



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:38 PM UTC

PDB ID : 4XS4 / pdb_00004xs4
Title : Salmonella typhimurium AhpC C165S mutant
Authors : Perkins, A.; Nelson, K.; Parsonage, D.; Poole, L.; Karplus, P.A.
Deposited on : 2015-01-21
Resolution : 2.65 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

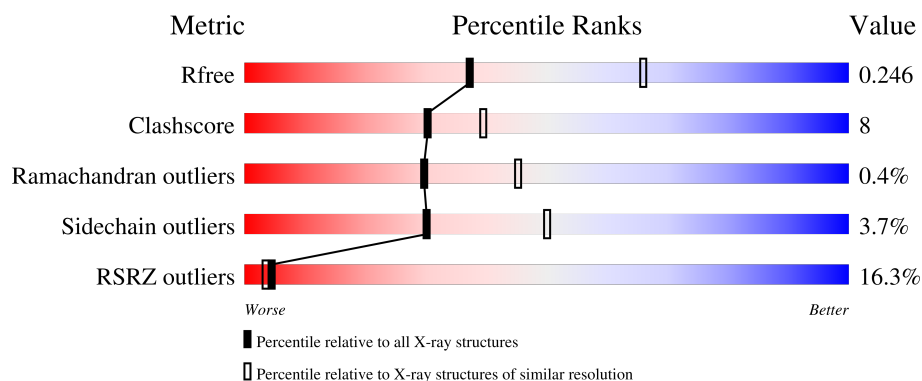
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	186	6% 74% 14% 10%
1	C	186	17% 77% 16% 7%
1	D	186	18% 82% 16% ..
1	E	186	25% 73% 22% 6%
2	B	186	15% 80% 16% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7688 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 Alkyl hydroperoxide reductase subunit C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	167	Total	C	N	O	S	0	10	0
			1389	884	228	273	4			
1	C	186	Total	C	N	O	S	0	2	0
			1473	938	244	288	3			
1	D	186	Total	C	N	O	S	0	1	0
			1462	931	242	286	3			
1	E	186	Total	C	N	O	S	0	1	0
			1464	932	242	287	3			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	165	SER	CYS	engineered mutation	UNP P0A251
C	165	SER	CYS	engineered mutation	UNP P0A251
D	165	SER	CYS	engineered mutation	UNP P0A251
E	165	SER	CYS	engineered mutation	UNP P0A251

- Molecule 2 is a protein called Alkyl hydroperoxide reductase subunit C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	186	Total	C	N	O	S	0	9	0
			1531	976	254	297	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	165	SER	CYS	engineered mutation	UNP P0A251

- Molecule 3 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total K 1 1	0	0
3	B	1	Total K 1 1	0	0
3	D	1	Total K 1 1	0	0

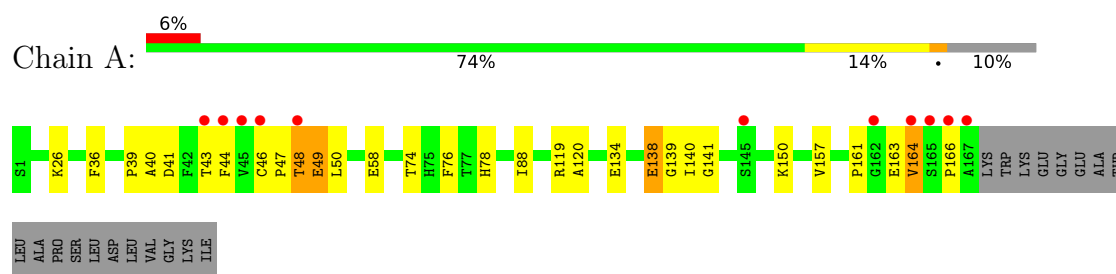
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	90	Total O 90 90	0	0
4	B	94	Total O 94 94	0	0
4	C	79	Total O 79 79	0	0
4	D	80	Total O 80 80	0	0
4	E	23	Total O 23 23	0	0

