



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:02 PM GMT

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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) 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

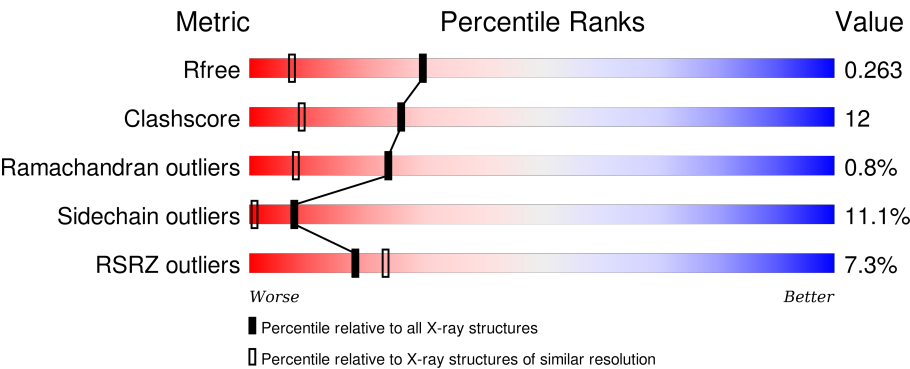
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R <sub>free</sub>	91344	1609 (1.76-1.76)
Clashscore	102246	1730 (1.76-1.76)
Ramachandran outliers	100387	1711 (1.76-1.76)
Sidechain outliers	100360	1711 (1.76-1.76)
RSRZ outliers	91569	1610 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . 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	 5% 70% 18% • 9%
1	B	200	 7% 64% 23% • • 9%
1	C	200	 5% 68% 21% • • 9%
1	D	200	 6% 69% 18% 5% • 9%
1	E	200	 10% 73% 19% 5% 5%

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Mol	Chain	Length	Quality of chain
1	F	200	<p>7% 65% 20% 6% 9%</p>

## 2 Entry composition

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.

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	182	Total	C	N	O	S	Se	0	3	0
			1357	854	235	259	5	4			
1	B	182	Total	C	N	O	S	Se	0	2	0
			1355	854	235	259	4	3			
1	C	182	Total	C	N	O	S	Se	0	2	0
			1355	853	235	259	4	4			
1	D	182	Total	C	N	O	S	Se	0	1	0
			1361	858	238	259	3	3			
1	E	191	Total	C	N	O	S	Se	0	0	0
			1423	895	249	272	3	4			
1	F	182	Total	C	N	O	S	Se	0	0	0
			1361	856	239	260	3	3			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	679	ALA	SER	ENGINEERED	UNP P0A9M0
B	679	ALA	SER	ENGINEERED	UNP P0A9M0
C	679	ALA	SER	ENGINEERED	UNP P0A9M0
D	679	ALA	SER	ENGINEERED	UNP P0A9M0
E	679	ALA	SER	ENGINEERED	UNP P0A9M0
F	679	ALA	SER	ENGINEERED	UNP P0A9M0

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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		

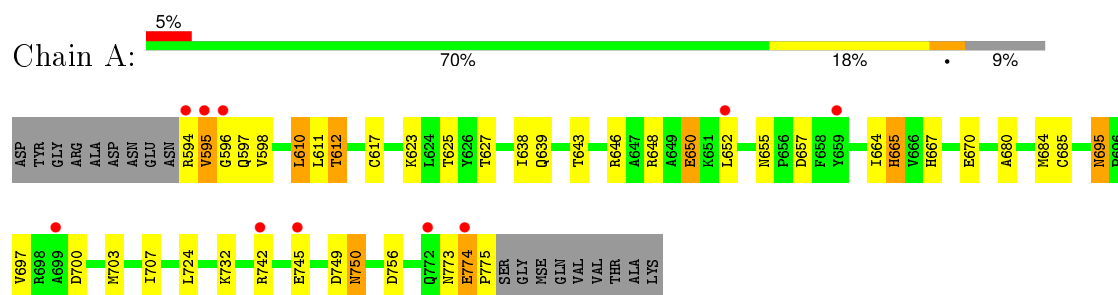
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	134	Total	O	0	0
			134	134		
3	B	129	Total	O	0	0
			129	129		
3	C	142	Total	O	0	0
			142	142		
3	D	109	Total	O	0	0
			109	109		
3	E	154	Total	O	0	0
			154	154		
3	F	124	Total	O	0	0
			124	124		

