



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 05:09 am BST

PDB ID : 3WU5
Title : Reduced E.coli Lon Proteolytic domain
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Yokoyama, S.
Deposited on : 2014-04-22
Resolution : 2.07 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 ⓘ](#)) 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 : 2.11
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) : 2.11

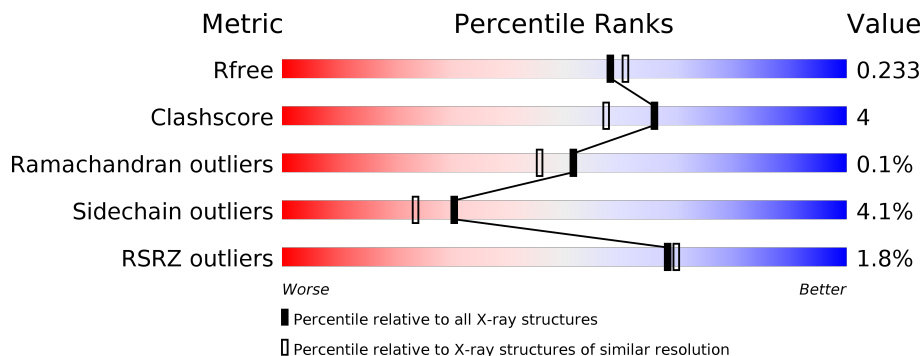
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.07 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	2684 (2.08-2.04)
Clashscore	141614	2801 (2.08-2.04)
Ramachandran outliers	138981	2768 (2.08-2.04)
Sidechain outliers	138945	2768 (2.08-2.04)
RSRZ outliers	127900	2646 (2.08-2.04)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	200	 84% 7% 9% 2%
1	B	200	 81% 9% 11% 2%
1	C	200	 83% 8% 10%
1	D	200	 80% 10% 10% 2%
1	E	200	 78% 16% 5% 6%
1	F	200	 73% 16% 11% 2%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8289 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
			Total	C	N	O	S			
1	A	182	1365	861	238	259	7	0	1	0
1	B	178	1325	837	230	252	6	0	0	0
1	C	181	1354	855	234	258	7	0	1	0
1	D	181	1349	851	234	258	6	0	0	0
1	E	191	1423	895	249	272	7	0	0	0
1	F	178	1325	837	230	252	6	0	0	0

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: O₄S).



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


- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	26	Total	O	0	0
			26	26		
3	B	19	Total	O	0	0
			19	19		
3	C	33	Total	O	0	0
			33	33		
3	D	14	Total	O	0	0
			14	14		
3	E	11	Total	O	0	0
			11	11		
3	F	20	Total	O	0	0
			20	20		

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 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.

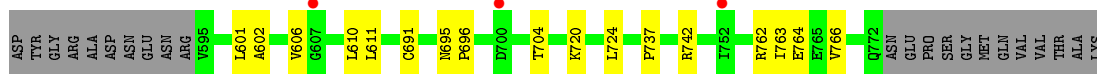
- Molecule 1: Lon protease

Chain A: 




- Molecule 1: Lon protease

Chain B: 




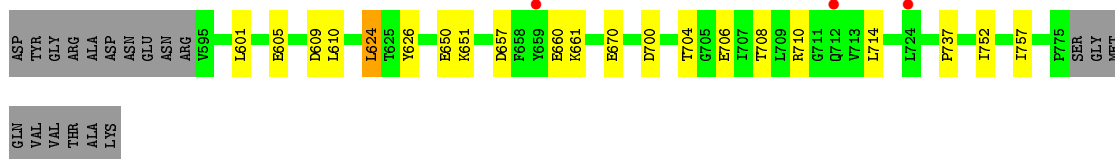
- Molecule 1: Lon protease

Chain C: 




- Molecule 1: Lon protease

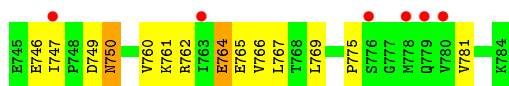
Chain D: 