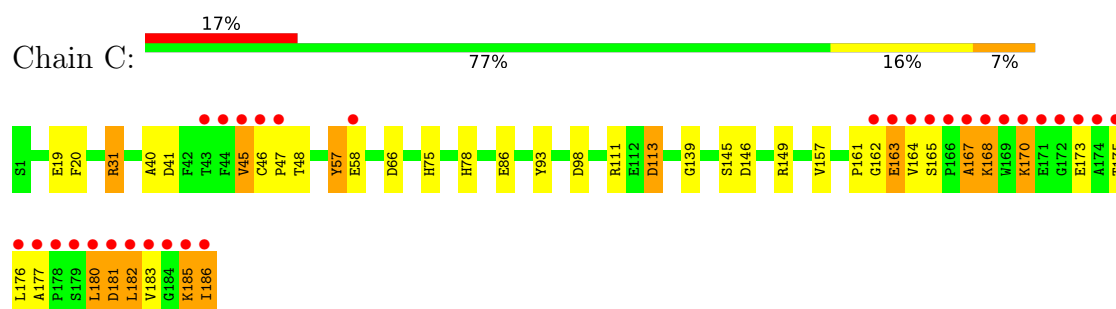
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

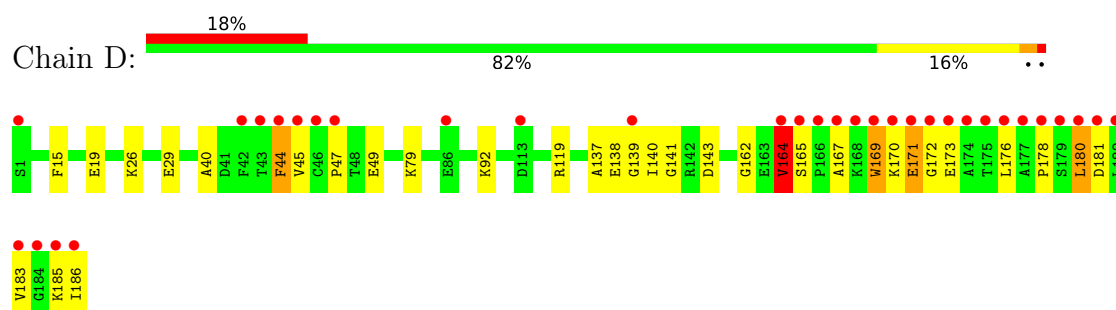
• Molecule 1: Alkyl hydroperoxide reductase subunit C



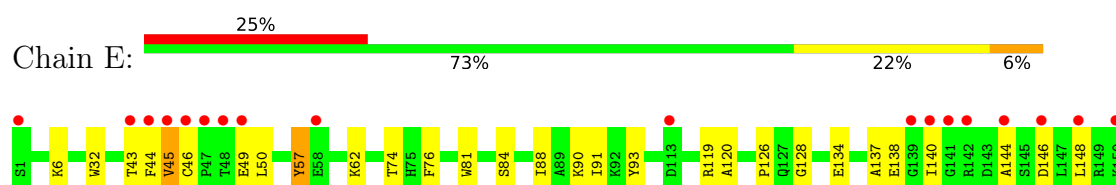
• Molecule 1: Alkyl hydroperoxide reductase subunit C

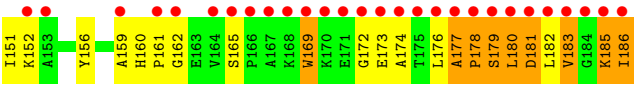


• Molecule 1: Alkyl hydroperoxide reductase subunit C

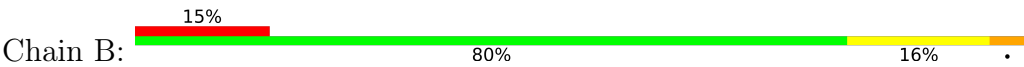


• Molecule 1: Alkyl hydroperoxide reductase subunit C





● Molecule 2: Alkyl hydroperoxide reductase subunit C



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	127.05Å 172.10Å 136.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	68.11 – 2.65 68.11 – 2.65	Depositor EDS
% Data completeness (in resolution range)	100.0 (68.11-2.65) 99.9 (68.11-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 2.65Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.202 , 0.245 0.206 , 0.246	Depositor DCC
R_{free} test set	2160 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	45.4	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 72.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7688	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OCS, K

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	0.81	1/1423 (0.1%)	1.10	7/1932 (0.4%)
1	C	0.82	0/1507	1.36	23/2041 (1.1%)
1	D	0.78	0/1496	1.18	8/2027 (0.4%)
1	E	0.75	1/1498 (0.1%)	1.41	25/2030 (1.2%)
2	B	0.87	2/1551 (0.1%)	1.48	25/2098 (1.2%)
All	All	0.81	4/7475 (0.1%)	1.32	88/10128 (0.9%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	183	VAL	CA-C	6.17	1.60	1.52
1	E	173	GLU	CA-C	5.83	1.61	1.53
2	B	137	ALA	CA-CB	-5.63	1.44	1.53
1	A	163	GLU	CA-C	-5.36	1.46	1.53