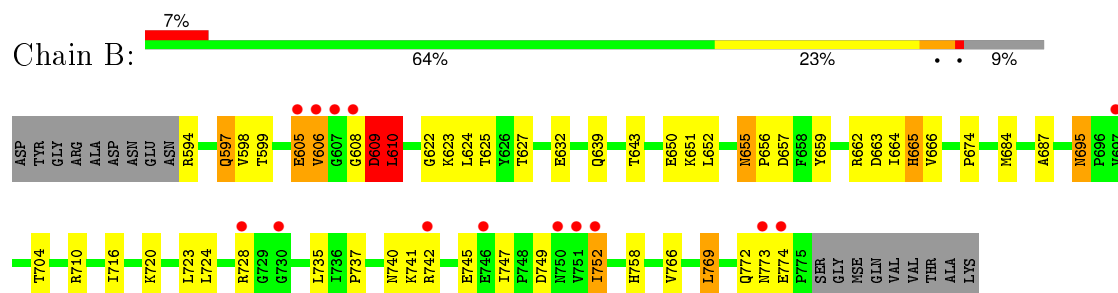
### 3 Residue-property plots [i](#)

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 ( $\text{RSRZ} > 2$ ). 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.

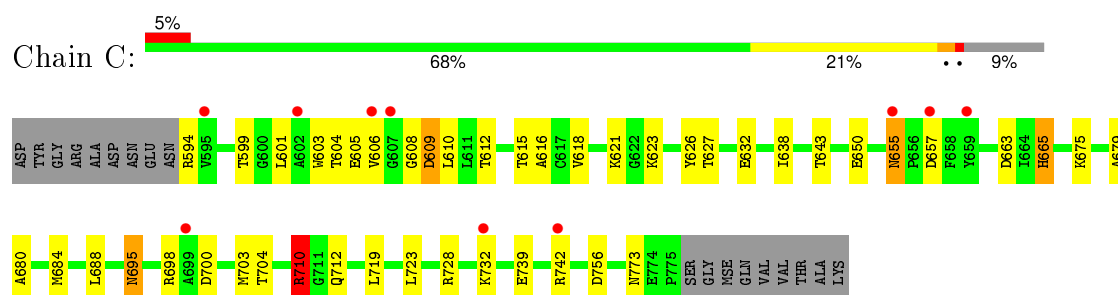
- Molecule 1: ATP-dependent protease La



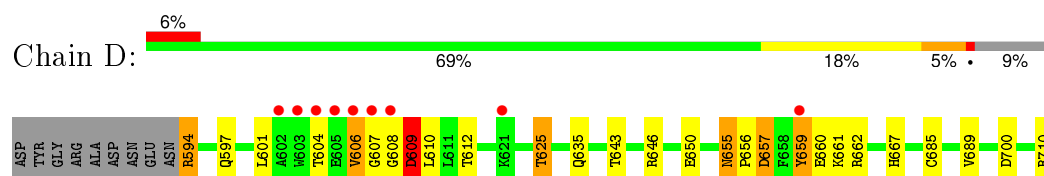
- Molecule 1: ATP-dependent protease La



- Molecule 1: ATP-dependent protease La

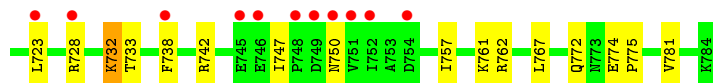
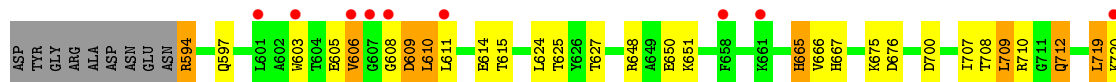


