Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:55 AM GMT

PDB ID	:	3CMM
Title	:	Crystal Structure of the Uba1-Ubiquitin Complex
Authors	:	Lee, I.; Schindelin, H.
Deposited on	:	2008-03-23
Resolution	:	2.70 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

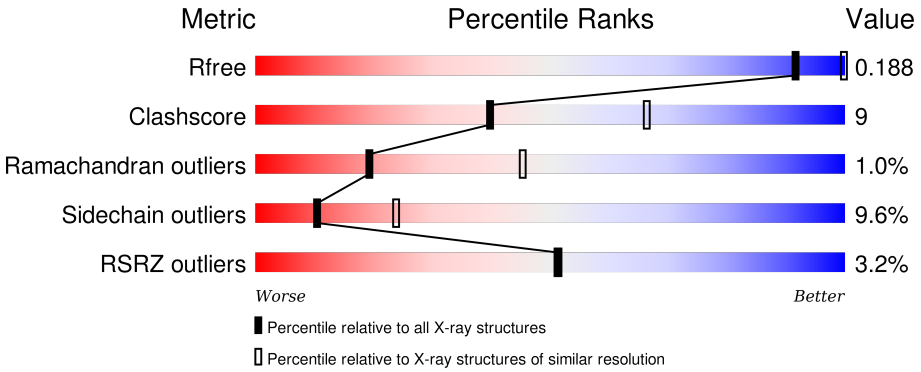
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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	1015	4% 75% 18% 5%
1	C	1015	2% 77% 18%
2	B	76	% 74% 22%
2	D	76	3% 88% 11%

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	PRO	A	5119	-	-	-	X
3	PRO	C	5129	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17241 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.

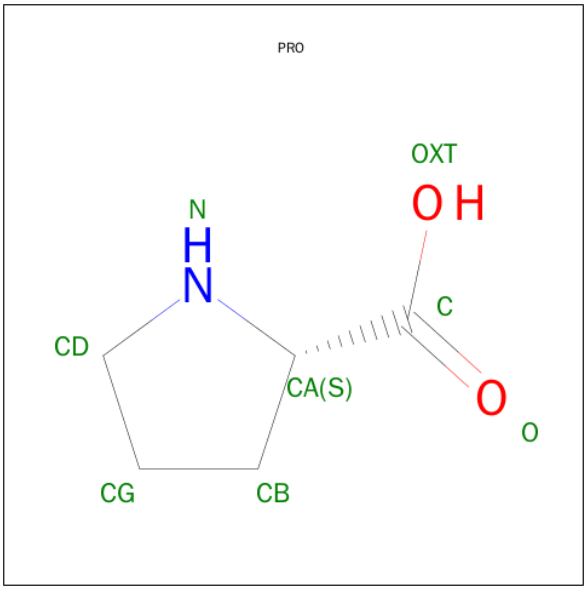
- Molecule 1 is a protein called Ubiquitin-activating enzyme E1 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1001	Total	C	N	O	S	0	0	0
			7911	5045	1306	1537	23			
1	C	1006	Total	C	N	O	S	0	0	0
			7938	5058	1312	1545	23			

- Molecule 2 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	76	Total	C	N	O	S	0	0	0
			601	375	105	120	1			
2	D	76	Total	C	N	O	S	0	0	0
			601	375	105	120	1			

- Molecule 3 is PROLINE (three-letter code: PRO) (formula: $C_5H_9NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			7	5	1	1		
3	C	1	Total	C	N	O	0	0
			7	5	1	1		

- Molecule 4 is water.

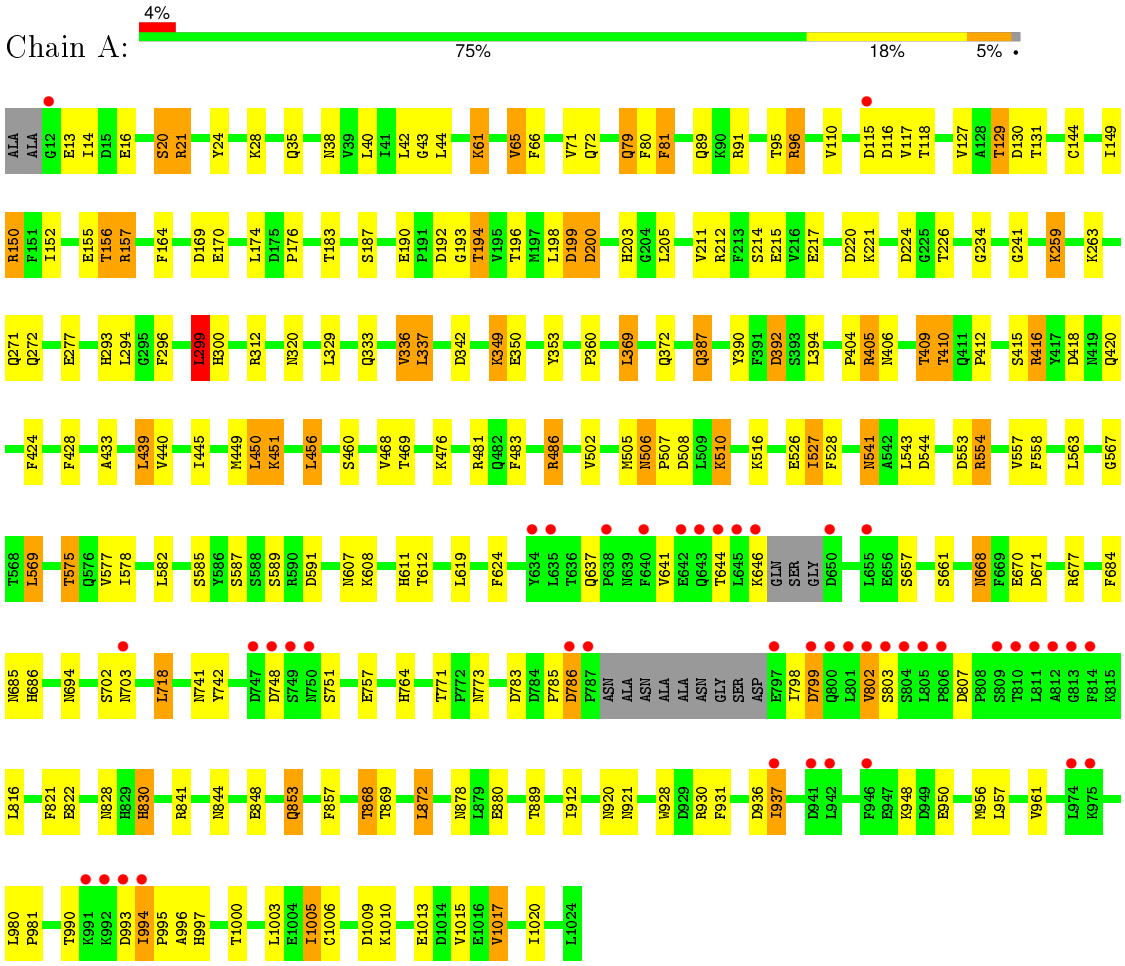
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	79	Total	O	0	0
			79	79		
4	B	4	Total	O	0	0
			4	4		
4	C	87	Total	O	0	0
			87	87		
4	D	6	Total	O	0	0
			6	6		