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	182	LEU	N-CA-C	22.71	140.66	113.18
2	B	182	LEU	CA-C-N	-12.94	104.29	122.92
2	B	182	LEU	C-N-CA	-12.94	104.29	122.92
1	E	177	ALA	CA-C-N	11.95	132.09	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	177	ALA	C-N-CA	11.95	132.09	119.90
2	B	182	LEU	N-CA-CB	-11.56	90.99	110.41
1	E	174	ALA	N-CA-C	10.69	125.58	110.50
2	B	184	GLY	N-CA-C	-10.52	101.38	115.36
2	B	180	LEU	N-CA-C	-10.42	99.29	114.39
2	B	177	ALA	N-CA-C	9.94	131.00	108.93
1	C	181	ASP	N-CA-C	9.50	122.63	111.71
1	A	140	ILE	N-CA-C	9.44	121.22	106.88
1	E	183	VAL	N-CA-C	8.98	121.06	108.93
2	B	183	VAL	N-CA-C	8.95	121.86	108.80
1	C	181	ASP	N-CA-CB	-8.87	96.57	110.22
2	B	183	VAL	CG1-CB-CG2	-8.68	91.71	110.80
1	D	172	GLY	N-CA-C	8.60	126.03	113.48
2	B	176	LEU	CA-CB-CG	-8.58	86.27	116.30
1	E	57	TYR	N-CA-C	8.34	120.45	111.36
2	B	183	VAL	CA-C-N	8.28	137.99	121.93
2	B	183	VAL	C-N-CA	8.28	137.99	121.93
1	C	167	ALA	N-CA-C	8.23	121.85	110.24
1	D	169	TRP	CA-C-N	7.96	136.19	122.82
1	D	169	TRP	C-N-CA	7.96	136.19	122.82
2	B	180	LEU	CA-C-N	7.59	133.39	120.72
2	B	180	LEU	C-N-CA	7.59	133.39	120.72
1	C	45	VAL	N-CA-C	7.56	118.35	110.72
1	E	160	HIS	CA-C-N	7.53	127.29	119.76
1	E	160	HIS	C-N-CA	7.53	127.29	119.76
1	D	44	PHE	N-CA-C	7.19	121.75	112.12
1	A	138	GLU	N-CA-C	7.16	120.92	111.75
1	C	180	LEU	N-CA-C	7.07	118.99	111.28
2	B	167	ALA	N-CA-C	-6.94	100.17	110.23
1	C	45	VAL	CB-CA-C	-6.92	102.66	112.22
1	E	172	GLY	N-CA-C	6.90	123.89	114.92
1	E	43	THR	CA-C-N	6.74	132.67	122.56
1	E	43	THR	C-N-CA	6.74	132.67	122.56
1	C	57	TYR	N-CA-C	6.68	118.64	111.36
1	A	26	LYS	CB-CG-CD	6.52	126.31	111.30
1	C	177	ALA	CA-C-N	-6.51	112.79	119.83
1	C	177	ALA	C-N-CA	-6.51	112.79	119.83
2	B	181	ASP	CA-C-N	6.35	133.97	121.58
2	B	181	ASP	C-N-CA	6.35	133.97	121.58
2	B	172	GLY	N-CA-C	6.18	122.05	114.69
1	D	183	VAL	N-CA-C	6.16	117.25	108.93
1	C	165	SER	CA-C-N	6.09	127.45	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	165	SER	C-N-CA	6.09	127.45	119.84
1	C	185	LYS	N-CA-C	6.09	120.87	112.90
2	B	182	LEU	CA-CB-CG	6.08	137.59	116.30
1	C	186	ILE	CG1-CB-CG2	-5.94	92.88	110.70
1	D	164	VAL	N-CA-C	5.93	118.74	108.95
1	E	45	VAL	N-CA-C	5.92	116.70	110.72
2	B	167	ALA	CA-C-O	-5.91	114.69	121.19
1	A	26	LYS	CA-CB-CG	-5.85	102.40	114.10
2	B	182	LEU	CB-CG-CD2	-5.83	93.22	110.70
1	E	183	VAL	CB-CA-C	-5.79	102.66	111.69
1	E	144	ALA	N-CA-C	5.77	119.42	112.38
1	A	161	PRO	CA-C-N	-5.68	113.17	122.20
1	A	161	PRO	C-N-CA	-5.68	113.17	122.20
1	D	40	ALA	N-CA-C	5.64	117.24	107.93
2	B	170	LYS	N-CA-C	-5.62	100.52	109.23
1	E	146[A]	ASP	N-CA-C	-5.58	105.19	111.28
1	E	146[B]	ASP	N-CA-C	-5.58	105.19	111.28
1	E	180	LEU	N-CA-C	5.58	122.69	110.80
1	E	44	PHE	N-CA-C	5.57	119.76	112.13
1	E	156	TYR	N-CA-C	-5.57	105.29	111.36
1	C	168	LYS	CB-CG-CD	5.54	124.05	111.30
2	B	181	ASP	CA-C-O	5.47	126.11	119.38
1	C	173	GLU	CA-C-N	5.46	128.47	120.71
1	C	173	GLU	C-N-CA	5.46	128.47	120.71
2	B	141	GLY	N-CA-C	5.46	118.97	111.54
1	E	173	GLU	N-CA-CB	-5.44	102.18	110.45
1	C	161	PRO	N-CA-C	5.43	123.65	112.47
1	E	151	ILE	N-CA-C	5.32	115.52	110.42
1	E	144	ALA	CA-C-N	-5.28	113.69	122.40
1	E	144	ALA	C-N-CA	-5.28	113.69	122.40
1	C	146	ASP	N-CA-C	-5.26	105.62	111.36
1	C	163	GLU	CB-CA-C	-5.26	98.97	109.33
1	D	44	PHE	CA-CB-CG	-5.23	108.57	113.80
1	A	49	GLU	N-CA-C	-5.21	105.66	111.23
1	C	145	SER	N-CA-C	5.20	116.94	111.28
1	C	40	ALA	N-CA-C	5.19	116.83	108.32
1	E	178	PRO	CA-C-O	-5.15	115.54	121.36
1	E	169	TRP	CB-CA-C	5.12	118.21	109.72
1	E	173	GLU	CB-CA-C	5.09	119.88	109.76
2	B	177	ALA	CA-C-O	-5.06	115.13	120.09
1	C	98	ASP	CA-C-N	-5.04	114.42	119.56
1	C	98	ASP	C-N-CA	-5.04	114.42	119.56

