZ-NH2	-7.81	116.40	120.30
1	D	295	ARG	NE-CZ-NH1	7.43	124.02	120.30
1	B	255	CYS	CA-CB-SG	-7.03	101.35	114.00
1	B	255	CYS	CB-CA-C	-6.66	97.08	110.40
1	B	242	CYS	N-CA-C	-6.55	93.32	111.00
1	A	170	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	A	111	ARG	NE-CZ-NH2	-6.23	117.19	120.30
1	B	317	ARG	NE-CZ-NH2	-6.23	117.19	120.30
1	B	448	ASP	CB-CG-OD2	-6.07	112.84	118.30
1	E	295	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	B	474	ASP	CB-CG-OD1	5.68	123.41	118.30
1	B	448	ASP	CB-CG-OD1	5.63	123.37	118.30
1	D	337	ASP	CB-CG-OD1	5.63	123.37	118.30
1	D	295	ARG	NE-CZ-NH2	-5.61	117.49	120.30
1	B	155	LEU	CB-CG-CD1	-5.51	101.63	111.00
1	B	392	ASP	CB-CG-OD1	5.46	123.21	118.30
1	D	111	ARG	NE-CZ-NH1	-5.44	117.58	120.30
1	D	111	ARG	NE-CZ-NH2	5.39	123.00	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	199	PHE	C-N-CA	-5.35	108.33	121.70
1	D	242	CYS	N-CA-C	-5.25	96.81	111.00
1	A	280	ASP	CB-CG-OD1	5.03	122.83	118.30
1	D	259	ARG	NE-CZ-NH1	-5.02	117.79	120.30
1	D	332	ASP	CB-CA-C	-5.02	100.36	110.40

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	429	PRO	Peptide
1	B	241	TYR	Peptide
1	B	430	GLU	Peptide
1	D	241	TYR	Peptide
1	D	259	ARG	Peptide
1	E	204	MET	Peptide

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	3218	0	3039	71	0
1	B	3173	0	3002	95	0
1	D	2909	0	2756	79	0
1	E	3143	0	2971	103	0
2	A	14	0	13	0	0
2	B	14	0	13	0	0
2	D	14	0	13	3	0
2	E	14	0	13	2	0
3	D	6	0	8	0	0
4	A	316	0	0	10	0
4	B	294	0	0	18	0
4	D	276	0	0	19	0
4	E	284	0	0	19	0
All	All	13675	0	11828	341	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 14.

All (341) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:CYS:CB	1:B:242:CYS:SG	2.02	1.48
1:D:242:CYS:CB	1:D:242:CYS:SG	2.04	1.44
1:D:398:SER:HB2	4:D:2254:HOH:O	1.25	1.30
1:E:119:ILE:HG13	4:E:2041:HOH:O	0.99	1.15
1:D:435:CYS:HB2	1:D:459:CYS:SG	1.88	1.14
1:E:431:THR:HA	1:E:434:GLN:NE2	1.66	1.09
1:B:426:PRO:N	1:B:427:PRO:HA	1.61	1.07
1:A:207:ASN:O	1:A:208:ASN:HB2	1.51	1.06
1:E:377:ASP:HB3	4:E:2243:HOH:O	1.52	1.05
1:E:199:PHE:O	1:E:200:LYS:HB2	1.62	0.97
1:A:144:THR:HG21	4:A:2079:HOH:O	1.65	0.96
1:E:319:GLU:H	1:E:323:GLN:NE2	1.63	0.95
1:B:430:GLU:HB3	1:B:434:GLN:NE2	1.81	0.94
1:B:211:THR:HG22	1:B:213:TYR:H	1.30	0.94
1:A:144:THR:HG22	1:A:147:GLU:H	1.32	0.93
1:B:211:THR:CG2	1:B:213:TYR:H	1.81	0.93
1:E:319:GLU:H	1:E:323:GLN:HE22	1.09	0.92
1:D:211:THR:HG23	1:D:213:TYR:H	1.33	0.91
1:B:203:ALA:O	1:B:211:THR:HB	1.70	0.90
1:B:349:SER:HB2	4:B:2218:HOH:O	1.72	0.90
1:E:105:VAL:HG22	1:E:211:THR:HG21	1.52	0.88
1:E:431:THR:HA	1:E:434:GLN:HE22	1.34	0.88
1:E:292:ARG:HG2	1:E:292:ARG:HH11	1.39	0.88
1:D:221:SER:HB2	1:D:267:HIS:O	1.76	0.86
1:A:379:THR:HG21	1:A:381:GLU:OE2	1.75	0.85
1:A:321:LYS:HE3	1:A:401:VAL:HG21	1.58	0.85
1:E:292:ARG:HD3	1:E:411:GLU:OE2	1.77	0.84
1:E:472:THR:HG22	1:E:475:GLU:H	1.39	0.84
