



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:49 PM UTC

PDB ID : 3WU4 / pdb_00003wu4
Title : Oxidized-form structure of 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 : 1.70 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

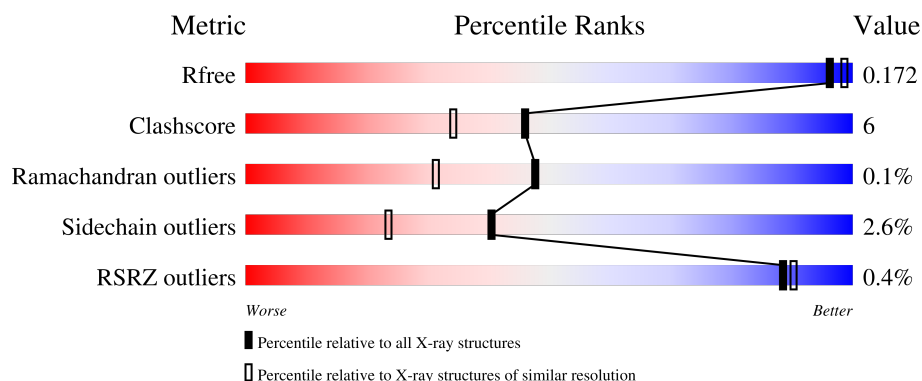
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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}	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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 of 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	
1	B	200	
1	C	200	
1	D	200	
1	E	200	

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Mol	Chain	Length	Quality of chain
1	F	200	78% 12% 10%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8497 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	178	Total	C	N	O	S	0	0	0
			1326	836	231	253	6			
1	B	180	Total	C	N	O	S	0	0	0
			1342	846	233	257	6			
1	C	181	Total	C	N	O	S	0	0	0
			1349	851	234	258	6			
1	D	182	Total	C	N	O	S	0	0	0
			1360	857	238	259	6			
1	E	194	Total	C	N	O	S	0	0	0
			1448	908	254	279	7			
1	F	179	Total	C	N	O	S	0	0	0
			1333	841	232	254	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 (CCD ID: 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		

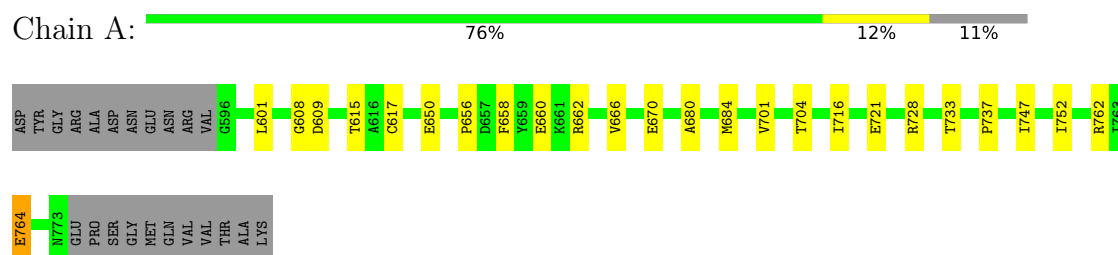
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	54	Total	O	0	0
			54	54		
3	B	45	Total	O	0	0
			45	45		
3	C	57	Total	O	0	0
			57	57		
3	D	42	Total	O	0	0
			42	42		
3	E	62	Total	O	0	0
			62	62		
3	F	54	Total	O	0	0
			54	54		

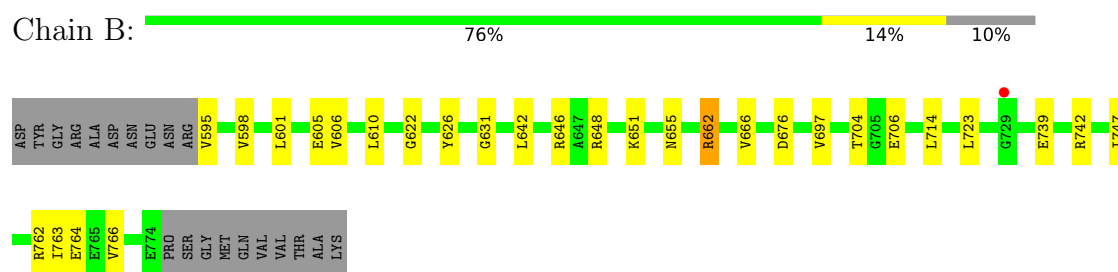
3 Residue-property plots [i](#)

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.