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	181	ASP	Peptide

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	1389	0	1327	23	0
1	C	1473	0	1433	34	0
1	D	1462	0	1422	38	0
1	E	1464	0	1421	37	0
2	B	1531	0	1483	16	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
4	A	90	0	0	3	0
4	B	94	0	0	0	1
4	C	79	0	0	1	0
4	D	80	0	0	0	1
4	E	23	0	0	0	0
All	All	7688	0	7086	121	1

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 8.

All (121) 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:A:49:GLU:HG2	2:B:167:ALA:HB2	1.48	0.94
1:C:45:VAL:HG22	1:D:164:VAL:HG11	1.53	0.90
1:E:182:LEU:HG	1:E:185:LYS:HD3	1.56	0.86
1:C:163:GLU:N	1:C:163:GLU:OE1	2.11	0.83
1:D:165:SER:HB3	1:D:169:TRP:CG	2.15	0.82
1:C:45:VAL:CG2	1:D:164:VAL:HG11	2.12	0.78
1:D:170:LYS:N	1:D:173:GLU:OE2	2.15	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:119:ARG:NH2	1:E:138:GLU:OE2	2.16	0.76
1:C:167:ALA:HB2	1:D:49:GLU:HG2	1.71	0.71
1:E:182:LEU:HD21	1:E:186:ILE:HG12	1.72	0.71
1:C:176:LEU:HD21	1:C:186:ILE:HD12	1.72	0.69
1:E:165:SER:HB3	1:E:169:TRP:NE1	2.07	0.69
2:B:162:GLY:O	2:B:178:PRO:HD2	1.92	0.69
1:E:182:LEU:HD23	1:E:182:LEU:O	1.93	0.69
1:C:183:VAL:HA	1:D:44:PHE:CE1	2.30	0.67
1:E:137:ALA:HB3	1:E:140:ILE:HD12	1.76	0.67
1:A:40:ALA:O	1:A:43[B]:THR:OG1	2.10	0.67
1:D:162:GLY:O	1:D:178:PRO:HD2	1.95	0.66
2:B:79:LYS:NZ	1:D:180:LEU:O	2.28	0.66
1:E:182:LEU:HD21	1:E:186:ILE:HG23	1.77	0.66
1:A:139:GLY:HA3	2:B:157:VAL:HG11	1.76	0.66
1:E:62:LYS:O	1:E:62:LYS:HD2	1.95	0.65
1:E:45:VAL:HG11	1:E:119:ARG:NH2	2.12	0.65
2:B:45[B]:VAL:HG11	2:B:138:GLU:OE1	1.97	0.64
1:A:44[B]:PHE:C	1:A:47[B]:PRO:HD2	2.23	0.63
1:C:183:VAL:HA	1:D:44:PHE:CZ	2.34	0.62
1:C:182:LEU:HG	1:D:44:PHE:CE1	2.34	0.62
1:E:50:LEU:HB3	1:E:91:ILE:HD11	1.82	0.61
1:E:6:LYS:NZ	1:E:128:GLY:HA3	2.16	0.60
2:B:15:PHE:CE1	2:B:79:LYS:HG3	2.36	0.60
1:C:182:LEU:HA	1:C:185:LYS:HD3	1.84	0.59
1:D:26:LYS:HA	1:D:29:GLU:HG3	1.83	0.59
1:D:119:ARG:NH2	1:D:138:GLU:OE1	2.36	0.59