1:E:135:ARG:NH1	4:E:2056:HOH:O	2.10	0.84
1:A:183:SER:HB2	4:A:2110:HOH:O	1.77	0.83
1:E:76:VAL:O	1:E:80:THR:HG22	1.77	0.83
1:E:237:GLU:OE1	1:E:340:HIS:HE1	1.62	0.82
1:A:207:ASN:C	1:A:207:ASN:ND2	2.32	0.82
1:E:199:PHE:O	1:E:200:LYS:CB	2.24	0.82
1:A:342:TYR:HB3	1:A:343:PRO:HD3	1.61	0.81
1:B:428:THR:HB	1:B:429:PRO:HD2	1.62	0.80
1:B:427:PRO:HD2	1:B:431:THR:HG23	1.63	0.79
1:E:240:LYS:HG3	4:E:2136:HOH:O	1.82	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:144:THR:HG22	1:D:147:GLU:H	1.49	0.78
1:D:467:THR:HG23	4:D:2270:HOH:O	1.82	0.77
1:A:90:HIS:HB2	4:A:2006:HOH:O	1.85	0.77
1:D:342:TYR:O	4:D:2206:HOH:O	2.02	0.77
1:E:379:THR:HG23	4:E:2243:HOH:O	1.84	0.77
1:A:207:ASN:C	1:A:207:ASN:HD22	1.89	0.76
1:E:165:THR:HG22	1:E:167:SER:H	1.48	0.76
1:A:207:ASN:O	1:A:208:ASN:CB	2.31	0.75
1:B:76:VAL:O	1:B:80:THR:HG23	1.87	0.75
1:D:89:HIS:HD2	2:D:1001:NAG:O6	1.70	0.74
1:E:284:SER:HB3	4:E:2173:HOH:O	1.87	0.74
1:D:223:LYS:HE2	4:D:2124:HOH:O	1.86	0.74
1:D:436:THR:HG22	4:D:2265:HOH:O	1.86	0.73
1:B:177:GLU:HG3	4:B:2085:HOH:O	1.88	0.73
1:A:73:GLN:HG3	1:A:79:LYS:HE2	1.70	0.73
1:A:211:THR:HG22	1:A:213:TYR:H	1.54	0.73
1:E:205:ASP:OD1	1:E:208:ASN:N	2.21	0.73
1:A:76:VAL:O	1:A:80:THR:HG23	1.88	0.73
1:D:398:SER:CB	4:D:2254:HOH:O	2.01	0.73
1:D:211:THR:CG2	1:D:213:TYR:H	2.01	0.73
1:A:165:THR:HG22	1:A:167:SER:H	1.55	0.72
1:E:166:PRO:O	4:E:2083:HOH:O	2.07	0.72
1:D:303:ARG:HE	1:D:467:THR:HG21	1.55	0.71
1:D:435:CYS:CB	1:D:459:CYS:SG	2.75	0.71
1:E:319:GLU:N	1:E:323:GLN:NE2	2.38	0.71
1:D:314:VAL:HG23	1:E:186:LYS:HE2	1.73	0.71
1:B:240:LYS:HE3	4:B:2128:HOH:O	1.91	0.70
1:D:237:GLU:OE1	1:D:340:HIS:HE1	1.73	0.70
1:B:252:THR:HG21	4:B:2218:HOH:O	1.90	0.70
1:B:239:LYS:HG3	1:B:248:PRO:HD3	1.74	0.70
1:E:145:GLU:HG3	1:E:350:TRP:CZ2	2.27	0.70
1:E:205:ASP:HB2	4:E:2112:HOH:O	1.93	0.69
1:B:155:LEU:HD11	1:B:350:TRP:CZ3	2.28	0.69
1:E:127:GLN:HE21	1:E:244:VAL:HG22	1.58	0.69
1:B:473:ALA:HA	1:B:476:GLN:NE2	2.07	0.68
1:E:344:LEU:HA	1:E:358:GLN:HE22	1.58	0.68
2:E:1001:NAG:O4	4:E:2280:HOH:O	2.07	0.68
1:E:155:LEU:HD11	1:E:350:TRP:CE3	2.28	0.68
1:E:155:LEU:HD11	1:E:350:TRP:HE3	1.59	0.68
1:D:242:CYS:CB	1:D:255:CYS:HB3	2.23	0.67
1:A:411:GLU:OE1	4:A:2264:HOH:O	2.13	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:242:CYS:HB2	1:D:255:CYS:HB3	1.75	0.67
1:B:165:THR:HG23	1:B:167:SER:H	1.60	0.67
1:D:463:GLN:HA	1:D:463:GLN:HE21	1.56	0.67
1:B:358:GLN:OE1	4:B:2227:HOH:O	2.13	0.66
1:A:203:ALA:O	1:A:211:THR:HB	1.95	0.66
1:A:379:THR:HG23	1:A:381:GLU:H	1.60	0.66
1:E:119:ILE:HD11	4:E:2021:HOH:O	1.95	0.66
1:B:144:THR:HG22	1:B:147:GLU:H	1.62	0.65
1:E:209:LYS:HG3	4:E:2116:HOH:O	1.96	0.65
1:A:240:LYS:NZ	4:A:2150:HOH:O	2.29	0.65
1:D:314:VAL:CG2	1:E:186:LYS:HE2	2.27	0.65
1:E:127:GLN:NE2	1:E:244:VAL:HG22	2.11	0.65
1:E:472:THR:CG2	1:E:475:GLU:H	2.10	0.64
1:D:236:MET:O	1:D:255:CYS:CB	2.45	0.64
