

Full wwPDB X-ray Structure Validation Report (i)

Oct 16, 2021 - 09:36 PM EDT

PDB ID	:	1RRE
Title	:	Crystal structure of E.coli Lon proteolytic domain
Authors	:	Botos, I.; Melnikov, E.E.; Cherry, S.; Tropea, J.E.; Khalatova, A.G.; Rasulova,
		F.; Dauter, Z.; Maurizi, M.R.; Rotanova, T.V.; Wlodawer, A.; Gustchina, A.
Deposited on	:	2003-12-08
Resolution	:	1.75 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 (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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
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)	:	2.23.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY\;DIFFRACTION$

The reported resolution of this entry is 1.75 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	2340(1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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 <=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		
			5%		
1	А	200	70%	18%	• 9%
			7%		
1	В	200	64%	22%	•• 9%
			5%		
1	С	200	68%	20%	• 9%
			6%		
1	D	200	68%	18%	• 9%
			10%		
1	E	200	72%	18%	• •



Mol	Chain	Length	Quality of chain	Quality of chain					
	-		6%						
1	F	200	65%	20%	6%	9%			



1RRE

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 9029 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.

Mol	Chain	Residues		_	Atom	IS			ZeroOcc	AltConf	Trace
1	Λ	189	Total	С	Ν	0	S	Se	0	2	0
1	Л	162	1357	854	235	259	5	4	0	5	0
1	В	199	Total	С	Ν	Ο	S	Se	0	2	0
1	D	102	1355	854	235	259	4	3	0	2	0
1	С	189	Total	С	Ν	Ο	\mathbf{S}	Se	0	9	0
1	U	162	1355	853	235	259	4	4	0	2	0
1	л	100	Total	С	Ν	Ο	\mathbf{S}	Se	0	1	0
1	D	102	1361	858	238	259	3	3	0	T	0
1	1 E	101	Total	С	Ν	Ο	\mathbf{S}	Se	0	0	0
1		191	1423	895	249	272	3	4	0	0	0
1	F	189	Total	С	Ν	0	\mathbf{S}	Se	0	0	0
	T,	102	1361	856	239	260	3	3	0		U

• Molecule 1 is a protein called ATP-dependent protease La.

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	679	ALA	SER	engineered mutation	UNP P0A9M0
В	679	ALA	SER	engineered mutation	UNP P0A9M0
С	679	ALA	SER	engineered mutation	UNP P0A9M0
D	679	ALA	SER	engineered mutation	UNP P0A9M0
Е	679	ALA	SER	engineered mutation	UNP P0A9M0
F	679	ALA	SER	engineered mutation	UNP P0A9M0

• Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	С	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	D	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	Е	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	F	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	134	Total O 134 134	0	0
3	В	129	Total O 129 129	0	0
3	С	142	Total O 142 142	0	0
3	D	109	Total O 109 109	0	0
3	Е	154	Total O 154 154	0	0
3	F	124	Total O 124 124	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: ATP-dependent protease La



18%



 \bullet Molecule 1: ATP-dependent protease La

Chain E:

72%

• Molecule 1: ATP-dependent protease La





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants	86.37Å 86.37Å 124.16Å	Deneriten
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	19.96 - 1.75	Depositor
Resolution (A)	19.94 - 1.75	EDS
% Data completeness	93.5 (19.96-1.75)	Depositor
(in resolution range)	$93.6\ (19.94-1.75)$	EDS
R _{merge}	0.07	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.83 (at 1.74 \text{\AA})$	Xtriage
Refinement program	REFMAC $5.1.24$	Depositor
B B.	0.205 , 0.263	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.209 , 0.263	DCC
R_{free} test set	9386 reflections (9.61%)	wwPDB-VP
Wilson B-factor $(Å^2)$	24.8	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.34 , 45.3	EDS
L-test for twinning ²	$< L > = 0.50, < L^2 > = 0.33$	Xtriage
	0.015 for -h,-k,l	
Estimated twinning fraction	0.034 for h,-h-k,-l	Xtriage
	0.017 for -k,-h,-l	
F_o, F_c correlation	0.95	EDS
Total number of atoms	9029	wwPDB-VP
Average B, all atoms $(Å^2)$	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 7.03% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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	Bo	nd lengths	B	ond angles
	Unain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.86	1/1390~(0.1%)	0.97	3/1883~(0.2%)
1	В	0.78	0/1384	0.95	5/1875~(0.3%)
1	С	0.88	1/1384~(0.1%)	0.98	6/1875~(0.3%)
1	D	0.74	0/1385	0.92	4/1876~(0.2%)
1	Е	0.76	0/1439	0.92	4/1946~(0.2%)
1	F	0.80	1/1377~(0.1%)	0.94	7/1865~(0.4%)
All	All	0.80	3/8359~(0.0%)	0.95	29/11320~(0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
1	А	703	MSE	SE-CE	-7.46	1.51	1.95
1	С	703	MSE	SE-CE	-6.12	1.59	1.95
1	F	751	VAL	CB-CG2	-5.00	1.42	1.52

