Full wwPDB X-ray Structure Validation Report (i)

Oct 24, 2024 – 09:57 AM EDT

PDB ID	:	3EFB
Title	:	Crystal Structure of Probable sor Operon Regulator from Shigella flexneri
Authors	:	Kim, Y.; Evdokimova, E.; Kudritska, M.; Savchenko, A.; Edwards, A.; Anderson, W.F.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on	:	2008-09-08
Resolution	:	2.00 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:

|		
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 2.00 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	Percentile Ranks	Value
Rfree		0.191
Clashscore		15
Ramachandran outliers		0.4%
Sidechain outliers		6.5%
RSRZ outliers		4.8%

Worse   *Better*

▊ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
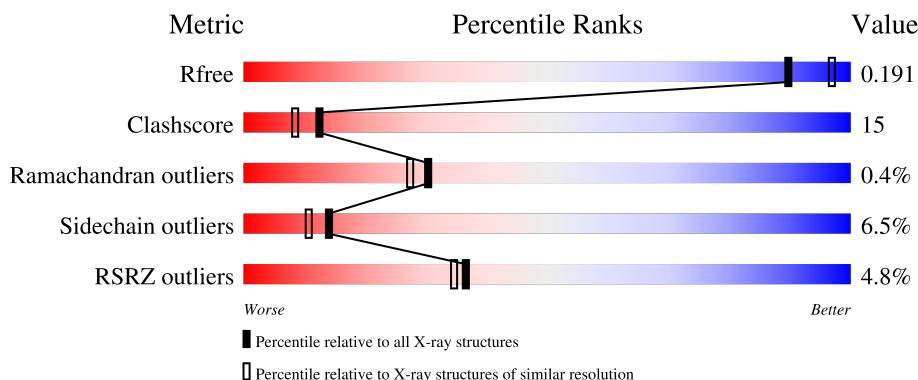
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	9409 (2.00-2.00)
Clashscore	180529	10737 (2.00-2.00)
Ramachandran outliers	177936	10628 (2.00-2.00)
Sidechain outliers	177891	10627 (2.00-2.00)
RSRZ outliers	164620	9409 (2.00-2.00)

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	266	% — 69% 22% • 8%
1	B	266	3% — 65% 21% • 12%
1	C	266	5% — 68% 17% • 12%
1	D	266	8% — 59% 30% • 7%
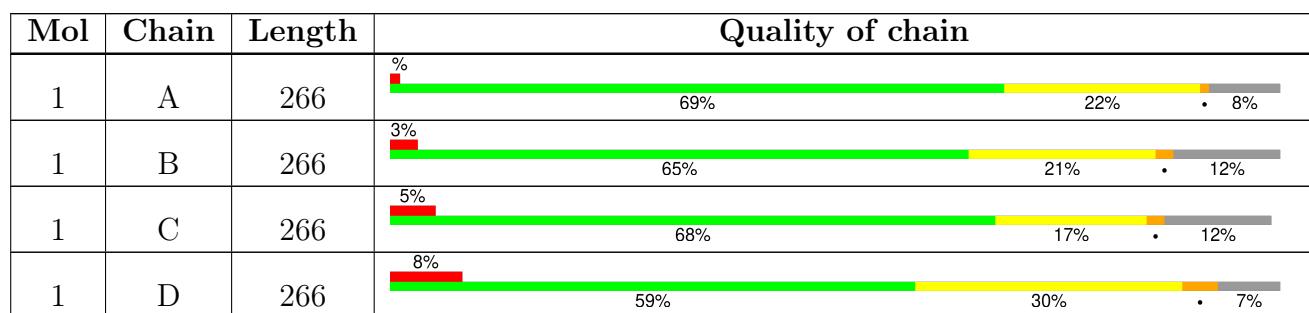
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ACY	B	266	-	-	X	-