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.

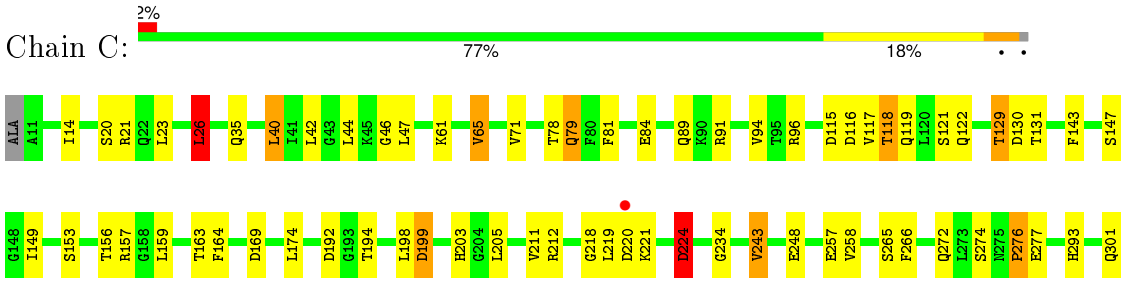
- Molecule 1: Ubiquitin-activating enzyme E1 1

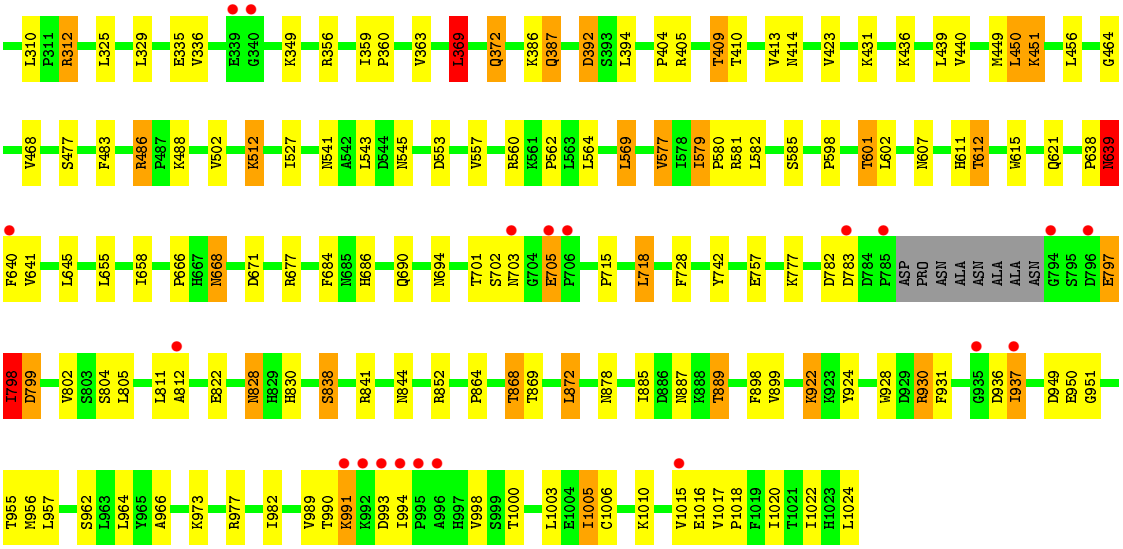
Chain A:



- Molecule 1: Ubiquitin-activating enzyme E1 1

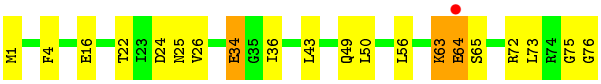
Chain C:





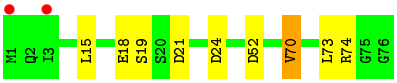
- Molecule 2: Ubiquitin

Chain B:



- Molecule 2: Ubiquitin

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	115.36Å 118.56Å 207.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70 47.54 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.5 (20.00-2.70) 98.5 (47.54-2.70)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.91 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.191 , 0.247 0.193 , 0.188	Depositor DCC
R_{free} test set	3897 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	44.3	Xtriage
Anisotropy	0.248	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 49.1	EDS
Estimated twinning fraction	0.014 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 77601 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	17241	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.34% 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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.57	2/8075 (0.0%)	0.66	2/10928 (0.0%)
1	C	0.55	2/8102 (0.0%)	0.66	6/10964 (0.1%)
2	B	0.98	2/606 (0.3%)	0.69	0/812
2	D	0.48	0/606	0.65	0/812
All	All	0.57	6/17389 (0.0%)	0.66	8/23516 (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	C	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	16	GLU	CD-OE1	15.74	1.43	1.25
2	B	16	GLU	CD-OE2	13.64	1.40	1.25
1	A	637	GLN	CD-OE1	7.75	1.41	1.24
1	C	922	LYS	CD-CE	6.80	1.68	1.51
1	C	922	LYS	CG-CD	6.71	1.75	1.52
1	A	646	LYS	C-O	6.70	1.36	1.23