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	С	663	ASP	CB-CG-OD2	7.79	125.31	118.30
1	В	609	ASP	CB-CG-OD2	7.57	125.11	118.30
1	В	610	LEU	CA-CB-CG	7.34	132.19	115.30
1	А	756	ASP	CB-CG-OD2	7.17	124.75	118.30
1	С	756	ASP	CB-CG-OD2	6.68	124.31	118.30
1	D	700	ASP	CB-CG-OD2	6.68	124.31	118.30
1	Е	610	LEU	CA-CB-CG	6.60	130.47	115.30
1	С	710	ARG	NE-CZ-NH2	-6.53	117.04	120.30
1	F	724	LEU	CA-CB-CG	6.49	130.22	115.30
1	D	657	ASP	CB-CG-OD2	6.34	124.01	118.30
1	С	609	ASP	CB-CG-OD2	6.34	124.00	118.30
1	С	710	ARG	NE-CZ-NH1	6.22	123.41	120.30



Mol	Chain	\mathbf{Res}	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	С	657	ASP	CB-CG-OD2	6.09	123.78	118.30
1	F	743	ASP	CB-CG-OD2	6.04	123.74	118.30
1	F	609	ASP	CB-CG-OD1	6.02	123.72	118.30
1	Ε	700	ASP	CB-CG-OD2	5.86	123.57	118.30
1	F	657	ASP	CB-CG-OD2	5.80	123.52	118.30
1	В	663	ASP	CB-CG-OD2	5.78	123.50	118.30
1	F	663	ASP	CB-CG-OD2	5.71	123.44	118.30
1	А	749	ASP	CB-CG-OD2	5.67	123.41	118.30
1	D	743	ASP	CB-CG-OD2	5.67	123.40	118.30
1	D	609	ASP	CB-CG-OD2	5.60	123.34	118.30
1	А	610	LEU	CA-CB-CG	5.60	128.18	115.30
1	В	749	ASP	CB-CG-OD2	5.52	123.27	118.30
1	Ε	609	ASP	CB-CG-OD2	5.38	123.14	118.30
1	В	710	ARG	NE-CZ-NH1	-5.31	117.64	120.30
1	Е	676	ASP	CB-CG-OD2	5.25	123.02	118.30
1	F	719	LEU	CB-CG-CD2	5.22	119.88	111.00
1	F	749	ASP	CB-CG-OD2	5.20	122.98	118.30

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	А	1357	0	1394	35	0
1	В	1355	0	1389	44	0
1	С	1355	0	1394	31	0
1	D	1361	0	1401	38	0
1	Е	1423	0	1472	29	0
1	F	1361	0	1403	42	0
2	В	5	0	0	0	0
2	С	5	0	0	0	0
2	D	5	0	0	0	0
2	Е	5	0	0	0	0
2	F	5	0	0	0	0
3	А	134	0	0	11	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	В	129	0	0	17	0
3	С	142	0	0	11	0
3	D	109	0	0	10	0
3	Е	154	0	0	7	0
3	F	124	0	0	12	0
All	All	9029	0	8453	207	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 12.

