



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:12 AM UTC

PDB ID : 5UCG / pdb_00005ucg
Title : Structure of the PP2C Phosphatase Domain and a Fragment of the Regulatory Domain of the Cell Fate Determinant SpoIIE from Bacillus Subtilis
Authors : Bradshaw, N.; Levnikov, V.; Zimanyi, C.; Gaudet, R.; Wilkinson, A.; Losick, R.
Deposited on : 2016-12-22
Resolution : 3.91 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
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

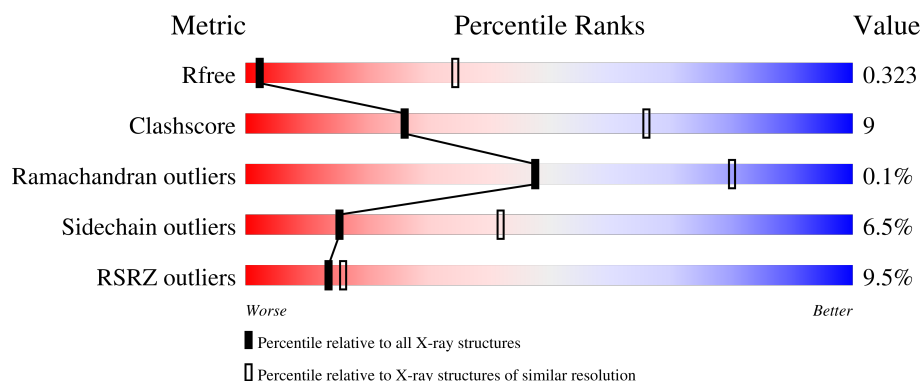
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.91 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	1270 (4.10-3.70)
Clashscore	190562	1034 (4.08-3.72)
Ramachandran outliers	187476	1251 (4.10-3.70)
Sidechain outliers	187428	1243 (4.10-3.70)
RSRZ outliers	180081	1269 (4.10-3.70)

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	345	7% 75% 23% .
1	B	345	12% 74% 21% ..
1	C	345	12% 68% 25% ..
1	D	345	10% 73% 21% ..
1	E	345	5% 75% 20% ..

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 13166 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.

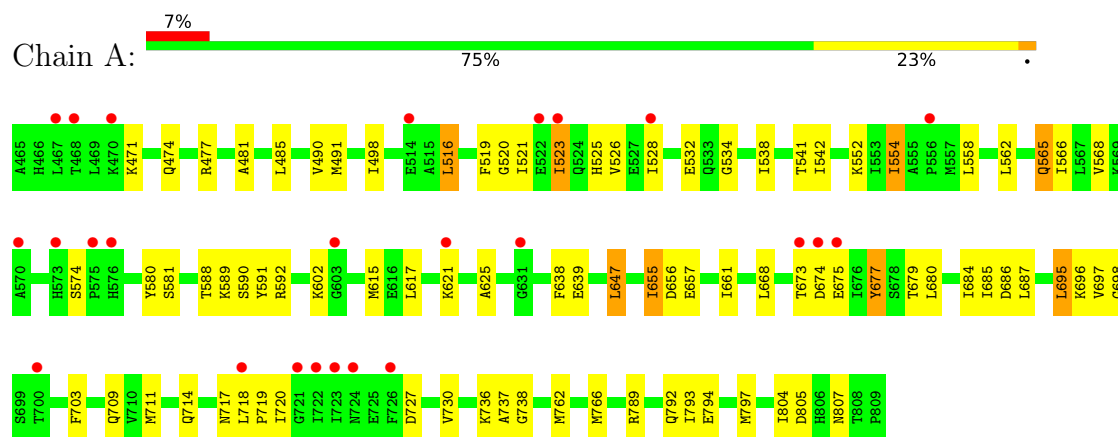
- Molecule 1 is a protein called Stage II sporulation protein E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	345	Total	C	N	O	S	0	0	0
			2690	1685	463	528	14			
1	E	338	Total	C	N	O	S	0	0	0
			2639	1654	451	520	14			
1	B	337	Total	C	N	O	S	0	0	0
			2631	1652	452	513	14			
1	C	331	Total	C	N	O	S	0	0	0
			2599	1631	444	511	13			
1	D	334	Total	C	N	O	S	0	0	0
			2607	1633	446	514	14			

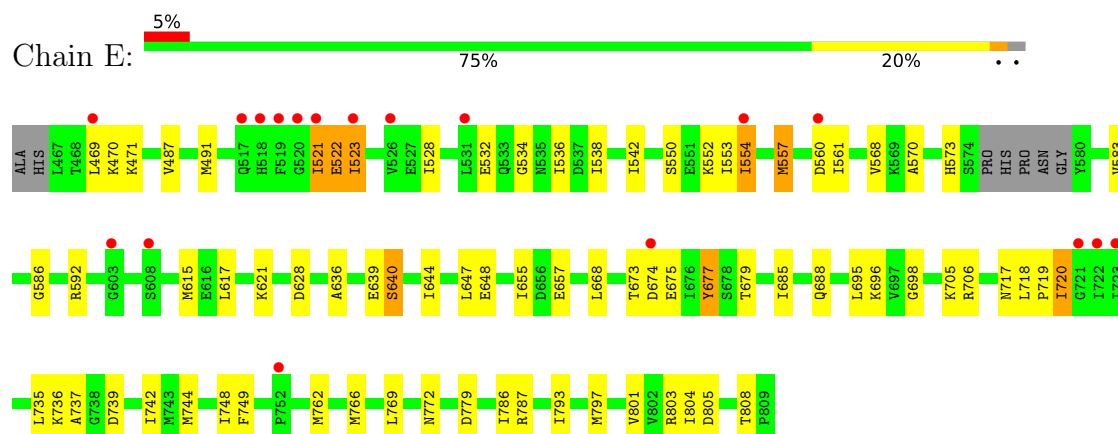
3 Residue-property plots [i](#)

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.