1:C:139:GLY:HA2	1:D:164:VAL:HG22	1.84	0.59
1:E:182:LEU:O	1:E:185:LYS:HB3	2.01	0.58
1:C:164:VAL:HG11	1:D:45:VAL:HG21	1.86	0.58
1:A:44[B]:PHE:O	1:A:47[B]:PRO:HD2	2.04	0.57
1:D:137:ALA:HB3	1:D:140:ILE:HD12	1.86	0.57
1:E:165:SER:HB3	1:E:169:TRP:CD1	2.39	0.57
1:E:181:ASP:HA	1:E:183:VAL:H	1.70	0.57
1:D:170:LYS:H	1:D:173:GLU:CD	2.13	0.56
1:A:39:PRO:HD2	1:A:46[B]:CYS:SG	2.45	0.56
1:C:182:LEU:HG	1:D:44:PHE:CD1	2.40	0.56
1:C:48:THR:HG22	1:D:167:ALA:HB3	1.88	0.55
1:A:164:VAL:HG11	2:B:45[B]:VAL:HG22	1.88	0.55
1:C:168:LYS:HE2	1:D:143:ASP:OD2	2.07	0.55
1:E:182:LEU:CD2	1:E:186:ILE:HG12	2.37	0.54
1:C:46:CYS:N	1:C:47:PRO:HD2	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47[B]:PRO:HB3	1:A:88:ILE:HD11	1.89	0.54
1:A:157:VAL:HG11	2:B:139:GLY:HA3	1.90	0.54
1:A:47[B]:PRO:HA	1:A:50:LEU:HD12	1.90	0.53
1:A:139:GLY:O	2:B:165:SER:HB2	2.09	0.53
1:E:57:TYR:CE1	1:E:93:TYR:HB3	2.43	0.52
1:E:181:ASP:HA	1:E:183:VAL:HG22	1.91	0.52
1:D:44:PHE:C	1:D:47:PRO:HD2	2.35	0.52
1:C:31:ARG:HD3	1:C:66:ASP:OD2	2.10	0.51
2:B:163:GLU:OE1	2:B:175:THR:HG21	2.11	0.50
1:E:6:LYS:HZ2	1:E:128:GLY:HA3	1.76	0.50
1:D:164:VAL:HG13	1:D:165:SER:N	2.27	0.50
1:D:181:ASP:O	1:D:185:LYS:HE2	2.11	0.50
1:A:36:PHE:HZ	1:A:49:GLU:HB3	1.76	0.50
1:C:47:PRO:HG3	1:D:186:ILE:CG2	2.42	0.50
1:E:32:TRP:CE2	1:E:126:PRO:HD3	2.47	0.50
1:E:183:VAL:HG23	1:E:183:VAL:O	2.12	0.49
1:C:180:LEU:HD12	1:C:181:ASP:N	2.27	0.49
1:D:170:LYS:CG	1:D:171:GLU:N	2.75	0.49
1:A:74:THR:OG1	1:A:76:PHE:HB2	2.11	0.49
1:E:46:CYS:O	1:E:49:GLU:HB2	2.12	0.49
1:E:120:ALA:HA	1:E:134:GLU:O	2.12	0.49
1:E:148:LEU:O	1:E:152:LYS:HG2	2.12	0.49
1:C:176:LEU:HD21	1:C:186:ILE:CD1	2.43	0.49
1:D:170:LYS:HG2	1:D:171:GLU:N	2.28	0.49
1:E:165:SER:HB3	1:E:169:TRP:HE1	1.77	0.49
1:D:15:PHE:CE1	1:D:79:LYS:HG3	2.48	0.48
1:A:119:ARG:HE	1:A:138:GLU:HA	1.78	0.48
1:D:19:GLU:HA	1:D:19:GLU:OE1	2.14	0.47
1:C:41:ASP:OD2	1:C:78:HIS:ND1	2.45	0.47
1:A:150:LYS:NZ	4:A:341:HOH:O	2.48	0.46
