



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 10:17 AM UTC

PDB ID : 3BFE / pdb_00003bfe
Title : Crystal Structure of the Class A beta-lactamase SED-1 from *Citrobacter sedlakii*
Authors : Pernot, L.; Petrella, S.; Sougakoff, W.
Deposited on : 2007-11-21
Resolution : 2.40 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

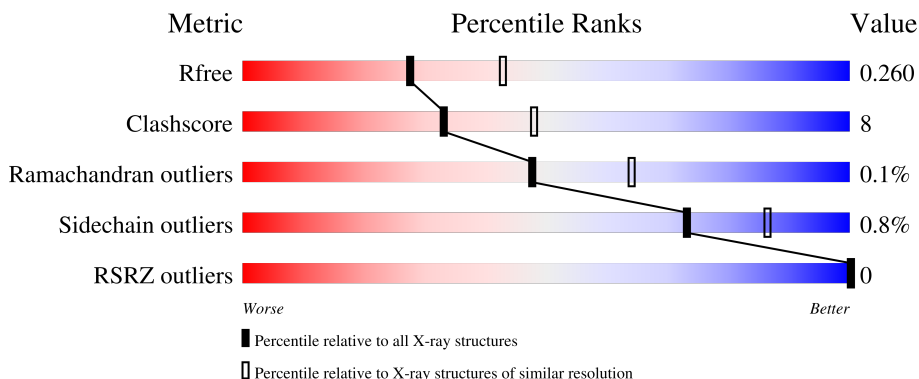
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


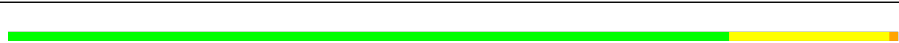


The reported resolution of this entry is 2.40 Å.

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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	262	 82% 18%
1	B	262	 81% 18% .
1	C	262	 79% 19% .
1	D	262	 81% 17% .

2 Entry composition [i](#)

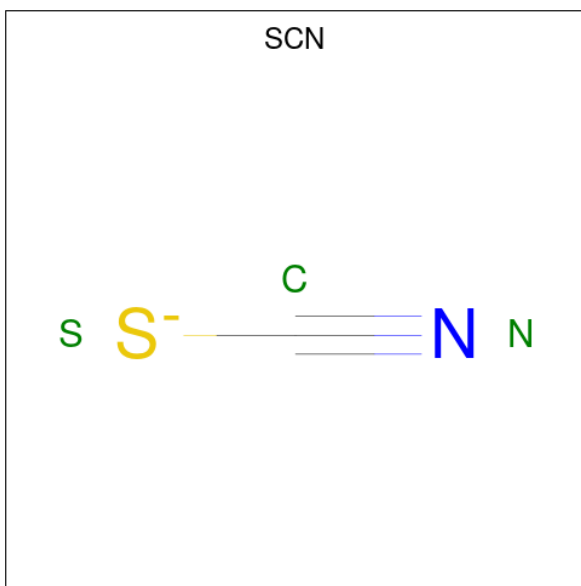
There are 3 unique types of molecules in this entry. The entry contains 8428 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Class A beta-lactamase Sed1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	262	Total 1985	C 1239	N 354	O 385	S 7	0	0	0
1	B	262	Total 1985	C 1239	N 354	O 385	S 7	0	0	0
1	C	262	Total 1985	C 1239	N 354	O 385	S 7	0	0	0
1	D	262	Total 1985	C 1239	N 354	O 385	S 7	0	0	0

- Molecule 2 is THIOCYANATE ION (CCD ID: SCN) (formula: CNS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	S		
2	A	1	Total 3	C 1	N 1	S 1	0	0

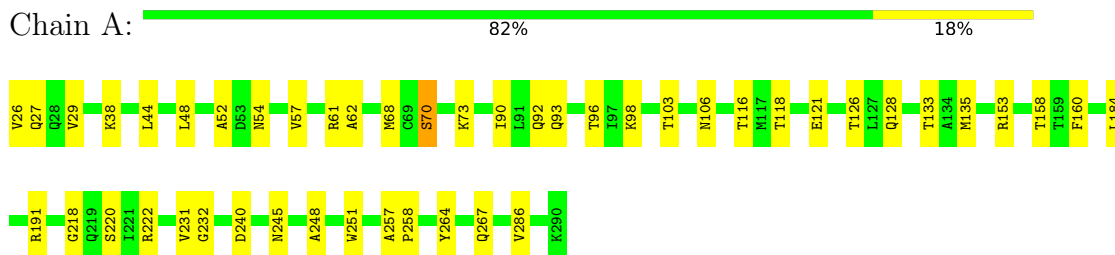
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	130	Total 130	O 130	0	0
3	B	122	Total 122	O 122	0	0
3	C	113	Total 113	O 113	0	0
3	D	120	Total 120	O 120	0	0