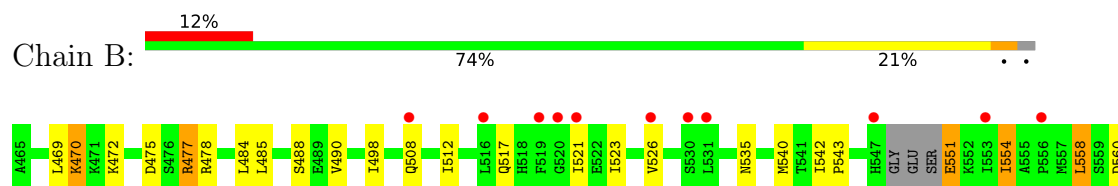
• Molecule 1: Stage II sporulation protein E

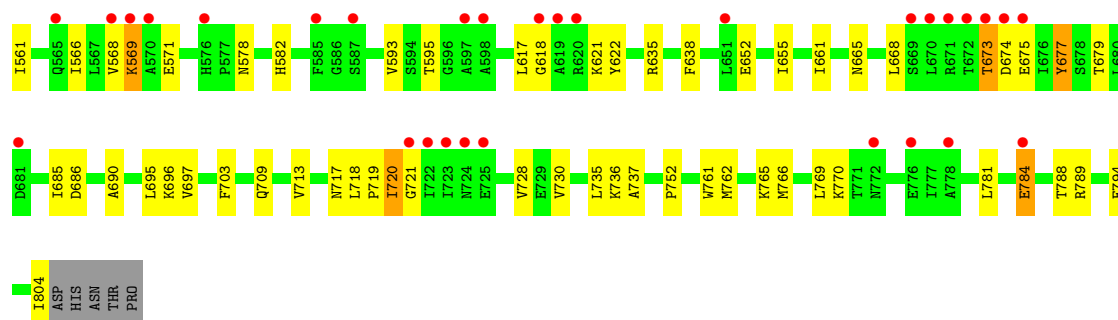


• Molecule 1: Stage II sporulation protein E

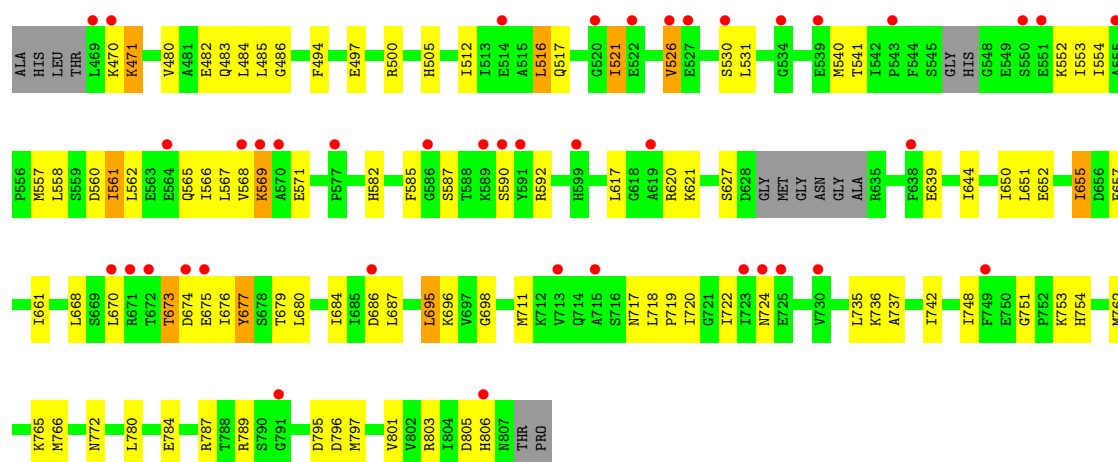


• Molecule 1: Stage II sporulation protein E

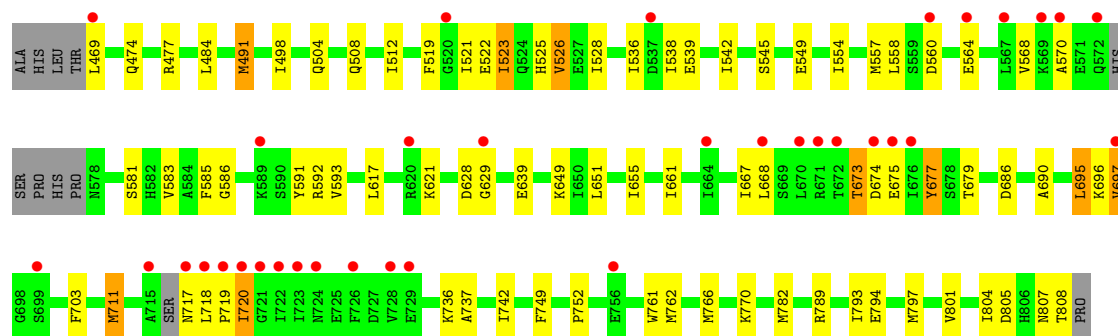
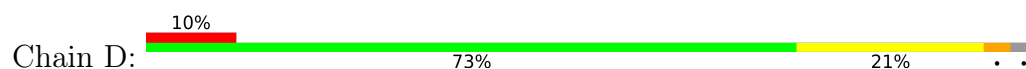




