Full wwPDB X-ray Structure Validation Report ⓘ

Sep 24, 2023 – 11:10 AM EDT

PDB ID	:	5UCG
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.; Levdikov, 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:

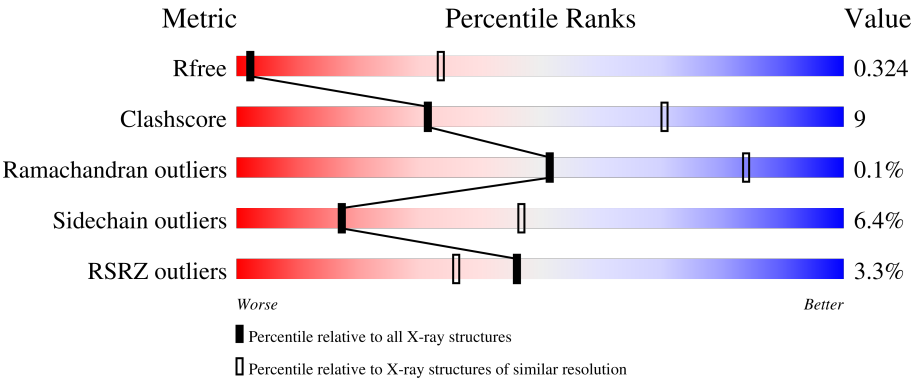
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 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}	130704	1002 (4.14-3.66)
Clashscore	141614	1004 (4.12-3.68)
Ramachandran outliers	138981	1021 (4.14-3.66)
Sidechain outliers	138945	1014 (4.14-3.66)
RSRZ outliers	127900	1275 (4.20-3.60)

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
1	A	345	3% 76% 22%
1	B	345	3% 74% 22%
1	C	345	4% 68% 26%
1	D	345	5% 74% 22%
1	E	345	2% 75% 21%

2 Entry composition (i)

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.

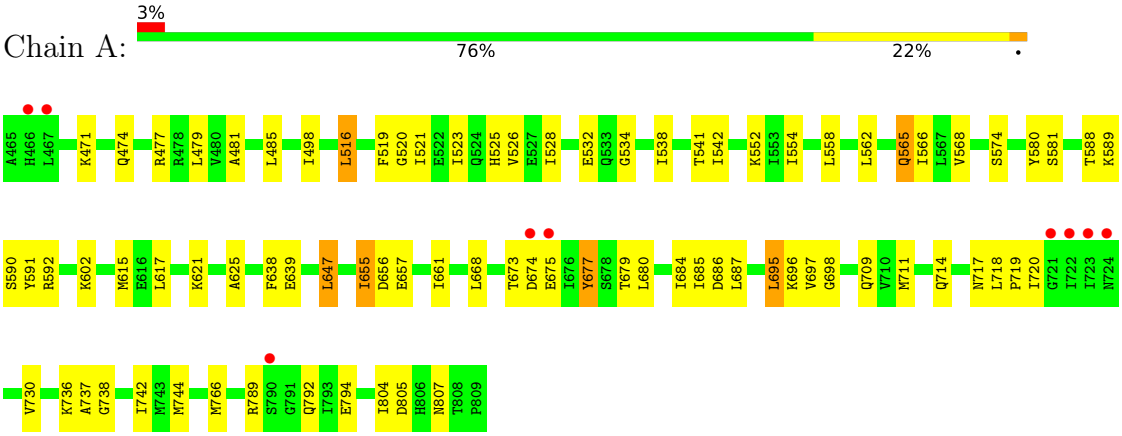
- Molecule 1 is a protein called Stage II sporulation protein E.