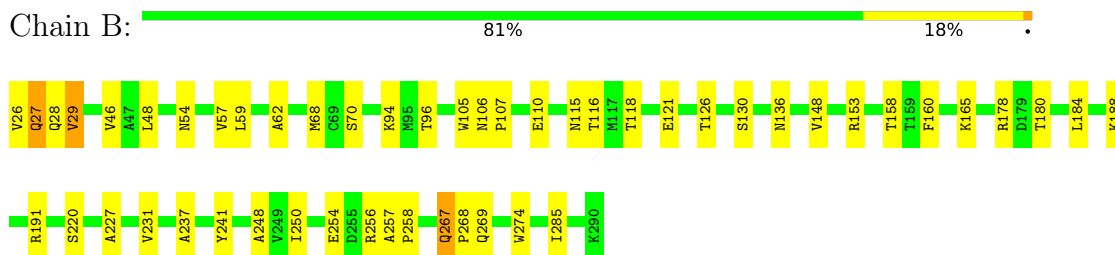
3 Residue-property plots

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.

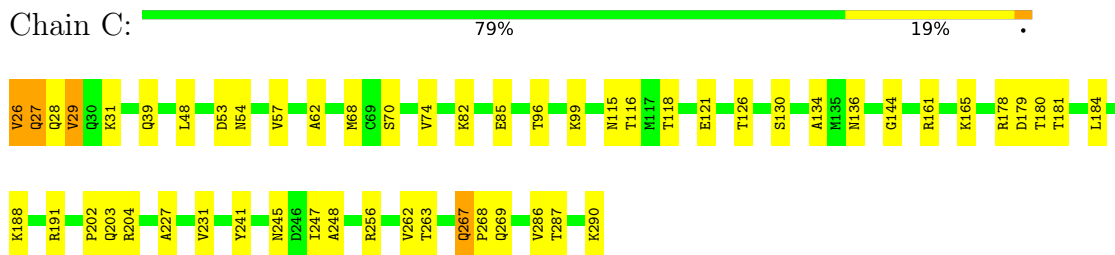
- Molecule 1: Class A beta-lactamase Sed1



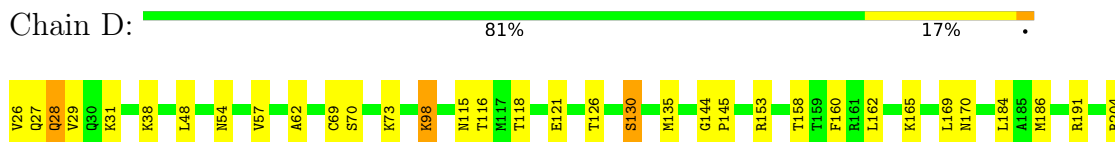
- Molecule 1: Class A beta-lactamase Sed1



- Molecule 1: Class A beta-lactamase Sed1



- Molecule 1: Class A beta-lactamase Sed1





4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	188.10Å 73.66Å 105.41Å 90.00° 121.67° 90.00°	Depositor
Resolution (Å)	29.31 – 2.40 29.31 – 2.40	Depositor EDS
% Data completeness (in resolution range)	88.7 (29.31-2.40) 88.7 (29.31-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.33 (at 2.39Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.223 , 0.260 0.223 , 0.260	Depositor DCC
R_{free} test set	2145 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	18.1	Xtrriage
Anisotropy	0.644	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 24.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.215 for -h-2*1,-k,l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8428	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 31.07 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1760e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: SCN

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	0.43	0/2016	0.97	9/2734 (0.3%)
1	B	0.43	0/2016	0.97	15/2734 (0.5%)
1	C	0.48	1/2016 (0.0%)	1.05	19/2734 (0.7%)
1	D	0.43	0/2016	1.00	12/2734 (0.4%)
All	All	0.44	1/8064 (0.0%)	1.00	55/10936 (0.5%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	263	THR	C-N	-9.49	1.20	1.33