- Molecule 1: ATP-dependent protease La

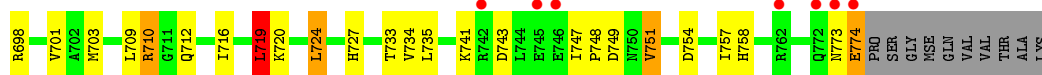




- Molecule 1: ATP-dependent protease La



- Molecule 1: ATP-dependent protease La



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.37Å 86.37Å 124.16Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.96 – 1.75 19.94 – 1.75	Depositor EDS
% Data completeness (in resolution range)	93.5 (19.96-1.75) 93.6 (19.94-1.75)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.83 (at 1.74Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.205 , 0.263 0.209 , 0.263	Depositor DCC
$R_{free}$ test set	9386 reflections (10.63%)	DCC
Wilson B-factor (Å <sup>2</sup> )	24.8	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 45.2	EDS
Estimated twinning fraction	0.015 for -h,-k,l 0.034 for h,-h-k,-l 0.017 for -k,-h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 97715 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9029	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.86	1/1390 (0.1%)	0.97	3/1883 (0.2%)
1	B	0.78	0/1384	0.95	5/1875 (0.3%)
1	C	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	E	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	Z	Observed(Å)	Ideal(Å)
1	A	703	MSE	SE-CE	-7.46	1.51	1.95
1	C	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(°)	Ideal(°)
1	C	663	ASP	CB-CG-OD2	7.79	125.31	118.30
1	B	609	ASP	CB-CG-OD2	7.57	125.11	118.30
1	B	610	LEU	CA-CB-CG	7.34	132.19	115.30
1	A	756	ASP	CB-CG-OD2	7.17	124.75	118.30
1	C	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	E	610	LEU	CA-CB-CG	6.60	130.47	115.30
1	C	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	C	609	ASP	CB-CG-OD2	6.34	124.00	118.30
1	C	710	ARG	NE-CZ-NH1	6.22	123.41	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	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	E	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	B	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	A	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	A	610	LEU	CA-CB-CG	5.60	128.18	115.30
1	B	749	ASP	CB-CG-OD2	5.52	123.27	118.30
1	E	609	ASP	CB-CG-OD2	5.38	123.14	118.30
1	B	710	ARG	NE-CZ-NH1	-5.31	117.64	120.30
1	E	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	A	1357	0	1394	35	0
1	B	1355	0	1389	44	0
1	C	1355	0	1394	31	0
1	D	1361	0	1401	38	0
1	E	1423	0	1472	29	0
1	F	1361	0	1403	42	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	134	0	0	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	129	0	0	17	0
3	C	142	0	0	11	0
3	D	109	0	0	10	0
3	E	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 distance (Å)	Clash 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:D:625:THR:HG23	3:D:1432:HOH:O	1.79	0.82
1:A:680:ALA:O	1:A:684[B]:MSE:HG3	1.80	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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:HD22	1:C:655:ASN:H	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:B:659:TYR:HB2	3:B:1307:HOH:O	1.94	0.67
1:A:596:GLY:HA2	3:A:905:HOH:O	1.95	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:D:656:PRO:O	1:D:659:TYR:CZ	2.52	0.62
1:A:665:HIS:HD2	1:B:643:THR:OG1	1.82	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:F:747:ILE:CG2	1:F:751:VAL:CG2	2.79	0.61
1:A:774:GLU:HB2	1:A:775:PRO:CD	2.30	0.61
1:B:666:VAL:CG1	1:B:684[A]:MSE:HE1	2.31	0.60
1:A:625:THR:HB	3:A:910:HOH:O	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:627:THR:OG1	1:E:665:HIS:HE1	1.88	0.57
1:D:752:ILE:HG21	3:D:1493:HOH:O	2.05	0.57
1:A:650:GLU:HG3	3:A:901:HOH:O	2.04	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:F:748:PRO:O	1:F:751:VAL:HG22	2.09	0.53
1:A:598:VAL:HG22	1:A:697:VAL:HG21	1.91	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:D:752:ILE:HG23	1:D:757:ILE:CD1	2.40	0.51
1:B:599:THR:HG23	1:B:610:LEU:HD13	1.92	0.51
1:B:655:ASN:C	1:B:655:ASN:HD22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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:F:773:ASN:O	1:F:774:GLU:CB	2.61	0.48
1:C:698:ARG:HD3	3:C:1428:HOH:O	2.12	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:F:712:GLN:NE2	3:F:1674:HOH:O	2.48	0.47
1:A:617[B]:CYS:HB3	1:A:664:ILE:HD12	1.97	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:F:598:VAL:CG2	1:F:703:MSE:HE3	2.45	0.46
1:E:728:ARG:HD3	3:E:1621:HOH:O	2.15	0.46
1:B:623:LYS:O	1:B:624:LEU:HD22	2.15	0.46
1:C:712:GLN:NE2	3:C:1333:HOH:O	2.49	0.46
1:A:617[A]:CYS:HB3	1:A:664:ILE:CD1	2.46	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:618:VAL:HG11	1:D:646:ARG:HB3	1.99	0.45
1:C:594:ARG:CA	3:C:1421:HOH:O	2.65	0.45
1:F:655:ASN:ND2	3:F:1683:HOH:O	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:627:THR:OG1	1:A:667:HIS:CD2	2.70	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:F:695:ASN:HD21	1:F:773:ASN:N	2.02	0.44
1:D:608:GLY:CA	3:D:1491:HOH:O	2.64	0.44
1:A:646:ARG:CD	3:F:1704:HOH:O	2.65	0.44
1:A:594:ARG:C	1:A:595:VAL:HG23	2.38	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:E:708:THR:HG22	1:E:712:GLN:O	2.18	0.44
1:B:624:LEU:HD13	1:B:664:ILE:HB	2.00	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:HG13	1:E:781:VAL:O	2.19	0.42
1:D:594:ARG:HA	1:D:594:ARG:HD3	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:HB3	1:D:741:LYS:HE3	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:C:688:LEU:HG	3:C:1431:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:737:PRO:HD2	1:B:740:ASN:HD22	1.86	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: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:611:LEU:HD22	1:E:675:LYS:HD3	2.04	0.40
1:E:738:PHE:CZ	1:E:761:LYS:NZ	2.86	0.40
1:C:638:ILE:HG12	1:C:684[A]:MSE:SE	2.71	0.40
1:A:750:ASN:HD22	1:A:750:ASN:N	2.18	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	183/200 (92%)	177 (97%)	4 (2%)	2 (1%)	17	4
1	B	182/200 (91%)	178 (98%)	3 (2%)	1 (0%)	34	14
1	C	182/200 (91%)	178 (98%)	4 (2%)	0	100	100
1	D	181/200 (90%)	174 (96%)	4 (2%)	3 (2%)	11	2
1	E	189/200 (94%)	183 (97%)	4 (2%)	2 (1%)	17	4
1	F	180/200 (90%)	175 (97%)	4 (2%)	1 (1%)	30	12
All	All	1097/1200 (91%)	1065 (97%)	23 (2%)	9 (1%)	24	8