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 8130 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 Probable sor-operon regulator.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	246	Total 2005	C 1256	N 348	O 390	S 3	Se 8	0	14	0
1	B	235	Total 1845	C 1170	N 318	O 347	S 3	Se 7	0	3	0
1	C	233	Total 1841	C 1162	N 319	O 350	S 3	Se 7	9	6	0
1	D	248	Total 1936	C 1221	N 332	O 373	S 3	Se 7	0	3	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP Q83PA8
B	0	GLY	-	expression tag	UNP Q83PA8
C	0	GLY	-	expression tag	UNP Q83PA8
D	0	GLY	-	expression tag	UNP Q83PA8

- Molecule 2 is ACETIC ACID (three-letter code: ACY) (formula: $C_2H_4O_2$).
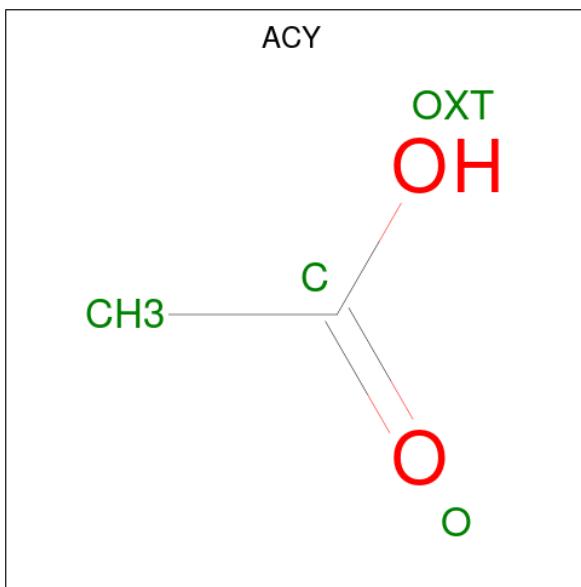
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total C O 4 2 2			0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	154	Total O 154 154		0	0
3	B	118	Total O 118 118		0	0
3	C	129	Total O 129 129		0	0
3	D	98	Total O 98 98		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: Probable sor-operon regulator
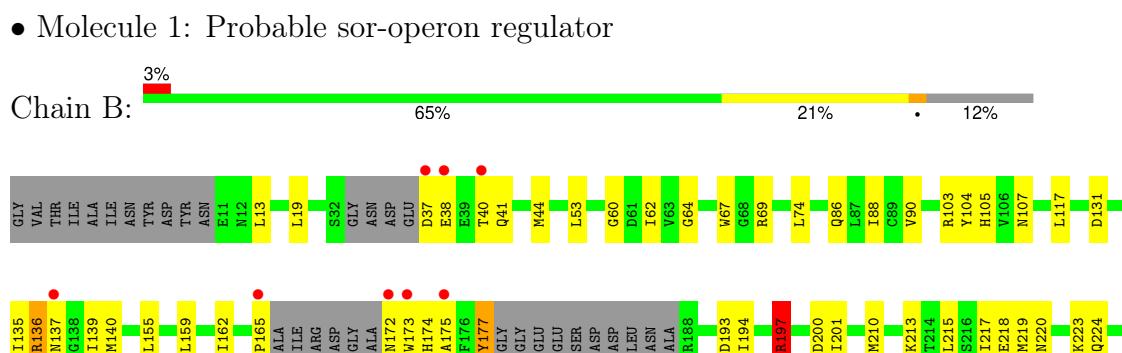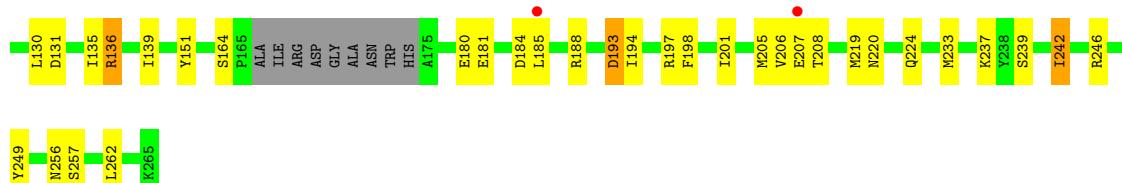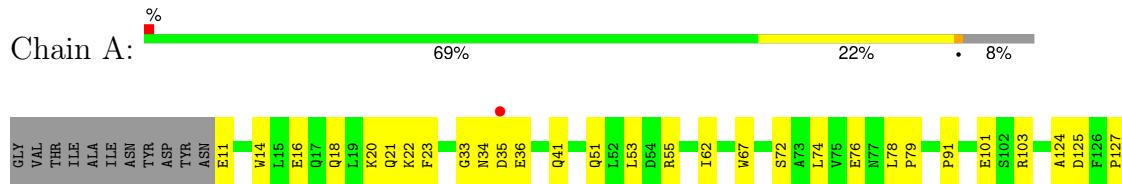
Chain A:

• Molecule 1: Probable sor-operon regulator

Chain B:

• Molecule 1: Probable sor-operon regulator

Chain C:

N256 T259 L264 LYS

• Molecule 1: Probable sor-operon regulator

Chain D:
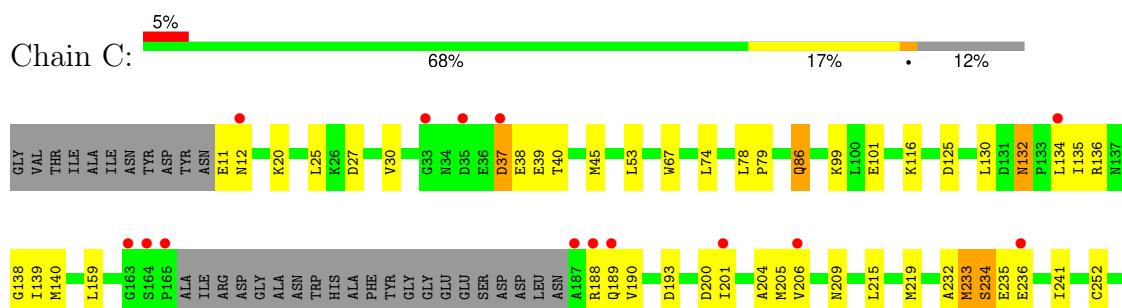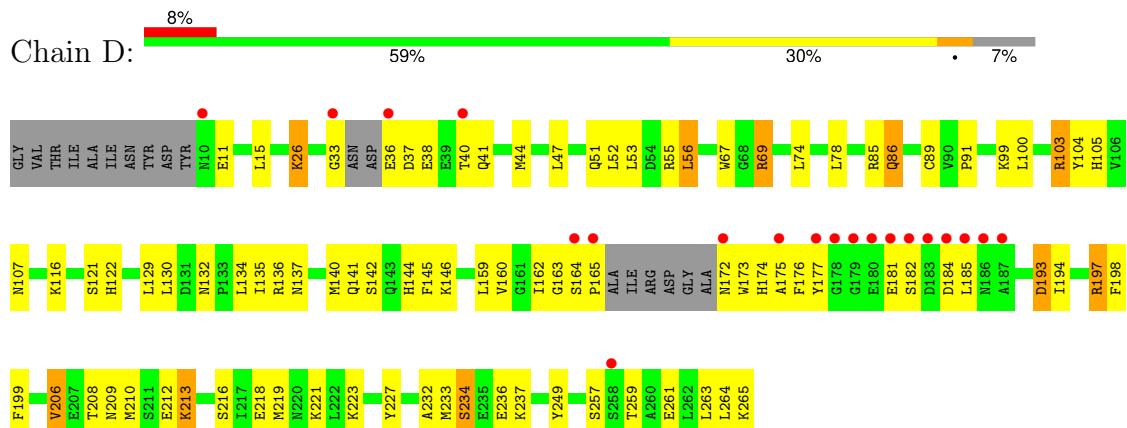
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	69.54Å 238.46Å 53.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.38 – 2.00 33.38 – 2.01	Depositor EDS
% Data completeness (in resolution range)	99.4 (33.38-2.00) 99.0 (33.38-2.01)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	3.55 (at 2.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine)/refmac5.5	Depositor
R, R_{free}	0.200 , 0.249 0.194 , 0.191	Depositor DCC
R_{free} test set	3049 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	36.7	Xtriage
Anisotropy	0.515	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 59.0	EDS
L-test for twinning[2]	$<\|L\|> = 0.49, <L^2> = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	8130	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 64.03 % 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 8.8222e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[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 ⓘ