- Molecule 1: Lon protease

Chain E: 





- Molecule 1: Lon protease



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	86.35Å 86.35Å 124.38Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.79 – 2.07 43.18 – 2.07	Depositor EDS
% Data completeness (in resolution range)	99.9 (40.79-2.07) 92.4 (43.18-2.07)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.23 (at 2.06Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.1_1168)	Depositor
R, R_{free}	0.183 , 0.234 0.184 , 0.233	Depositor DCC
R_{free} test set	3211 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	38.8	Xtriage
Anisotropy	0.609	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 36.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.063 for -h,-k,l 0.052 for h,-h-k,-l 0.036 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8289	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.46% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.40	0/1388	0.56	1/1885 (0.1%)
1	B	0.39	0/1344	0.55	0/1826
1	C	0.37	0/1377	0.53	0/1871
1	D	0.35	0/1369	0.54	1/1861 (0.1%)
1	E	0.35	0/1443	0.53	0/1958
1	F	0.37	0/1344	0.53	0/1826
All	All	0.37	0/8265	0.54	2/11227 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	624	LEU	CA-CB-CG	5.69	128.38	115.30
1	A	610	LEU	CA-CB-CG	5.01	126.82	115.30

There are no chirality outliers.

There are no planarity outliers.

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	1365	0	1415	7	0
1	B	1325	0	1374	6	0
1	C	1354	0	1402	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1349	0	1393	11	0
1	E	1423	0	1474	20	0
1	F	1325	0	1374	16	0
2	B	5	0	0	0	0
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	26	0	0	0	0
3	B	19	0	0	0	0
3	C	33	0	0	0	0
3	D	14	0	0	0	0
3	E	11	0	0	0	0
3	F	20	0	0	0	0
All	All	8289	0	8432	66	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 (66) 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	1.28	0.81
1:E:715:PRO:HG3	1:E:739:GLU:HB2	1.73	0.71
1:F:601:LEU:HB2	1:F:704:THR:HB	1.78	0.65
1:B:602:ALA:HB3	1:B:611:LEU:HD12	1.79	0.65
1:E:750:ASN:OD1	1:E:750:ASN:N	2.32	0.62
1:E:760:VAL:HG21	1:E:766:VAL:HG23	1.84	0.60
1:B:601:LEU:HB2	1:B:704:THR:HB	1.85	0.59
1:F:700:ASP:HB2	1:F:732:LYS:HB3	1.84	0.59
1:E:762:ARG:HB3	1:E:764:GLU:HG2	1.85	0.59
1:C:670:GLU:CD	1:C:670:GLU:H	2.06	0.58
1:E:611:LEU:HD22	1:E:675:LYS:HD3	1.85	0.58
1:F:715:PRO:HG3	1:F:739:GLU:HB2	1.86	0.57
1:F:744:LEU:HA	1:F:747:ILE:HD13	1.87	0.57
1:D:601:LEU:HB2	1:D:704:THR:HB	1.86	0.56
1:E:760:VAL:HG23	1:E:765:GLU:HB2	1.88	0.56
1:D:609:ASP:OD1	1:D:610:LEU:N	2.39	0.56