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	774	GLU

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Mol	Chain	Res	Type
1	B	609	ASP
1	D	609	ASP
1	E	606	VAL
1	E	609	ASP
1	A	595	VAL
1	D	606	VAL
1	F	606	VAL
1	D	607	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	148/156 (95%)	133 (90%)	15 (10%)	9	1
1	B	147/156 (94%)	130 (88%)	17 (12%)	7	1
1	C	147/156 (94%)	127 (86%)	20 (14%)	5	0
1	D	147/156 (94%)	130 (88%)	17 (12%)	7	1
1	E	153/156 (98%)	136 (89%)	17 (11%)	8	1
1	F	146/156 (94%)	134 (92%)	12 (8%)	14	2
All	All	888/936 (95%)	790 (89%)	98 (11%)	8	1

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

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

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Mol	Chain	Res	Type
1	A	700	ASP
1	A	724	LEU
1	A	732	LYS
1	A	742	ARG
1	A	750	ASN
1	B	597	GLN
1	B	605	GLU
1	B	606	VAL
1	B	610	LEU
1	B	652	LEU
1	B	655	ASN
1	B	665	HIS
1	B	695	ASN
1	B	720	LYS
1	B	723	LEU
1	B	724	LEU
1	B	728	ARG
1	B	741	LYS
1	B	745	GLU
1	B	752	ILE
1	B	769	LEU
1	B	772	GLN
1	C	599	THR
1	C	605	GLU
1	C	606	VAL
1	C	609	ASP
1	C	610	LEU
1	C	612	THR
1	C	621	LYS
1	C	623	LYS
1	C	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	C	732	LYS
1	C	742	ARG