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

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	0.48	0/2027	0.61	0/2719
1	B	0.44	0/1869	0.63	2/2509 (0.1%)
1	C	0.46	0/1862	0.60	0/2500
1	D	0.41	0/1961	0.55	0/2635
All	All	0.45	0/7719	0.60	2/10363 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	197	ARG	NE-CZ-NH1	6.23	123.42	120.30
1	B	197	ARG	NE-CZ-NH2	-5.29	117.65	120.30

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	2005	0	1982	52	0
1	B	1845	0	1846	56	0
1	C	1841	0	1855	48	0
1	D	1936	0	1917	80	0
2	B	4	0	3	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	154	0	0	7	0
3	B	118	0	0	4	0
3	C	129	0	0	8	0
3	D	98	0	0	7	0
All	All	8130	0	7603	231	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 15.

All (231) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:45:MSE:SE	1:C:233:MSE:HG2	1.94	1.17
1:B:37:ASP:HB3	1:B:40:THR:OG1	1.44	1.16
1:B:194:ILE:HB	1:B:219:MSE:HE1	1.25	1.13
1:A:194:ILE:HB	1:A:219:MSE:HE1	1.34	1.03
1:D:194:ILE:HB	1:D:219:MSE:HE1	1.36	1.02
1:C:132:ASN:C	1:C:132:ASN:HD22	1.71	0.92
1:B:37:ASP:OD1	1:B:40:THR:HG23	1.70	0.92
1:B:105:HIS:HD2	1:B:107:ASN:H	1.18	0.91
1:D:105:HIS:HD2	1:D:107:ASN:H	1.22	0.87
1:C:190:VAL:HG22	1:C:206:VAL:HG21	1.57	0.87
1:C:201:ILE:HD12	1:C:201:ILE:H	1.41	0.85
1:C:37:ASP:OD1	1:C:40:THR:HG23	1.78	0.84
1:A:130[A]:LEU:HD11	1:A:139:ILE:HD12	1.61	0.82
1:D:103:ARG:HD2	1:D:104:TYR:CE1	2.15	0.82
1:D:130:LEU:O	1:D:213:LYS:HB2	1.80	0.81
1:D:69:ARG:HD3	1:D:104:TYR:CZ	2.17	0.80
1:B:37:ASP:OD1	1:B:40:THR:CG2	2.30	0.79
1:A:130[B]:LEU:HD21	1:A:139:ILE:HD12	1.66	0.76
1:B:37:ASP:CB	1:B:40:THR:OG1	2.30	0.74
1:B:197:ARG:HB2	1:B:219:MSE:HE2	1.71	0.72
1:A:33:GLY:HA3	1:A:41:GLN:OE1	1.92	0.69
1:C:136:ARG:HG3	1:C:215:LEU:CD1	2.22	0.69
1:D:182:SER:HA	1:D:185:LEU:HD12	1.75	0.68
1:A:125:ASP:OD1	1:D:105:HIS:HE1	1.76	0.68
1:A:237:LYS:HA	1:A:262:LEU:HG	1.75	0.68
1:D:177:TYR:HA	1:D:210:MSE:HE1	1.75	0.68