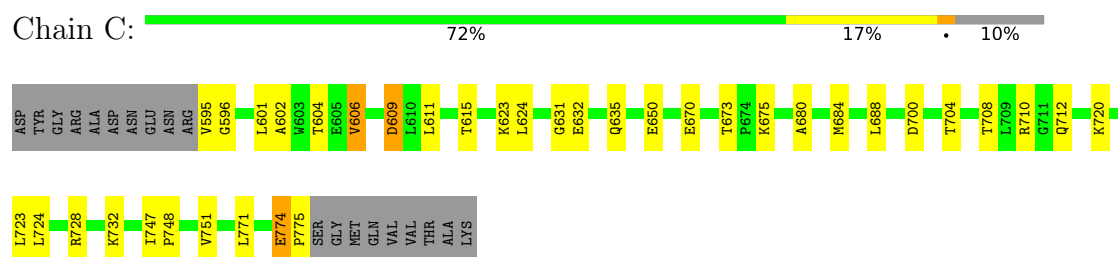
• Molecule 1: Lon protease



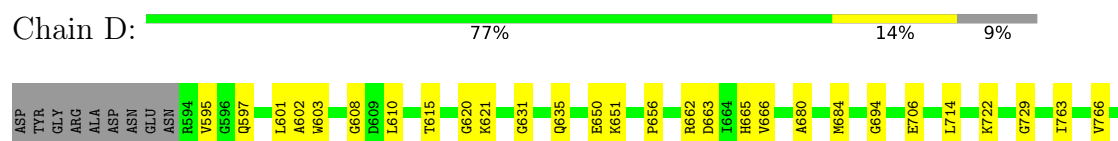
• Molecule 1: Lon protease



• Molecule 1: Lon protease

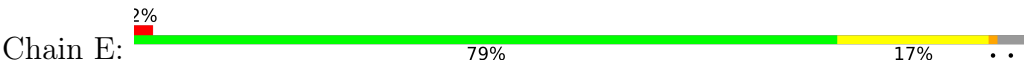


• Molecule 1: Lon protease



P775
SER
GLY
MET
GLN
VAL
THR
ALA
LYS

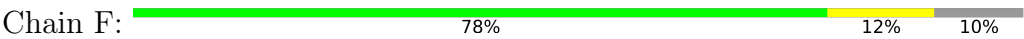
● Molecule 1: Lon protease



ASP	TYR	GLY	ARG	ALA	ASP	R591	R594	V603	T604	E605	V606	G607	G608	D609	L610	E614	T615	A616	C617	G622	K623	L624	T625	Y626	L642	T643	R646	K651	N655	F658	R662	Y666	E670	P674	K675	A680	M684	C691	P696	D700
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L719	K732	T733	N740	V751	L757	L767	P775	K784
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● Molecule 1: Lon protease



ASP	TTR	GLY	ARG	ALA	ASN	ASN	ASN	ARG	V595	V598	L610	L611	T612	G620	A640	V644	R648	D657	F658	Y659	R662	D663	P669	G694	N695	P696	V697	D700	V701	T708	L709	R710	V713	A726	T733	V734	L735	E764	N773	GLU	PRO
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SER	GLY	MET	GLN	VAL	THR	ALA	LYS
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4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	86.39Å 86.39Å 124.37Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	37.41 – 1.70 37.41 – 1.70	Depositor EDS
% Data completeness (in resolution range)	97.5 (37.41-1.70) 93.2 (37.41-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 1.70Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.1_1168)	Depositor
R, R_{free}	0.152 , 0.177 0.150 , 0.172	Depositor DCC
R_{free} test set	5566 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	23.6	Xtriage
Anisotropy	0.759	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 41.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.338 for -h,-k,l 0.117 for h,-h-k,-l 0.118 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	8497	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% 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	0.49	0/1345	0.83	1/1827 (0.1%)
1	B	0.50	0/1361	0.85	2/1849 (0.1%)
1	C	0.50	0/1369	0.84	1/1861 (0.1%)
1	D	0.47	0/1380	0.82	0/1875
1	E	0.49	0/1468	0.81	0/1992
1	F	0.51	0/1352	0.81	0/1837
All	All	0.49	0/8275	0.83	4/11241 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	655	ASN	CA-C-N	6.21	126.40	119.32
1	B	655	ASN	C-N-CA	6.21	126.40	119.32
1	C	609	ASP	N-CA-C	5.64	116.00	108.38
1	A	660	GLU	N-CA-C	-5.44	106.81	113.50

