



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:38 AM UTC

PDB ID : 1RRE / pdb_00001rre
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 ⓘ 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:

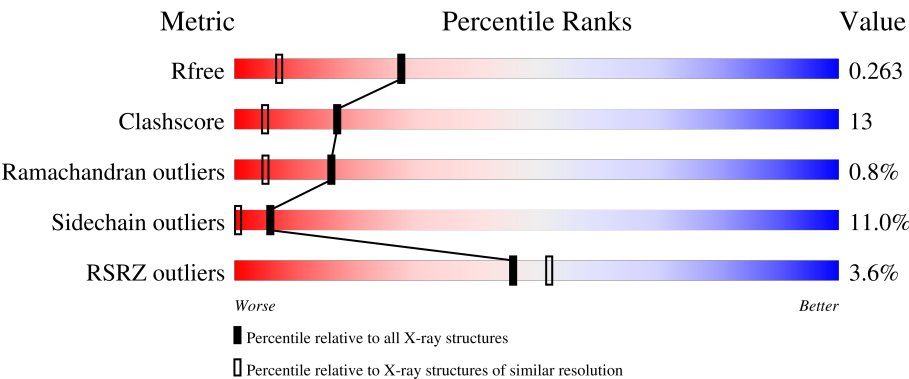
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance 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 _{free}	180053	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (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 $\leq 5\%$. 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	2% 70% 17% • 9%
1	B	200	5% 64% 23% • 9%
1	C	200	2% 68% 22% • 9%
1	D	200	4% 68% 18% 6% 9%
1	E	200	4% 72% 20% • •

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Mol	Chain	Length	Quality of chain
1	F	200	% 64%22%•9%

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.

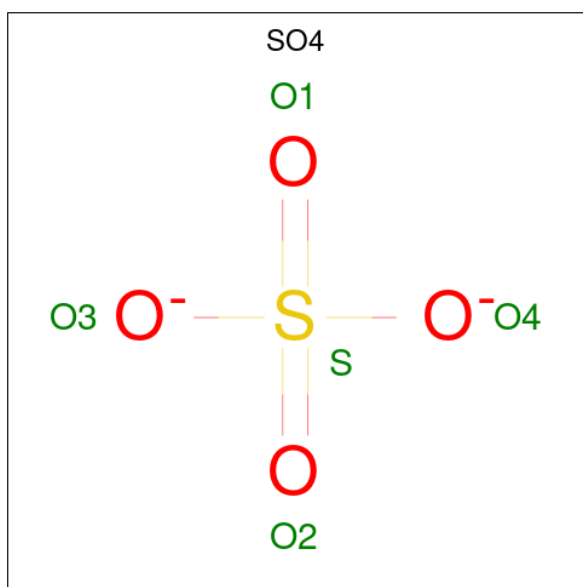
- Molecule 1 is a protein called ATP-dependent protease La.

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 mutation	UNP P0A9M0
B	679	ALA	SER	engineered mutation	UNP P0A9M0
C	679	ALA	SER	engineered mutation	UNP P0A9M0
D	679	ALA	SER	engineered mutation	UNP P0A9M0
E	679	ALA	SER	engineered mutation	UNP P0A9M0
F	679	ALA	SER	engineered mutation	UNP P0A9M0

- 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		

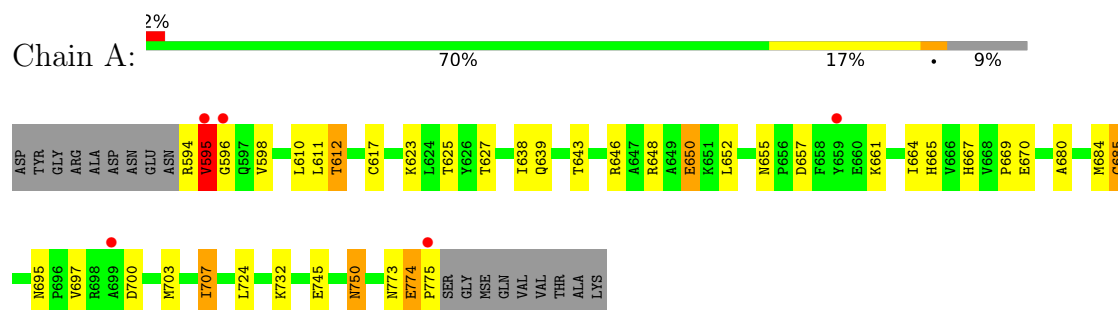
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	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		