1:B:105:HIS:CD2	1:B:107:ASN:H	2.07	0.68
1:B:237:LYS:HE2	2:B:266:ACY:O	1.93	0.67
1:A:130[A]:LEU:HD12	1:A:136:ARG:HA	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:ASP:O	1:B:41:GLN:CG	2.43	0.67
1:D:53:LEU:HD22	1:D:159:LEU:HD21	1.77	0.66
1:D:136:ARG:NE	1:D:140:MSE:HE3	2.10	0.66
1:A:127:PRO:HG2	1:A:130[A]:LEU:HD21	1.77	0.66
1:B:194:ILE:CB	1:B:219:MSE:HE1	2.15	0.66
1:D:105:HIS:CD2	1:D:107:ASN:H	2.09	0.66
1:A:130[A]:LEU:HD13	1:A:135:ILE:HG22	1.78	0.65
1:B:197:ARG:HD2	1:B:217:ILE:O	1.97	0.65
1:D:164:SER:HB2	1:D:237:LYS:HG3	1.80	0.64
1:D:194:ILE:HB	1:D:219:MSE:CE	2.20	0.64
1:B:44:MSE:HA	1:B:44:MSE:HE2	1.79	0.64
1:D:142:SER:OG	3:D:315:HOH:O	2.14	0.64
1:B:218:GLU:HG3	3:B:355:HOH:O	1.99	0.62
1:D:184:ASP:HB3	3:D:323:HOH:O	1.98	0.62
1:D:33:GLY:HA3	1:D:41:GLN:HE21	1.64	0.62
1:C:136:ARG:HG3	1:C:215:LEU:HD13	1.81	0.62
1:A:51:GLN:O	1:A:55[B]:ARG:HG3	1.99	0.62
1:C:201:ILE:H	1:C:201:ILE:CD1	2.12	0.61
1:D:26:LYS:HG2	1:D:227:TYR:HE1	1.66	0.61
1:C:140:MSE:HE3	1:C:215:LEU:HD12	1.82	0.61
1:B:135:ILE:HG12	1:C:138:GLY:HA3	1.83	0.61
1:B:105:HIS:HE1	1:C:125:ASP:OD1	1.83	0.61
1:C:130:LEU:HD13	1:C:136:ARG:HA	1.82	0.61
1:A:242:ILE:O	1:A:246:ARG:HG3	2.01	0.60
1:A:130[B]:LEU:HD23	1:A:135:ILE:HG22	1.81	0.60
1:A:205[B]:MSE:HE2	1:A:249:TYR:HE1	1.66	0.60
1:C:201:ILE:HD12	1:C:201:ILE:N	2.15	0.60
1:B:162:ILE:O	1:B:237:LYS:HE3	2.02	0.60
1:A:184:ASP:O	1:A:188:ARG:HG3	2.02	0.59
1:B:37:ASP:O	1:B:41:GLN:HG3	2.01	0.59
1:A:72:SER:O	1:A:76:GLU:HG3	2.03	0.59
1:B:177:TYR:CD2	1:B:210:MSE:HE1	2.38	0.59
1:C:78:LEU:HB2	1:C:116:LYS:HD3	1.84	0.59
1:D:213:LYS:NZ	1:D:213:LYS:HB3	2.18	0.59
1:A:130[A]:LEU:HD12	1:A:136:ARG:CA	2.33	0.57
1:A:55[A]:ARG:HG2	1:A:55[A]:ARG:HH11	1.69	0.57
1:C:79:PRO:CD	3:C:367:HOH:O	2.52	0.57
1:A:130[B]:LEU:HD23	1:A:135:ILE:CG2	2.35	0.57
1:B:37:ASP:O	1:B:41:GLN:HG2	2.04	0.57
1:D:144:HIS:N	3:D:315:HOH:O	2.36	0.57
1:C:132:ASN:C	1:C:132:ASN:ND2	2.45	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:HIS:HD2	1:B:107:ASN:N	1.97	0.56