All (207) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:C:704:THR:HB	3:C:1401:HOH:O	1.27	1.34
1:B:735:LEU:HD13	3:B:1328:HOH:O	1.55	1.07
1:B:606:VAL:HB	3:B:1231:HOH:O	1.56	1.05
1:C:615:THR:HG21	1:C:688:LEU:HD23	1.45	0.99
1:C:739:GLU:HG3	3:C:1409:HOH:O	1.63	0.97
1:A:685[B]:CYS:SG	1:A:707:ILE:CD1	2.56	0.94
1:C:704:THR:CB	3:C:1401:HOH:O	1.92	0.93
1:C:601:LEU:O	1:C:704:THR:HG23	1.71	0.91
1:B:716:ILE:H	1:B:740:ASN:HD21	1.19	0.90
1:A:685[B]:CYS:SG	1:A:707:ILE:HD12	2.16	0.85
1:A:695:ASN:HD21	1:A:773:ASN:H	1.23	0.85
1:F:695:ASN:HD21	1:F:773:ASN:H	1.23	0.85
1:B:766:VAL:HA	3:B:1328:HOH:O	1.75	0.85
1:B:695:ASN:HD21	1:B:773:ASN:H	1.26	0.84
1:A:680:ALA:O	1:A:684[B]:MSE:HG3	1.80	0.82
1:D:625:THR:HG23	3:D:1432:HOH:O	1.79	0.82
1:A:612:THR:HB	3:A:870:HOH:O	1.78	0.82
1:E:723:LEU:HD12	1:E:747:ILE:HD13	1.63	0.81
1:B:665:HIS:HD2	1:C:643:THR:OG1	1.67	0.78
1:C:695:ASN:HD21	1:C:773:ASN:H	1.30	0.77
1:F:747:ILE:HG22	1:F:751:VAL:CG2	2.15	0.76
1:F:639:GLN:NE2	3:F:1713:HOH:O	2.19	0.76
1:B:608:GLY:O	1:B:609:ASP:O	2.05	0.74
1:F:609:ASP:HB3	3:F:1705:HOH:O	1.88	0.74
1:C:680:ALA:O	1:C:684[A]:MSE:HG3	1.89	0.73
1:A:680:ALA:O	1:A:684[A]:MSE:HG2	1.90	0.72
1:F:609:ASP:OD2	3:F:1695:HOH:O	2.07	0.71
1:B:758:HIS:HD2	3:B:1310:HOH:O	1.74	0.71



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:685[B]:CYS:SG	1:A:707:ILE:HD13	2.31	0.69
1:F:727:HIS:HD2	1:F:754:ASP:OD2	1.74	0.69
1:D:646:ARG:NE	1:D:659:TYR:CD2	2.61	0.69
1:C:655:ASN:H	1:C:655:ASN:HD22	1.40	0.69
1:D:655:ASN:HD22	1:D:656:PRO:HD2	1.57	0.69
1:F:598:VAL:HG11	1:F:683:ALA:O	1.91	0.69
1:E:648:ARG:CZ	3:E:1537:HOH:O	2.40	0.68
1:A:596:GLY:HA2	3:A:905:HOH:O	1.95	0.67
1:B:659:TYR:HB2	3:B:1307:HOH:O	1.94	0.67
1:E:648:ARG:NE	3:E:1537:HOH:O	2.28	0.67
1:B:632:GLU:CD	3:B:1306:HOH:O	2.34	0.66
1:D:717:GLY:O	1:D:722:LYS:NZ	2.26	0.66
1:C:680:ALA:O	1:C:684[B]:MSE:HG2	1.95	0.66
1:B:632:GLU:CG	3:B:1306:HOH:O	2.42	0.65
1:D:612:THR:HG23	3:D:1506:HOH:O	1.96	0.65
1:F:655:ASN:CB	3:F:1720:HOH:O	2.46	0.64
1:F:627:THR:OG1	1:F:665:HIS:HE1	1.81	0.64
1:C:665:HIS:HD2	1:D:643:THR:OG1	1.80	0.64
1:D:635:GLN:OE1	3:D:1504:HOH:O	2.15	0.64
1:B:655:ASN:HD22	1:B:656:PRO:N	1.96	0.64
1:B:774:GLU:O	3:B:1317:HOH:O	2.15	0.64
1:D:594:ARG:HH12	1:D:772:GLN:NE2	1.95	0.63
1:A:665:HIS:HD2	1:B:643:THR:OG1	1.82	0.62
1:D:656:PRO:O	1:D:659:TYR:CZ	2.52	0.62
1:C:627:THR:OG1	1:C:665:HIS:HE1	1.82	0.62
1:A:745:GLU:HG2	3:A:909:HOH:O	1.99	0.62
1:A:774:GLU:HB2	1:A:775:PRO:CD	2.30	0.61
1:F:747:ILE:CG2	1:F:751:VAL:CG2	2.79	0.61
1:A:625:THR:HB	3:A:910:HOH:O	1.99	0.60
1:B:666:VAL:CG1	1:B:684[A]:MSE:HE1	2.31	0.60
1:B:625:THR:HG23	3:B:1210:HOH:O	2.02	0.60
1:B:639:GLN:HG2	3:B:1316:HOH:O	2.00	0.60
1:B:605:GLU:OE1	1:B:674:PRO:HG2	2.02	0.60
1:A:655:ASN:ND2	1:A:657:ASP:OD2	2.35	0.60
1:B:606:VAL:CG1	3:B:1231:HOH:O	2.51	0.59
1:E:615:THR:HG22	1:E:666:VAL:HB	1.85	0.58
1:D:685:CYS:O	1:D:689:VAL:HG12	2.02	0.58
1:F:657:ASP:CG	3:F:1640:HOH:O	2.41	0.58
1:D:608:GLY:O	1:D:609:ASP:HB2	2.03	0.58
1:D:752:ILE:HD12	1:D:757:ILE:HD11	1.85	0.58
1:C:594:ARG:N	3:C:1419:HOH:O	2.36	0.58