• Molecule 1: Stage II sporulation protein E



• Molecule 1: Stage II sporulation protein E



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	125.62Å 125.62Å 330.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.05 – 3.91 50.05 – 3.91	Depositor EDS
% Data completeness (in resolution range)	86.6 (50.05-3.91) 81.7 (50.05-3.91)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.78 (at 3.88Å)	Xtriage
Refinement program	PHENIX 1.11.1 _2575	Depositor
R, R_{free}	0.276 , 0.323 0.278 , 0.323	Depositor DCC
R_{free} test set	1091 reflections (4.38%)	wwPDB-VP
Wilson B-factor (Å ²)	33.8	Xtriage
Anisotropy	0.278	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 53.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.80	EDS
Total number of atoms	13166	wwPDB-VP
Average B, all atoms (Å ²)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% 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](#)

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	0.12	0/2729	0.34	1/3672 (0.0%)
1	B	0.11	0/2667	0.31	0/3585
1	C	0.11	0/2633	0.32	0/3538
1	D	0.11	0/2638	0.32	0/3541
1	E	0.11	0/2673	0.32	0/3592
All	All	0.11	0/13340	0.32	1/17928 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	727	ASP	CB-CA-C	-5.72	108.99	115.79

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	2690	0	2701	55	0
1	B	2631	0	2655	51	0
1	C	2599	0	2616	62	0
1	D	2607	0	2624	57	0
1	E	2639	0	2658	46	0
All	All	13166	0	13254	249	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 9.