1:D:700:ASP:OD2	1:D:700:ASP:N	2.37	0.55
1:F:738:PHE:O	1:F:741:LYS:HB2	2.07	0.55
1:C:597:GLN:NE2	1:D:710:ARG:HH11	2.01	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:617:CYS:O	1:E:662:ARG:NH2	2.40	0.53
1:F:673:THR:O	1:F:675:LYS:HG3	2.08	0.53
1:C:597:GLN:NE2	1:D:710:ARG:HD3	2.24	0.52
1:D:704:THR:O	1:D:737:PRO:HD3	2.11	0.51
1:F:708:THR:OG1	1:F:710:ARG:HG2	2.11	0.50
1:E:746:GLU:OE1	1:E:746:GLU:N	2.45	0.50
1:F:704:THR:O	1:F:737:PRO:HD3	2.11	0.49
1:A:595:VAL:HA	1:A:615:THR:O	2.13	0.49
1:D:706:GLU:HB3	1:D:714:LEU:HB2	1.95	0.49
1:A:601:LEU:HB2	1:A:704:THR:HB	1.95	0.49
1:E:765:GLU:O	1:E:769:LEU:HG	2.14	0.48
1:A:601:LEU:CD2	1:A:610:LEU:HD22	2.44	0.47
1:D:752:ILE:HG23	1:D:757:ILE:HD12	1.97	0.47
1:E:735:LEU:HD21	1:E:769:LEU:HB2	1.96	0.47
1:F:612:THR:O	1:F:669:PRO:HD2	2.14	0.47
1:B:704:THR:O	1:B:737:PRO:HD3	2.15	0.47
1:B:720:LYS:O	1:B:724:LEU:HG	2.15	0.46
1:E:723:LEU:HD12	1:E:747:ILE:HD13	1.98	0.46
1:F:648:ARG:HH21	1:F:762:ARG:NH2	2.14	0.46
1:C:597:GLN:NE2	1:C:614:GLU:OE2	2.49	0.45
1:E:744:LEU:HD23	1:E:747:ILE:HD12	1.98	0.45
1:E:700:ASP:HB3	1:E:732:LYS:HG3	1.99	0.45
1:F:718:GLY:O	1:F:721:GLU:HG2	2.17	0.45
1:A:626:TYR:HA	1:A:666:VAL:O	2.17	0.44
1:C:602:ALA:HB3	1:C:611:LEU:HD12	1.99	0.44
1:C:680:ALA:O	1:C:684[A]:MET:HG2	2.17	0.44
1:E:723:LEU:HD12	1:E:747:ILE:CD1	2.48	0.44
1:A:720:LYS:O	1:A:724:LEU:HG	2.18	0.43
1:E:601:LEU:HB2	1:E:704:THR:HB	2.00	0.43
1:A:650:GLU:HG3	1:A:656:PRO:HG3	2.00	0.42
1:A:723:LEU:HD23	1:A:723:LEU:HA	1.86	0.42
1:E:760:VAL:CG2	1:E:765:GLU:HB2	2.50	0.42
1:E:641:ALA:O	1:E:645:VAL:HG23	2.20	0.42
1:D:657:ASP:O	1:D:660:GLU:HG2	2.19	0.42
1:B:763:ILE:O	1:B:766:VAL:HB	2.19	0.42
1:C:704:THR:O	1:C:737:PRO:HD3	2.19	0.42
1:F:710:ARG:HG3	1:F:712:GLN:HG3	2.02	0.41
1:F:723:LEU:HD12	1:F:747:ILE:HG12	2.00	0.41
1:F:695:ASN:ND2	1:F:771:LEU:HB3	2.34	0.41
1:E:738:PHE:CD1	1:E:761:LYS:HE3	2.54	0.41
1:E:767:LEU:HB3	1:E:775:PRO:HG3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:719:LEU:HD22	1:E:740:ASN:HB3	2.02	0.41
1:F:595:VAL:HB	1:F:615:THR:O	2.20	0.41
1:B:695:ASN:HA	1:B:696:PRO:HD3	1.91	0.41
1:C:682:ILE:HG13	1:C:703:MET:HG3	2.02	0.41
1:F:750:ASN:N	1:F:750:ASN:OD1	2.54	0.41
1:D:708:THR:OG1	1:D:710:ARG:HG2	2.20	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	181/200 (90%)	179 (99%)	2 (1%)	0	100	100
1	B	176/200 (88%)	173 (98%)	3 (2%)	0	100	100
1	C	180/200 (90%)	176 (98%)	4 (2%)	0	100	100
1	D	179/200 (90%)	176 (98%)	3 (2%)	0	100	100
1	E	189/200 (94%)	180 (95%)	8 (4%)	1 (0%)	29	19
1	F	176/200 (88%)	174 (99%)	2 (1%)	0	100	100
All	All	1081/1200 (90%)	1058 (98%)	22 (2%)	1 (0%)	51	45