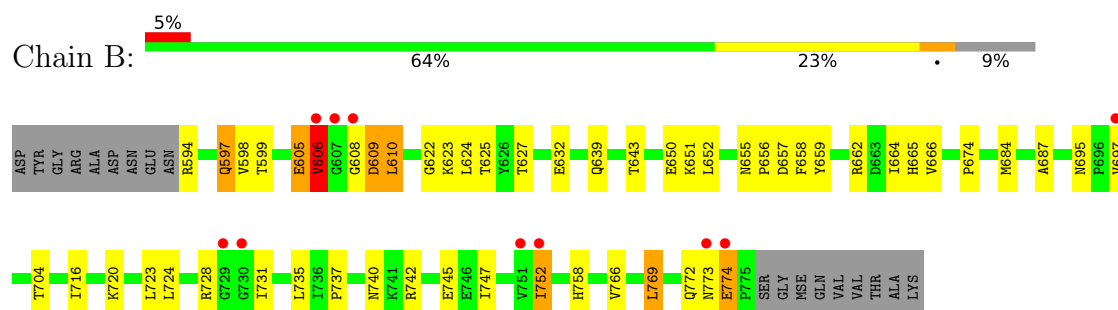
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

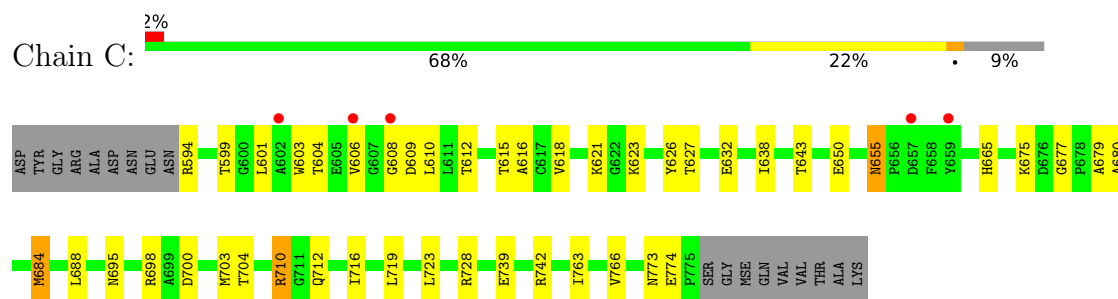
- Molecule 1: ATP-dependent protease La



- Molecule 1: ATP-dependent protease La

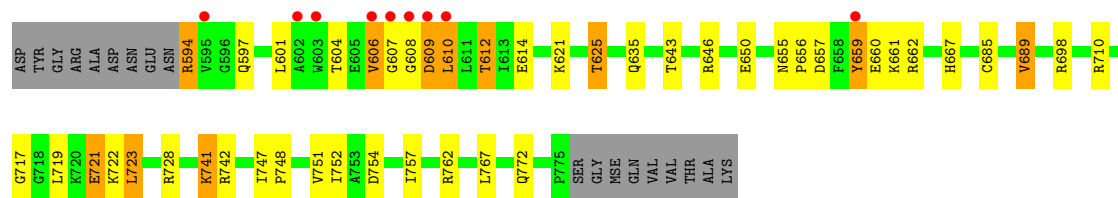


- Molecule 1: ATP-dependent protease La

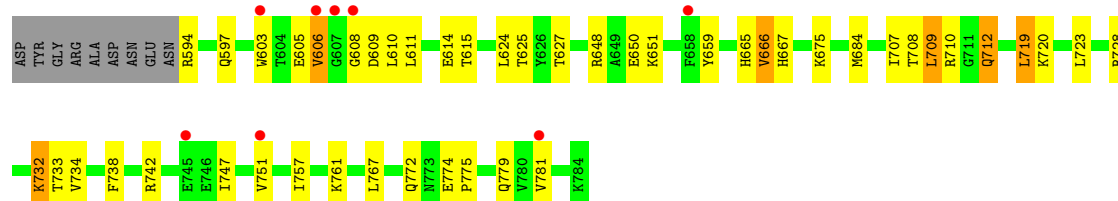


- Molecule 1: ATP-dependent protease La

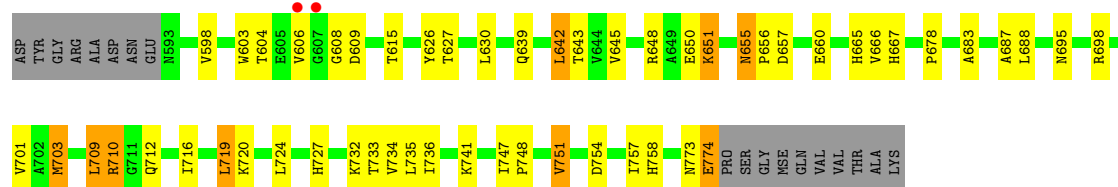




• Molecule 1: ATP-dependent protease La



• Molecule 1: ATP-dependent protease La



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	86.37Å 86.37Å 124.16Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.96 – 1.75 19.96 – 1.75	Depositor EDS
% Data completeness (in resolution range)	93.5 (19.96-1.75) 93.5 (19.96-1.75)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 (9.61%)	wwPDB-VP
Wilson B-factor (Å ²)	24.8	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 39.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.015 for -h,-k,l 0.034 for h,-h-k,-l 0.017 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	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.*

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	1.16	3/1390 (0.2%)	1.12	3/1883 (0.2%)
1	B	1.01	0/1384	1.06	2/1875 (0.1%)
1	C	1.20	5/1384 (0.4%)	1.17	3/1875 (0.2%)
1	D	1.00	0/1385	1.05	0/1876
1	E	0.99	1/1439 (0.1%)	1.02	0/1946