All (249) 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:D:697:VAL:HG21	1:D:720:ILE:HG13	1.55	0.88
1:A:525:HIS:HB3	1:A:541:THR:HB	1.57	0.84
1:C:696:LYS:O	1:C:717:ASN:ND2	2.17	0.73
1:A:679:THR:HG22	1:A:719:PRO:HB3	1.71	0.72
1:A:696:LYS:O	1:A:717:ASN:ND2	2.19	0.72
1:B:697:VAL:HG11	1:B:720:ILE:HG13	1.72	0.72
1:A:668:LEU:HB3	1:A:677:TYR:HD1	1.54	0.71
1:C:620:ARG:HH12	1:D:477:ARG:HH22	1.41	0.69
1:C:679:THR:HG22	1:C:719:PRO:HB3	1.73	0.69
1:B:679:THR:HG22	1:B:719:PRO:HB3	1.75	0.68
1:B:668:LEU:HB3	1:B:677:TYR:HD1	1.58	0.68
1:E:668:LEU:HB3	1:E:677:TYR:HD1	1.59	0.68
1:E:679:THR:HG22	1:E:719:PRO:HB3	1.75	0.68
1:D:639:GLU:HG3	1:D:677:TYR:HE2	1.59	0.67
1:B:558:LEU:HD23	1:B:566:ILE:HG12	1.76	0.67
1:A:498:ILE:HG21	1:B:485:LEU:HD11	1.77	0.66
1:D:668:LEU:HB3	1:D:677:TYR:HD1	1.60	0.66
1:A:639:GLU:HB2	1:A:677:TYR:HE2	1.58	0.66
1:E:628:ASP:O	1:E:640:SER:OG	2.14	0.66
1:E:705:LYS:NZ	1:E:769:LEU:O	2.29	0.66
1:B:571:GLU:OE2	1:C:765:LYS:NZ	2.30	0.64
1:E:521:ILE:HD13	1:E:542:ILE:HG22	1.79	0.64
1:C:784:GLU:OE2	1:C:787:ARG:NH1	2.30	0.63
1:E:762:MET:HG3	1:E:766:MET:HE3	1.81	0.63
1:A:647:LEU:HD13	1:A:680:LEU:HD21	1.81	0.63
1:C:675:GLU:HG2	1:C:719:PRO:HG3	1.81	0.63
1:D:793:ILE:HG23	1:D:797:MET:HE2	1.82	0.62
1:D:696:LYS:O	1:D:717:ASN:ND2	2.27	0.62
1:A:639:GLU:HB2	1:A:677:TYR:CE2	2.35	0.61
1:A:485:LEU:HD11	1:B:498:ILE:HG21	1.82	0.61
1:D:679:THR:HG22	1:D:719:PRO:HB3	1.83	0.61
1:C:751:GLY:O	1:C:789:ARG:NH2	2.34	0.61
1:E:675:GLU:HG2	1:E:719:PRO:HG3	1.82	0.61
1:D:570:ALA:HA	1:D:583:VAL:HG12	1.83	0.60
1:A:621:LYS:HG2	1:A:686:ASP:HA	1.85	0.59
1:D:545:SER:OG	1:D:549:GLU:OE1	2.19	0.59
1:E:696:LYS:O	1:E:717:ASN:ND2	2.25	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:568:VAL:HG23	1:D:585:PHE:HE1	1.67	0.59
1:E:592:ARG:N	1:E:805:ASP:O	2.36	0.59
1:C:621:LYS:HG2	1:C:686:ASP:HA	1.85	0.58
1:A:625:ALA:HB1	1:A:680:LEU:HD11	1.83	0.58
1:C:517:GLN:HB3	1:C:521:ILE:HG13	1.85	0.58
1:B:675:GLU:HG2	1:B:719:PRO:HG3	1.84	0.57
1:C:661:ILE:HG13	1:C:695:LEU:HG	1.85	0.57
1:C:668:LEU:HB3	1:C:677:TYR:HD1	1.68	0.57
1:D:536:ILE:O	1:D:586:GLY:HA2	2.04	0.57
1:D:675:GLU:HG2	1:D:719:PRO:HG3	1.86	0.57
1:C:620:ARG:HH12	1:D:477:ARG:NH2	2.03	0.57
1:D:528:ILE:HG13	1:D:538:ILE:HG22	1.87	0.57
1:B:526:VAL:HG23	1:B:540:MET:HG2	1.87	0.56
1:D:542:ILE:O	1:D:581:SER:N	2.33	0.56
1:C:530:SER:HB3	1:D:474:GLN:HG2	1.88	0.56
1:D:639:GLU:HG3	1:D:677:TYR:CE2	2.41	0.56
1:A:516:LEU:HD12	1:A:523:ILE:HG12	1.87	0.55
1:D:668:LEU:HB3	1:D:677:TYR:CD1	2.39	0.55
1:C:772:ASN:HB3	1:C:803:ARG:HH11	1.71	0.55
1:A:675:GLU:HG2	1:A:719:PRO:HG3	1.88	0.55
1:B:472:LYS:HD2	1:B:475:ASP:HB2	1.88	0.54
1:A:574:SER:HB2	1:A:580:TYR:HB2	1.90	0.54
1:B:752:PRO:HB3	1:B:788:THR:HG21	1.90	0.54
1:D:762:MET:HG3	1:D:766:MET:HE3	1.89	0.54
1:E:470:LYS:HD3	1:E:471:LYS:HG2	1.90	0.54
1:E:560:ASP:OD1	1:E:561:ILE:N	2.40	0.53
1:B:621:LYS:HG2	1:B:686:ASP:HA	1.88	0.53
1:D:519:PHE:HD1	1:D:521:ILE:H	1.56	0.53
1:D:661:ILE:HG21	1:D:695:LEU:HD11	1.90	0.53
1:B:696:LYS:O	1:B:717:ASN:ND2	2.39	0.53
1:C:679:THR:HB	1:C:698:GLY:HA3	1.91	0.53
1:B:665:ASN:OD1	1:B:721:GLY:N	2.30	0.53
1:D:526:VAL:HG23	1:D:539:GLU:O	2.08	0.53
1:E:639:GLU:HB2	1:E:677:TYR:CE2	2.44	0.53
1:E:706:ARG:NH2	1:E:739:ASP:OD2	2.38	0.53
1:C:651:LEU:HD11	1:C:684:ILE:HD11	1.91	0.53
1:A:661:ILE:HG13	1:A:695:LEU:HG	1.91	0.52
1:C:592:ARG:N	1:C:805:ASP:O	2.42	0.52
1:C:485:LEU:HD11	1:D:498:ILE:HG21	1.90	0.52
1:B:765:LYS:HD2	1:C:571:GLU:OE2	2.09	0.52
1:D:677:TYR:HB3	1:D:720:ILE:HG22	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:569:LYS:HD2	1:C:780:LEU:HD13	1.90	0.52
1:C:480:VAL:HG21	1:D:649:LYS:HD2	1.91	0.52
1:A:657:GLU:HG2	1:A:684:ILE:HD12	1.90	0.52
1:E:673:THR:HG22	1:E:674:ASP:H	1.75	0.51
1:A:696:LYS:HE3	1:A:714:GLN:HA	1.92	0.51
1:E:749:PHE:HA	1:E:762:MET:HE3	1.92	0.51