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	1326	0	1369	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1342	0	1384	14	0
1	C	1349	0	1391	21	0
1	D	1360	0	1404	15	0
1	E	1448	0	1490	21	0
1	F	1333	0	1378	13	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	54	0	0	5	0
3	B	45	0	0	1	0
3	C	57	0	0	2	0
3	D	42	0	0	0	0
3	E	62	0	0	2	0
3	F	54	0	0	3	0
All	All	8497	0	8416	97	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 6.

All (97) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:764:GLU:OE2	3:A:849:HOH:O	2.01	0.79
1:A:615:THR:HG22	1:A:666:VAL:HG22	1.69	0.72
1:A:650:GLU:HG3	1:A:656:PRO:HG3	1.74	0.68
1:C:673:THR:O	1:C:675:LYS:NZ	2.28	0.66
1:A:670:GLU:OE1	3:A:830:HOH:O	2.11	0.66
1:F:700:ASP:OD1	3:F:952:HOH:O	2.13	0.66
1:A:601:LEU:HB2	1:A:704:THR:HB	1.81	0.63
1:E:603:TRP:HA	1:E:608:GLY:HA2	1.82	0.62
1:F:713:VAL:O	3:F:940:HOH:O	2.15	0.61
1:D:706:GLU:HB3	1:D:714:LEU:HB2	1.83	0.61
1:E:605:GLU:HB2	1:E:674:PRO:HD2	1.84	0.59
1:A:728:ARG:NH1	3:A:850:HOH:O	2.36	0.58
1:D:610:LEU:HD11	1:D:729:GLY:HA3	1.85	0.58
1:B:648:ARG:NH1	1:B:764:GLU:OE2	2.34	0.57
1:E:700:ASP:HB3	1:E:732:LYS:HG2	1.85	0.57
1:C:771:LEU:HD12	1:C:775:PRO:HG3	1.87	0.57
1:C:602:ALA:HB3	1:C:611:LEU:HD12	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:655:ASN:HB3	1:E:658:PHE:HB3	1.87	0.56
1:D:650:GLU:HG3	1:D:656:PRO:HG3	1.88	0.56
1:A:762:ARG:NH2	3:A:835:HOH:O	2.36	0.55
1:D:680:ALA:O	1:D:684:MET:HG2	2.10	0.52
1:F:648:ARG:NH1	1:F:764:GLU:OE2	2.29	0.52
1:B:739:GLU:OE1	3:B:910:HOH:O	2.19	0.52
1:C:700:ASP:HB2	1:C:732:LYS:HB3	1.93	0.51
1:E:615:THR:HG22	1:E:666:VAL:HG22	1.92	0.51
1:D:615:THR:HG22	1:D:666:VAL:HG22	1.93	0.51
1:E:642:LEU:O	1:E:646:ARG:HG3	2.11	0.51
1:C:632:GLU:HG3	3:C:936:HOH:O	2.10	0.50
1:C:631:GLY:O	1:C:635:GLN:HG3	2.12	0.50
1:C:673:THR:OG1	3:C:953:HOH:O	2.20	0.50
1:A:650:GLU:CD	1:A:650:GLU:H	2.20	0.49
1:C:615:THR:HG21	1:C:688:LEU:HD23	1.94	0.49
1:E:651:LYS:HD2	1:E:651:LYS:H	1.77	0.49
1:F:640:ALA:O	1:F:644:VAL:HG23	2.13	0.48
1:C:680:ALA:O	1:C:684:MET:HG2	2.12	0.48
1:E:680:ALA:O	1:E:684:MET:HG2	2.14	0.48
1:A:658:PHE:HB2	1:A:662:ARG:HH21	1.79	0.48
1:B:706:GLU:HB3	1:B:714:LEU:HB2	1.95	0.47
1:E:604:THR:HG22	1:E:675:LYS:HG2	1.97	0.47
1:D:763:ILE:HD12	1:D:766:VAL:HB	1.97	0.47
1:B:642:LEU:O	1:B:646:ARG:HG3	2.15	0.47
1:A:747:ILE:HB	1:A:752:ILE:HD11	1.97	0.46
1:D:665:HIS:ND1	1:E:643:THR:OG1	2.44	0.46
1:E:719:LEU:HD22	1:E:740:ASN:HB3	1.96	0.46
1:A:609:ASP:OD2	3:A:820:HOH:O	2.21	0.46
1:E:609:ASP:OD1	1:E:610:LEU:N	2.39	0.46
1:E:767:LEU:HB3	1:E:775:PRO:HG3	1.97	0.46
1:B:622:GLY:HA2	1:B:662:ARG:O	2.17	0.45