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	27	GLN	N-CA-C	-13.12	97.17	113.97
1	C	27	GLN	N-CA-C	-10.07	103.14	114.62
1	C	27	GLN	OE1-CD-NE2	-9.97	112.62	122.60
1	D	28	GLN	OE1-CD-NE2	-9.96	112.64	122.60
1	A	27	GLN	OE1-CD-NE2	-9.95	112.65	122.60
1	D	27	GLN	OE1-CD-NE2	-9.28	113.32	122.60
1	C	28	GLN	OE1-CD-NE2	-9.20	113.40	122.60
1	C	263	THR	CA-C-N	9.13	136.16	122.93
1	C	263	THR	C-N-CA	9.13	136.16	122.93
1	A	27	GLN	N-CA-C	-7.31	104.39	113.38
1	B	248	ALA	N-CA-C	7.01	119.51	108.79
1	A	27	GLN	CG-CD-NE2	6.71	126.47	116.40
1	B	28	GLN	N-CA-C	-6.69	105.11	113.28
1	B	29	VAL	N-CA-C	-6.69	103.96	110.72
1	C	231	VAL	N-CA-C	6.64	118.28	108.45
1	C	27	GLN	CG-CD-NE2	6.56	126.24	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	27	GLN	N-CA-C	-6.54	105.33	113.38
1	D	28	GLN	CG-CD-NE2	6.44	126.07	116.40
1	A	248	ALA	N-CA-C	6.42	117.97	108.60
1	B	267	GLN	CA-C-N	6.42	126.34	119.28
1	B	267	GLN	C-N-CA	6.42	126.34	119.28
1	D	248	ALA	N-CA-C	6.28	118.39	108.79
1	C	28	GLN	CG-CD-NE2	6.25	125.77	116.40
1	D	27	GLN	CG-CD-NE2	6.20	125.70	116.40
1	B	231	VAL	N-CA-C	6.18	117.59	108.45
1	A	267	GLN	CA-C-N	6.16	125.56	118.85
1	A	267	GLN	C-N-CA	6.16	125.56	118.85
1	A	220	SER	N-CA-C	6.03	113.72	108.78
1	C	248	ALA	N-CA-C	5.78	117.64	108.79
1	A	218	GLY	N-CA-C	5.74	119.83	112.83
1	C	267	GLN	CA-C-N	5.73	125.26	119.19
1	C	267	GLN	C-N-CA	5.73	125.26	119.19
1	C	144	GLY	CA-C-N	5.72	125.84	119.32
1	C	144	GLY	C-N-CA	5.72	125.84	119.32
1	B	250	ILE	N-CA-C	5.71	116.10	108.11
1	C	29	VAL	N-CA-C	-5.66	104.83	111.00
1	D	144	GLY	CA-C-N	5.61	125.14	119.19
1	D	144	GLY	C-N-CA	5.61	125.14	119.19
1	D	267	GLN	CA-C-N	5.61	125.13	119.19
1	D	267	GLN	C-N-CA	5.61	125.13	119.19
1	D	227	ALA	N-CA-C	5.60	118.92	111.75
1	C	227	ALA	N-CA-C	5.58	118.89	111.75
1	C	286	VAL	N-CA-C	5.57	118.90	111.44
1	B	59	LEU	N-CA-C	5.55	118.44	109.40
1	B	46	VAL	N-CA-C	5.53	116.24	108.17
1	B	220	SER	N-CA-C	5.51	113.30	108.78
1	B	285	ILE	N-CA-C	5.49	115.69	110.42
1	B	148	VAL	N-CA-C	-5.40	105.11	111.00
1	B	94	LYS	N-CA-C	5.26	118.30	110.52
1	D	231	VAL	N-CA-C	5.17	116.09	108.45
1	A	68	MET	N-CA-C	5.04	116.78	111.28
1	C	26	VAL	CA-C-N	5.04	131.25	121.63
1	C	26	VAL	C-N-CA	5.04	131.25	121.63
1	C	245	ASN	N-CA-C	5.03	117.06	109.41
1	B	227	ALA	N-CA-C	5.01	118.16	111.75

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	1985	0	2011	28	0
1	B	1985	0	2011	29	0
1	C	1985	0	2010	30	0
1	D	1985	0	2011	40	0
2	A	3	0	0	0	0
3	A	130	0	0	3	0
3	B	122	0	0	0	0
3	C	113	0	0	4	0
3	D	120	0	0	2	0
All	All	8428	0	8043	125	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 8.