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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	E	594	ARG
1	E	605	GLU
1	E	606	VAL
1	E	610	LEU
1	E	624	LEU
1	E	650	GLU
1	E	651	LYS
1	E	665	HIS
1	E	709	LEU
1	E	712	GLN
1	E	719	LEU
1	E	720	LYS
1	E	732	LYS
1	E	742	ARG
1	E	750	ASN
1	E	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

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

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

Mol	Chain	Res	Type
1	A	665	HIS
1	A	667	HIS
1	A	695	ASN
1	A	750	ASN
1	B	655	ASN
1	B	665	HIS
1	B	695	ASN
1	B	740	ASN
1	B	758	HIS
1	B	773	ASN
1	C	655	ASN
1	C	665	HIS
1	C	695	ASN
1	D	597	GLN
1	D	655	ASN
1	D	772	GLN
1	E	639	GLN
1	E	665	HIS
1	E	750	ASN
1	E	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 ⓘ

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 ⓘ

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	B	1201	-	4,4,4	0.73	0	6,6,6	0.58	0
2	SO4	C	1301	-	4,4,4	0.57	0	6,6,6	0.97	0
2	SO4	D	1401	-	4,4,4	0.57	0	6,6,6	1.21	1 (16%)
2	SO4	E	1501	-	4,4,4	0.34	0	6,6,6	0.45	0
2	SO4	F	1601	-	4,4,4	0.52	0	6,6,6	0.29	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
2	SO4	B	1201	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1301	-	-	0/0/0/0	0/0/0/0
2	SO4	D	1401	-	-	0/0/0/0	0/0/0/0
2	SO4	E	1501	-	-	0/0/0/0	0/0/0/0
2	SO4	F	1601	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1401	SO4	O2-S-O1	2.64	117.87	109.50

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 ⓘ

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 ⓘ

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	179/200 (89%)	0.41	10 (5%) 28 33	9, 19, 36, 49	0
1	B	179/200 (89%)	0.62	14 (7%) 16 20	12, 23, 42, 49	0
1	C	179/200 (89%)	0.48	10 (5%) 28 33	11, 20, 38, 42	0
1	D	179/200 (89%)	0.77	11 (6%) 25 29	15, 24, 43, 56	0
1	E	187/200 (93%)	0.64	20 (10%) 8 10	14, 24, 45, 51	0
1	F	179/200 (89%)	0.55	14 (7%) 16 20	18, 28, 44, 54	0
All	All	1082/1200 (90%)	0.58	79 (7%) 18 23	9, 23, 42, 56	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	607	GLY	8.2
1	D	607	GLY	8.0
1	D	603	TRP	7.5
1	E	606	VAL	7.4
1	C	606	VAL	6.7
1	D	608	GLY	6.6
1	E	607	GLY	6.1
1	F	606	VAL	5.6
1	D	659	TYR	5.1
1	A	595	VAL	5.0
1	B	607	GLY	4.7
1	B	606	VAL	4.7
1	D	606	VAL	4.5
1	B	751	VAL	4.4
1	B	750	ASN	4.3
1	C	659	TYR	4.2
1	D	605	GLU	4.1
1	B	774	GLU	4.0
1	E	658	PHE	3.8

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

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Mol	Chain	Res	Type	RSRZ
1	A	745	GLU	2.3
1	D	621	LYS	2.3
1	C	699	ALA	2.3
1	E	611	LEU	2.3
1	E	601	LEU	2.2
1	F	742	ARG	2.2
1	F	772	GLN	2.2
1	A	652	LEU	2.2
1	E	661	LYS	2.2
1	E	720	LYS	2.2
1	D	752	ILE	2.2
1	A	659	TYR	2.2
1	F	762	ARG	2.1
1	E	754	ASP	2.1
1	D	604	THR	2.1
1	F	745	GLU	2.1
1	E	749	ASP	2.1
1	F	621	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 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	SO4	F	1601	5/5	0.96	0.12	1.97	34,37,43,45	0
2	SO4	B	1201	5/5	0.96	0.12	1.05	25,31,34,37	0
2	SO4	E	1501	5/5	0.92	0.14	1.01	44,48,50,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	D	1401	5/5	0.95	0.14	-0.03	39,40,44,45	0
2	SO4	C	1301	5/5	0.98	0.07	-0.37	27,28,35,36	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.