1:C:596:GLY:N	1:C:615:THR:O	2.37	0.45
1:C:724:LEU:O	1:C:728:ARG:HG3	2.17	0.45
1:C:708:THR:OG1	1:C:710:ARG:HG2	2.16	0.45
1:E:617:CYS:N	1:E:691:CYS:SG	2.89	0.45
1:B:648:ARG:HH22	1:B:762:ARG:NH2	2.15	0.45
1:C:604:THR:OG1	1:C:606:VAL:HG22	2.17	0.44
1:E:614:GLU:OE2	1:F:710:ARG:HG2	2.17	0.44
1:C:720:LYS:HA	1:C:747:ILE:HG12	1.98	0.44
1:E:622:GLY:HA2	3:E:928:HOH:O	2.18	0.44
1:F:708:THR:OG1	1:F:710:ARG:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:595:VAL:HA	1:C:615:THR:O	2.18	0.44
1:F:610:LEU:HD12	1:F:726:ALA:HA	1.99	0.44
1:C:723:LEU:HD12	1:C:747:ILE:HD13	1.99	0.43
1:E:732:LYS:HG3	1:E:733:THR:N	2.33	0.43
1:D:602:ALA:HA	1:D:722:LYS:HE3	2.00	0.43
1:E:626:TYR:HA	1:E:666:VAL:O	2.19	0.43
1:D:603:TRP:HA	1:D:608:GLY:HA2	2.00	0.43
1:A:704:THR:O	1:A:737:PRO:HD3	2.19	0.43
1:C:774:GLU:HA	1:C:775:PRO:HD3	1.91	0.43
1:B:631:GLY:HA3	1:B:676:ASP:CG	2.44	0.43
1:D:631:GLY:O	1:D:635:GLN:HG3	2.19	0.43
1:C:710:ARG:HE	1:C:712:GLN:CD	2.26	0.43
1:D:601:LEU:CD2	1:D:610:LEU:HD23	2.50	0.42
1:F:657:ASP:OD1	3:F:943:HOH:O	2.21	0.42
1:F:620:GLY:HA3	1:F:663:ASP:CG	2.45	0.42
1:B:601:LEU:HB2	1:B:704:THR:HB	2.01	0.42
1:D:620:GLY:HA3	1:D:663:ASP:OD1	2.20	0.42
1:B:648:ARG:O	1:B:651:LYS:HG2	2.20	0.42
1:C:601:LEU:HB2	1:C:704:THR:HB	2.02	0.42
1:E:662:ARG:NH2	3:E:927:HOH:O	2.45	0.42
1:F:612:THR:O	1:F:669:PRO:HD2	2.20	0.42
1:A:701:VAL:HG22	1:A:733:THR:HB	2.02	0.41
1:E:624:LEU:HD22	1:E:642:LEU:HD23	2.02	0.41
1:C:623:LYS:HD2	1:C:624:LEU:H	1.85	0.41
1:C:748:PRO:HB2	1:C:751:VAL:HG23	2.01	0.41
1:D:595:VAL:HG11	1:D:694:GLY:HA2	2.01	0.41
1:F:694:GLY:O	1:F:696:PRO:HD3	2.21	0.41
1:A:680:ALA:O	1:A:684:MET:HG2	2.21	0.41
1:B:763:ILE:HD12	1:B:766:VAL:HB	2.01	0.41
1:F:598:VAL:HG22	1:F:697:VAL:HG11	2.03	0.41
1:A:608:GLY:H	1:A:721:GLU:CD	2.28	0.41
1:B:723:LEU:HD12	1:B:747:ILE:HD13	2.03	0.41
1:B:626:TYR:HA	1:B:666:VAL:O	2.21	0.41
1:E:594:ARG:HB2	1:E:696:PRO:HB3	2.02	0.41
1:F:701:VAL:HG22	1:F:733:THR:HB	2.03	0.41
1:B:598:VAL:HG22	1:B:697:VAL:HG21	2.02	0.40
1:D:620:GLY:HA3	1:D:663:ASP:CG	2.47	0.40
1:D:621:LYS:N	1:D:663:ASP:OD1	2.51	0.40
1:B:648:ARG:HB3	1:B:651:LYS:HD3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	176/200 (88%)	170 (97%)	6 (3%)	0	100	100
1	B	178/200 (89%)	171 (96%)	7 (4%)	0	100	100
1	C	179/200 (90%)	173 (97%)	6 (3%)	0	100	100
1	D	180/200 (90%)	173 (96%)	7 (4%)	0	100	100
1	E	192/200 (96%)	187 (97%)	4 (2%)	1 (0%)	24	12
1	F	177/200 (88%)	175 (99%)	2 (1%)	0	100	100
All	All	1082/1200 (90%)	1049 (97%)	32 (3%)	1 (0%)	48	31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	608	GLY