1	F	1.09	3/1377 (0.2%)	1.05	1/1865 (0.1%)
All	All	1.08	12/8359 (0.1%)	1.08	9/11320 (0.1%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	703	MSE	SE-CE	-14.67	1.51	1.95
1	C	703	MSE	SE-CE	-12.04	1.59	1.95
1	F	703	MSE	SE-CE	-8.50	1.70	1.95
1	C	684[A]	MSE	SE-CE	6.98	2.16	1.95
1	C	684[B]	MSE	SE-CE	6.98	2.16	1.95
1	E	684	MSE	SE-CE	-6.34	1.76	1.95
1	F	736	ILE	CA-CB	-5.59	1.49	1.55
1	C	684[A]	MSE	C-O	-5.41	1.17	1.24
1	C	684[B]	MSE	C-O	-5.41	1.17	1.24
1	A	595	VAL	CA-C	5.37	1.59	1.52
1	A	707	ILE	CG1-CD1	-5.24	1.31	1.51
1	F	678	PRO	CA-C	5.01	1.58	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	606	VAL	CB-CA-C	5.41	118.75	111.94
1	A	669	PRO	CA-C-O	-5.40	115.17	122.08
1	C	677	GLY	CA-C-N	5.31	127.32	120.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	677	GLY	C-N-CA	5.31	127.32	120.89
1	A	685[A]	CYS	CB-CA-C	-5.31	102.55	110.88
1	A	685[B]	CYS	CB-CA-C	-5.31	102.55	110.88
1	C	763	ILE	N-CA-C	5.12	115.84	110.62
1	B	731	ILE	N-CA-C	-5.08	102.95	109.30
1	F	630	LEU	N-CA-C	5.06	117.81	109.76

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1357	0	1394	36	0
1	B	1355	0	1389	47	0
1	C	1355	0	1394	31	0
1	D	1361	0	1401	39	0
1	E	1423	0	1472	31	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
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	213	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 13.