All (125) 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:153:ARG:HE	1:D:158:THR:HA	1.38	0.86
1:B:54:ASN:ND2	1:B:191:ARG:HH12	1.78	0.82
1:C:26:VAL:N	1:C:29:VAL:HG23	1.98	0.78
1:D:28:GLN:HB3	1:D:31:LYS:HE2	1.64	0.77
1:C:54:ASN:HD21	1:C:191:ARG:HH22	1.31	0.76
1:D:28:GLN:O	1:D:31:LYS:HG2	1.87	0.74
1:A:70:SER:HB2	3:A:301:HOH:O	1.90	0.71
1:D:54:ASN:HD21	1:D:191:ARG:HH22	1.36	0.71
1:D:115:ASN:ND2	1:D:116:THR:H	1.92	0.67
1:A:54:ASN:HD21	1:A:191:ARG:HH22	1.43	0.66
1:B:54:ASN:HD21	1:B:191:ARG:HH22	1.44	0.66
1:D:98:LYS:HZ3	1:D:98:LYS:HA	1.61	0.66
1:A:26:VAL:N	1:A:29:VAL:HG23	2.11	0.66
1:A:153:ARG:HE	1:A:158:THR:HA	1.59	0.66
1:B:153:ARG:HE	1:B:158:THR:HA	1.65	0.61
1:A:92:GLN:HG3	3:A:366:HOH:O	2.00	0.61
1:D:26:VAL:HA	1:D:29:VAL:HG23	1.84	0.59
1:B:136:ASN:OD1	1:B:165:LYS:HB2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:26:VAL:O	1:D:26:VAL:HG12	2.03	0.58
1:C:204:ARG:HD3	3:C:293:HOH:O	2.04	0.57
1:C:202:PRO:HG2	1:C:203:GLN:OE1	2.05	0.56
1:A:222:ARG:HG3	3:A:293:HOH:O	2.04	0.56
1:B:54:ASN:HD21	1:B:191:ARG:HH12	1.50	0.56
1:B:105:TRP:CE2	1:B:107:PRO:HG3	2.41	0.56
1:D:126:THR:O	1:D:130:SER:HA	2.06	0.56
1:C:115:ASN:ND2	1:C:116:THR:H	2.04	0.55
1:C:126:THR:HG22	1:C:134:ALA:HB3	1.89	0.55
1:A:90:ILE:HG13	1:A:93:GLN:NE2	2.22	0.54
1:D:145:PRO:HD2	3:D:352:HOH:O	2.07	0.54
1:C:27:GLN:O	1:C:31:LYS:HG3	2.07	0.54
1:B:26:VAL:N	1:B:29:VAL:HG23	2.22	0.54
1:A:48:LEU:HB3	1:A:57:VAL:HB	1.90	0.54
1:C:247:ILE:HG22	1:C:262:VAL:HG13	1.90	0.53
1:D:98:LYS:HA	1:D:98:LYS:NZ	2.23	0.53
1:C:126:THR:O	1:C:130:SER:HA	2.09	0.52
1:C:68:MET:HG2	1:C:181:THR:HG22	1.91	0.52
1:D:247:ILE:HG22	1:D:262:VAL:HG13	1.91	0.52
1:A:52:ALA:HB2	1:A:257:ALA:HB3	1.92	0.52
1:A:73:LYS:HD3	1:A:126:THR:OG1	2.11	0.51
1:C:48:LEU:HB3	1:C:57:VAL:HB	1.92	0.51
1:A:245:ASN:HB3	1:A:264:TYR:CD1	2.46	0.51
1:B:267:GLN:HB3	1:B:268:PRO:HD2	1.93	0.51
1:D:204:ARG:HD3	3:D:327:HOH:O	2.11	0.50
1:A:73:LYS:HE3	1:A:135:MET:HB2	1.94	0.50
1:D:26:VAL:O	1:D:26:VAL:CG1	2.59	0.50
1:D:118:THR:OG1	1:D:121:GLU:HG3	2.12	0.50
1:A:128:GLN:HE22	1:C:99:LYS:NZ	2.09	0.49
1:D:28:GLN:CB	1:D:31:LYS:HE2	2.38	0.49
1:B:48:LEU:HB3	1:B:57:VAL:HB	1.94	0.49
1:B:106:ASN:HB2	1:B:110:GLU:HB3	1.94	0.49
1:D:281:ALA:O	1:D:285:ILE:HG13	2.11	0.49
1:B:153:ARG:NE	1:B:158:THR:HA	2.27	0.49
1:D:48:LEU:HB3	1:D:57:VAL:HB	1.94	0.48
1:D:115:ASN:HD22	1:D:116:THR:N	2.11	0.48
1:C:241:TYR:HA	1:C:269:GLN:O	2.13	0.48
1:B:118:THR:OG1	1:B:121:GLU:HG3	2.13	0.48
1:D:241:TYR:HA	1:D:269:GLN:O	2.14	0.48
1:D:160:PHE:C	1:D:160:PHE:CD1	2.92	0.48
1:A:96:THR:HG22	1:A:116:THR:HG22	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:184:LEU:HD11	1:C:188:LYS:HE3	1.95	0.47
1:C:54:ASN:ND2	1:C:191:ARG:HH12	2.13	0.47
1:D:54:ASN:ND2	1:D:191:ARG:HH12	2.13	0.47
1:B:26:VAL:HG12	1:B:27:GLN:N	2.30	0.47
1:B:54:ASN:HD21	1:B:191:ARG:NH2	2.09	0.47
1:C:62:ALA:HB1	1:C:184:LEU:HB2	1.96	0.47
1:B:54:ASN:ND2	1:B:191:ARG:NH1	2.57	0.47