1:D:319:GLU:OE2	4:D:2185:HOH:O	2.15	0.64
1:B:339:PRO:HG2	1:B:342:TYR:CD2	2.32	0.63
1:D:312:ASP:CB	1:E:183:SER:HB3	2.29	0.63
1:D:464:ILE:HD13	4:D:2273:HOH:O	1.98	0.63
1:E:377:ASP:CB	4:E:2243:HOH:O	2.27	0.62
1:B:155:LEU:HD11	1:B:350:TRP:HZ3	1.63	0.62
1:B:135:ARG:NH1	4:B:2050:HOH:O	2.31	0.62
1:D:203:ALA:O	1:D:211:THR:HB	1.99	0.62
1:D:312:ASP:HB3	1:E:183:SER:HB3	1.80	0.62
2:D:1001:NAG:H2	4:D:2274:HOH:O	2.00	0.62
1:E:211:THR:HG23	4:E:2029:HOH:O	1.99	0.62
1:B:428:THR:OG1	1:B:430:GLU:HG2	2.00	0.62
1:E:358:GLN:H	1:E:361:GLN:NE2	1.97	0.62
1:E:144:THR:HG23	1:E:147:GLU:H	1.65	0.61
1:B:75:ASN:HD21	1:B:78:MET:HB2	1.65	0.61
1:A:144:THR:HG22	1:A:147:GLU:N	2.12	0.61
1:D:436:THR:CG2	4:D:2265:HOH:O	2.45	0.61
1:E:379:THR:O	1:E:379:THR:OG1	2.17	0.61
1:B:430:GLU:HB3	1:B:434:GLN:CD	2.22	0.60
1:E:89:HIS:HD2	2:E:1001:NAG:O6	1.85	0.60
1:D:221:SER:OG	1:D:416:PHE:CZ	2.54	0.60
1:E:248:PRO:HG2	1:E:251:LEU:HD12	1.82	0.60
1:D:236:MET:O	1:D:255:CYS:HB2	2.01	0.60
1:D:212:LYS:NZ	1:D:214:ARG:HH12	1.99	0.60
1:B:418:ILE:HG21	1:D:379:THR:HA	1.82	0.60
1:B:240:LYS:HG3	4:B:2128:HOH:O	2.03	0.59
1:E:73:GLN:HA	1:E:79:LYS:HG3	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:THR:CG2	1:A:213:TYR:H	2.14	0.59
1:B:427:PRO:HD2	1:B:431:THR:CG2	2.32	0.59
1:E:126:LEU:HG	1:E:254:TYR:CE1	2.38	0.59
1:E:211:THR:CG2	4:E:2029:HOH:O	2.50	0.58
1:D:221:SER:OG	1:D:416:PHE:CE1	2.57	0.58
1:B:436:THR:O	1:B:439:LYS:N	2.36	0.58
1:A:144:THR:CG2	1:A:147:GLU:H	2.12	0.58
1:D:258:PRO:O	1:D:259:ARG:HD3	2.03	0.58
1:B:161:LEU:HD11	1:B:163:PHE:CD2	2.39	0.58
1:A:342:TYR:CB	1:A:343:PRO:HD3	2.34	0.57
1:D:298:VAL:HA	1:D:392:ASP:OD1	2.04	0.57
1:E:292:ARG:HG2	1:E:292:ARG:NH1	2.14	0.57
1:B:460:VAL:CG2	1:B:465:GLN:HG3	2.35	0.57
1:E:207:ASN:N	1:E:207:ASN:OD1	2.38	0.57
1:B:183:SER:HB2	4:B:2094:HOH:O	2.05	0.57
1:B:70:ASN:ND2	1:B:72:PHE:H	2.02	0.56
1:A:237:GLU:HG3	4:A:2146:HOH:O	2.05	0.56
1:A:377:ASP:HB3	1:A:379:THR:HG22	1.87	0.56
1:A:103:LYS:HD2	1:A:212:LYS:HB3	1.85	0.56
1:D:165:THR:HG22	1:D:169:GLN:H	1.71	0.56
1:D:126:LEU:HG	1:D:254:TYR:CE1	2.41	0.56
1:E:205:ASP:OD1	1:E:208:ASN:HA	2.05	0.56
1:B:75:ASN:N	1:B:75:ASN:HD22	2.03	0.56
1:B:321:LYS:HD3	4:B:2107:HOH:O	2.05	0.56
1:B:304:CYS:H	1:B:455:GLN:NE2	2.04	0.56
1:D:236:MET:O	1:D:255:CYS:HB3	2.06	0.56
1:B:428:THR:CB	1:B:429:PRO:HD2	2.34	0.56
1:E:120:TRP:O	1:E:260:LYS:HE2	2.05	0.56
1:E:292:ARG:CG	1:E:292:ARG:HH11	2.15	0.55
1:A:209:LYS:HG2	1:D:415:ASN:HB3	1.88	0.55
1:A:304:CYS:H	1:A:455:GLN:NE2	2.03	0.55
1:E:431:THR:HA	1:E:434:GLN:HE21	1.62	0.55
1:E:303:ARG:NH2	1:E:309:GLU:OE1	2.36	0.55
1:E:145:GLU:HG3	1:E:350:TRP:HZ2	1.68	0.55
1:D:303:ARG:NH1	1:D:305:LEU:HD11	2.20	0.55
1:E:237:GLU:OE1	1:E:340:HIS:CE1	2.52	0.55
1:D:396:SER:OG	1:D:464:ILE:HA	2.06	0.55
1:B:295:ARG:HG2	1:B:373:PHE:CE2	2.41	0.55
1:D:435:CYS:O	1:D:436:THR:CB	2.55	0.54
