Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 12:31 PM BST

PDB ID	:	3WU6
Title	:	Oxidized E.coli Lon Proteolytic domain
Authors	:	Nishii, W.; Kukimoto-Niino, M.; Terada, T.; Shirouzu, M.; Muramatsu, T.; Yokoyama, S.
Deposited on	:	2014-04-22
Resolution	:	1.80 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

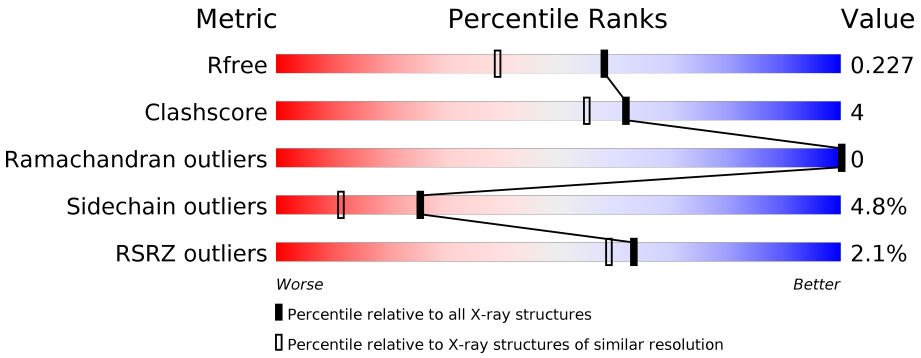
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 1.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	200	3% 82% 10% • 8%
1	B	200	3% 81% 10% • 10%
1	C	200	2% 77% 13% • 9%
1	D	200	2% 80% 11% • 9%
1	E	200	3% 84% 15% ••
1	F	200	83% 6% • 10%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8625 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.

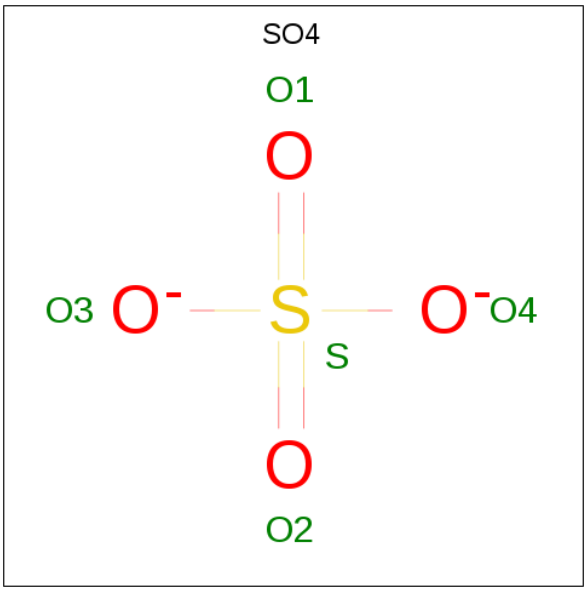
- Molecule 1 is a protein called Lon protease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	185	Total	C	N	O	S	0	2	0
			1393	876	243	266	8			
1	B	181	Total	C	N	O	S	0	2	0
			1360	857	238	257	8			
1	C	182	Total	C	N	O	S	0	1	0
			1365	861	238	259	7			
1	D	182	Total	C	N	O	S	0	0	0
			1360	857	238	259	6			
1	E	198	Total	C	N	O	S	0	0	0
			1476	923	261	285	7			
1	F	180	Total	C	N	O	S	0	0	0
			1344	847	236	255	6			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	679	ALA	SER	ENGINEERED MUTATION	UNP C9QQ79
B	679	ALA	SER	ENGINEERED MUTATION	UNP C9QQ79
C	679	ALA	SER	ENGINEERED MUTATION	UNP C9QQ79
D	679	ALA	SER	ENGINEERED MUTATION	UNP C9QQ79
E	679	ALA	SER	ENGINEERED MUTATION	UNP C9QQ79
F	679	ALA	SER	ENGINEERED MUTATION	UNP C9QQ79

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0

- Molecule 3 is water.