1:B:96:THR:HA	1:B:116:THR:HG22	1.96	0.47
1:B:184:LEU:HD11	1:B:188:LYS:HE3	1.96	0.47
1:C:178:ARG:O	1:C:180:THR:HG23	2.15	0.47
1:C:287:THR:O	1:C:290:LYS:HG2	2.14	0.47
1:B:54:ASN:HD21	1:B:191:ARG:NH1	2.14	0.46
1:C:96:THR:HG22	1:C:116:THR:HG22	1.97	0.46
1:D:186:MET:O	1:D:186:MET:HE3	2.15	0.46
1:A:251:TRP:CD1	1:A:258:PRO:HG3	2.50	0.46
1:D:115:ASN:ND2	1:D:116:THR:N	2.62	0.46
1:D:275:ARG:HB3	1:D:278:VAL:HG23	1.97	0.46
1:C:118:THR:OG1	1:C:121:GLU:HG3	2.15	0.46
1:D:69:CYS:HA	1:D:170:ASN:ND2	2.31	0.46
1:A:54:ASN:ND2	1:A:191:ARG:HH12	2.14	0.46
1:A:70:SER:OG	1:A:73:LYS:NZ	2.43	0.45
1:A:128:GLN:HE22	1:C:99:LYS:HZ1	1.64	0.45
1:C:39:GLN:HG3	3:C:325:HOH:O	2.16	0.45
1:D:145:PRO:HB3	1:D:162:LEU:HG	1.99	0.45
1:B:126:THR:O	1:B:130:SER:HA	2.17	0.45
1:B:62:ALA:HB1	1:B:184:LEU:HB2	1.99	0.45
1:D:73:LYS:HE2	1:D:135:MET:HB2	1.99	0.45
1:D:62:ALA:HB1	1:D:184:LEU:HB2	1.98	0.44
1:D:233:ASP:CB	1:D:248:ALA:HB2	2.47	0.44
1:D:69:CYS:HA	1:D:170:ASN:HD22	1.83	0.44
1:A:62:ALA:HB1	1:A:184:LEU:HB2	1.99	0.44
1:D:233:ASP:HB2	1:D:248:ALA:HB2	1.99	0.44
1:B:115:ASN:ND2	1:B:116:THR:H	2.15	0.44
1:D:28:GLN:C	1:D:31:LYS:HG2	2.42	0.43
1:A:38:LYS:HE3	1:A:38:LYS:HB2	1.71	0.43
1:C:82:LYS:O	1:C:85:GLU:HB2	2.18	0.43
1:C:136:ASN:OD1	1:C:165:LYS:HB2	2.18	0.43
1:D:26:VAL:HA	1:D:29:VAL:CG2	2.47	0.43
1:D:70:SER:HB2	1:D:236:GLY:HA2	1.99	0.43
1:C:74:VAL:HG21	1:C:247:ILE:HD11	2.00	0.43
1:D:269:GLN:N	1:D:269:GLN:CD	2.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:169:LEU:C	1:D:169:LEU:HD12	2.44	0.42
1:D:241:TYR:CD1	1:D:270:GLN:HA	2.55	0.42
1:A:118:THR:OG1	1:A:121:GLU:HG3	2.19	0.42
1:C:267:GLN:HB3	1:C:268:PRO:CD	2.50	0.42
1:A:160:PHE:CD1	1:A:160:PHE:C	2.97	0.42
1:B:257:ALA:HA	1:B:258:PRO:HD3	1.89	0.42
1:D:38:LYS:HB2	1:D:38:LYS:HE3	1.87	0.42
1:A:57:VAL:HG11	1:A:286:VAL:HG12	2.02	0.42
1:A:245:ASN:HB3	1:A:264:TYR:CE1	2.55	0.42
1:A:90:ILE:HG13	1:A:93:GLN:CD	2.45	0.41
1:B:237:ALA:HB1	1:B:274:TRP:CE2	2.55	0.41
1:B:178:ARG:O	1:B:180:THR:HG23	2.20	0.41
1:B:241:TYR:HA	1:B:269:GLN:O	2.19	0.41
1:B:254:GLU:OE1	1:B:256:ARG:NH1	2.51	0.41
1:B:153:ARG:NH2	1:B:160:PHE:O	2.53	0.41
1:D:269:GLN:CD	1:D:269:GLN:H	2.29	0.41
1:A:103:THR:HG22	1:A:133:THR:OG1	2.19	0.41
1:B:54:ASN:HD22	1:B:54:ASN:HA	1.65	0.41
1:C:53:ASP:O	1:C:54:ASN:HB2	2.21	0.41
1:C:70:SER:HB2	3:C:362:HOH:O	2.20	0.41
1:C:161:ARG:O	1:C:179:ASP:HA	2.21	0.41
1:A:44:LEU:O	1:A:61:ARG:HD2	2.21	0.40
1:A:231:VAL:HG12	1:A:232:GLY:N	2.36	0.40
1:B:68:MET:SD	1:B:160:PHE:CE2	3.15	0.40
1:C:256:ARG:HD3	3:C:309:HOH:O	2.21	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	260/262 (99%)	248 (95%)	11 (4%)	1 (0%)	30 43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	260/262 (99%)	246 (95%)	14 (5%)	0	100	100
1	C	260/262 (99%)	248 (95%)	12 (5%)	0	100	100
1	D	260/262 (99%)	249 (96%)	11 (4%)	0	100	100
All	All	1040/1048 (99%)	991 (95%)	48 (5%)	1 (0%)	48	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	240	ASP