1:E:786:ILE:HD11	1:E:797:MET:HE1	1.93	0.50
1:A:655:ILE:HG12	1:A:656:ASP:N	2.27	0.50
1:C:558:LEU:HD11	1:C:565:GLN:HA	1.92	0.50
1:C:673:THR:HG22	1:C:674:ASP:H	1.75	0.50
1:D:521:ILE:HD12	1:D:542:ILE:HG12	1.93	0.50
1:B:789:ARG:NH2	1:B:794:GLU:OE1	2.45	0.50
1:D:789:ARG:NH2	1:D:794:GLU:OE1	2.45	0.50
1:A:762:MET:HG3	1:A:766:MET:HE3	1.94	0.50
1:D:538:ILE:HG13	1:D:585:PHE:HD2	1.77	0.49
1:A:532:GLU:HG3	1:A:534:GLY:H	1.77	0.49
1:A:793:ILE:HG23	1:A:797:MET:HE2	1.93	0.49
1:C:668:LEU:HB3	1:C:677:TYR:CD1	2.46	0.49
1:D:673:THR:HG22	1:D:674:ASP:H	1.78	0.49
1:D:522:GLU:HG2	1:D:523:ILE:H	1.78	0.49
1:B:673:THR:HG22	1:B:674:ASP:H	1.77	0.49
1:C:512:ILE:O	1:C:516:LEU:HB2	2.12	0.48
1:D:592:ARG:HB2	1:D:807:ASN:HB3	1.95	0.48
1:A:673:THR:HG22	1:A:674:ASP:H	1.78	0.48
1:E:685:ILE:HD13	1:E:804:ILE:HD11	1.96	0.48
1:C:657:GLU:HG2	1:C:684:ILE:HD12	1.94	0.48
1:A:718:LEU:HB3	1:A:719:PRO:HD2	1.96	0.48
1:C:494:PHE:HE1	1:C:655:ILE:HG21	1.78	0.48
1:C:753:LYS:HG2	1:C:754:HIS:CD2	2.49	0.48
1:E:668:LEU:HD12	1:E:720:ILE:HG21	1.96	0.48
1:D:749:PHE:HA	1:D:762:MET:HE3	1.96	0.48
1:C:639:GLU:HG3	1:C:677:TYR:CE2	2.49	0.48
1:A:592:ARG:N	1:A:805:ASP:O	2.46	0.48
1:A:679:THR:HB	1:A:698:GLY:CA	2.45	0.47
1:B:761:TRP:O	1:B:765:LYS:HG2	2.14	0.47
1:C:557:MET:SD	1:C:566:ILE:HG21	2.54	0.47
1:E:639:GLU:HB2	1:E:677:TYR:HE2	1.79	0.47
1:D:736:LYS:HG3	1:D:737:ALA:H	1.78	0.47
1:E:718:LEU:HB3	1:E:719:PRO:HD2	1.95	0.47
1:B:784:GLU:HG2	1:C:571:GLU:OE2	2.14	0.47
1:A:481:ALA:O	1:A:485:LEU:N	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:738:GLY:N	1:A:804:ILE:O	2.38	0.47
1:B:770:LYS:H	1:C:569:LYS:HG2	1.80	0.47
1:A:565:GLN:HG2	1:A:588:THR:HG21	1.97	0.47
1:E:742:ILE:HG22	1:E:801:VAL:HG13	1.96	0.47
1:B:551:GLU:HB3	1:B:568:VAL:HG21	1.96	0.47
1:E:679:THR:HB	1:E:698:GLY:HA3	1.97	0.47
1:D:703:PHE:CG	1:D:766:MET:HE1	2.49	0.47
1:A:668:LEU:HB3	1:A:677:TYR:CD1	2.43	0.47
1:C:650:ILE:HG12	1:D:484:LEU:HD11	1.97	0.47
1:A:552:LYS:HD3	1:A:552:LYS:HA	1.62	0.46
1:C:540:MET:HG3	1:C:585:PHE:HE2	1.79	0.46
1:C:661:ILE:HG21	1:C:695:LEU:HD11	1.97	0.46
1:D:554:ILE:HA	1:D:557:MET:HB3	1.97	0.46
1:A:680:LEU:O	1:A:698:GLY:N	2.49	0.46
1:C:505:HIS:CE1	1:C:531:LEU:HB3	2.50	0.46
1:E:532:GLU:HG3	1:E:534:GLY:H	1.80	0.46
1:A:736:LYS:HG3	1:A:737:ALA:H	1.81	0.46
1:C:736:LYS:HG3	1:C:737:ALA:H	1.80	0.46
1:E:744:MET:HB2	1:E:748:ILE:HB	1.98	0.46
1:C:627:SER:HB3	1:C:644:ILE:HD11	1.97	0.46
1:B:685:ILE:HD13	1:B:804:ILE:HD11	1.98	0.46
1:E:772:ASN:O	1:E:803:ARG:HD3	2.16	0.45
1:B:761:TRP:CZ2	1:B:765:LYS:HE3	2.51	0.45
1:C:590:SER:O	1:C:687:LEU:HB3	2.16	0.45
1:E:522:GLU:HG2	1:E:523:ILE:N	2.31	0.45
1:C:497:GLU:OE1	1:C:500:ARG:NH1	2.50	0.45
1:A:789:ARG:HD3	1:A:792:GLN:HB2	1.98	0.45
1:B:521:ILE:HB	1:B:543:PRO:HD2	1.99	0.45
1:B:769:LEU:HA	1:C:569:LYS:HD3	1.98	0.45
1:E:636:ALA:HA	1:E:639:GLU:HG2	1.97	0.45
1:B:560:ASP:OD1	1:B:561:ILE:N	2.50	0.45
1:C:718:LEU:H	1:C:724:ASN:ND2	2.15	0.45
1:C:762:MET:HG3	1:C:766:MET:HE3	1.99	0.45
1:D:621:LYS:HG2	1:D:686:ASP:HA	1.99	0.45
1:B:718:LEU:HB3	1:B:719:PRO:HD2	1.99	0.45
1:B:736:LYS:HG3	1:B:737:ALA:H	1.82	0.45
1:E:736:LYS:HD2	1:E:736:LYS:HA	1.87	0.44
1:B:766:MET:HA	1:B:769:LEU:HG	1.98	0.44
1:C:652:GLU:O	1:D:477:ARG:NE	2.49	0.44
1:D:717:ASN:OD1	1:D:717:ASN:N	2.49	0.44
1:A:655:ILE:HG12	1:A:656:ASP:H	1.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:560:ASP:OD1	1:C:561:ILE:N	2.51	0.44
1:D:508:GLN:O	1:D:512:ILE:HG12	2.17	0.44
1:E:554:ILE:HA	1:E:557:MET:HB3	1.99	0.44
1:A:680:LEU:HB3	1:A:697:VAL:CG1	2.48	0.44
1:C:748:ILE:HD11	1:C:797:MET:HB3	1.99	0.44
1:A:477:ARG:HG3	1:B:652:GLU:O	2.18	0.44
1:A:516:LEU:HD22	1:A:521:ILE:HD12	1.99	0.44
1:B:762:MET:HG3	1:B:766:MET:HE3	1.99	0.44
1:E:787:ARG:CZ	1:E:787:ARG:HB3	2.47	0.44
1:D:628:ASP:OD1	1:D:629:GLY:N	2.51	0.44
1:D:742:ILE:HG22	1:D:801:VAL:HG22	1.99	0.44