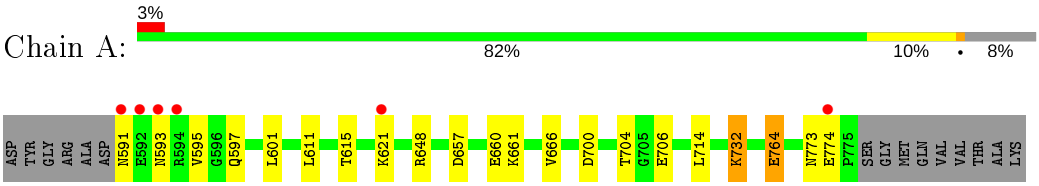
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	57	Total O 57 57	0	0
3	B	53	Total O 53 53	0	0
3	C	54	Total O 54 54	0	0
3	D	37	Total O 37 37	0	0
3	E	49	Total O 49 49	0	0
3	F	52	Total O 52 52	0	0

3 Residue-property plots (i)

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

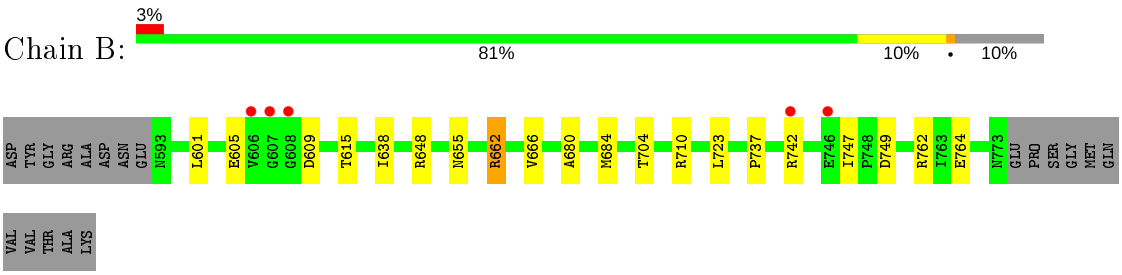
- Molecule 1: Lon protease

Chain A:



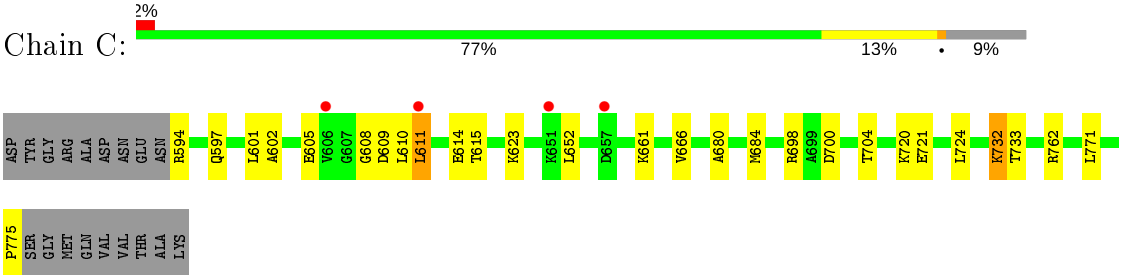
- Molecule 1: Lon protease

Chain B:



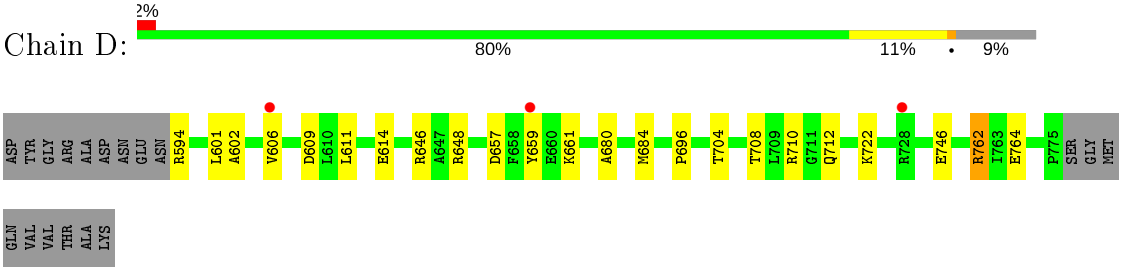
- Molecule 1: Lon protease

Chain C:



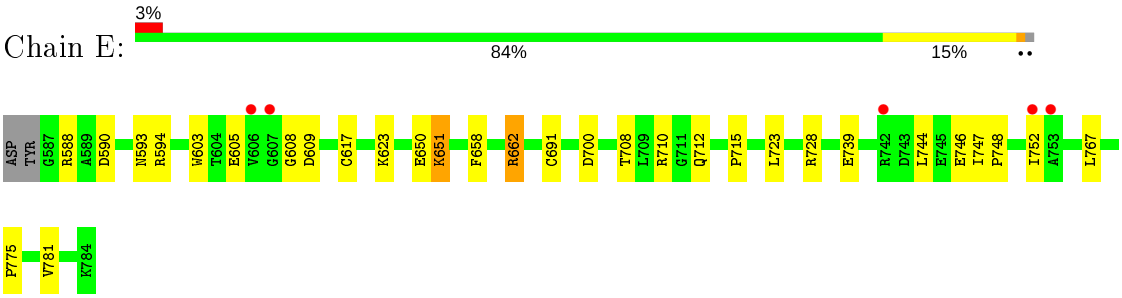
- Molecule 1: Lon protease

Chain D:



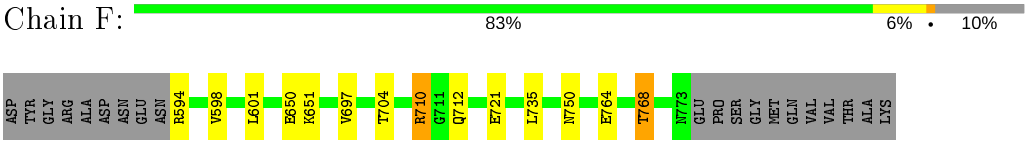
- Molecule 1: Lon protease

Chain E:



• Molecule 1: Lon protease

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	86.44Å 86.44Å 124.94Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	32.11 – 1.80 32.11 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (32.11-1.80) 93.0 (32.11-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	1.61 (at 1.80Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.1_1168)	Depositor
R, R_{free}	0.189 , 0.226 0.189 , 0.227	Depositor DCC
R_{free} test set	4818 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	24.2	Xtriage
Anisotropy	0.671	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 29.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.093 for -h,-k,l 0.057 for h,-h-k,-l 0.043 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	8625	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.76% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.34	0/1419	0.54	0/1927
1	B	0.32	0/1385	0.53	0/1880
1	C	0.33	0/1388	0.53	0/1885
1	D	0.32	0/1380	0.52	0/1875
1	E	0.32	0/1496	0.52	0/2029
1	F	0.31	0/1363	0.53	0/1851
All	All	0.32	0/8431	0.53	0/11447

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1393	0	1435	10	0
1	B	1360	0	1410	16	0
1	C	1365	0	1413	17	0
1	D	1360	0	1404	20	0
1	E	1476	0	1515	13	0
1	F	1344	0	1391	5	0
2	B	5	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
3	A	57	0	0	0	0
3	B	53	0	0	0	0
3	C	54	0	0	0	0
3	D	37	0	0	0	0
3	E	49	0	0	1	0
3	F	52	0	0	0	0
All	All	8625	0	8568	74	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 4.