1:E:184:ASN:O	1:E:186:LYS:HD2	2.07	0.54
1:E:70:ASN:ND2	1:E:72:PHE:H	2.06	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:ARG:HD3	1:E:109:LEU:HD22	1.89	0.54
1:A:76:VAL:O	1:A:80:THR:CG2	2.56	0.53
1:B:209:LYS:N	4:B:2108:HOH:O	2.42	0.53
1:B:211:THR:HG22	1:B:213:TYR:N	2.12	0.53
1:A:317:ARG:HD2	1:A:383:LYS:HE2	1.90	0.53
1:B:148:TYR:OH	1:B:252:THR:HB	2.08	0.53
1:E:165:THR:HG23	1:E:166:PRO:HD2	1.90	0.53
1:E:173:PRO:HB3	1:E:227:HIS:CE1	2.44	0.53
1:A:301:LYS:NZ	1:A:450:GLN:HE21	2.07	0.53
1:A:209:LYS:HG2	1:D:415:ASN:CB	2.39	0.52
1:B:165:THR:HG22	1:B:169:GLN:N	2.24	0.52
1:A:145:GLU:CD	4:A:2080:HOH:O	2.46	0.52
1:A:431:THR:HA	1:A:434:GLN:HE21	1.74	0.52
2:D:1001:NAG:H83	2:D:1001:NAG:H3	1.92	0.52
1:B:78:MET:HE1	1:B:432:ALA:O	2.09	0.52
1:A:148:TYR:OH	1:A:153:ASN:ND2	2.41	0.52
1:D:303:ARG:HB3	1:D:455:GLN:HB2	1.92	0.52
1:B:189:THR:HG21	1:B:283:ILE:HD11	1.90	0.52
1:D:345:THR:H	1:D:358:GLN:NE2	2.08	0.52
1:E:304:CYS:H	1:E:455:GLN:NE2	2.08	0.52
1:D:252:THR:HG21	4:D:2212:HOH:O	2.09	0.51
1:A:415:ASN:HA	1:A:418:ILE:HD12	1.91	0.51
1:D:90:HIS:ND1	1:D:285:LYS:HB3	2.25	0.51
1:E:184:ASN:O	1:E:186:LYS:CD	2.59	0.51
1:B:262:VAL:HG22	4:B:2139:HOH:O	2.10	0.51
1:E:316:GLU:OE1	1:E:327:LYS:HE3	2.11	0.51
1:A:358:GLN:H	1:A:361:GLN:NE2	2.09	0.51
4:D:2181:HOH:O	1:E:186:LYS:HE3	2.10	0.51
1:E:91:HIS:CE1	1:E:115:GLY:HA3	2.46	0.51
1:B:155:LEU:HD21	4:B:2220:HOH:O	2.09	0.51
1:D:252:THR:HG23	4:D:2146:HOH:O	2.09	0.51
1:B:430:GLU:CB	1:B:434:GLN:NE2	2.64	0.51
1:B:75:ASN:H	1:B:75:ASN:HD22	1.58	0.50
1:B:184:ASN:ND2	4:B:2093:HOH:O	2.38	0.50
1:A:233:MET:SD	1:A:236:MET:CE	3.00	0.50
1:A:342:TYR:CB	1:A:343:PRO:CD	2.88	0.50
1:A:298:VAL:CG2	1:A:310:LEU:HD11	2.42	0.50
1:B:189:THR:CG2	1:B:283:ILE:HD11	2.41	0.50
1:B:429:PRO:O	1:B:433:LEU:N	2.31	0.50
1:B:473:ALA:HA	1:B:476:GLN:HE22	1.77	0.50
1:E:295:ARG:HG2	1:E:373:PHE:CD2	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:GLU:O	1:A:182:ASN:N	2.46	0.49
4:D:2181:HOH:O	1:E:186:LYS:CE	2.60	0.49
1:D:377:ASP:O	1:D:379:THR:N	2.46	0.49
1:B:144:THR:CG2	1:B:147:GLU:H	2.26	0.49
1:E:372:GLY:HA2	1:E:385:ALA:O	2.11	0.49
1:A:69:GLY:N	4:A:2001:HOH:O	2.45	0.49
1:A:347:GLN:NE2	4:A:2220:HOH:O	2.45	0.49
1:D:444:PHE:HD1	1:D:454:ARG:NH1	2.10	0.49
1:A:81:PHE:O	1:A:84:ARG:HD2	2.13	0.49
1:B:288:ASN:O	1:B:408:SER:HB2	2.12	0.49
1:B:321:LYS:HD2	1:B:401:VAL:HG21	1.94	0.48
1:D:351:ASN:ND2	1:D:353:TRP:HE1	2.11	0.48
1:E:143:PRO:HG3	1:E:155:LEU:HG	1.95	0.48
1:B:301:LYS:NZ	1:B:450:GLN:HE21	2.11	0.48
1:E:211:THR:HG22	1:E:212:LYS:N	2.28	0.48
1:B:144:THR:HG22	1:B:147:GLU:HG3	1.95	0.48
1:B:237:GLU:HA	1:B:255:CYS:SG	2.53	0.48
1:E:448:ASP:C	1:E:448:ASP:OD1	2.52	0.48
1:A:426:PRO:HB2	4:A:2278:HOH:O	2.12	0.48
1:E:472:THR:O	1:E:476:GLN:HG3	2.13	0.48
1:B:165:THR:HG23	1:B:167:SER:N	2.28	0.48
1:E:289:GLN:HE22	1:E:417:ILE:HD11	1.78	0.48