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:E:627:THR:OG1	1:E:665:HIS:HE1	1.88	0.57
1:A:650:GLU:HG3	3:A:901:HOH:O	2.04	0.57
1:D:752:ILE:HG21	3:D:1493:HOH:O	2.05	0.57
1:F:747:ILE:CG2	1:F:751:VAL:HG21	2.35	0.57
1:C:655:ASN:H	1:C:655:ASN:ND2	2.02	0.57
1:F:655:ASN:HB2	3:F:1720:HOH:O	2.05	0.57
1:A:667:HIS:HE1	3:B:1202:HOH:O	1.88	0.56
1:D:655:ASN:HD22	1:D:656:PRO:CD	2.17	0.56
1:B:735:LEU:CD1	3:B:1328:HOH:O	2.32	0.56
1:D:728:ARG:HB2	3:D:1499:HOH:O	2.06	0.56
1:B:655:ASN:HD22	1:B:656:PRO:CD	2.19	0.56
1:D:721:GLU:OE1	1:D:721:GLU:N	2.38	0.55
1:E:625:THR:HG21	3:E:1651:HOH:O	2.06	0.55
1:A:750:ASN:HD22	1:A:750:ASN:H	1.54	0.55
1:B:769:LEU:HB2	3:B:1328:HOH:O	2.06	0.55
1:D:752:ILE:HD12	1:D:757:ILE:CD1	2.37	0.55
1:B:666:VAL:HG11	1:B:684[A]:MSE:HE1	1.88	0.55
1:A:612:THR:CB	3:A:870:HOH:O	2.47	0.55
1:A:774:GLU:HB2	1:A:775:PRO:HD3	1.88	0.55
1:D:656:PRO:O	1:D:659:TYR:CE2	2.60	0.54
1:B:594:ARG:N	3:B:1324:HOH:O	2.40	0.54
1:A:643:THR:OG1	1:F:665:HIS:HD2	1.89	0.54
1:C:603:TRP:HA	1:C:608:GLY:HA2	1.91	0.53
1:C:712:GLN:HG3	3:C:1407:HOH:O	2.08	0.53
1:F:598:VAL:HG12	1:F:687:ALA:HB2	1.89	0.53
1:A:598:VAL:HG22	1:A:697:VAL:HG21	1.91	0.53
1:F:748:PRO:O	1:F:751:VAL:HG22	2.09	0.53
1:D:601:LEU:CD2	1:D:610:LEU:HD12	2.39	0.53
1:D:762:ARG:HD3	3:D:1492:HOH:O	2.08	0.53
1:A:646:ARG:HD2	3:F:1704:HOH:O	2.09	0.52
1:E:603:TRP:HA	1:E:608:GLY:HA2	1.92	0.52
1:D:689:VAL:HG11	1:D:767:LEU:HD22	1.90	0.52
1:B:598:VAL:CG1	1:B:687:ALA:HB2	2.40	0.51
1:B:599:THR:HG23	1:B:610:LEU:HD13	1.92	0.51
1:D:752:ILE:HG23	1:D:757:ILE:CD1	2.40	0.51
1:B:655:ASN:HD22	1:B:655:ASN:C	2.13	0.51
1:E:665:HIS:HD2	1:F:643:THR:OG1	1.93	0.51
1:A:627:THR:OG1	1:A:667:HIS:HD2	1.93	0.51
1:C:655:ASN:HB2	3:C:1411:HOH:O	2.11	0.50
1:E:738:PHE:CE1	1:E:761:LYS:NZ	2.74	0.50
1:D:601:LEU:HA	1:D:609:ASP:O	2.11	0.50