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	142/160 (89%)	139 (98%)	3 (2%)	47	30
1	B	144/160 (90%)	138 (96%)	6 (4%)	26	11
1	C	145/160 (91%)	140 (97%)	5 (3%)	32	16
1	D	146/160 (91%)	143 (98%)	3 (2%)	47	30
1	E	156/160 (98%)	153 (98%)	3 (2%)	50	34
1	F	143/160 (89%)	140 (98%)	3 (2%)	47	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	876/960 (91%)	853 (97%)	23 (3%)	40	23

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	617	CYS
1	A	716	ILE
1	A	764	GLU
1	B	595	VAL
1	B	605	GLU
1	B	606	VAL
1	B	610	LEU
1	B	662	ARG
1	B	742	ARG
1	C	606	VAL
1	C	609	ASP
1	C	650	GLU
1	C	670	GLU
1	C	774	GLU
1	D	597	GLN
1	D	651	LYS
1	D	662	ARG
1	E	606	VAL
1	E	670	GLU
1	E	732	LYS
1	F	659	TYR
1	F	662	ARG
1	F	735	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	750	ASN
1	B	639	GLN
1	C	639	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 oligosaccharides 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	E	801	-	4,4,4	0.23	0	6,6,6	0.11	0
2	SO4	B	801	-	4,4,4	0.26	0	6,6,6	0.15	0
2	SO4	F	801	-	4,4,4	0.23	0	6,6,6	0.24	0
2	SO4	C	801	-	4,4,4	0.27	0	6,6,6	0.19	0
2	SO4	D	801	-	4,4,4	0.25	0	6,6,6	0.20	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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	178/200 (89%)	-0.89	0 100 100	19, 30, 53, 64	0
1	B	180/200 (90%)	-0.72	1 (0%) 85 88	20, 33, 59, 82	0
1	C	181/200 (90%)	-0.85	0 100 100	21, 32, 54, 68	0
1	D	182/200 (91%)	-0.67	0 100 100	24, 37, 61, 89	0
1	E	194/200 (97%)	-0.58	3 (1%) 72 76	23, 36, 64, 95	0
1	F	179/200 (89%)	-0.85	0 100 100	20, 31, 53, 95	0
All	All	1094/1200 (91%)	-0.76	4 (0%) 88 90	19, 33, 59, 95	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	757	ILE	3.1
1	B	729	GLY	2.9
1	E	733	THR	2.2
1	E	751	VAL	2.1

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 oligosaccharides 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	0.97	0.08	58,59,64,66	0
2	SO4	E	801	5/5	0.98	0.07	70,70,72,73	0
2	SO4	C	801	5/5	0.98	0.05	34,46,48,51	0
2	SO4	B	801	5/5	0.99	0.03	34,40,42,43	0
2	SO4	D	801	5/5	0.99	0.05	39,45,47,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.