1:B:472:THR:OG1	1:B:475:GLU:HG3	2.14	0.48
1:E:369[A]:ARG:HG3	1:E:387:SER:C	2.34	0.47
1:A:142:VAL:HG23	1:A:162:ASN:ND2	2.30	0.47
1:E:205:ASP:OD1	1:E:208:ASN:CA	2.62	0.47
1:D:257:LYS:HE3	1:D:259:ARG:HE	1.80	0.47
1:A:418:ILE:O	1:A:419:PRO:C	2.51	0.47
1:A:319:GLU:H	1:A:323:GLN:NE2	2.12	0.47
1:A:160:ASN:ND2	1:A:172:SER:OG	2.42	0.47
1:B:426:PRO:N	1:B:427:PRO:CA	2.49	0.47
1:E:431:THR:CA	1:E:434:GLN:NE2	2.58	0.47
1:D:377:ASP:HB2	1:D:383:LYS:HD2	1.96	0.47
1:D:202:VAL:HG12	1:D:214:ARG:HG2	1.96	0.46
1:B:372:GLY:HA2	1:B:385:ALA:O	2.15	0.46
1:E:351:ASN:HA	4:E:2220:HOH:O	2.15	0.46
1:B:240:LYS:CE	4:B:2128:HOH:O	2.56	0.46
1:B:298:VAL:CG2	1:B:310:LEU:HD21	2.45	0.46
1:A:207:ASN:ND2	1:A:207:ASN:O	2.42	0.46
1:E:144:THR:HG22	1:E:147:GLU:CG	2.46	0.46
1:B:211:THR:HG23	1:B:213:TYR:H	1.71	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:148:TYR:OH	1:D:252:THR:HB	2.14	0.46
1:E:172:SER:HG	1:E:228:ILE:H	1.63	0.46
1:A:73:GLN:O	1:A:79:LYS:HE2	2.16	0.46
1:B:298:VAL:HG21	1:B:310:LEU:HD21	1.97	0.46
1:D:338:GLN:N	1:D:339:PRO:HD3	2.31	0.46
1:B:460:VAL:HG23	1:B:465:GLN:HG3	1.98	0.45
1:D:344:LEU:HA	1:D:358:GLN:HE22	1.82	0.45
1:A:220:ASP:C	1:A:220:ASP:OD1	2.55	0.45
1:A:175:PRO:HA	1:A:225:LEU:HD23	1.98	0.45
1:D:242:CYS:SG	1:D:242:CYS:CA	3.01	0.45
1:B:242:CYS:SG	1:B:242:CYS:CA	2.99	0.45
1:E:151:SER:OG	1:E:156:PRO:HD3	2.17	0.45
1:A:70:ASN:ND2	1:A:72:PHE:H	2.14	0.45
1:D:160:ASN:ND2	1:D:172:SER:OG	2.50	0.45
1:A:241:TYR:OH	1:A:342:TYR:N	2.46	0.45
1:D:144:THR:HG21	4:D:2068:HOH:O	2.17	0.45
1:E:262:VAL:HG23	1:E:263:THR:HG23	1.99	0.45
1:D:242:CYS:C	1:D:242:CYS:SG	2.95	0.45
1:B:296:PHE:CE1	1:B:402:SER:HB3	2.52	0.45
1:E:397:ASP:C	1:E:397:ASP:OD1	2.56	0.45
1:E:472:THR:HG22	1:E:475:GLU:N	2.19	0.44
1:E:295:ARG:HG2	1:E:373:PHE:CE2	2.53	0.44
1:A:144:THR:HG23	1:A:146:LYS:H	1.83	0.44
1:E:145:GLU:HG2	4:E:2219:HOH:O	2.18	0.44
1:B:75:ASN:ND2	1:B:75:ASN:N	2.64	0.44
1:B:295:ARG:HG2	1:B:373:PHE:CD2	2.53	0.44
1:B:155:LEU:HA	1:B:155:LEU:HD12	1.67	0.44
1:B:410:SER:OG	1:E:104:GLU:OE1	2.28	0.44
1:D:103:LYS:HD2	1:D:212:LYS:HB3	2.00	0.44
1:B:460:VAL:HB	1:B:465:GLN:HG3	2.00	0.44
1:B:155:LEU:HD11	1:B:350:TRP:CE3	2.53	0.43
1:B:78:MET:HB2	1:B:78:MET:HE3	1.72	0.43
1:E:321:LYS:HE2	1:E:401:VAL:HG21	1.99	0.43
1:E:379:THR:OG1	1:E:381:GLU:HG3	2.18	0.43
1:A:160:ASN:ND2	1:A:172:SER:HG	2.16	0.43
1:A:205:ASP:OD1	1:A:208:ASN:N	2.25	0.43
1:B:460:VAL:HB	1:B:465:GLN:CG	2.48	0.43
1:E:70:ASN:HD21	1:E:72:PHE:HB2	1.83	0.43
1:E:259:ARG:HD2	1:E:330:GLU:OE1	2.18	0.43
1:A:233:MET:SD	1:A:236:MET:HE1	2.58	0.43
1:D:369:ARG:NH1	4:D:2236:HOH:O	2.38	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:LYS:CE	1:B:450:GLN:HE21	2.31	0.43
1:B:259:ARG:NH1	1:B:330:GLU:OE1	2.41	0.43
1:A:342:TYR:HB3	1:A:343:PRO:CD	2.38	0.43
1:D:204:MET:CE	1:D:208:ASN:O	2.66	0.43
1:A:241:TYR:CE2	1:A:342:TYR:CD2	3.07	0.42