	At and D	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:D:719:LEU:HG	1:D:723:LEU:HD22	1.93	0.50
1:B:650:GLU:HB2	1:B:651:LYS:HE3	1.94	0.50
1:F:603:TRP:HA	1:F:608:GLY:HA3	1.93	0.50
1:A:627:THR:OG1	1:A:665:HIS:HE1	1.94	0.50
1:A:625:THR:HG23	3:A:865:HOH:O	2.10	0.50
1:D:752:ILE:HG23	1:D:757:ILE:HD12	1.94	0.50
1:A:774:GLU:CB	1:A:775:PRO:CD	2.89	0.49
1:B:655:ASN:ND2	1:B:657:ASP:H	2.11	0.49
1:E:719:LEU:HD22	1:E:723:LEU:HG	1.95	0.49
1:F:604:THR:H	1:F:608:GLY:HA2	1.78	0.49
1:B:666:VAL:HG11	1:B:684[A]:MSE:CE	2.43	0.49
1:D:667:HIS:HB3	1:E:709:LEU:HD22	1.95	0.49
1:D:655:ASN:ND2	1:D:656:PRO:HD2	2.25	0.49
1:C:604:THR:HG22	1:C:675:LYS:HG2	1.94	0.49
1:C:698:ARG:HD3	3:C:1428:HOH:O	2.12	0.48
1:F:773:ASN:O	1:F:774:GLU:CB	2.61	0.48
3:A:786:HOH:O	1:F:667:HIS:HE1	1.95	0.48
1:F:720:LYS:HG3	3:F:1719:HOH:O	2.13	0.48
1:A:625:THR:CB	3:A:910:HOH:O	2.59	0.48
1:C:679:ALA:HB1	1:C:704:THR:HG22	1.95	0.47
1:E:712:GLN:HG2	3:E:1642:HOH:O	2.15	0.47
1:B:655:ASN:HD22	1:B:656:PRO:HD2	1.79	0.47
1:D:597:GLN:HE22	1:E:710:ARG:HD3	1.79	0.47
1:B:704:THR:O	1:B:737:PRO:HD3	2.14	0.47
1:B:742:ARG:NH2	3:B:1311:HOH:O	2.47	0.47
1:A:639:GLN:NE2	3:A:867:HOH:O	2.40	0.47
1:A:617[B]:CYS:HB3	1:A:664:ILE:HD12	1.97	0.47
1:F:712:GLN:NE2	3:F:1674:HOH:O	2.48	0.47
1:C:594:ARG:O	1:C:616:ALA:HA	2.14	0.47
1:F:645:VAL:HG21	1:F:688:LEU:HD23	1.97	0.47
1:E:728:ARG:HD3	3:E:1621:HOH:O	2.15	0.46
1:F:598:VAL:CG2	1:F:703:MSE:HE3	2.45	0.46
1:B:623:LYS:O	1:B:624:LEU:HD22	2.15	0.46
1:A:617[A]:CYS:HB3	1:A:664:ILE:CD1	2.46	0.46
1:C:712:GLN:NE2	3:C:1333:HOH:O	2.49	0.46
1:D:742:ARG:HD2	3:D:1488:HOH:O	2.17	0.45
1:B:627:THR:OG1	1:B:665:HIS:HE1	1.98	0.45
1:E:648:ARG:NH2	3:E:1537:HOH:O	2.47	0.45
1:C:594:ARG:CA	3:C:1421:HOH:O	2.65	0.45
1:C:618:VAL:HG11	1:D:646:ARG:HB3	1.99	0.45
1:A:627:THR:OG1	1:A:667:HIS:CD2	2.70	0.45