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	369	LEU	CA-CB-CG	6.90	131.18	115.30
1	A	872	LEU	CA-CB-CG	6.45	130.13	115.30
1	A	299	LEU	CA-CB-CG	6.34	129.89	115.30
1	C	872	LEU	CA-CB-CG	6.22	129.61	115.30
1	C	922	LYS	CB-CG-CD	-5.84	96.42	111.60
1	C	26	LEU	CA-CB-CG	5.73	128.48	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	922	LYS	CD-CE-NZ	-5.10	99.97	111.70
1	C	468	VAL	CB-CA-C	-5.02	101.86	111.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	386	LYS	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	7911	0	7820	146	0
1	C	7938	0	7843	146	0
2	B	601	0	625	15	0
2	D	601	0	625	4	0
3	A	7	0	7	1	0
3	C	7	0	7	1	0
4	A	79	0	0	4	0
4	B	4	0	0	0	0
4	C	87	0	0	13	0
4	D	6	0	0	0	0
All	All	17241	0	16927	299	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (299) 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:922:LYS:CD	1:C:922:LYS:CG	1.75	1.59
1:A:558:PHE:HZ	1:A:1000:THR:HG21	1.11	1.13
1:C:46:GLY:HA3	1:C:78:THR:HG22	1.11	1.07
1:A:558:PHE:CZ	1:A:1000:THR:HG21	1.91	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:GLY:HA3	1:C:78:THR:CG2	1.88	1.03
1:A:469:THR:HG22	1:A:516:LYS:HB2	1.46	0.94
1:C:46:GLY:CA	1:C:78:THR:HG22	1.99	0.92
1:A:1005:ILE:HD12	1:A:1020:ILE:HD11	1.51	0.91
1:C:922:LYS:CD	1:C:922:LYS:CB	2.49	0.91
1:A:203:HIS:HD2	1:A:205:LEU:H	1.21	0.89
1:C:887:ASN:HB3	4:C:5206:HOH:O	1.75	0.86
1:A:372:GLN:OE1	1:A:868:THR:HG21	1.75	0.85
1:C:203:HIS:HD2	1:C:205:LEU:H	1.24	0.84
1:C:272:GLN:NE2	1:C:276:PRO:O	2.13	0.81
1:C:922:LYS:CG	1:C:922:LYS:CE	2.60	0.80
1:A:607:ASN:H	1:A:611:HIS:HD2	1.30	0.79
1:C:607:ASN:H	1:C:611:HIS:HD2	1.31	0.78
1:C:797:GLU:O	1:C:799:ASP:N	2.17	0.78
1:A:42:LEU:O	1:A:129:THR:HB	1.84	0.77
1:C:221:LYS:O	1:C:224:ASP:HB2	1.84	0.77
1:C:852:ARG:HD3	4:C:5201:HOH:O	1.85	0.75
1:C:581:ARG:HD3	4:C:5200:HOH:O	1.85	0.75
1:A:221:LYS:O	1:A:224:ASP:HB2	1.87	0.74
1:C:638:PRO:O	1:C:639:ASN:HB3	1.88	0.74
1:A:44:LEU:HD13	1:A:65:VAL:HG13	1.69	0.74
1:A:445:ILE:HD12	2:B:76:GLY:HA3	1.69	0.73
1:C:192:ASP:OD1	1:C:194:THR:HG22	1.87	0.73
1:A:349:LYS:HD3	1:A:353:TYR:CE1	2.25	0.72
1:A:272:GLN:HE22	1:A:277:GLU:H	1.36	0.72
1:C:116:ASP:OD1	1:C:118:THR:HB	1.90	0.72
1:A:203:HIS:CD2	1:A:205:LEU:H	2.07	0.71
1:C:372:GLN:HG2	1:C:868:THR:CG2	2.20	0.71
1:A:822:GLU:H	1:A:830:HIS:CD2	2.09	0.71
1:C:42:LEU:O	1:C:129:THR:HB	1.89	0.71
1:A:1005:ILE:CD1	1:A:1020:ILE:HD11	2.21	0.71
1:A:822:GLU:H	1:A:830:HIS:HD2	1.36	0.70
1:C:701:THR:HG22	1:C:702:SER:H	1.54	0.70
1:C:822:GLU:H	1:C:830:HIS:HD2	1.38	0.70
1:C:163:THR:HG21	1:C:369:LEU:HD11	1.73	0.70
1:A:203:HIS:HE1	1:A:234:GLY:O	1.75	0.70
1:A:416:ARG:HH11	1:A:416:ARG:HG3	1.57	0.69
1:C:668:ASN:ND2	1:C:671:ASP:H	1.90	0.69
1:A:612:THR:HG22	1:A:841:ARG:HG2	1.76	0.68
1:A:1005:ILE:HD12	1:A:1020:ILE:CD1	2.23	0.68
1:A:404:PRO:O	1:A:409:THR:HG21	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:558:PHE:HZ	1:A:1000:THR:CG2	2.00	0.67
1:C:372:GLN:HG2	1:C:868:THR:HG21	1.78	0.66
2:B:34:GLU:HB3	2:B:36:ILE:HD12	1.75	0.66
1:C:684:PHE:HB3	1:C:718:LEU:HD22	1.77	0.66
1:C:409:THR:HG22	1:C:410:THR:HG23	1.77	0.66
1:A:369:LEU:O	1:A:369:LEU:HD22	1.97	0.65
1:A:333:GLN:HB2	1:A:336:VAL:HG22	1.79	0.64
1:C:962:SER:HB3	4:C:5172:HOH:O	1.97	0.64
1:C:483:PHE:O	1:C:486:ARG:NH2	2.31	0.64
1:C:169:ASP:O	1:C:265:SER:HB3	1.99	0.63
1:A:449:MET:CE	1:A:878:ASN:HD21	2.13	0.62
1:C:404:PRO:O	1:C:409:THR:HG21	2.00	0.61
1:C:203:HIS:CD2	1:C:205:LEU:H	2.11	0.61
1:C:164:PHE:HE1	1:C:272:GLN:HG2	1.65	0.61
1:A:506:ASN:C	1:A:506:ASN:HD22	2.02	0.61
1:A:449:MET:HE3	1:A:878:ASN:HD21	1.66	0.60