All (213) 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: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:632:GLU:CD	3:B:1306:HOH:O	2.34	0.71
1:B:758:HIS:HD2	3:B:1310:HOH:O	1.74	0.71
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:657:ASP:CG	3:F:1640:HOH:O	2.41	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: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
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:B:655:ASN:HD22	1:B:655:ASN:C	2.13	0.55
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:D:608:GLY:C	3:D:1491:HOH:O	2.55	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:594:ARG:C	1:A:595:VAL:HG23	2.38	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:D:657:ASP:OD2	1:D:657:ASP:C	2.58	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
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:F:642:LEU:HD23	1:F:688:LEU:HD21	2.00	0.44
1:A:695:ASN:C	1:A:695:ASN:HD22	2.25	0.44
1:B:655:ASN:C	1:B:655:ASN:ND2	2.74	0.44
1:E:659:TYR:CD1	1:E:659:TYR:C	2.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:658:PHE:CD1	1:B:658:PHE:C	2.97	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:B:657:ASP:OD1	1:B:657:ASP:C	2.61	0.42
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:614:GLU:CD	1:E:708:THR:OG1	2.62	0.42
1:D:594:ARG:HD3	1:D:594:ARG:HA	1.81	0.42
1:E:781:VAL:O	1:E:781:VAL:HG13	2.19	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:732:LYS:HG3	1:E:733:THR:N	2.35	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	Percentiles	
1	A	183/200 (92%)	177 (97%)	4 (2%)	2 (1%)	11	2
1	B	182/200 (91%)	178 (98%)	3 (2%)	1 (0%)	24	11
1	C	182/200 (91%)	178 (98%)	4 (2%)	0	100	100
1	D	181/200 (90%)	174 (96%)	4 (2%)	3 (2%)	7	1
1	E	189/200 (94%)	183 (97%)	4 (2%)	2 (1%)	11	2
1	F	180/200 (90%)	175 (97%)	4 (2%)	1 (1%)	21	8
All	All	1097/1200 (91%)	1065 (97%)	23 (2%)	9 (1%)	16	5

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	774	GLU
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%)	135 (91%)	13 (9%)	9	1
1	B	147/156 (94%)	132 (90%)	15 (10%)	7	1
1	C	147/156 (94%)	128 (87%)	19 (13%)	4	0
1	D	147/156 (94%)	127 (86%)	20 (14%)	3	0
1	E	153/156 (98%)	136 (89%)	17 (11%)	6	0
1	F	146/156 (94%)	133 (91%)	13 (9%)	9	1
All	All	888/936 (95%)	791 (89%)	97 (11%)	6	0

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	595	VAL
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	661	LYS
1	A	670	GLU
1	A	700	ASP
1	A	724	LEU
1	A	732	LYS
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	697	VAL
1	B	720	LYS
1	B	723	LEU
1	B	724	LEU

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Mol	Chain	Res	Type
1	B	728	ARG
1	B	745	GLU
1	B	752	ILE
1	B	769	LEU
1	B	772	GLN
1	B	774	GLU
1	C	599	THR
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	710	ARG
1	C	716	ILE
1	C	719	LEU
1	C	723	LEU
1	C	728	ARG
1	C	742	ARG
1	C	766	VAL
1	C	774	GLU
1	D	594	ARG
1	D	604	THR
1	D	606	VAL
1	D	610	LEU
1	D	612	THR
1	D	621	LYS
1	D	625	THR
1	D	650	GLU
1	D	659	TYR
1	D	660	GLU
1	D	661	LYS
1	D	662	ARG
1	D	689	VAL
1	D	698	ARG
1	D	710	ARG
1	D	721	GLU
1	D	723	LEU