1:E:248:PRO:HA	1:E:249:PRO:HD3	1.69	0.42
1:B:259:ARG:HD2	1:B:330:GLU:OE1	2.19	0.42
1:B:321:LYS:HG3	4:B:2191:HOH:O	2.18	0.42
1:E:75:ASN:HB2	4:E:2011:HOH:O	2.19	0.42
1:B:305:LEU:N	1:B:305:LEU:HD12	2.34	0.42
1:E:260:LYS:HD3	1:E:325:TRP:CZ2	2.54	0.42
1:A:448:ASP:O	1:A:452:CYS:N	2.52	0.42
1:A:379:THR:HG23	1:A:381:GLU:HG3	2.00	0.42
1:D:250:ASP:HB3	4:D:2144:HOH:O	2.19	0.42
1:D:199:PHE:CZ	1:D:277:GLU:HG3	2.54	0.42
1:E:78:MET:O	1:E:82:MET:HG2	2.20	0.42
1:A:160:ASN:HD21	1:A:172:SER:HG	1.61	0.42
1:D:127:GLN:HG2	1:D:244:VAL:HG13	2.02	0.42
1:A:104:GLU:OE1	1:D:410:SER:OG	2.29	0.41
1:D:315:ILE:CG2	1:D:383:LYS:HD3	2.50	0.41
1:E:321:LYS:HG3	1:E:403:TYR:OH	2.20	0.41
1:E:90:HIS:ND1	1:E:285:LYS:HB3	2.35	0.41
1:B:91:HIS:CE1	1:B:115:GLY:HA3	2.55	0.41
1:B:252:THR:HG22	4:B:2134:HOH:O	2.20	0.41
1:E:90:HIS:HB3	4:E:2175:HOH:O	2.20	0.41
1:D:317:ARG:NH2	4:D:2244:HOH:O	2.52	0.41
1:D:459:CYS:HA	1:D:463:GLN:HB3	2.01	0.41
1:E:252:THR:HG23	4:E:2146:HOH:O	2.18	0.41
1:A:235:LEU:HD23	1:A:338:GLN:HG2	2.02	0.41
1:D:171:ILE:HD13	1:D:171:ILE:N	2.35	0.41
1:A:70:ASN:HD22	1:A:71:PRO:HD2	1.86	0.41
1:E:128:GLN:HB3	1:E:129:PRO:HD2	2.03	0.41
1:D:248:PRO:HA	1:D:249:PRO:HD3	1.92	0.41
1:D:389:GLN:NE2	4:D:2249:HOH:O	2.54	0.41
1:A:165:THR:HG22	1:A:167:SER:N	2.30	0.41
1:B:358:GLN:HG2	4:B:2226:HOH:O	2.20	0.41
1:B:339:PRO:HG2	1:B:342:TYR:CG	2.56	0.41
1:A:126:LEU:HG	1:A:254:TYR:CE1	2.56	0.41
1:D:161:LEU:HD21	1:D:163:PHE:HB2	2.03	0.41
1:B:99:LEU:HB3	1:B:111:ARG:HB3	2.03	0.41
1:D:207:ASN:O	1:D:208:ASN:CB	2.68	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:222:LYS:HE2	1:E:222:LYS:HB2	1.90	0.41
1:B:144:THR:HG22	1:B:147:GLU:CG	2.51	0.41
1:B:72:PHE:HA	1:B:78:MET:HG2	2.03	0.41
1:B:321:LYS:HB3	1:B:403:TYR:OH	2.21	0.41
1:A:172:SER:HA	1:A:173:PRO:C	2.41	0.41
1:E:294:TYR:CE2	1:E:433:LEU:HD13	2.56	0.41
1:E:205:ASP:O	1:E:209:LYS:HB3	2.21	0.40
1:B:259:ARG:HA	1:B:259:ARG:HD2	1.76	0.40
1:B:211:THR:CG2	1:B:213:TYR:N	2.65	0.40
1:D:212:LYS:HZ2	1:D:214:ARG:HH12	1.66	0.40
1:E:202:VAL:HG12	1:E:214:ARG:HG2	2.03	0.40
1:B:242:CYS:C	1:B:242:CYS:SG	2.99	0.40
1:B:252:THR:HG23	4:B:2136:HOH:O	2.22	0.40
1:D:172:SER:HA	1:D:173:PRO:C	2.40	0.40
1:A:172:SER:HG	1:A:228:ILE:H	1.68	0.40
1:D:143:PRO:HB3	1:D:156:PRO:HG2	2.03	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	402/456 (88%)	387 (96%)	14 (4%)	1 (0%)	52	48
1	B	391/456 (86%)	378 (97%)	12 (3%)	1 (0%)	46	41
1	D	352/456 (77%)	337 (96%)	14 (4%)	1 (0%)	46	41
1	E	387/456 (85%)	370 (96%)	16 (4%)	1 (0%)	46	41
All	All	1532/1824 (84%)	1472 (96%)	56 (4%)	4 (0%)	46	41

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	208	ASN
1	B	427	PRO
1	E	208	ASN
1	D	332	ASP

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	356/388 (92%)	327 (92%)	29 (8%)	15	9
1	B	351/388 (90%)	321 (92%)	30 (8%)	13	8