1:E:182:LEU:HD21	1:E:186:ILE:CG1	2.44	0.46
1:C:183:VAL:CG2	1:D:44:PHE:HZ	2.29	0.46
1:A:58:GLU:HB2	4:A:349:HOH:O	2.16	0.45
1:C:111:ARG:HB3	1:C:113[A]:ASP:OD2	2.16	0.45
1:E:74:THR:OG1	1:E:76:PHE:HB2	2.16	0.45
1:E:81:TRP:CE2	1:E:88:ILE:HG13	2.51	0.45
1:E:176:LEU:HD23	1:E:177:ALA:N	2.32	0.45
1:A:120:ALA:HA	1:A:134:GLU:O	2.17	0.45
2:B:109:ASN:OD1	2:B:118:ASP:HB2	2.17	0.45
1:C:181:ASP:C	1:C:181:ASP:OD1	2.59	0.45
1:C:183:VAL:HG22	1:D:44:PHE:HZ	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:177:ALA:HA	1:E:178:PRO:HD2	1.69	0.45
1:A:46[A]:CYS:O	1:A:48[A]:THR:N	2.48	0.45
1:C:149:ARG:NH2	1:D:141:GLY:O	2.37	0.45
1:C:183:VAL:HA	1:D:44:PHE:HE1	1.79	0.44
2:B:16:LYS:O	2:B:19:GLU:HG3	2.17	0.44
1:E:182:LEU:CG	1:E:185:LYS:HD3	2.40	0.44
1:E:6:LYS:HZ3	1:E:128:GLY:HA3	1.83	0.44
2:B:162:GLY:O	2:B:178:PRO:CD	2.63	0.43
1:E:159:ALA:C	1:E:161:PRO:HD3	2.43	0.43
1:C:162:GLY:N	1:C:163:GLU:OE1	2.52	0.43
1:D:169:TRP:HA	1:D:173:GLU:OE2	2.18	0.43
1:C:164:VAL:HG13	1:D:139:GLY:HA2	2.01	0.43
1:C:57:TYR:CE1	1:C:93:TYR:HB3	2.54	0.43
1:A:141:GLY:O	2:B:149:ARG:NH2	2.29	0.42
1:C:139:GLY:N	4:C:230:HOH:O	2.34	0.42
1:E:119:ARG:HE	1:E:138:GLU:HA	1.84	0.42
1:A:139:GLY:N	4:A:338:HOH:O	2.38	0.42
1:C:168:LYS:O	1:C:170:LYS:HE2	2.19	0.42
1:D:92:LYS:HB3	1:D:92:LYS:HE2	1.86	0.42
1:E:62:LYS:HD2	1:E:62:LYS:C	2.44	0.42
1:C:20:PHE:CD1	1:C:75:HIS:HD2	2.38	0.42
1:A:166:PRO:O	2:B:46[A]:OCS:HB3	2.20	0.41
1:E:178:PRO:O	1:E:179:SER:OG	2.25	0.41
1:A:41:ASP:OD2	1:A:78:HIS:ND1	2.39	0.41
1:C:157:VAL:HG11	1:D:139:GLY:HA3	2.03	0.41
1:E:162:GLY:O	1:E:178:PRO:HD2	2.21	0.41
1:D:169:TRP:HA	1:D:173:GLU:CD	2.46	0.41
1:A:40:ALA:HB3	1:A:43[A]:THR:HG21	2.03	0.40
1:C:164:VAL:CG1	1:D:139:GLY:HA2	2.51	0.40
1:D:169:TRP:HA	1:D:173:GLU:OE1	2.22	0.40
2:B:32:TRP:CE2	2:B:126:PRO:HD3	2.56	0.40
1:E:45:VAL:HG13	1:E:46:CYS:N	2.37	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:307:HOH:O	4:D:302:HOH:O[8_457]	2.17	0.03