All (74) 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:597:GLN:HE22	1:D:710:ARG:HH11	1.11	0.93
1:E:723:LEU:HD12	1:E:747:ILE:HD13	1.62	0.80
1:D:648:ARG:HH22	1:D:762:ARG:HH22	1.41	0.69
1:C:623:LYS:NZ	1:D:659:TYR:OH	2.26	0.68
1:B:666:VAL:HG11	1:B:684[B]:MET:HE1	1.77	0.65
1:E:744:LEU:HA	1:E:747:ILE:HD12	1.77	0.65
1:C:597:GLN:NE2	1:D:710:ARG:HD3	2.11	0.65
1:B:615:THR:HG22	1:B:666:VAL:HG22	1.79	0.64
1:D:710:ARG:NE	1:D:712:GLN:OE1	2.31	0.62
1:A:700:ASP:HB3	1:A:732:LYS:HB3	1.82	0.62
1:F:764:GLU:O	1:F:768:THR:HG22	1.99	0.61
1:D:648:ARG:HH22	1:D:762:ARG:NH2	1.97	0.61
1:E:708:THR:OG1	1:E:710:ARG:HG2	2.01	0.61
1:A:591:ASN:HB2	1:B:648:ARG:HG2	1.84	0.58
1:C:609:ASP:OD1	1:C:610:LEU:N	2.37	0.57
1:C:700:ASP:HB2	1:C:732:LYS:HG2	1.87	0.57
1:D:601:LEU:HB2	1:D:704:THR:HB	1.87	0.56
1:B:680:ALA:O	1:B:684[B]:MET:HG2	2.07	0.55
1:B:762:ARG:HB3	1:B:764:GLU:OE2	2.07	0.55
1:D:708:THR:OG1	1:D:710:ARG:HG2	2.08	0.53
1:D:648:ARG:NH2	1:D:762:ARG:HH22	2.06	0.53
1:D:710:ARG:HG3	1:D:712:GLN:HG3	1.90	0.53
1:F:598:VAL:HG22	1:F:697:VAL:HG21	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:762:ARG:NH1	1:D:764:GLU:H	2.09	0.51
1:E:712:GLN:NE2	3:E:948:HOH:O	2.44	0.50
1:E:767:LEU:HB3	1:E:775:PRO:HG2	1.94	0.50
1:B:666:VAL:CG1	1:B:684[B]:MET:HE1	2.41	0.50
1:E:658:PHE:O	1:E:662:ARG:HG2	2.11	0.50
1:B:704:THR:O	1:B:737:PRO:HD3	2.13	0.49
1:C:732:LYS:HG3	1:C:733:THR:N	2.29	0.48
1:A:648:ARG:NH1	1:A:764:GLU:OE1	2.44	0.48
1:C:597:GLN:HE22	1:D:710:ARG:HD3	1.77	0.48
1:B:601:LEU:HB2	1:B:704:THR:HB	1.95	0.48
1:B:723:LEU:HD12	1:B:747:ILE:HD12	1.96	0.48
1:D:762:ARG:CZ	1:D:762:ARG:HB2	2.43	0.47
1:E:590:ASP:O	1:E:594:ARG:HG3	2.14	0.47
1:A:601:LEU:HB2	1:A:704:THR:HB	1.97	0.47
1:C:680:ALA:O	1:C:684[A]:MET:HG2	2.15	0.46
1:C:602:ALA:HB3	1:C:611:LEU:HD21	1.98	0.46
1:D:602:ALA:HA	1:D:722:LYS:HE3	1.98	0.46
1:A:657:ASP:O	1:A:660:GLU:HG2	2.16	0.46
1:A:595:VAL:HA	1:A:615:THR:O	2.15	0.46
1:B:684[B]:MET:HE3	1:B:684[B]:MET:HA	1.98	0.45
1:F:601:LEU:HB2	1:F:704:THR:HB	1.97	0.45
1:C:597:GLN:NE2	1:C:614:GLU:HG2	2.31	0.45
1:C:698:ARG:HB3	1:C:700:ASP:OD1	2.17	0.45
1:D:646:ARG:HD2	1:D:659:TYR:CD2	2.52	0.45
1:E:715:PRO:HB3	1:E:739:GLU:HB2	2.00	0.44
1:A:774:GLU:H	1:A:774:GLU:CD	2.20	0.44
1:C:615:THR:HG22	1:C:666:VAL:HG22	2.00	0.44
1:B:764:GLU:H	1:B:764:GLU:CD	2.20	0.44
1:B:666:VAL:HG11	1:B:684[B]:MET:CE	2.47	0.43
1:C:720:LYS:O	1:C:724:LEU:HG	2.19	0.43
1:C:608:GLY:N	1:C:721:GLU:OE1	2.43	0.43
1:E:617:CYS:N	1:E:691:CYS:SG	2.92	0.43
1:A:661:LYS:HE2	1:A:661:LYS:HB3	1.89	0.43
1:D:594:ARG:HB2	1:D:696:PRO:HB3	2.01	0.43
1:B:638:ILE:HG12	1:B:684[B]:MET:HE2	2.01	0.43
1:B:710:ARG:HB2	1:B:710:ARG:HE	1.72	0.42
1:A:615:THR:HG22	1:A:666:VAL:HG22	2.02	0.42
1:D:657:ASP:O	1:D:661:LYS:HG2	2.19	0.42
1:E:650:GLU:HB2	1:E:651:LYS:HE2	2.02	0.42
1:C:597:GLN:NE2	1:D:710:ARG:HH11	1.95	0.42
1:D:680:ALA:O	1:D:684:MET:HG2	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:601:LEU:HB2	1:C:704:THR:HB	2.01	0.42
1:F:710:ARG:NE	1:F:712:GLN:OE1	2.46	0.42
1:B:648:ARG:NH1	1:B:764:GLU:OE1	2.39	0.41
1:E:603:TRP:HA	1:E:608:GLY:HA2	2.01	0.41
1:C:771:LEU:HD12	1:C:775:PRO:HG3	2.03	0.41
1:E:748:PRO:O	1:E:752:ILE:HG12	2.20	0.41
1:D:614:GLU:OE2	1:E:710:ARG:HD3	2.21	0.41
1:F:651:LYS:NZ	1:F:651:LYS:H	2.18	0.41
1:A:706:GLU:HB3	1:A:714:LEU:HB2	2.02	0.41
1:B:662:ARG:HD2	1:B:662:ARG:HA	1.89	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	185/200 (92%)	180 (97%)	5 (3%)	0	100	100
1	B	181/200 (90%)	179 (99%)	2 (1%)	0	100	100
1	C	181/200 (90%)	179 (99%)	2 (1%)	0	100	100
1	D	180/200 (90%)	176 (98%)	4 (2%)	0	100	100
1	E	196/200 (98%)	190 (97%)	6 (3%)	0	100	100
1	F	178/200 (89%)	175 (98%)	3 (2%)	0	100	100
All	All	1101/1200 (92%)	1079 (98%)	22 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	151/160 (94%)	144 (95%)	7 (5%)	27 13
1	B	147/160 (92%)	141 (96%)	6 (4%)	30 16
1	C	147/160 (92%)	140 (95%)	7 (5%)	25 11
1	D	146/160 (91%)	141 (97%)	5 (3%)	37 22
1	E	158/160 (99%)	147 (93%)	11 (7%)	15 5
1	F	144/160 (90%)	137 (95%)	7 (5%)	25 11
All	All	893/960 (93%)	850 (95%)	43 (5%)	25 11