	At and 0	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:F:655:ASN:ND2	3:F:1683:HOH:O	2.50	0.45
1:B:747:ILE:CG2	1:B:752:ILE:HD12	2.47	0.45
1:D:747:ILE:HG23	1:D:748:PRO:HD2	1.99	0.45
1:E:767:LEU:HB3	1:E:775:PRO:HG2	1.99	0.45
1:D:597:GLN:HE22	1:E:710:ARG:NH1	2.14	0.45
1:D:608:GLY:C	3:D:1491:HOH:O	2.55	0.44
1:F:642:LEU:HD23	1:F:688:LEU:HD21	2.00	0.44
1:F:734:VAL:CG2	1:F:757:ILE:HG12	2.47	0.44
1:E:707:ILE:HG13	1:E:708:THR:N	2.33	0.44
1:A:594:ARG:C	1:A:595:VAL:HG23	2.38	0.44
1:A:646:ARG:CD	3:F:1704:HOH:O	2.65	0.44
1:D:608:GLY:CA	3:D:1491:HOH:O	2.64	0.44
1:F:695:ASN:HD21	1:F:773:ASN:N	2.02	0.44
1:F:650:GLU:HG2	1:F:656:PRO:HG3	2.00	0.44
1:B:598:VAL:HG11	1:B:687:ALA:HB2	2.00	0.44
1:B:624:LEU:HD13	1:B:664:ILE:HB	2.00	0.44
1:E:708:THR:HG22	1:E:712:GLN:O	2.18	0.44
1:E:723:LEU:HD12	1:E:747:ILE:CD1	2.40	0.44
1:F:701:VAL:HG12	1:F:733:THR:HB	1.99	0.43
1:E:667:HIS:HB3	1:F:709:LEU:HD22	1.99	0.43
1:C:698:ARG:HB3	1:C:700:ASP:OD2	2.18	0.43
1:E:774:GLU:HA	1:E:775:PRO:HD3	1.89	0.43
1:A:638:ILE:HG12	1:A:684[B]:MSE:SE	2.68	0.43
1:B:632:GLU:HG3	3:B:1306:HOH:O	2.14	0.43
1:C:700:ASP:HA	3:C:1442:HOH:O	2.17	0.43
1:F:758:HIS:CE1	3:F:1709:HOH:O	2.72	0.43
1:F:598:VAL:CG1	1:F:687:ALA:HB2	2.49	0.43
1:A:648:ARG:NH1	3:A:834:HOH:O	2.19	0.42
1:F:648:ARG:HA	1:F:651:LYS:CE	2.50	0.42
1:F:615:THR:HG22	1:F:666:VAL:HG22	2.01	0.42
1:D:657:ASP:OD2	1:D:657:ASP:C	2.58	0.42
1:E:781:VAL:O	1:E:781:VAL:HG13	2.19	0.42
1:D:594:ARG:HD3	1:D:594:ARG:HA	1.81	0.42
1:E:614:GLU:OE2	1:F:710:ARG:HG3	2.20	0.42
1:B:666:VAL:HG13	1:B:684[A]:MSE:HE1	2.00	0.41
1:D:741:LYS:HE3	1:D:741:LYS:HB3	1.93	0.41
1:B:622:GLY:HA2	1:B:662:ARG:O	2.20	0.41
1:D:646:ARG:HD2	3:D:1467:HOH:O	2.19	0.41
1:F:626:TYR:HA	1:F:666:VAL:O	2.19	0.41
1:F:698:ARG:O	1:F:701:VAL:HG22	2.20	0.41
1:B:737:PRO:HD2	1:B:740:ASN:HD22	1.86	0.41



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:688:LEU:HG	3:C:1431:HOH:O	2.20	0.41
1:E:594:ARG:HB3	1:E:597:GLN:HB3	2.03	0.41
1:F:604:THR:N	1:F:608:GLY:HA2	2.35	0.41
1:B:597:GLN:OE1	1:C:710:ARG:HD3	2.20	0.40
1:E:732:LYS:HG3	1:E:733:THR:N	2.35	0.40
1:E:772:GLN:NE2	3:E:1586:HOH:O	2.53	0.40
1:E:611:LEU:HD22	1:E:675:LYS:HD3	2.04	0.40
1:F:627:THR:OG1	1:F:667:HIS:HD2	2.04	0.40
1:F:716:ILE:HD11	1:F:719:LEU:HD23	2.03	0.40
1:E:738:PHE:CZ	1:E:761:LYS:NZ	2.86	0.40
1:A:750:ASN:HD22	1:A:750:ASN:N	2.18	0.40
1:C:638:ILE:HG12	1:C:684[A]:MSE:SE	2.71	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	Perce	ntiles
1	А	183/200~(92%)	177 (97%)	4 (2%)	2 (1%)	14	3
1	В	182/200~(91%)	178 (98%)	3 (2%)	1 (0%)	29	12
1	С	182/200~(91%)	178 (98%)	4 (2%)	0	100	100
1	D	181/200 (90%)	174 (96%)	4 (2%)	3 (2%)	9	1
1	Ε	189/200~(94%)	183 (97%)	4 (2%)	2 (1%)	14	3
1	F	180/200~(90%)	175 (97%)	4 (2%)	1 (1%)	25	10
All	All	1097/1200~(91%)	1065 (97%)	23 (2%)	9 (1%)	19	6