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			

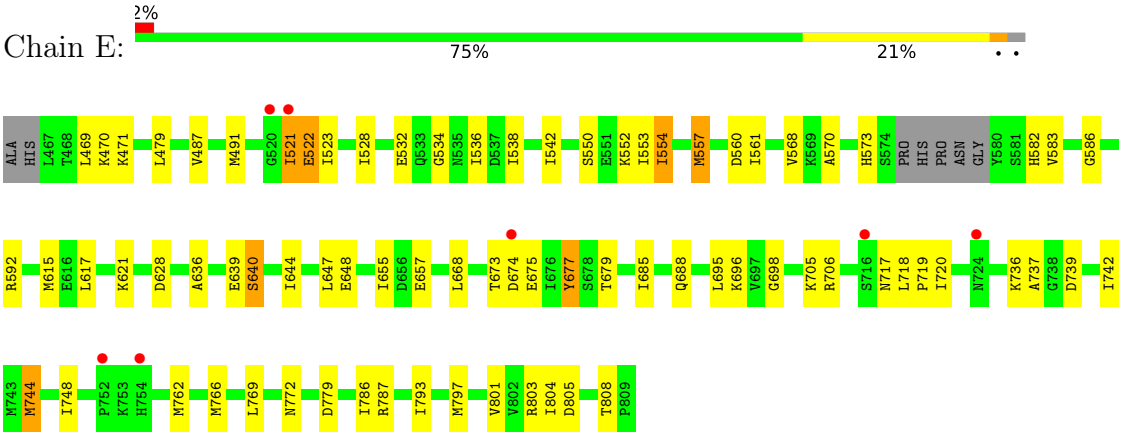
3 Residue-property plots (i)

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.

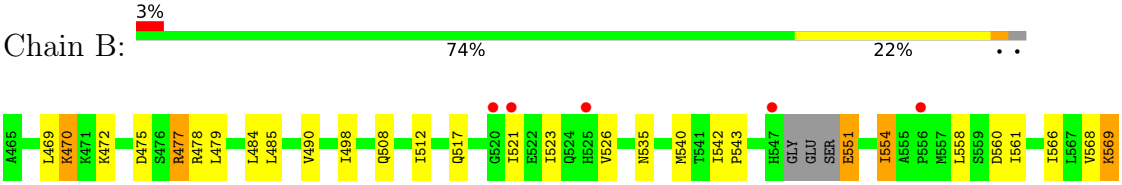
• Molecule 1: Stage II sporulation protein E