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	175/186 (94%)	168 (96%)	7 (4%)	0	100	100
1	C	186/186 (100%)	181 (97%)	5 (3%)	0	100	100
1	D	185/186 (100%)	181 (98%)	4 (2%)	0	100	100
1	E	185/186 (100%)	178 (96%)	5 (3%)	2 (1%)	11	19
2	B	191/186 (103%)	188 (98%)	1 (0%)	2 (1%)	12	20
All	All	922/930 (99%)	896 (97%)	22 (2%)	4 (0%)	30	45

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	179	SER
1	E	180	LEU
2	B	168	LYS
2	B	178	PRO

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	149/154 (97%)	146 (98%)	3 (2%)	48	69
1	C	156/154 (101%)	147 (94%)	9 (6%)	18	31
1	D	155/154 (101%)	151 (97%)	4 (3%)	40	63
1	E	155/154 (101%)	151 (97%)	4 (3%)	40	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	160/153 (105%)	149 (93%)	11 (7%)	14	24
All	All	775/769 (101%)	744 (96%)	31 (4%)	30	47

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48[A]	THR
1	A	48[B]	THR
1	A	164	VAL
2	B	19	GLU
2	B	45[A]	VAL
2	B	45[B]	VAL
2	B	86	GLU
2	B	164	VAL
2	B	168	LYS
2	B	173	GLU
2	B	175	THR
2	B	179	SER
2	B	182	LEU
2	B	185	LYS
1	C	19	GLU
1	C	31	ARG
1	C	58	GLU
1	C	86	GLU
1	C	113[A]	ASP
1	C	113[B]	ASP
1	C	170	LYS
1	C	175	THR
1	C	182	LEU
1	D	164	VAL
1	D	171	GLU
1	D	176	LEU
1	D	180	LEU
1	E	84	SER
1	E	90	LYS
1	E	185	LYS
1	E	186	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	GLN
2	B	160	HIS
1	C	160	HIS
1	E	12	ASN
1	E	61	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues 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	OCS	B	46[A]	2	6,8,9	0.77	0	7,11,13	1.53	2 (28%)
2	OCS	B	46[B]	2	4,5,9	0.82	0	1,5,13	0.50	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	OCS	B	46[A]	2	-	1/4/7/9	-
2	OCS	B	46[B]	2	-	1/1/4/9	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	46[A]	OCS	OD3-SG-CB	2.17	110.00	106.76
2	B	46[A]	OCS	OD1-SG-CB	2.04	109.80	106.76

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	46[A]	OCS	N-CA-CB-SG
2	B	46[B]	OCS	N-CA-CB-SG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	46[A]	OCS	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

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	167/186 (89%)	0.02	11 (6%)	24 18	16, 40, 76, 142	10 (5%)
1	C	186/186 (100%)	0.83	31 (16%)	4 3	16, 52, 113, 199	24 (12%)
1	D	186/186 (100%)	0.78	33 (17%)	4 2	30, 52, 110, 150	23 (12%)
1	E	186/186 (100%)	1.43	46 (24%)	2 1	47, 79, 134, 188	23 (12%)
2	B	185/186 (99%)	1.08	27 (14%)	6 4	14, 39, 66, 160	31 (16%)
All	All	910/930 (97%)	0.84	148 (16%)	4 3	14, 52, 118, 199	111 (12%)

All (148) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	176	LEU	15.3
2	B	169	TRP	14.7
1	E	180	LEU	12.6
2	B	167	ALA	12.4
2	B	174	ALA	12.3
2	B	182	LEU	11.9
2	B	180	LEU	11.7
2	B	177	ALA	11.7
2	B	171	GLU	11.6
2	B	166	PRO	11.5
2	B	164	VAL	11.5
1	C	180	LEU	11.3
2	B	178	PRO	11.1
1	C	176	LEU	10.9
2	B	185	LYS	10.6
1	A	44[A]	PHE	10.3
2	B	172	GLY	10.2
2	B	186	ILE	9.8
2	B	168	LYS	9.8
1	C	182	LEU	9.6