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	208/208 (100%)	205 (99%)	3 (1%)	59	79
1	B	208/208 (100%)	207 (100%)	1 (0%)	81	91
1	C	208/208 (100%)	208 (100%)	0	100	100
1	D	208/208 (100%)	205 (99%)	3 (1%)	59	79
All	All	832/832 (100%)	825 (99%)	7 (1%)	73	86

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	SER
1	A	98	LYS
1	A	106	ASN
1	B	70	SER
1	D	98	LYS
1	D	130	SER
1	D	165	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	93	GLN
1	A	128	GLN
1	A	147	ASN
1	B	54	ASN
1	B	92	GLN
1	B	93	GLN
1	B	115	ASN
1	B	219	GLN
1	C	54	ASN
1	C	93	GLN
1	C	115	ASN
1	C	147	ASN
1	C	170	ASN
1	C	270	GLN
1	D	28	GLN
1	D	54	ASN
1	D	93	GLN
1	D	115	ASN
1	D	170	ASN
1	D	219	GLN

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](#)

1 ligand is 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	SCN	A	1	-	1,2,2	0.03	0	0,1,1	-	-

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	262/262 (100%)	-1.79	0 100 100	7, 15, 32, 51	0
1	B	262/262 (100%)	-1.76	0 100 100	7, 16, 34, 58	0
1	C	262/262 (100%)	-1.78	0 100 100	6, 17, 35, 48	0
1	D	262/262 (100%)	-1.78	0 100 100	7, 17, 34, 50	0
All	All	1048/1048 (100%)	-1.78	0 100 100	6, 16, 35, 58	0

There are no RSRZ outliers to report.

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(Å ²)	Q<0.9
2	SCN	A	1	3/3	1.00	0.02	32,32,33,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.