1:E:570:ALA:HA	1:E:583:VAL:HG12	2.00	0.44
1:E:636:ALA:O	1:E:640:SER:HB2	2.17	0.43
1:B:521:ILE:HD12	1:B:542:ILE:HG22	2.00	0.43
1:D:661:ILE:HG13	1:D:695:LEU:HG	2.00	0.43
1:C:742:ILE:HG22	1:C:801:VAL:HG13	2.01	0.43
1:A:519:PHE:O	1:A:521:ILE:N	2.51	0.43
1:B:695:LEU:HD21	1:B:730:VAL:HG12	2.01	0.43
1:C:484:LEU:HD12	1:C:484:LEU:HA	1.89	0.43
1:A:685:ILE:HD13	1:A:804:ILE:HD11	2.00	0.43
1:B:554:ILE:HD12	1:B:554:ILE:HA	1.78	0.43
1:C:737:ALA:HB2	1:C:806:HIS:CE1	2.54	0.43
1:E:536:ILE:O	1:E:586:GLY:HA2	2.19	0.43
1:E:568:VAL:O	1:D:770:LYS:HB2	2.19	0.43
1:E:786:ILE:HD12	1:E:793:ILE:HG12	2.01	0.43
1:A:679:THR:HB	1:A:698:GLY:HA2	2.00	0.43
1:E:487:VAL:O	1:E:491:MET:HG2	2.19	0.43
1:E:554:ILE:HA	1:E:554:ILE:HD12	1.79	0.43
1:A:491:MET:HE3	1:B:488:SER:HB2	2.01	0.42
1:A:542:ILE:O	1:A:581:SER:HB3	2.18	0.42
1:D:491:MET:HE1	1:D:667:ILE:HD11	2.01	0.42
1:A:565:GLN:HG3	1:A:566:ILE:N	2.33	0.42
1:C:553:ILE:HG13	1:C:554:ILE:HD13	2.02	0.42
1:C:718:LEU:HB3	1:C:719:PRO:HD2	2.01	0.42
1:C:552:LYS:HD3	1:C:552:LYS:HA	1.61	0.42
1:D:504:GLN:O	1:D:508:GLN:HG2	2.18	0.42
1:D:568:VAL:HG23	1:D:585:PHE:CE1	2.51	0.42
1:B:717:ASN:OD1	1:B:717:ASN:N	2.53	0.42
1:A:602:LYS:NZ	1:A:794:GLU:O	2.53	0.42
1:B:595:THR:HG21	1:B:622:TYR:OH	2.20	0.42
1:C:483:GLN:OE1	1:C:722:ILE:HG12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:718:LEU:HB3	1:D:719:PRO:HD2	2.01	0.42
1:C:639:GLU:HG3	1:C:677:TYR:CD2	2.54	0.42
1:D:782:MET:SD	1:D:797:MET:HE3	2.60	0.42
1:A:805:ASP:OD1	1:A:805:ASP:N	2.53	0.42
1:E:528:ILE:HA	1:E:538:ILE:HG22	2.02	0.42
1:A:528:ILE:HG23	1:A:538:ILE:HG22	2.00	0.42
1:E:469:LEU:O	1:E:471:LYS:N	2.44	0.42
1:E:573:HIS:CE1	1:D:761:TRP:HE1	2.37	0.42
1:B:508:GLN:O	1:B:512:ILE:HG12	2.20	0.42
1:B:696:LYS:HE3	1:B:713:VAL:O	2.20	0.42
1:B:717:ASN:ND2	1:B:728:VAL:HG23	2.35	0.42
1:E:644:ILE:O	1:E:648:GLU:HB2	2.20	0.41
1:C:621:LYS:HE2	1:C:686:ASP:HB2	2.02	0.41
1:B:517:GLN:HA	1:B:523:ILE:HG23	2.01	0.41
1:C:470:LYS:HG2	1:C:471:LYS:HG3	2.03	0.41
1:C:558:LEU:CD1	1:C:565:GLN:HA	2.50	0.41
1:D:558:LEU:HB2	1:D:564:GLU:O	2.21	0.41
1:A:590:SER:O	1:A:687:LEU:HB3	2.20	0.41
1:B:477:ARG:HH21	1:B:478:ARG:HG3	1.86	0.41
1:E:736:LYS:HG3	1:E:737:ALA:H	1.86	0.41
1:B:484:LEU:HD12	1:B:484:LEU:HA	1.86	0.41
1:B:661:ILE:HG13	1:B:695:LEU:HD13	2.02	0.41
1:A:474:GLN:OE1	1:A:477:ARG:NH1	2.53	0.41
1:A:638:PHE:CE1	1:B:635:ARG:HA	2.56	0.41
1:B:470:LYS:CD	1:B:470:LYS:H	2.34	0.41
1:D:519:PHE:CD1	1:D:521:ILE:HG12	2.55	0.41
1:D:649:LYS:HD3	1:D:649:LYS:HA	1.88	0.41
1:A:589:LYS:O	1:A:807:ASN:ND2	2.53	0.41
1:E:677:TYR:HD2	1:E:677:TYR:HA	1.70	0.41
1:B:535:ASN:HD21	1:B:618:GLY:HA3	1.86	0.41
1:B:690:ALA:HB1	1:B:735:LEU:HD12	2.03	0.41
1:B:703:PHE:CG	1:B:766:MET:HE1	2.56	0.41
1:C:482:GLU:O	1:C:486:GLY:N	2.50	0.41
1:C:795:ASP:OD1	1:C:796:ASP:N	2.54	0.41
1:C:526:VAL:HG12	1:C:540:MET:HA	2.03	0.41
1:E:779:ASP:OD2	1:C:470:LYS:HG3	2.21	0.40
1:E:803:ARG:NH2	1:E:805:ASP:OD2	2.54	0.40
1:C:670:LEU:O	1:C:676:ILE:HD13	2.22	0.40
1:D:591:TYR:HB3	1:D:804:ILE:HG23	2.02	0.40
1:D:752:PRO:HG3	1:D:761:TRP:CE3	2.56	0.40
1:E:621:LYS:NZ	1:E:657:GLU:OE2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:711:MET:HE2	1:D:711:MET:HB3	1.73	0.40
1:A:558:LEU:HG	1:A:565:GLN:HA	2.02	0.40
1:A:638:PHE:HB3	1:B:638:PHE:CG	2.57	0.40
1:A:703:PHE:CG	1:A:766:MET:HE1	2.56	0.40
1:A:554:ILE:HD13	1:A:554:ILE:HA	1.75	0.40
1:A:695:LEU:HD23	1:A:730:VAL:HG12	2.03	0.40
1:D:591:TYR:CE2	1:D:690:ALA:HB2	2.57	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	343/345 (99%)	313 (91%)	28 (8%)	2 (1%)	21	55
1	B	333/345 (96%)	303 (91%)	30 (9%)	0	100	100
1	C	325/345 (94%)	306 (94%)	19 (6%)	0	100	100
1	D	328/345 (95%)	306 (93%)	22 (7%)	0	100	100
1	E	334/345 (97%)	310 (93%)	24 (7%)	0	100	100
All	All	1663/1725 (96%)	1538 (92%)	123 (7%)	2 (0%)	48	80