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	593	ASN
1	A	597	GLN
1	A	611	LEU
1	A	621	LYS
1	A	732	LYS
1	A	764	GLU
1	A	773	ASN
1	B	605	GLU
1	B	609	ASP
1	B	655	ASN
1	B	662	ARG
1	B	742	ARG
1	B	749	ASP
1	C	594	ARG
1	C	605	GLU
1	C	611	LEU
1	C	652	LEU
1	C	661	LYS
1	C	732	LYS
1	C	762	ARG
1	D	606	VAL
1	D	609	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	611	LEU
1	D	746	GLU
1	D	762	ARG
1	E	588	ARG
1	E	593	ASN
1	E	605	GLU
1	E	609	ASP
1	E	623	LYS
1	E	651	LYS
1	E	662	ARG
1	E	700	ASP
1	E	728	ARG
1	E	746	GLU
1	E	781	VAL
1	F	594	ARG
1	F	650	GLU
1	F	710	ARG
1	F	721	GLU
1	F	735	LEU
1	F	750	ASN
1	F	768	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	597	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides 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	SO4	D	801	-	4,4,4	0.16	0	6,6,6	0.22	0
2	SO4	F	801	-	4,4,4	0.18	0	6,6,6	0.28	0
2	SO4	C	801	-	4,4,4	0.19	0	6,6,6	0.33	0
2	SO4	E	801	-	4,4,4	0.20	0	6,6,6	0.22	0
2	SO4	B	801	-	4,4,4	0.13	0	6,6,6	0.24	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (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	185/200 (92%)	-0.23	6 (3%) 47 41	15, 27, 58, 98	0
1	B	181/200 (90%)	-0.14	5 (2%) 53 47	16, 31, 64, 78	0
1	C	182/200 (91%)	-0.23	4 (2%) 62 57	18, 30, 54, 68	0
1	D	182/200 (91%)	-0.16	3 (1%) 72 68	19, 35, 58, 77	0
1	E	198/200 (99%)	-0.14	5 (2%) 57 52	19, 34, 68, 80	0
1	F	180/200 (90%)	-0.35	0 100 100	16, 29, 55, 82	0
All	All	1108/1200 (92%)	-0.21	23 (2%) 63 59	15, 32, 61, 98	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	593	ASN	7.5
1	B	607	GLY	6.1
1	E	606	VAL	5.6
1	C	606	VAL	4.9
1	E	752	ILE	4.6
1	A	592	GLU	4.1
1	B	606	VAL	3.6
1	A	774	GLU	3.2
1	A	591	ASN	3.2
1	E	607	GLY	3.0
1	E	753	ALA	2.9
1	A	594	ARG	2.4
1	A	621	LYS	2.4
1	C	611	LEU	2.4
1	B	608	GLY	2.4
1	B	742	ARG	2.4
1	D	659	TYR	2.4
1	C	657	ASP	2.3
1	E	742	ARG	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	746	GLU	2.3
1	D	728	ARG	2.1
1	D	606	VAL	2.1
1	C	651	LYS	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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{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	B-factors(Å^2)	Q<0.9
2	SO4	F	801	5/5	0.88	0.14	27,29,45,59	0
2	SO4	C	801	5/5	0.94	0.16	23,28,39,52	0
2	SO4	B	801	5/5	0.95	0.08	29,34,44,48	0
2	SO4	E	801	5/5	0.98	0.09	42,44,57,58	0
2	SO4	D	801	5/5	0.98	0.09	36,44,48,55	0

6.5 Other polymers (i)

There are no such residues in this entry.