1:A:449:MET:HE1	1:A:878:ASN:ND2	2.17	0.60
1:C:71:VAL:HG22	1:C:91:ARG:HG2	1.83	0.60
1:A:930:ARG:HD3	4:A:5182:HOH:O	2.01	0.60
1:C:372:GLN:OE1	1:C:868:THR:HG21	2.03	0.59
1:A:203:HIS:HD2	1:A:205:LEU:N	1.97	0.59
1:C:405:ARG:HD2	1:C:423:VAL:O	2.02	0.59
1:A:296:PHE:HA	1:A:299:LEU:CD2	2.32	0.59
1:A:80:PHE:O	1:A:505:MET:HG2	2.03	0.59
1:A:506:ASN:ND2	1:A:508:ASP:H	2.00	0.58
1:C:569:LEU:HB3	2:D:73:LEU:HD22	1.85	0.58
1:C:615:TRP:CE3	1:C:841:ARG:HD2	2.38	0.58
1:A:469:THR:HG21	1:A:528:PHE:HZ	1.68	0.58
1:C:312:ARG:HA	1:C:356:ARG:HE	1.68	0.58
1:A:990:THR:HB	1:A:993:ASP:HB2	1.86	0.58
1:C:581:ARG:HG2	4:C:5200:HOH:O	2.03	0.58
1:C:868:THR:HG22	1:C:869:THR:H	1.68	0.57
1:C:560:ARG:HD2	1:C:930:ARG:CZ	2.33	0.57
1:C:79:GLN:C	1:C:79:GLN:HE21	2.08	0.57
1:A:657:SER:O	1:A:661:SER:HB2	2.03	0.57
2:D:18:GLU:O	2:D:21:ASP:HB2	2.04	0.57
1:C:44:LEU:HD22	1:C:65:VAL:HG13	1.85	0.57
1:A:575:THR:HG21	4:A:5154:HOH:O	2.05	0.57
1:A:912:ILE:HD11	2:B:49:GLN:OE1	2.05	0.56
1:C:312:ARG:HB2	4:C:5152:HOH:O	2.04	0.56
1:C:956:MET:HB2	1:C:1006:CYS:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:PHE:O	1:C:147:SER:HB2	2.05	0.56
1:C:121:SER:HA	1:C:149:ILE:HD11	1.88	0.56
1:C:868:THR:CG2	1:C:869:THR:N	2.70	0.55
1:C:203:HIS:HE1	1:C:234:GLY:O	1.90	0.55
1:C:701:THR:HG22	1:C:702:SER:N	2.19	0.55
1:A:449:MET:CE	1:A:878:ASN:ND2	2.69	0.55
1:C:989:VAL:C	1:C:991:LYS:H	2.10	0.55
1:A:451:LYS:HG3	1:A:483:PHE:HZ	1.72	0.54
1:C:638:PRO:O	1:C:639:ASN:CB	2.54	0.54
1:A:612:THR:CG2	1:A:841:ARG:HG2	2.36	0.54
1:C:598:PRO:HB2	1:C:601:THR:HG23	1.90	0.54
1:C:553:ASP:OD2	1:C:585:SER:HB2	2.08	0.54
1:A:176:PRO:HD2	1:A:259:LYS:HG2	1.89	0.54
1:C:828:ASN:HD22	1:C:828:ASN:C	2.10	0.54
1:C:272:GLN:NE2	1:C:387:GLN:CB	2.72	0.53
1:A:156:THR:C	1:A:157:ARG:HG2	2.28	0.53
1:A:557:VAL:HA	1:A:928:TRP:CZ3	2.44	0.53
1:A:931:PHE:HE1	1:A:1017:VAL:HG13	1.72	0.53
1:A:440:VAL:HG12	1:A:543:LEU:HD21	1.90	0.53
1:A:203:HIS:CE1	1:A:234:GLY:O	2.60	0.53
1:C:413:VAL:HG12	1:C:414:ASN:H	1.74	0.53
2:B:26:VAL:HG21	2:B:56:LEU:HD21	1.90	0.53
1:A:544:ASP:HA	2:B:75:GLY:HA2	1.91	0.53
1:A:624:PHE:HA	1:A:741:ASN:HD21	1.74	0.53
1:C:822:GLU:H	1:C:830:HIS:CD2	2.24	0.52
1:C:129:THR:HG23	1:C:130:ASP:H	1.73	0.52
1:A:79:GLN:NE2	1:A:81:PHE:H	2.08	0.52
1:C:640:PHE:HE2	1:C:658:ILE:HD11	1.75	0.52
1:C:957:LEU:HD21	1:C:1003:LEU:HD13	1.91	0.52
2:B:22:THR:OG1	2:B:25:ASN:HB2	2.10	0.52
1:A:155:GLU:OE1	1:A:300:HIS:HE1	1.92	0.52
1:C:129:THR:HG23	1:C:130:ASP:N	2.25	0.52
1:A:127:VAL:HA	1:A:152:ILE:O	2.10	0.52
1:A:320:ASN:OD1	3:A:5119:PRO:HB2	2.09	0.51
1:C:44:LEU:HD22	1:C:65:VAL:CG1	2.40	0.51
1:A:71:VAL:HG22	1:A:91:ARG:HG2	1.92	0.51
1:C:450:LEU:HB3	1:C:502:VAL:HG21	1.92	0.51
1:C:668:ASN:HD22	1:C:668:ASN:C	2.14	0.51
1:C:440:VAL:HG12	1:C:543:LEU:HD21	1.92	0.51
1:A:469:THR:HG21	1:A:528:PHE:CZ	2.45	0.51
1:A:406:ASN:O	1:A:410:THR:HB	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:203:HIS:HD2	1:C:205:LEU:N	2.01	0.51
1:A:554:ARG:NH1	4:A:5146:HOH:O	2.43	0.51
1:A:798:ILE:O	1:A:802:VAL:HG23	2.10	0.50
1:A:912:ILE:HD11	2:B:49:GLN:CD	2.31	0.50
2:B:43:LEU:HB3	2:B:50:LEU:HD12	1.93	0.50
1:C:956:MET:O	1:C:1005:ILE:HG13	2.12	0.50
1:C:924:TYR:CD1	1:C:1018:PRO:HG3	2.46	0.50
1:A:433:ALA:O	1:A:460:SER:O	2.29	0.50
1:A:607:ASN:OD1	1:A:608:LYS:HE3	2.11	0.50
1:A:558:PHE:O	1:A:930:ARG:NH1	2.43	0.49
1:A:224:ASP:HB3	1:A:226:THR:H	1.77	0.49
1:C:828:ASN:ND2	1:C:830:HIS:H	2.10	0.49
1:A:742:TYR:CE1	1:A:816:LEU:HD21	2.46	0.49
1:C:219:LEU:HD22	1:C:243:VAL:HG13	1.93	0.49
1:C:129:THR:HG21	4:C:5132:HOH:O	2.11	0.49
1:A:96:ARG:HG3	1:A:110:VAL:HG23	1.95	0.49