1	D	321/388 (83%)	295 (92%)	26 (8%)	15	9
1	E	347/388 (89%)	319 (92%)	28 (8%)	15	9
All	All	1375/1552 (89%)	1262 (92%)	113 (8%)	14	9

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	ASN
1	A	75	ASN
1	A	76	VAL
1	A	80	THR
1	A	84	ARG
1	A	126	LEU
1	A	138	PHE
1	A	144	THR
1	A	169	GLN
1	A	186	LYS
1	A	191	LEU
1	A	207	ASN
1	A	209	LYS
1	A	211	THR
1	A	212	LYS
1	A	239	LYS
1	A	240	LYS
1	A	245	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	250	ASP
1	A	310	LEU
1	A	311	THR
1	A	317	ARG
1	A	338	GLN
1	A	342	TYR
1	A	347	GLN
1	A	419	PRO
1	A	430	GLU
1	A	436	THR
1	A	439	LYS
1	B	70	ASN
1	B	75	ASN
1	B	80	THR
1	B	84	ARG
1	B	109	LEU
1	B	116	LEU
1	B	126	LEU
1	B	138	PHE
1	B	144	THR
1	B	149	LYS
1	B	155	LEU
1	B	166	PRO
1	B	167	SER
1	B	170	ARG
1	B	191	LEU
1	B	211	THR
1	B	222	LYS
1	B	239	LYS
1	B	240	LYS
1	B	242	CYS
1	B	252	THR
1	B	255	CYS
1	B	259	ARG
1	B	292	ARG
1	B	310	LEU
1	B	319	GLU
1	B	349	SER
1	B	379	THR
1	B	430	GLU
1	B	476	GLN
1	D	84	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	109	LEU
1	D	126	LEU
1	D	127	GLN
1	D	138	PHE
1	D	144	THR
1	D	165	THR
1	D	169	GLN
1	D	191	LEU
1	D	211	THR
1	D	221	SER
1	D	242	CYS
1	D	245	LYS
1	D	252	THR
1	D	259	ARG
1	D	303	ARG
1	D	305	LEU
1	D	310	LEU
1	D	312	ASP
1	D	317	ARG
1	D	351	ASN
1	D	442	ASP
1	D	444	PHE
1	D	454	ARG
1	D	463	GLN
1	D	471	CYS
1	E	70	ASN
1	E	79	LYS
1	E	80	THR
1	E	116	LEU
1	E	126	LEU
1	E	135	ARG
1	E	138	PHE
1	E	155	LEU
1	E	171	ILE
1	E	183	SER
1	E	191	LEU
1	E	207	ASN
1	E	212	LYS
1	E	245	LYS
1	E	252	THR
1	E	259	ARG
1	E	291	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	292	ARG
1	E	317	ARG
1	E	377	ASP
1	E	379	THR
1	E	408	SER
1	E	411	GLU
1	E	434	GLN
1	E	438	ASP
1	E	439	LYS
1	E	472	THR
1	E	478	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	ASN
1	A	75	ASN
1	A	90	HIS
1	A	92	GLN
1	A	123	HIS
1	A	153	ASN
1	A	160	ASN
1	A	207	ASN
1	A	208	ASN
1	A	289	GLN
1	A	323	GLN
1	A	338	GLN
1	A	358	GLN
1	A	361	GLN
1	A	434	GLN
1	A	450	GLN
1	A	455	GLN
1	A	476	GLN
1	B	70	ASN
1	B	73	GLN
1	B	75	ASN
1	B	123	HIS
1	B	127	GLN
1	B	160	ASN
1	B	169	GLN
1	B	289	GLN
1	B	338	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	361	GLN
1	B	434	GLN
1	B	450	GLN
1	B	455	GLN
1	B	476	GLN
1	D	89	HIS
1	D	123	HIS
1	D	127	GLN
1	D	160	ASN
1	D	169	GLN
1	D	289	GLN
1	D	338	GLN
1	D	340	HIS
1	D	351	ASN
1	D	358	GLN
1	D	455	GLN
1	D	463	GLN
1	D	465	GLN
1	E	70	ASN
1	E	75	ASN
1	E	89	HIS
1	E	101	GLN
1	E	123	HIS
1	E	127	GLN
1	E	160	ASN
1	E	184	ASN
1	E	207	ASN
1	E	265	ASN
1	E	289	GLN
1	E	323	GLN
1	E	338	GLN
1	E	340	HIS
1	E	358	GLN
1	E	361	GLN
1	E	434	GLN
1	E	455	GLN

5.3.3 RNA

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)

5 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	NAG	A	1001	1	14,14,15	0.80	0	15,19,21	2.05	3 (20%)
2	NAG	B	1001	1	14,14,15	1.09	1 (7%)	15,19,21	1.29	2 (13%)
2	NAG	D	1001	1	14,14,15	0.61	0	15,19,21	2.26	6 (40%)