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	729	GLY

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	147/160 (92%)	142 (97%)	5 (3%)	37	30
1	B	142/160 (89%)	136 (96%)	6 (4%)	30	23
1	C	146/160 (91%)	142 (97%)	4 (3%)	44	39
1	D	145/160 (91%)	138 (95%)	7 (5%)	25	18
1	E	153/160 (96%)	144 (94%)	9 (6%)	19	11
1	F	142/160 (89%)	137 (96%)	5 (4%)	36	29
All	All	875/960 (91%)	839 (96%)	36 (4%)	30	23

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	610	LEU
1	A	650	GLU
1	A	662	ARG
1	A	742	ARG
1	A	755	LEU
1	B	606	VAL
1	B	610	LEU
1	B	691	CYS
1	B	742	ARG
1	B	762	ARG
1	B	764	GLU
1	C	606	VAL
1	C	626	TYR
1	C	659	TYR
1	C	762	ARG
1	D	605	GLU
1	D	624	LEU
1	D	626	TYR
1	D	650	GLU
1	D	651	LYS
1	D	661	LYS
1	D	670	GLU
1	E	609	ASP
1	E	621	LYS
1	E	700	ASP
1	E	712	GLN

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Mol	Chain	Res	Type
1	E	732	LYS
1	E	749	ASP
1	E	750	ASN
1	E	764	GLU
1	E	781	VAL
1	F	595	VAL
1	F	610	LEU
1	F	650	GLU
1	F	651	LYS
1	F	659	TYR

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 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	SO4	C	801	-	4,4,4	0.16	0	6,6,6	0.43	0
2	SO4	F	801	-	4,4,4	0.16	0	6,6,6	0.37	0
2	SO4	D	801	-	4,4,4	0.13	0	6,6,6	0.13	0
2	SO4	B	801	-	4,4,4	0.11	0	6,6,6	0.14	0
2	SO4	E	801	-	4,4,4	0.15	0	6,6,6	0.11	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q < 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	182/200 (91%)	-0.14	0 100 100	19, 36, 69, 87	0
1	B	178/200 (89%)	-0.02	3 (1%) 70 71	23, 47, 81, 104	0
1	C	181/200 (90%)	-0.09	0 100 100	23, 39, 70, 82	0
1	D	181/200 (90%)	0.04	3 (1%) 70 71	30, 53, 82, 122	0
1	E	191/200 (95%)	0.32	11 (5%) 23 24	32, 63, 108, 125	0
1	F	178/200 (89%)	0.10	3 (1%) 70 71	20, 50, 79, 101	0
All	All	1091/1200 (90%)	0.04	20 (1%) 68 70	19, 48, 84, 125	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	607	GLY	6.2
1	E	779	GLN	5.1
1	D	659	TYR	4.0
1	E	747	ILE	3.8
1	E	658	PHE	2.9
1	B	700	ASP	2.8
1	B	607	GLY	2.7
1	E	776	SER	2.7
1	E	778	MET	2.6
1	E	724	LEU	2.6
1	B	752	ILE	2.5
1	E	606	VAL	2.5
1	F	747	ILE	2.3
1	D	712	GLN	2.2
1	D	724	LEU	2.1
1	E	763	ILE	2.1
1	E	692	LEU	2.1
1	F	611	LEU	2.0
1	E	780	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	F	754	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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SO4	F	801	5/5	0.87	0.11	67,68,73,76	0
2	SO4	C	801	5/5	0.92	0.10	38,57,59,61	0
2	SO4	E	801	5/5	0.94	0.18	82,90,92,94	0
2	SO4	B	801	5/5	0.98	0.09	47,58,66,68	0
2	SO4	D	801	5/5	0.98	0.08	45,63,71,79	0

6.5 Other polymers [i](#)

There are no such residues in this entry.