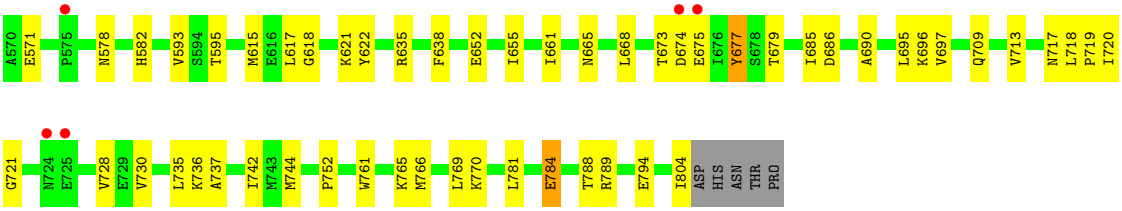


• Molecule 1: Stage II sporulation protein E

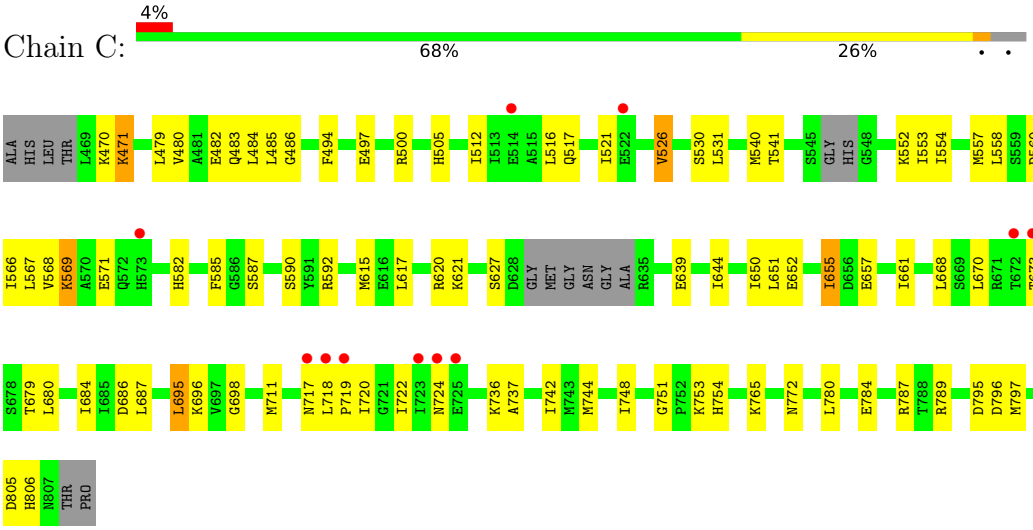


• Molecule 1: Stage II sporulation protein E

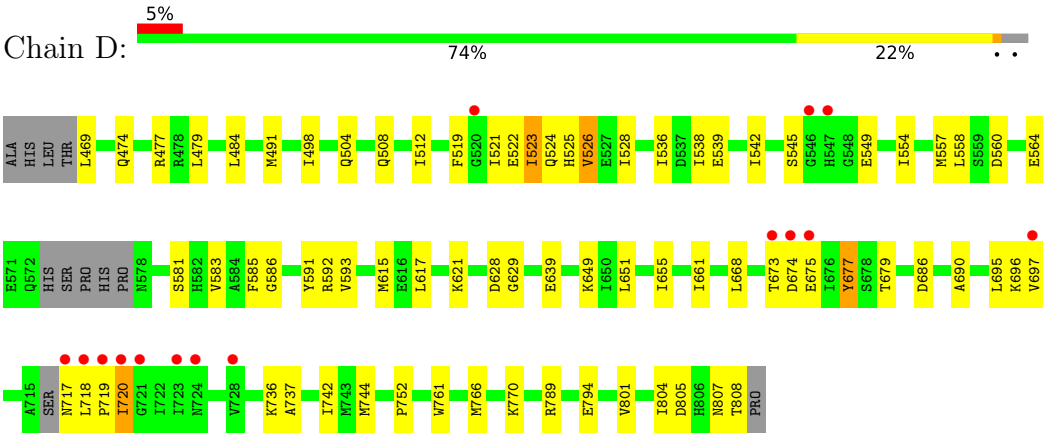




• Molecule 1: Stage II sporulation protein E



• Molecule 1: Stage II sporulation protein E



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	2.78 (at 3.88Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.276 , 0.323 0.276 , 0.324	Depositor DCC
R_{free} test set	1091 reflections (5.06%)	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)	0.28 , 38.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.79	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.24	0/2729	0.44	0/3672
1	B	0.24	0/2667	0.43	0/3585
1	C	0.24	0/2633	0.43	0/3538
1	D	0.24	0/2638	0.44	0/3541
1	E	0.24	0/2673	0.44	0/3592
All	All	0.24	0/13340	0.44	0/17928

There are no bond length outliers.

There are no bond angle outliers.

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	2690	0	2701	52	0
1	B	2631	0	2655	49	0
1	C	2599	0	2616	61	0
1	D	2607	0	2624	51	0
1	E	2639	0	2658	46	0
All	All	13166	0	13254	238	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 (238) 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: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: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:B:571:GLU:OE2	1:C:765:LYS:NZ	2.30	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:786:ILE:HD11	1:E:797:MET:HE1	1.90	0.54
1:B:752:PRO:HB3	1:B:788:THR:HG21	1.90	0.54
1:D:742:ILE:HD11	1:D:766:MET:HE1	1.90	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
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:B:742:ILE:HD11	1:B:766:MET:HE1	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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
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:E:742:ILE:HD11	1:E:766:MET:HE1	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:742:ILE:HD11	1:A:766:MET:HE1	1.98	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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:542:ILE:O	1:A:581:SER:HB3	2.18	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
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:E:762:MET:HG3	1:E:766:MET:HE3	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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%)	25 63
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%)	51 84

All (2) Ramachandran outliers are listed below:

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

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	Percentiles
1	A	298/298 (100%)	281 (94%)	17 (6%)	20 50
1	B	291/298 (98%)	272 (94%)	19 (6%)	17 46
1	C	290/298 (97%)	270 (93%)	20 (7%)	15 45
1	D	288/298 (97%)	269 (93%)	19 (7%)	16 46
1	E	293/298 (98%)	274 (94%)	19 (6%)	17 46
All	All	1460/1490 (98%)	1366 (94%)	94 (6%)	17 47