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Mol	Chain	Res	Type	RSRZ
2	B	183	VAL	9.6
1	C	175	THR	9.0
1	E	174	ALA	8.8
2	B	175	THR	8.6
2	B	170	LYS	8.5
2	B	179	SER	8.4
1	E	184	GLY	8.2
1	C	186	ILE	8.1
1	D	176	LEU	8.1
1	D	167	ALA	8.0
1	D	180	LEU	8.0
1	C	174	ALA	7.9
1	E	169	TRP	7.8
1	D	169	TRP	7.6
1	D	186	ILE	7.6
1	D	184	GLY	7.5
1	C	185	LYS	6.9
1	D	182	LEU	6.9
1	C	169	TRP	6.9
1	D	177	ALA	6.8
2	B	173	GLU	6.8
1	D	183	VAL	6.8
1	C	167	ALA	6.6
2	B	184	GLY	6.4
1	C	184	GLY	6.3
1	C	165	SER	6.3
1	E	176	LEU	6.3
1	A	46[A]	CYS	6.3
1	E	183	VAL	6.2
1	E	170	LYS	6.1
1	D	178	PRO	6.1
2	B	165	SER	6.1
1	D	44	PHE	6.0
1	A	165	SER	6.0
1	A	45[A]	VAL	6.0
1	D	179	SER	6.0
1	E	164	VAL	5.9
1	D	172	GLY	5.9
2	B	181	ASP	5.8
1	C	166	PRO	5.6
1	C	179	SER	5.6
1	C	164	VAL	5.6

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Mol	Chain	Res	Type	RSRZ
1	D	174	ALA	5.5
1	E	182	LEU	5.5
1	E	45	VAL	5.5
1	E	175	THR	5.4
1	C	170	LYS	5.3
1	E	186	ILE	5.3
1	C	172	GLY	5.2
1	E	177	ALA	5.1
1	C	168	LYS	5.1
1	D	185	LYS	5.1
1	D	166	PRO	5.0
1	A	164	VAL	5.0
1	E	166	PRO	4.9
1	E	46	CYS	4.8
1	C	177	ALA	4.7
1	E	185	LYS	4.7
1	C	171	GLU	4.7
1	E	173	GLU	4.6
1	E	44	PHE	4.6
1	E	165	SER	4.6
1	A	166	PRO	4.4
1	E	168	LYS	4.4
1	D	165	SER	4.3
1	E	179	SER	4.3
1	D	175	THR	4.3
1	D	47	PRO	4.2
1	D	46	CYS	4.2
1	E	172	GLY	4.2
1	E	178	PRO	4.1
1	D	164	VAL	4.1
1	C	178	PRO	4.1
1	E	139	GLY	3.9
1	C	183	VAL	3.9
1	D	170	LYS	3.8
1	D	45	VAL	3.8
1	C	163	GLU	3.8
1	C	44	PHE	3.8
1	E	167	ALA	3.7
1	C	162	GLY	3.7
1	D	181	ASP	3.7
1	E	148	LEU	3.6
1	A	167	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	168	LYS	3.6
1	C	45	VAL	3.6
1	E	144	ALA	3.6
1	C	181	ASP	3.5
1	D	1	SER	3.4
1	C	46	CYS	3.4
1	E	171	GLU	3.4
1	E	181	ASP	3.2
1	D	171	GLU	3.0
1	E	140	ILE	2.9
1	E	162	GLY	2.9
1	E	150	LYS	2.9
1	E	43	THR	2.8
1	D	113	ASP	2.8
1	E	49	GLU	2.7
1	D	173	GLU	2.7
2	B	163	GLU	2.7
1	D	42	PHE	2.7
1	C	173	GLU	2.6
1	E	152	LYS	2.6
2	B	44[A]	PHE	2.5
1	D	43	THR	2.5
1	E	161	PRO	2.4
1	E	113	ASP	2.4
1	E	153	ALA	2.4
1	E	146[A]	ASP	2.3
1	E	141	GLY	2.3
1	E	159	ALA	2.2
1	A	48[A]	THR	2.2
1	C	58	GLU	2.2
1	E	1	SER	2.2
1	A	43[A]	THR	2.2
2	B	4	ASN	2.2
2	B	162	GLY	2.2
1	E	58	GLU	2.1
1	E	48	THR	2.1
1	D	139	GLY	2.1
1	D	86	GLU	2.1
1	C	47	PRO	2.1
1	C	43	THR	2.1
1	A	162	GLY	2.1
1	E	47	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	142	ARG	2.0
1	A	145	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
2	OCS	B	46[A]	9/10	0.88	0.18	41,49,79,79	9
2	OCS	B	46[B]	6/10	0.88	0.18	24,31,34,35	6

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(Å ²)	Q<0.9
3	K	A	201	1/1	0.86	0.16	52,52,52,52	1
3	K	B	201	1/1	0.93	0.13	73,73,73,73	0
3	K	D	201	1/1	0.94	0.18	105,105,105,105	0

6.5 Other polymers [i](#)

There are no such residues in this entry.