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	774	GLU
	<i>a</i>	1	



Contre	Contentaca from prettous page								
Mol	Chain	Res	Type						
1	В	609	ASP						
1	D	609	ASP						
1	Ε	606	VAL						
1	Е	609	ASP						
1	А	595	VAL						
1	D	606	VAL						
1	F	606	VAL						
1	D	607	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	Pe	erce	ntil	es
1	А	148/156~(95%)	133~(90%)	15 (10%)		7	1	
1	В	147/156~(94%)	130~(88%)	17~(12%)		5	0	
1	С	147/156~(94%)	127~(86%)	20 (14%)		3	0	
1	D	147/156~(94%)	130~(88%)	17~(12%)		5	0	
1	Ε	153/156~(98%)	136~(89%)	17 (11%)		6	1	
1	F	146/156~(94%)	134~(92%)	12 (8%)		11	1	
All	All	888/936~(95%)	790 (89%)	98 (11%)		6	1	

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	597	GLN
1	А	610	LEU
1	А	611	LEU
1	А	612	THR
1	А	623	LYS
1	А	650	GLU
1	А	652	LEU
1	А	665	HIS
1	А	670	GLU
1	А	695	ASN



Mol	Chain	Res	Type
1	А	700	ASP
1	А	724	LEU
1	А	732	LYS
1	А	742	ARG
1	А	750	ASN
1	В	597	GLN
1	В	605	GLU
1	В	606	VAL
1	В	610	LEU
1	В	652	LEU
1	В	655	ASN
1	В	665	HIS
1	В	695	ASN
1	В	720	LYS
1	В	723	LEU
1	В	724	LEU
1	В	728	ARG
1	В	741	LYS
1	В	745	GLU
1	В	752	ILE
1	В	769	LEU
1	В	772	GLN
1	С	599	THR
1	С	605	GLU
1	С	606	VAL
1	С	609	ASP
1	С	610	LEU
1	С	612	THR
1	С	621	LYS
1	С	623	LYS
1	С	626	TYR
1	C	632	GLU
1	C	650	GLU
1	C	655	ASN
1	C	665	HIS
1	C	695	ASN
1	C	710	ARG
1	C	719	LEU
1	C	723	LEU
1	C	728	ARG
1	С	732	LYS
1	С	742	ARG



Mol	Chain	Res	Type
1	D	594	ARG
1	D	604	THR
1	D	606	VAL
1	D	609	ASP
1	D	625	THR
1	D	650	GLU
1	D	655	ASN
1	D	659	TYR
1	D	660	GLU
1	D	661	LYS
1	D	662	ARG
1	D	710	ARG
1	D	721	GLU
1	D	723	LEU
1	D	741	LYS
1	D	751	VAL
1	D	754	ASP
1	Е	594	ARG
1	Е	605	GLU
1	Е	606	VAL
1	Е	610	LEU
1	Е	624	LEU
1	Е	650	GLU
1	Е	651	LYS
1	Е	665	HIS
1	Е	709	LEU
1	Е	712	GLN
1	Е	719	LEU
1	Е	720	LYS
1	Е	732	LYS
1	Е	742	ARG
1	Е	750	ASN
1	Е	757	ILE
1	E	762	ARG
1	F	626	TYR
1	F	642	LEU
1	F	651	LYS
1	F	655	ASN
1	F	665	HIS
1	F	695	ASN
1	F	710	ARG
1	F	719	LEU



Continued from previous page...

Mol	Chain	Res	Type
1	F	724	LEU
1	F	735	LEU
1	F	741	LYS
1	F	774	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	665	HIS
1	А	667	HIS
1	А	695	ASN
1	А	750	ASN
1	В	655	ASN
1	В	665	HIS
1	В	695	ASN
1	В	740	ASN
1	В	758	HIS
1	В	773	ASN
1	С	655	ASN
1	С	665	HIS
1	С	695	ASN
1	D	597	GLN
1	D	655	ASN
1	D	772	GLN
1	Е	639	GLN
1	Ε	665	HIS
1	Е	750	ASN
1	Е	779	GLN
1	F	635	GLN
1	F	665	HIS
1	F	667	HIS
1	F	695	ASN
1	F	727	HIS

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).