1:C:703:ASN:ND2	1:C:705:GLU:HB2	2.28	0.49
1:A:199:ASP:O	1:A:200:ASP:HB3	2.13	0.49
2:D:24:ASP:OD2	2:D:52:ASP:O	2.31	0.49
1:C:129:THR:CG2	1:C:130:ASP:N	2.75	0.49
1:C:23:LEU:O	1:C:26:LEU:O	2.31	0.49
1:C:889:THR:O	1:C:889:THR:CG2	2.60	0.49
1:A:21:ARG:HG3	1:A:481:ARG:NH1	2.27	0.49
1:A:350:GLU:OE1	1:A:405:ARG:NH2	2.45	0.49
1:A:44:LEU:CD1	1:A:65:VAL:HG13	2.42	0.48
1:C:349:LYS:HD3	3:C:5129:PRO:HG3	1.95	0.48
1:C:569:LEU:HD13	1:C:864:PRO:HD2	1.94	0.48
1:A:79:GLN:HE21	1:A:79:GLN:C	2.16	0.48
1:C:798:ILE:O	1:C:802:VAL:HG23	2.13	0.48
1:C:868:THR:CG2	1:C:869:THR:H	2.26	0.48
1:A:506:ASN:C	1:A:506:ASN:ND2	2.66	0.48
1:C:557:VAL:HA	1:C:928:TRP:CZ3	2.49	0.48
1:C:40:LEU:HD13	1:C:42:LEU:HD21	1.96	0.48
1:A:193:GLY:HA3	1:A:241:GLY:O	2.14	0.47
1:C:405:ARG:HA	1:C:409:THR:HG21	1.96	0.47
1:A:214:SER:HB3	1:A:215:GLU:HG3	1.96	0.47
1:A:961:VAL:HG13	1:A:961:VAL:O	2.15	0.47
1:A:412:PRO:HA	1:A:418:ASP:HB2	1.96	0.47
1:C:405:ARG:CD	1:C:423:VAL:O	2.62	0.47
1:C:218:GLY:HA3	1:C:248:GLU:O	2.15	0.47
1:C:922:LYS:CD	1:C:922:LYS:HB2	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:615:TRP:CD2	1:C:841:ARG:HD2	2.50	0.47
1:A:483:PHE:O	1:A:486:ARG:NH2	2.48	0.47
1:C:78:THR:HG21	1:C:363:VAL:HG21	1.97	0.46
1:A:868:THR:CG2	1:A:869:THR:N	2.79	0.46
1:C:78:THR:CG2	1:C:363:VAL:HG11	2.45	0.46
1:C:372:GLN:CG	1:C:868:THR:HG21	2.45	0.46
1:A:841:ARG:O	1:A:844:ASN:HB2	2.16	0.46
1:A:957:LEU:HD11	1:A:1003:LEU:HD13	1.96	0.46
1:C:889:THR:HG22	4:C:5137:HOH:O	2.15	0.46
1:A:424:PHE:HB3	1:A:428:PHE:CD2	2.50	0.46
1:C:640:PHE:CE2	1:C:658:ILE:HD11	2.50	0.46
1:A:591:ASP:OD2	2:B:72:ARG:HB2	2.16	0.46
1:C:564:LEU:HD23	1:C:577:VAL:HG12	1.98	0.46
1:C:272:GLN:NE2	1:C:387:GLN:HB3	2.30	0.46
1:A:553:ASP:OD2	1:A:585:SER:HB2	2.16	0.46
1:A:42:LEU:HD23	1:A:66:PHE:HB3	1.98	0.46
1:A:821:PHE:HA	1:A:830:HIS:CD2	2.50	0.46
1:C:464:GLY:O	1:C:512:LYS:NZ	2.46	0.45
1:A:190:GLU:HB2	1:A:194:THR:HG23	1.98	0.45
1:C:955:THR:O	1:C:966:ALA:HA	2.16	0.45
1:A:129:THR:HG23	1:A:130:ASP:H	1.81	0.45
1:A:192:ASP:OD1	1:A:194:THR:HG22	2.16	0.45
1:A:684:PHE:HB3	1:A:718:LEU:HD22	1.98	0.45
1:A:450:LEU:HB3	1:A:502:VAL:HG21	1.98	0.45
1:A:369:LEU:C	1:A:369:LEU:HD22	2.37	0.45
1:A:507:PRO:O	1:A:510:LYS:HG3	2.16	0.45
1:C:153:SER:HB3	1:C:164:PHE:HB3	1.99	0.45
1:A:868:THR:HG22	1:A:869:THR:N	2.31	0.45
1:A:349:LYS:HD3	1:A:353:TYR:CZ	2.52	0.45
1:A:668:ASN:C	1:A:668:ASN:HD22	2.19	0.45
1:A:569:LEU:HB3	2:B:73:LEU:HD22	1.99	0.45
1:C:937:ILE:HG22	1:C:982:ILE:HD11	1.98	0.45
1:C:973:LYS:O	1:C:977:ARG:HG3	2.17	0.45
1:C:449:MET:HE3	1:C:878:ASN:HD21	1.83	0.44
2:B:1:MET:HB2	2:B:63:LYS:HB2	1.98	0.44
1:C:655:LEU:HD22	1:C:805:LEU:HD11	1.98	0.44
1:C:715:PRO:HA	1:C:844:ASN:O	2.18	0.44
1:A:420:GLN:HE22	1:A:456:LEU:HA	1.83	0.44
1:C:936:ASP:HB3	1:C:1024:LEU:HD23	1.99	0.44
1:C:372:GLN:HG2	1:C:868:THR:HG23	1.97	0.44
1:C:257:GLU:HG2	1:C:258:VAL:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:607:ASN:H	1:A:611:HIS:CD2	2.20	0.44
1:A:544:ASP:HB2	2:B:75:GLY:HA2	2.00	0.44
1:C:198:LEU:O	1:C:199:ASP:C	2.56	0.44
1:C:79:GLN:NE2	1:C:81:PHE:H	2.16	0.43
1:A:38:ASN:HD21	1:A:61:LYS:HG2	1.83	0.43
1:C:96:ARG:NH2	4:C:5190:HOH:O	2.50	0.43
1:A:558:PHE:CZ	1:A:1000:THR:CG2	2.81	0.43
1:A:961:VAL:CG1	1:A:961:VAL:O	2.66	0.43
1:C:541:ASN:HB3	4:C:5216:HOH:O	2.17	0.43
2:B:4:PHE:HE1	2:B:64:GLU:HG3	1.84	0.43
1:C:159:LEU:O	1:C:392:ASP:HA	2.19	0.43
1:C:431:LYS:HD3	1:C:885:ILE:HG22	1.99	0.43
1:C:335:GLU:CD	1:C:335:GLU:H	2.22	0.43
1:A:587:SER:C	1:A:589:SER:H	2.21	0.43
1:C:569:LEU:CD1	1:C:864:PRO:HD2	2.49	0.43
1:A:702:SER:O	1:A:703:ASN:HB2	2.19	0.43