1:A:233:MSE:HE3	1:A:256:ASN:ND2	2.19	0.56
1:D:165:PRO:HG3	1:D:173:TRP:CE2	2.40	0.56
1:A:233:MSE:HE3	1:A:256:ASN:HD21	1.70	0.56
1:B:74:LEU:HD22	1:B:159:LEU:CD2	2.36	0.56
1:B:240:GLY:HA3	3:B:383:HOH:O	2.06	0.56
1:D:99:LYS:HE3	1:D:176:PHE:HA	1.88	0.55
1:B:69:ARG:HG2	1:B:104:TYR:CZ	2.41	0.55
1:C:256:ASN:ND2	1:C:259:THR:OG1	2.38	0.55
1:A:130[B]:LEU:CD2	1:A:135:ILE:HG22	2.36	0.55
1:A:193:ASP:HB3	1:A:198:PHE:CD2	2.42	0.55
1:C:136:ARG:CG	1:C:215:LEU:CD1	2.85	0.55
1:D:177:TYR:O	1:D:181:GLU:HB2	2.07	0.55
1:B:242:ILE:HG23	1:B:263:LEU:HD23	1.88	0.54
1:D:142:SER:CB	3:D:315:HOH:O	2.55	0.54
1:A:205[A]:MSE:HE2	3:A:384:HOH:O	2.06	0.54
1:A:130[B]:LEU:HD21	1:A:139:ILE:CD1	2.37	0.54
1:B:137:ASN:HB2	3:B:385:HOH:O	2.08	0.54
1:D:177:TYR:CD2	1:D:210:MSE:SE	3.11	0.53
1:A:62:ILE:HD13	1:A:151:TYR:HD1	1.72	0.53
1:C:12:ASN:OD1	1:C:30:VAL:HG12	2.07	0.53
1:A:53:LEU:HD23	1:A:78:LEU:HD21	1.90	0.53
1:D:185:LEU:HD23	1:D:208:THR:HG21	1.91	0.53
1:D:172:ASN:HA	1:D:175:ALA:HB3	1.90	0.53
1:B:136:ARG:HD3	1:B:215:LEU:HD21	1.90	0.53
1:D:99:LYS:HE2	1:D:176:PHE:HD2	1.74	0.53
1:A:239:SER:H	1:A:242:ILE:HD11	1.74	0.52
1:C:79:PRO:HD3	3:C:367:HOH:O	2.09	0.52
1:D:208:THR:C	1:D:210:MSE:H	2.12	0.52
1:D:165:PRO:HA	1:D:173:TRP:CG	2.45	0.52
1:A:205[B]:MSE:HE2	1:A:249:TYR:CE1	2.44	0.52
1:C:86:GLN:NE2	3:C:322:HOH:O	2.38	0.52
1:A:130[A]:LEU:HD12	1:A:136:ARG:CB	2.40	0.51
1:B:238:TYR:O	1:B:242:ILE:HG12	2.09	0.51
1:D:232:ALA:HB1	1:D:237:LYS:HD2	1.92	0.51
1:A:205[A]:MSE:HG2	1:A:249:TYR:OH	2.10	0.50
1:D:163:GLY:HA3	1:D:193:ASP:OD1	2.11	0.50
1:D:213:LYS:HB3	1:D:213:LYS:HZ2	1.76	0.50
1:B:131:ASP:O	1:B:213:LYS:HE3	2.11	0.50
1:B:242:ILE:HG23	1:B:263:LEU:CD2	2.42	0.50
1:D:33:GLY:C	1:D:36:GLU:HB2	2.32	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:188:ARG:O	1:C:189:GLN:HB2	2.11	0.50
1:D:55:ARG:NH2	3:D:338:HOH:O	2.25	0.50
1:D:136:ARG:CD	1:D:140:MSE:HE3	2.41	0.50