Mal	Turne	Chain	Dec	Tink	В	ond leng	gths	E	Bond ang	gles
INIOI	туре	Unain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	C	1301	-	4,4,4	0.37	0	$6,\!6,\!6$	1.01	0
2	SO4	В	1201	-	4,4,4	0.26	0	6,6,6	0.65	0
2	SO4	F	1601	-	4,4,4	0.24	0	6,6,6	0.44	0
2	SO4	Е	1501	-	4,4,4	0.11	0	6,6,6	0.44	0
2	SO4	D	1401	-	4,4,4	0.24	0	6,6,6	0.82	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 (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, 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	А	179/200~(89%)	0.39	10 (5%) 24	30	9, 19, 36, 49	0
1	В	179/200~(89%)	0.60	14 (7%) 13	17	12, 23, 42, 49	0
1	С	179/200~(89%)	0.46	10 (5%) 24	30	11, 20, 38, 42	0
1	D	179/200~(89%)	0.74	11 (6%) 21	26	15, 24, 43, 56	0
1	Е	187/200~(93%)	0.62	20 (10%) 6	8	14, 24, 45, 51	0
1	F	179/200~(89%)	0.52	13 (7%) 15	20	18, 28, 44, 54	0
All	All	1082/1200~(90%)	0.55	78 (7%) 15	20	9, 23, 42, 56	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	607	GLY	8.2
1	D	607	GLY	7.8
1	Е	606	VAL	7.4
1	D	603	TRP	7.4
1	С	606	VAL	6.7
1	D	608	GLY	6.6
1	Е	607	GLY	6.0
1	F	606	VAL	5.6
1	D	659	TYR	5.0
1	А	595	VAL	5.0
1	В	606	VAL	4.7
1	В	607	GLY	4.7
1	D	606	VAL	4.4
1	В	751	VAL	4.4
1	В	750	ASN	4.2
1	C	659	TYR	4.1
1	D	605	GLU	4.1
1	В	774	GLU	4.0
1	Е	658	PHE	3.8



Mol	Chain	Res	Type	RSRZ
1	С	602	ALA	3.6
1	А	699	ALA	3.6
1	D	602	ALA	3.5
1	Е	728	ARG	3.5
1	В	728	ARG	3.4
1	В	746	GLU	3.4
1	А	594	ARG	3.4
1	А	774	GLU	3.4
1	F	593	ASN	3.3
1	В	752	ILE	3.3
1	Е	748	PRO	3.2
1	С	657	ASP	3.2
1	Е	603	TRP	3.2
1	В	773	ASN	3.1
1	В	697	VAL	3.1
1	Е	751	VAL	3.0
1	Е	750	ASN	3.0
1	С	732	LYS	2.9
1	F	651	LYS	2.9
1	Е	745	GLU	2.8
1	D	742	ARG	2.8
1	В	605	GLU	2.7
1	Е	746	GLU	2.7
1	А	772	GLN	2.7
1	В	608	GLY	2.7
1	Е	723	LEU	2.7
1	С	607	GLY	2.6
1	Е	738	PHE	2.6
1	А	742	ARG	2.5
1	Е	752	ILE	2.5
1	Е	608	GLY	2.5
1	С	655	ASN	2.4
1	В	742	ARG	2.4
1	F	774	GLU	2.4
1	F	660	GLU	2.4
1	В	730	GLY	2.4
1	F	746	GLU	2.4
1	А	596	GLY	2.4
1	С	595	VAL	2.3
1	С	742	ARG	2.3
1	F	773	ASN	2.3
1	F	623	LYS	2.3



Mol	Chain	Res	Type	RSRZ
1	А	745	GLU	2.3
1	D	621	LYS	2.3
1	F	742	ARG	2.2
1	F	772	GLN	2.2
1	С	699	ALA	2.2
1	Ε	661	LYS	2.2
1	Е	611	LEU	2.2
1	Ε	720	LYS	2.2
1	А	652	LEU	2.2
1	Ε	601	LEU	2.2
1	F	762	ARG	2.1
1	D	752	ILE	2.1
1	Е	754	ASP	2.1
1	А	659	TYR	2.1
1	F	745	GLU	2.1
1	D	604	THR	2.1
1	Е	749	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 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	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
2	SO4	Е	1501	5/5	0.92	0.14	44,48,50,52	0
2	SO4	D	1401	5/5	0.95	0.14	39,40,44,45	0
2	SO4	В	1201	5/5	0.96	0.12	25,31,34,37	0
2	SO4	F	1601	5/5	0.96	0.12	34,37,43,45	0
2	SO4	С	1301	5/5	0.98	0.07	27,28,35,36	0



6.5 Other polymers (i)

There are no such residues in this entry.