1:A:272:GLN:NE2	1:A:277:GLU:H	2.11	0.43
1:C:666:PRO:HD2	1:C:742:TYR:CE1	2.54	0.43
1:C:581:ARG:CD	4:C:5200:HOH:O	2.56	0.43
1:C:451:LYS:HG3	1:C:483:PHE:HZ	1.83	0.43
1:A:117:VAL:HG21	1:C:728:PHE:CE2	2.53	0.43
1:A:79:GLN:HE22	1:A:81:PHE:HB2	1.83	0.43
1:C:690:GLN:HE21	1:C:694:ASN:HD21	1.67	0.43
1:A:129:THR:CG2	1:A:130:ASP:N	2.81	0.42
1:C:35:GLN:O	1:C:61:LYS:HB2	2.20	0.42
1:A:129:THR:HG23	1:A:130:ASP:N	2.35	0.42
1:C:116:ASP:HB3	1:C:119:GLN:HE21	1.84	0.42
1:A:296:PHE:HA	1:A:299:LEU:HD22	2.00	0.42
1:A:742:TYR:CD1	1:A:816:LEU:HD21	2.54	0.42
1:C:266:PHE:N	1:C:266:PHE:CD1	2.87	0.42
1:C:931:PHE:CE2	1:C:950:GLU:HG2	2.54	0.42
1:C:272:GLN:NE2	1:C:387:GLN:HB2	2.35	0.42
1:A:293:HIS:HA	1:A:390:TYR:CZ	2.54	0.42
1:C:79:GLN:HE22	1:C:81:PHE:HB2	1.84	0.42
1:A:199:ASP:O	1:A:200:ASP:CB	2.67	0.42
1:C:276:PRO:O	1:C:277:GLU:HB3	2.20	0.42
1:A:43:GLY:HA3	1:A:131:THR:OG1	2.19	0.42
1:A:980:LEU:HA	1:A:981:PRO:HD3	1.94	0.42
1:A:16:GLU:O	1:A:20:SER:HB2	2.20	0.42
1:C:579:ILE:HA	1:C:580:PRO:HD3	1.86	0.42
1:A:360:PRO:HG2	1:A:456:LEU:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:619:LEU:HD12	1:A:619:LEU:HA	1.88	0.42
1:C:951:GLY:HA3	1:C:1010:LYS:HE3	2.02	0.42
1:A:994:ILE:HA	1:A:995:PRO:HD2	1.94	0.42
1:C:272:GLN:CD	1:C:276:PRO:O	2.57	0.42
1:C:219:LEU:HD22	1:C:243:VAL:CG1	2.50	0.42
1:A:526:GLU:HB2	1:A:997:HIS:CE1	2.55	0.42
1:A:170:GLU:HB3	1:A:263:LYS:HE2	2.01	0.42
1:A:799:ASP:OD1	1:A:799:ASP:N	2.53	0.42
1:C:301:GLN:HE21	1:C:325:LEU:HD22	1.85	0.42
1:A:44:LEU:HD11	1:A:65:VAL:HG22	2.01	0.41
1:A:456:LEU:HD12	1:A:456:LEU:HA	1.93	0.41
1:C:47:LEU:HA	1:C:363:VAL:HG13	2.01	0.41
1:A:187:SER:HB2	1:A:198:LEU:HA	2.01	0.41
1:A:527:ILE:HD11	1:A:528:PHE:CZ	2.56	0.41
1:A:294:LEU:HD22	1:A:337:LEU:HD13	2.02	0.41
1:A:541:ASN:HB3	4:A:5152:HOH:O	2.21	0.41
1:A:544:ASP:CA	2:B:75:GLY:HA2	2.51	0.41
1:A:668:ASN:ND2	1:A:671:ASP:H	2.18	0.41
1:C:562:PRO:HA	1:C:580:PRO:HD3	2.02	0.41
1:C:641:VAL:O	1:C:645:LEU:HG	2.20	0.41
1:A:144:CYS:HB3	1:A:149:ILE:O	2.20	0.41
1:C:192:ASP:OD1	1:C:192:ASP:C	2.59	0.41
1:A:392:ASP:C	1:A:392:ASP:OD2	2.59	0.41
1:A:785:PRO:HA	1:A:786:ASP:HA	1.89	0.41
1:A:44:LEU:HD23	1:A:95:THR:HG21	2.02	0.41
1:A:506:ASN:HA	1:A:507:PRO:HD2	1.77	0.41
1:A:853:GLN:H	1:A:853:GLN:NE2	2.19	0.41
1:C:129:THR:CG2	4:C:5132:HOH:O	2.67	0.41
1:C:841:ARG:O	1:C:844:ASN:HB2	2.21	0.41
1:C:898:PHE:CD2	2:D:70:VAL:HG13	2.56	0.41
1:A:956:MET:HB3	1:A:1006:CYS:HB2	2.02	0.41
1:C:1020:ILE:HG22	1:C:1022:ILE:HD12	2.03	0.41
1:C:359:ILE:HA	1:C:360:PRO:HD3	1.96	0.41
1:A:563:LEU:HD23	1:A:578:ILE:HD13	2.01	0.41
1:C:1015:VAL:HG12	1:C:1016:GLU:O	2.21	0.41
1:C:957:LEU:CD2	1:C:964:LEU:HD12	2.51	0.40
1:C:276:PRO:HG3	1:C:293:HIS:NE2	2.35	0.40
1:A:567:GLY:HA3	2:B:73:LEU:O	2.21	0.40
1:A:150:ARG:H	1:A:150:ARG:HD2	1.85	0.40
1:A:439:LEU:HB3	1:A:468:VAL:HG13	2.03	0.40
1:A:164:PHE:HA	1:A:387:GLN:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:272:GLN:HE21	1:C:387:GLN:CB	2.33	0.40
1:A:506:ASN:HD22	1:A:508:ASP:H	1.68	0.40
1:C:310:LEU:O	1:C:356:ARG:NH2	2.54	0.40
1:A:668:ASN:ND2	1:A:670:GLU:HB3	2.37	0.40
1:C:156:THR:CG2	4:C:5134:HOH:O	2.70	0.40
1:A:920:ASN:OD1	1:A:1009:ASP:HB2	2.21	0.40
1:C:612:THR:HG23	1:C:838:SER:OG	2.21	0.40
1:A:24:TYR:CZ	1:A:857:PHE:HB2	2.55	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	995/1015 (98%)	926 (93%)	60 (6%)	9 (1%)	21	49
1	C	1002/1015 (99%)	935 (93%)	55 (6%)	12 (1%)	16	39
2	B	74/76 (97%)	72 (97%)	2 (3%)	0	100	100
2	D	74/76 (97%)	74 (100%)	0	0	100	100
All	All	2145/2182 (98%)	2007 (94%)	117 (6%)	21 (1%)	19	45