3	GOL	D	1472	-	5,5,5	0.33	0	5,5,5	0.47	0
2	NAG	E	1001	1	14,14,15	0.67	0	15,19,21	1.19	2 (13%)

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	NAG	A	1001	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1001	1	-	0/6/23/26	0/1/1/1
2	NAG	D	1001	1	-	0/6/23/26	0/1/1/1
3	GOL	D	1472	-	-	0/4/4/4	0/0/0/0
2	NAG	E	1001	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1001	NAG	O5-C1	-3.11	1.38	1.43

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1001	NAG	O7-C7-C8	-4.21	114.33	122.06
2	A	1001	NAG	C3-C2-N2	-2.77	103.93	110.56
2	B	1001	NAG	C3-C2-N2	-2.59	104.36	110.56
2	D	1001	NAG	C3-C2-N2	-2.56	104.43	110.56
2	E	1001	NAG	O3-C3-C2	-2.43	104.30	109.11
2	E	1001	NAG	O5-C5-C6	2.29	112.30	107.35
2	B	1001	NAG	C4-C3-C2	2.43	115.00	111.23
2	A	1001	NAG	O4-C4-C3	2.58	116.15	110.34
2	D	1001	NAG	C2-N2-C7	3.18	127.12	123.04
2	D	1001	NAG	C4-C3-C2	3.21	116.22	111.23
2	D	1001	NAG	O5-C5-C6	3.43	114.77	107.35
2	D	1001	NAG	C8-C7-N2	3.66	123.11	116.11
2	A	1001	NAG	C2-N2-C7	5.79	130.48	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1001	NAG	3	0
2	E	1001	NAG	2	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^{th} 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	407/456 (89%)	-0.24	9 (2%)	65	66	12, 22, 45, 57	0
1	B	401/456 (87%)	-0.21	4 (0%)	84	84	10, 23, 46, 56	0
1	D	367/456 (80%)	-0.05	25 (6%)	20	22	12, 22, 56, 67	0
1	E	396/456 (86%)	-0.19	10 (2%)	61	61	12, 24, 42, 59	0
All	All	1571/1824 (86%)	-0.18	48 (3%)	52	53	10, 23, 46, 67	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	444	PHE	5.9
1	E	440	PHE	5.1
1	E	74	ALA	4.1
1	E	76	VAL	4.0
1	D	443	SER	3.8
1	B	166	PRO	3.7
1	D	467	THR	3.6
1	D	300	LYS	3.6
1	A	342	TYR	3.5
1	D	468	SER	3.5
1	D	435	CYS	3.4
1	D	299	TRP	3.2
1	D	380	GLY	3.2
1	B	428	THR	3.2
1	D	457	THR	3.2
1	D	456	LYS	3.1
1	A	420	SER	3.1
1	D	454	ARG	2.9
1	A	241	TYR	2.9
1	A	346	SER	2.8
1	D	166	PRO	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	302	GLY	2.7
1	D	303	ARG	2.7
1	D	446	ALA	2.7
1	E	300	LYS	2.6
1	D	453	LYS	2.5
1	D	442	ASP	2.5
1	A	183	SER	2.4
1	D	458	SER	2.4
1	A	207	ASN	2.4
1	E	75	ASN	2.4
1	B	169	GLN	2.3
1	A	347	GLN	2.3
1	D	445	GLY	2.3
1	B	474	ASP	2.3
1	D	452	CYS	2.2
1	D	465	GLN	2.2
1	E	479	CYS	2.2
1	A	473	ALA	2.2
1	D	471	CYS	2.1
1	E	474	ASP	2.1
1	D	305	LEU	2.1
1	D	183	SER	2.1
1	E	377	ASP	2.1
1	A	477	ASN	2.1
1	D	447	CYS	2.1
1	E	311	THR	2.0
1	E	299	TRP	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, 95^{th} 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
2	NAG	E	1001	14/15	0.89	0.16	2.44	28,32,37,37	0
2	NAG	A	1001	14/15	0.95	0.11	1.02	18,24,28,30	0
3	GOL	D	1472	6/6	0.96	0.10	0.20	20,25,26,26	0
2	NAG	B	1001	14/15	0.87	0.13	0.16	22,27,34,38	0
2	NAG	D	1001	14/15	0.86	0.20	-	35,38,42,43	0

6.5 Other polymers (i)

There are no such residues in this entry.