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	520	GLY
1	A	591	TYR

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	298/298 (100%)	280 (94%)	18 (6%)	17	44
1	B	291/298 (98%)	272 (94%)	19 (6%)	15	42
1	C	290/298 (97%)	269 (93%)	21 (7%)	13	39
1	D	288/298 (97%)	270 (94%)	18 (6%)	16	42
1	E	293/298 (98%)	274 (94%)	19 (6%)	15	42
All	All	1460/1490 (98%)	1365 (94%)	95 (6%)	15	42

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	471	LYS
1	A	490	VAL
1	A	516	LEU
1	A	523	ILE
1	A	526	VAL
1	A	554	ILE
1	A	562	LEU
1	A	565	GLN
1	A	568	VAL
1	A	615	MET
1	A	617	LEU
1	A	647	LEU
1	A	655	ILE
1	A	677	TYR
1	A	695	LEU
1	A	709	GLN
1	A	711	MET
1	A	720	ILE
1	E	521	ILE
1	E	522	GLU
1	E	523	ILE
1	E	550	SER
1	E	552	LYS

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Mol	Chain	Res	Type
1	E	553	ILE
1	E	554	ILE
1	E	557	MET
1	E	615	MET
1	E	617	LEU
1	E	640	SER
1	E	647	LEU
1	E	655	ILE
1	E	677	TYR
1	E	688	GLN
1	E	695	LEU
1	E	720	ILE
1	E	735	LEU
1	E	808	THR
1	B	469	LEU
1	B	470	LYS
1	B	477	ARG
1	B	490	VAL
1	B	551	GLU
1	B	554	ILE
1	B	558	LEU
1	B	569	LYS
1	B	578	ASN
1	B	582	HIS
1	B	593	VAL
1	B	617	LEU
1	B	655	ILE
1	B	673	THR
1	B	677	TYR
1	B	709	GLN
1	B	720	ILE
1	B	781	LEU
1	B	784	GLU
1	C	471	LYS
1	C	516	LEU
1	C	521	ILE
1	C	526	VAL
1	C	541	THR
1	C	561	ILE
1	C	562	LEU
1	C	567	LEU
1	C	568	VAL

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Mol	Chain	Res	Type
1	C	569	LYS
1	C	582	HIS
1	C	587	SER
1	C	617	LEU
1	C	655	ILE
1	C	673	THR
1	C	677	TYR
1	C	680	LEU
1	C	695	LEU
1	C	711	MET
1	C	720	ILE
1	C	735	LEU
1	D	469	LEU
1	D	491	MET
1	D	523	ILE
1	D	525	HIS
1	D	526	VAL
1	D	560	ASP
1	D	593	VAL
1	D	617	LEU
1	D	651	LEU
1	D	655	ILE
1	D	673	THR
1	D	677	TYR
1	D	695	LEU
1	D	697	VAL
1	D	711	MET
1	D	720	ILE
1	D	805	ASP
1	D	808	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	632	ASN
1	A	806	HIS
1	E	572	GLN
1	B	533	GLN
1	B	547	HIS
1	B	709	GLN
1	B	758	HIS
1	B	775	GLN

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Mol	Chain	Res	Type
1	C	758	HIS
1	D	599	HIS
1	D	641	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	345/345 (100%)	0.65	25 (7%)	21	20	25, 74, 132, 181	0
1	B	337/345 (97%)	0.94	41 (12%)	8	12	62, 97, 153, 203	0
1	C	331/345 (95%)	1.07	41 (12%)	8	11	67, 107, 159, 223	0
1	D	334/345 (96%)	0.86	35 (10%)	11	14	26, 88, 143, 176	0
1	E	338/345 (97%)	0.74	18 (5%)	32	25	23, 79, 133, 169	0
All	All	1685/1725 (97%)	0.85	160 (9%)	14	16	23, 90, 147, 223	0