1:A:207[B]:GLU:HG3	1:A:208:THR:N	2.26	0.49
1:B:44:MSE:HG3	3:B:370:HOH:O	2.11	0.49
1:D:136:ARG:CZ	1:D:140:MSE:HE1	2.42	0.49
1:D:136:ARG:NE	1:D:140:MSE:CE	2.75	0.49
1:D:223:LYS:HE3	1:D:249:TYR:CE1	2.48	0.49
1:B:103:ARG:HG3	1:B:103:ARG:HH11	1.77	0.49
1:D:33:GLY:H	1:D:44:MSE:HE1	1.78	0.49
1:D:91:PRO:HD3	1:D:122:HIS:O	2.13	0.49
1:D:136:ARG:CZ	1:D:140:MSE:CE	2.90	0.49
1:A:197:ARG:HB3	1:A:205[A]:MSE:HE1	1.95	0.48
1:D:37:ASP:O	1:D:41:GLN:HG3	2.13	0.48
1:C:134[B]:LEU:HD12	3:C:387:HOH:O	2.13	0.48
1:B:53:LEU:HD22	1:B:159:LEU:HD21	1.94	0.48
1:B:201:ILE:HD11	1:B:242:ILE:HD11	1.96	0.48
1:D:99:LYS:NZ	1:D:129:LEU:HD12	2.28	0.48
1:D:103:ARG:HD2	1:D:104:TYR:CZ	2.48	0.48
1:D:259:THR:O	1:D:263:LEU:HG	2.13	0.48
1:D:162:ILE:O	1:D:237:LYS:HD3	2.14	0.48
1:C:200:ASP:OD2	1:C:204:ALA:HB3	2.14	0.48
1:C:132:ASN:HD21	1:C:135:ILE:HG13	1.78	0.47
1:C:136:ARG:CG	1:C:215:LEU:HD11	2.44	0.47
1:C:20[B]:LYS:HB2	1:C:20[B]:LYS:HE3	1.55	0.47
1:D:141:GLN:O	1:D:146:LYS:HE3	2.14	0.47
1:D:193:ASP:HB3	1:D:198:PHE:CD2	2.50	0.47
1:A:74:LEU:C	1:A:74:LEU:HD23	2.35	0.47
1:A:11:GLU:N	3:A:554:HOH:O	2.48	0.46
1:A:14:TRP:O	1:A:18:GLN:HG2	2.15	0.46
1:C:101:GLU:HG3	3:C:277:HOH:O	2.14	0.46
1:D:105:HIS:HD2	1:D:107:ASN:N	2.01	0.46
1:C:74:LEU:HD23	1:C:74:LEU:C	2.36	0.46
1:B:233:MSE:O	1:B:234:SER:CB	2.63	0.46
1:D:172:ASN:HB3	1:D:176:PHE:CE1	2.50	0.46
1:C:53:LEU:HD23	1:C:78:LEU:HD21	1.96	0.46
1:A:201:ILE:HG13	3:A:595:HOH:O	2.16	0.46
1:A:101:GLU:HG3	3:A:577:HOH:O	2.16	0.46
1:A:55[A]:ARG:HG2	1:A:55[A]:ARG:NH1	2.29	0.46
1:B:139:ILE:HD11	1:C:139:ILE:HD11	1.98	0.46
1:D:257:SER:O	1:D:261:GLU:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:PRO:HA	1:B:173:TRP:CG	2.51	0.46
1:C:37:ASP:OD1	1:C:40:THR:CG2	2.57	0.45
1:C:233:MSE:O	1:C:234:SER:CB	2.65	0.45
1:A:131:ASP:OD2	1:D:142:SER:HA	2.17	0.45
1:D:233:MSE:O	1:D:234:SER:CB	2.63	0.45
1:D:197:ARG:NH1	1:D:216:SER:O	2.49	0.45
1:B:64:GLY:HA2	1:B:90:VAL:O	2.17	0.45
1:B:60:GLY:HA2	1:B:86:GLN:O	2.17	0.45