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	387	GLN
1	A	937	ILE
1	C	224	ASP
1	C	387	GLN
1	C	639	ASN
1	C	798	ILE
1	A	20	SER

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Mol	Chain	Res	Type
1	A	996	ALA
1	A	199	ASP
1	A	200	ASP
1	A	807	ASP
1	C	20	SER
1	C	199	ASP
1	C	797	GLU
1	C	812	ALA
1	C	994	ILE
1	C	991	LYS
1	A	14	ILE
1	C	990	THR
1	C	276	PRO
1	A	802	VAL

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	885/892 (99%)	788 (89%)	97 (11%)	8 18
1	C	887/892 (99%)	809 (91%)	78 (9%)	12 28
2	B	69/69 (100%)	64 (93%)	5 (7%)	18 41
2	D	69/69 (100%)	65 (94%)	4 (6%)	25 52
All	All	1910/1922 (99%)	1726 (90%)	184 (10%)	10 24

All (184) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	GLU
1	A	21	ARG
1	A	28	LYS
1	A	35	GLN
1	A	40	LEU
1	A	61	LYS
1	A	65	VAL

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Mol	Chain	Res	Type
1	A	72	GLN
1	A	79	GLN
1	A	81	PHE
1	A	89	GLN
1	A	96	ARG
1	A	115	ASP
1	A	116	ASP
1	A	118	THR
1	A	129	THR
1	A	150	ARG
1	A	156	THR
1	A	157	ARG
1	A	169	ASP
1	A	174	LEU
1	A	183	THR
1	A	194	THR
1	A	196	THR
1	A	211	VAL
1	A	212	ARG
1	A	217	GLU
1	A	220	ASP
1	A	259	LYS
1	A	271	GLN
1	A	299	LEU
1	A	312	ARG
1	A	329	LEU
1	A	336	VAL
1	A	337	LEU
1	A	342	ASP
1	A	349	LYS
1	A	369	LEU
1	A	392	ASP
1	A	394	LEU
1	A	405	ARG
1	A	409	THR
1	A	410	THR
1	A	415	SER
1	A	416	ARG
1	A	439	LEU
1	A	450	LEU
1	A	451	LYS
1	A	456	LEU

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Mol	Chain	Res	Type
1	A	476	LYS
1	A	486	ARG
1	A	506	ASN
1	A	510	LYS
1	A	527	ILE
1	A	541	ASN
1	A	554	ARG
1	A	569	LEU
1	A	575	THR
1	A	577	VAL
1	A	582	LEU
1	A	641	VAL
1	A	644	THR
1	A	668	ASN
1	A	677	ARG
1	A	685	ASN
1	A	686	HIS
1	A	694	ASN
1	A	718	LEU
1	A	748	ASP
1	A	751	SER
1	A	757	GLU
1	A	764	HIS
1	A	771	THR
1	A	773	ASN
1	A	783	ASP
1	A	786	ASP
1	A	799	ASP
1	A	803	SER
1	A	828	ASN
1	A	830	HIS
1	A	848	GLU
1	A	853	GLN
1	A	868	THR
1	A	872	LEU
1	A	880	GLU
1	A	889	THR
1	A	921	ASN
1	A	936	ASP
1	A	937	ILE
1	A	948	LYS
1	A	950	GLU

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Mol	Chain	Res	Type
1	A	994	ILE
1	A	1005	ILE
1	A	1010	LYS
1	A	1013	GLU
1	A	1015	VAL
1	A	1017	VAL
1	C	14	ILE
1	C	21	ARG
1	C	26	LEU
1	C	40	LEU
1	C	65	VAL
1	C	79	GLN
1	C	84	GLU
1	C	89	GLN
1	C	94	VAL
1	C	115	ASP
1	C	117	VAL
1	C	118	THR
1	C	122	GLN
1	C	129	THR
1	C	131	THR
1	C	157	ARG
1	C	174	LEU
1	C	211	VAL
1	C	212	ARG
1	C	220	ASP
1	C	224	ASP
1	C	243	VAL
1	C	274	SER
1	C	312	ARG
1	C	329	LEU
1	C	336	VAL
1	C	369	LEU
1	C	372	GLN
1	C	392	ASP
1	C	394	LEU
1	C	409	THR
1	C	436	LYS
1	C	439	LEU
1	C	450	LEU
1	C	451	LYS
1	C	456	LEU