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Mol	Chain	Res	Type
1	D	741	LYS
1	D	751	VAL
1	D	754	ASP
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	666	VAL
1	E	709	LEU
1	E	712	GLN
1	E	719	LEU
1	E	720	LYS
1	E	732	LYS
1	E	734	VAL
1	E	742	ARG
1	E	751	VAL
1	E	757	ILE
1	E	779	GLN
1	F	642	LEU
1	F	651	LYS
1	F	655	ASN
1	F	660	GLU
1	F	709	LEU
1	F	710	ARG
1	F	719	LEU
1	F	724	LEU
1	F	732	LYS
1	F	735	LEU
1	F	741	LYS
1	F	751	VAL
1	F	774	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) 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	A	773	ASN

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Mol	Chain	Res	Type
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	C	772	GLN
1	C	773	ASN
1	D	597	GLN
1	D	639	GLN
1	D	655	ASN
1	D	772	GLN
1	D	773	ASN
1	E	597	GLN
1	E	639	GLN
1	E	665	HIS
1	E	750	ASN
1	E	779	GLN
1	F	597	GLN
1	F	635	GLN
1	F	665	HIS
1	F	667	HIS
1	F	695	ASN
1	F	727	HIS
1	F	750	ASN

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 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	1501	-	4,4,4	0.17	0	6,6,6	0.46	0
2	SO4	F	1601	-	4,4,4	0.25	0	6,6,6	0.44	0
2	SO4	B	1201	-	4,4,4	0.17	0	6,6,6	0.63	0
2	SO4	D	1401	-	4,4,4	0.21	0	6,6,6	0.85	0
2	SO4	C	1301	-	4,4,4	0.41	0	6,6,6	1.02	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	179/200 (89%)	0.02	5 (2%)	55 61	9, 19, 36, 49	2 (1%)
1	B	179/200 (89%)	0.40	10 (5%)	30 34	12, 23, 42, 49	1 (0%)
1	C	179/200 (89%)	0.18	5 (2%)	55 61	11, 20, 38, 42	1 (0%)
1	D	179/200 (89%)	0.36	9 (5%)	34 39	15, 24, 43, 56	0
1	E	187/200 (93%)	0.37	8 (4%)	40 46	14, 24, 45, 51	0
1	F	179/200 (89%)	0.45	2 (1%)	78 83	18, 28, 44, 54	0
All	All	1082/1200 (90%)	0.30	39 (3%)	46 52	9, 23, 42, 56	4 (0%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	606	VAL	6.3
1	F	606	VAL	6.2
1	F	607	GLY	5.0
1	C	606	VAL	4.3
1	D	602	ALA	4.3
1	D	603	TRP	4.1
1	E	607	GLY	4.0
1	B	606	VAL	3.8
1	C	659	TYR	3.8
1	D	608	GLY	3.6
1	E	658	PHE	3.5
1	C	602	ALA	3.5
1	B	752	ILE	3.5
1	D	659	TYR	3.4
1	C	608	GLY	3.2
1	D	607	GLY	3.2
1	D	606	VAL	3.2
1	A	595	VAL	2.9
1	A	699	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	751	VAL	2.7
1	A	596	GLY	2.6
1	B	608	GLY	2.6
1	B	773	ASN	2.6
1	E	608	GLY	2.5
1	B	774	GLU	2.5
1	B	607	GLY	2.5
1	C	657	ASP	2.5
1	A	775	PRO	2.5
1	B	751	VAL	2.4
1	A	659	TYR	2.3
1	B	730	GLY	2.3
1	B	697	VAL	2.3
1	E	781	VAL	2.2
1	D	595	VAL	2.1
1	E	745	GLU	2.1
1	E	603	TRP	2.1
1	D	610	LEU	2.0
1	B	729	GLY	2.0
1	D	609	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 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($\text{\AA}^2$)	Q<0.9
2	SO4	E	1501	5/5	0.87	0.11	44,48,50,52	0
2	SO4	D	1401	5/5	0.91	0.15	39,40,44,45	0
2	SO4	F	1601	5/5	0.91	0.12	34,37,43,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	B	1201	5/5	0.94	0.13	25,31,34,37	0
2	SO4	C	1301	5/5	0.95	0.09	27,28,35,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.