All (160) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	720	ILE	7.2
1	B	520	GLY	5.8
1	D	717	ASN	5.7
1	E	521	ILE	5.6
1	D	728	VAL	4.5
1	A	723	ILE	4.5
1	E	520	GLY	4.5
1	D	719	PRO	4.3
1	B	675	GLU	4.3
1	A	721	GLY	4.3
1	D	715	ALA	4.2
1	C	570	ALA	4.1
1	C	674	ASP	4.0
1	A	675	GLU	4.0
1	A	722	ILE	3.8
1	B	556	PRO	3.7
1	C	723	ILE	3.7
1	C	564	GLU	3.6
1	B	516	LEU	3.5
1	C	469	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	670	LEU	3.4
1	A	556	PRO	3.4
1	C	670	LEU	3.3
1	A	467	LEU	3.3
1	A	603	GLY	3.3
1	A	724	ASN	3.2
1	C	672	THR	3.2
1	B	618	GLY	3.2
1	E	526	VAL	3.2
1	B	670	LEU	3.2
1	B	547	HIS	3.2
1	B	521	ILE	3.1
1	B	619	ALA	3.1
1	D	756	GLU	3.1
1	D	697	VAL	3.0
1	C	591	TYR	3.0
1	E	674	ASP	3.0
1	A	523	ILE	2.9
1	C	675	GLU	2.9
1	C	724	ASN	2.9
1	D	620	ARG	2.9
1	D	569	LYS	2.9
1	C	470	LYS	2.9
1	C	568	VAL	2.8
1	D	668	LEU	2.8
1	B	674	ASP	2.8
1	A	673	THR	2.8
1	A	528	ILE	2.8
1	D	722	ILE	2.8
1	D	724	ASN	2.8
1	E	531	LEU	2.7
1	D	537	ASP	2.7
1	D	570	ALA	2.7
1	E	722	ILE	2.7
1	D	675	GLU	2.7
1	D	729	GLU	2.7
1	E	469	LEU	2.7
1	C	522	GLU	2.6
1	B	724	ASN	2.6
1	C	543	PRO	2.6
1	B	681	ASP	2.6
1	C	539	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	608	SER	2.6
1	D	560	ASP	2.6
1	E	519	PHE	2.6
1	D	672	THR	2.5
1	C	569	LYS	2.5
1	D	664	ILE	2.5
1	C	590	SER	2.5
1	B	776	GLU	2.5
1	B	585	PHE	2.5
1	D	721	GLY	2.5
1	A	470	LYS	2.5
1	C	577	PRO	2.5
1	C	715	ALA	2.5
1	B	530	SER	2.5
1	C	555	ALA	2.4
1	B	620	ARG	2.4
1	C	749	PHE	2.4
1	A	570	ALA	2.4
1	C	638	PHE	2.4
1	C	713	VAL	2.4
1	A	674	ASP	2.4
1	B	778	ALA	2.4
1	A	631	GLY	2.4
1	C	534	GLY	2.4
1	A	726	PHE	2.4
1	C	730	VAL	2.4
1	A	718	LEU	2.4
1	B	725	GLU	2.4
1	C	551	GLU	2.4
1	D	564	GLU	2.4
1	E	752	PRO	2.4
1	C	791	GLY	2.4
1	A	700	THR	2.4
1	B	531	LEU	2.4
1	B	671	ARG	2.4
1	B	721	GLY	2.3
1	D	718	LEU	2.3
1	C	589	LYS	2.3
1	D	589	LYS	2.3
1	E	523	ILE	2.3
1	B	672	THR	2.3
1	B	598	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	723	ILE	2.3
1	B	669	SER	2.3
1	C	530	SER	2.3
1	A	468	THR	2.3
1	D	671	ARG	2.3
1	B	519	PHE	2.3
1	A	575	PRO	2.3
1	C	806	HIS	2.3
1	C	619	ALA	2.2
1	B	569	LYS	2.2
1	B	784	GLU	2.2
1	B	553	ILE	2.2
1	C	527	GLU	2.2
1	E	518	HIS	2.2
1	B	508	GLN	2.2
1	A	573	HIS	2.2
1	D	572	GLN	2.2
1	D	469	LEU	2.2
1	A	522	GLU	2.2
1	E	721	GLY	2.2
1	B	576	HIS	2.2
1	E	517	GLN	2.2
1	C	586	GLY	2.1
1	B	673	THR	2.1
1	B	651	LEU	2.1
1	B	597	ALA	2.1
1	E	560	ASP	2.1
1	C	514	GLU	2.1
1	C	599	HIS	2.1
1	D	674	ASP	2.1
1	C	520	GLY	2.1
1	A	514	GLU	2.1
1	E	554	ILE	2.1
1	B	526	VAL	2.1
1	D	726	PHE	2.1
1	A	576	HIS	2.1
1	B	570	ALA	2.1
1	C	671	ARG	2.1
1	E	723	ILE	2.1
1	B	723	ILE	2.1
1	D	699	SER	2.1
1	D	567	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	603	GLY	2.0
1	C	686	ASP	2.0
1	A	621	LYS	2.0
1	B	565	GLN	2.0
1	B	568	VAL	2.0
1	D	520	GLY	2.0
1	D	629	GLY	2.0
1	B	722	ILE	2.0
1	B	587	SER	2.0
1	C	550	SER	2.0
1	B	772	ASN	2.0
1	D	676	ILE	2.0
1	C	725	GLU	2.0
1	C	526	VAL	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.