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Mol	Chain	Res	Type
1	C	477	SER
1	C	486	ARG
1	C	488	LYS
1	C	512	LYS
1	C	527	ILE
1	C	545	ASN
1	C	569	LEU
1	C	577	VAL
1	C	579	ILE
1	C	582	LEU
1	C	601	THR
1	C	602	LEU
1	C	612	THR
1	C	621	GLN
1	C	639	ASN
1	C	668	ASN
1	C	677	ARG
1	C	686	HIS
1	C	705	GLU
1	C	718	LEU
1	C	757	GLU
1	C	777	LYS
1	C	782	ASP
1	C	783	ASP
1	C	798	ILE
1	C	799	ASP
1	C	804	SER
1	C	811	LEU
1	C	828	ASN
1	C	838	SER
1	C	868	THR
1	C	872	LEU
1	C	889	THR
1	C	899	VAL
1	C	930	ARG
1	C	937	ILE
1	C	949	ASP
1	C	993	ASP
1	C	998	VAL
1	C	1000	THR
1	C	1005	ILE
1	C	1017	VAL

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Mol	Chain	Res	Type
2	B	24	ASP
2	B	34	GLU
2	B	63	LYS
2	B	64	GLU
2	B	65	SER
2	D	15	LEU
2	D	19	SER
2	D	70	VAL
2	D	74	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	79	GLN
1	A	203	HIS
1	A	272	GLN
1	A	300	HIS
1	A	419	ASN
1	A	420	GLN
1	A	429	GLN
1	A	506	ASN
1	A	541	ASN
1	A	611	HIS
1	A	668	ASN
1	A	685	ASN
1	A	725	ASN
1	A	741	ASN
1	A	773	ASN
1	A	828	ASN
1	A	830	HIS
1	A	853	GLN
1	A	878	ASN
1	A	979	ASN
1	A	997	HIS
1	C	79	GLN
1	C	119	GLN
1	C	201	ASN
1	C	203	HIS
1	C	272	GLN
1	C	541	ASN
1	C	611	HIS

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Mol	Chain	Res	Type
1	C	621	GLN
1	C	639	ASN
1	C	668	ASN
1	C	685	ASN
1	C	694	ASN
1	C	828	ASN
1	C	830	HIS
1	C	853	GLN
2	B	40	GLN
2	B	49	GLN
2	B	62	GLN
2	D	40	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

2 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	$\#\|Z\| > 2$
3	PRO	A	5119	-	6,7,8	0.70	0	7,8,10	1.38	0
3	PRO	C	5129	-	6,7,8	0.48	0	7,8,10	1.39	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	PRO	A	5119	-	-	0/0/9/11	0/1/1/1
3	PRO	C	5129	-	-	0/0/9/11	0/1/1/1

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	5119	PRO	1	0
3	C	5129	PRO	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^{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	1001/1015 (98%)	0.22	45 (4%) 37 36	29, 38, 46, 56	0
1	C	1006/1015 (99%)	0.18	21 (2%) 67 68	29, 37, 46, 61	0
2	B	76/76 (100%)	0.08	1 (1%) 79 79	31, 38, 41, 42	0
2	D	76/76 (100%)	0.50	2 (2%) 59 59	31, 38, 41, 43	0
All	All	2159/2182 (98%)	0.21	69 (3%) 51 51	29, 38, 46, 61	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	655	LEU	5.2
1	A	991	LYS	5.1
1	A	644	THR	5.0
1	A	801	LEU	4.7
1	A	975	LYS	4.6
1	A	803	SER	4.3
1	A	813	GLY	4.0
1	A	646	LYS	4.0
1	C	991	LYS	3.8
1	C	794	GLY	3.6
1	A	809	SER	3.6
1	A	797	GLU	3.6
1	A	937	ILE	3.5
1	A	811	LEU	3.5
1	A	749	SER	3.5
1	C	995	PRO	3.5
1	A	642	GLU	3.4
1	A	810	THR	3.4
1	A	635	LEU	3.4
1	A	638	PRO	3.4
1	A	115	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	993	ASP	3.3
1	A	992	LYS	3.2
1	C	812	ALA	3.2
1	A	806	PRO	3.2
1	C	339	GLU	3.2
1	A	643	GLN	3.2
1	C	937	ILE	3.1
1	C	785	PRO	3.1
1	A	645	LEU	3.1
1	A	747	ASP	3.1
1	C	992	LYS	2.9
1	C	994	ILE	2.8
2	D	1	MET	2.8
1	A	786	ASP	2.7
1	A	799	ASP	2.7
1	C	796	ASP	2.7
1	A	812	ALA	2.7
1	A	787	PRO	2.7
1	A	703	ASN	2.6
1	A	640	PHE	2.6
1	C	783	ASP	2.6
1	A	12	GLY	2.5
1	A	802	VAL	2.5
2	D	3	ILE	2.5
1	A	800	GLN	2.5
1	C	996	ALA	2.4
1	A	941	ASP	2.4
1	A	814	PHE	2.3
1	A	650	ASP	2.3
1	A	974	LEU	2.3
1	A	634	TYR	2.3
1	C	340	GLY	2.3
1	C	220	ASP	2.2
1	C	706	PRO	2.2
2	B	64	GLU	2.2
1	C	993	ASP	2.2
1	A	946	PHE	2.2
1	A	994	ILE	2.2
1	A	805	LEU	2.2
1	A	942	LEU	2.1
1	C	705	GLU	2.1
1	C	1015	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	750	ASN	2.1
1	C	703	ASN	2.1
1	A	804	SER	2.1
1	C	640	PHE	2.1
1	C	935	GLY	2.1
1	A	748	ASP	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
3	PRO	C	5129	7/8	0.91	0.38	11.26	61,62,62,62	0
3	PRO	A	5119	7/8	0.83	0.25	7.86	61,62,62,62	0

6.5 Other polymers (i)

There are no such residues in this entry.