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	471	LYS
1	A	479	LEU

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Mol	Chain	Res	Type
1	A	516	LEU
1	A	526	VAL
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	A	744	MET
1	E	479	LEU
1	E	521	ILE
1	E	522	GLU
1	E	550	SER
1	E	552	LYS
1	E	553	ILE
1	E	554	ILE
1	E	557	MET
1	E	582	HIS
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	744	MET
1	E	808	THR
1	B	469	LEU
1	B	470	LYS
1	B	477	ARG
1	B	479	LEU
1	B	490	VAL
1	B	551	GLU
1	B	554	ILE
1	B	569	LYS

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Mol	Chain	Res	Type
1	B	578	ASN
1	B	582	HIS
1	B	593	VAL
1	B	615	MET
1	B	617	LEU
1	B	655	ILE
1	B	677	TYR
1	B	709	GLN
1	B	744	MET
1	B	781	LEU
1	B	784	GLU
1	C	471	LYS
1	C	479	LEU
1	C	526	VAL
1	C	541	THR
1	C	561	ILE
1	C	562	LEU
1	C	567	LEU
1	C	568	VAL
1	C	569	LYS
1	C	582	HIS
1	C	587	SER
1	C	615	MET
1	C	617	LEU
1	C	655	ILE
1	C	677	TYR
1	C	680	LEU
1	C	695	LEU
1	C	711	MET
1	C	720	ILE
1	C	744	MET
1	D	469	LEU
1	D	479	LEU
1	D	491	MET
1	D	523	ILE
1	D	524	GLN
1	D	525	HIS
1	D	526	VAL
1	D	560	ASP
1	D	593	VAL
1	D	615	MET
1	D	617	LEU

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Mol	Chain	Res	Type
1	D	651	LEU
1	D	655	ILE
1	D	677	TYR
1	D	711	MET
1	D	720	ILE
1	D	744	MET
1	D	805	ASP
1	D	808	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	572	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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^{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	A	345/345 (100%)	-0.00	9 (2%)	56	45	25, 74, 132, 181	0
1	B	337/345 (97%)	0.24	10 (2%)	50	38	62, 97, 153, 203	0
1	C	331/345 (95%)	0.43	13 (3%)	39	30	67, 107, 159, 223	0
1	D	334/345 (96%)	0.16	16 (4%)	30	25	26, 88, 143, 176	0
1	E	338/345 (97%)	0.02	7 (2%)	63	53	23, 79, 133, 169	0
All	All	1685/1725 (97%)	0.17	55 (3%)	46	36	23, 90, 147, 223	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	717	ASN	7.6
1	C	724	ASN	7.3
1	D	720	ILE	7.1
1	D	719	PRO	6.5
1	B	520	GLY	5.3
1	C	674	ASP	5.3
1	A	723	ILE	4.9
1	E	521	ILE	4.7
1	B	675	GLU	4.6
1	B	521	ILE	4.5
1	D	675	GLU	4.3
1	D	674	ASP	4.2
1	B	674	ASP	4.1
1	C	723	ILE	3.8
1	C	719	PRO	3.8
1	A	724	ASN	3.7
1	D	724	ASN	3.7
1	D	718	LEU	3.5
1	D	723	ILE	3.5
1	D	547	HIS	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	672	THR	3.4
1	B	724	ASN	3.3
1	A	721	GLY	3.2
1	C	675	GLU	3.2
1	E	716	SER	3.1
1	A	466	HIS	3.1
1	C	718	LEU	3.1
1	C	725	GLU	3.1
1	B	725	GLU	3.1
1	E	520	GLY	3.1
1	B	547	HIS	3.1
1	C	673	THR	2.9
1	A	674	ASP	2.8
1	A	722	ILE	2.7
1	B	525	HIS	2.6
1	C	514	GLU	2.6
1	D	721	GLY	2.6
1	C	522	GLU	2.5
1	A	790	SER	2.5
1	A	467	LEU	2.5
1	C	573	HIS	2.4
1	C	717	ASN	2.4
1	E	724	ASN	2.4
1	E	674	ASP	2.3
1	D	697	VAL	2.3
1	B	556	PRO	2.3
1	B	575	PRO	2.3
1	D	546	GLY	2.2
1	A	675	GLU	2.2
1	D	728	VAL	2.1
1	E	752	PRO	2.1
1	E	754	HIS	2.1
1	D	520	GLY	2.1
1	D	699	SER	2.0
1	D	673	THR	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.