1:C:20[B]:LYS:HG3	1:C:25:LEU:O	2.17	0.45
1:D:78:LEU:O	1:D:116:LYS:HD2	2.17	0.45
1:C:27:ASP:O	1:C:252:CYS:HA	2.16	0.45
1:D:74:LEU:HD22	1:D:159:LEU:CD2	2.47	0.45
1:B:37:ASP:HB3	1:B:40:THR:HG1	1.69	0.44
1:D:181:GLU:OE1	1:D:181:GLU:HA	2.16	0.44
1:B:173:TRP:CZ3	1:B:193:ASP:OD1	2.70	0.44
1:C:232:ALA:HB1	1:C:241:ILE:HD11	1.98	0.44
1:B:220:ASN:O	1:B:224:GLN:HG3	2.18	0.44
1:B:237:LYS:CE	2:B:266:ACY:O	2.61	0.44
1:C:235:GLU:HG2	3:C:396:HOH:O	2.17	0.44
1:D:164:SER:CB	1:D:237:LYS:HG3	2.45	0.44
1:B:19:LEU:HD23	1:B:264:LEU:HD13	2.00	0.44
1:B:172:ASN:HA	1:B:175:ALA:HB3	1.99	0.44
1:A:16:GLU:O	1:A:20:LYS:HG3	2.18	0.44
1:B:248:LYS:HB2	1:B:248:LYS:HE3	1.69	0.43
1:C:132:ASN:ND2	1:C:132:ASN:O	2.48	0.43
1:C:99:LYS:HA	1:C:99:LYS:HD3	1.75	0.43
1:D:26:LYS:HG2	1:D:227:TYR:CE1	2.51	0.43
1:D:199:PHE:HA	1:D:206:VAL:HG12	2.00	0.43
1:C:136:ARG:HG2	1:C:215:LEU:HD11	1.99	0.43
1:D:47:LEU:O	1:D:51:GLN:HG3	2.19	0.43
1:D:52:LEU:HG	1:D:56:LEU:HD22	2.00	0.43
1:A:242:ILE:H	1:A:242:ILE:HG13	1.53	0.43
1:C:130:LEU:CD1	1:C:136:ARG:HA	2.47	0.43
1:D:33:GLY:N	1:D:44:MSE:HE1	2.34	0.43
1:B:200:ASP:OD2	1:B:200:ASP:C	2.56	0.43
1:D:145:PHE:N	3:D:315:HOH:O	2.22	0.43
1:D:132:ASN:HB3	1:D:135:ILE:HG12	2.00	0.43
1:D:221:LYS:HA	1:D:221:LYS:HD3	1.85	0.43
1:A:181:GLU:O	1:A:185:LEU:HG	2.19	0.43
1:D:56:LEU:HG	1:D:227:TYR:CE2	2.54	0.43
1:D:218:GLU:HG3	3:D:368:HOH:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130[B]:LEU:HD22	1:A:136:ARG:HA	2.01	0.43
1:C:219:MSE:HA	1:C:219:MSE:HE2	2.01	0.43
1:D:37:ASP:OD2	1:D:38:GLU:N	2.48	0.43
1:A:22:LYS:NZ	3:A:325:HOH:O	2.31	0.42
1:A:224:GLN:NE2	3:A:423:HOH:O	2.52	0.42
1:B:62:ILE:CD1	1:B:88:ILE:HD12	2.49	0.42
1:C:205:MSE:SE	1:C:219:MSE:HG3	2.69	0.42
1:D:40:THR:O	1:D:44:MSE:HG3	2.20	0.42
1:D:74:LEU:C	1:D:74:LEU:HD23	2.39	0.42
1:D:185:LEU:CD2	1:D:208:THR:HG21	2.49	0.42
1:D:210:MSE:C	1:D:212:GLU:H	2.23	0.42
1:A:34:ASN:C	1:A:36:GLU:N	2.73	0.42
1:B:233:MSE:HE3	1:B:233:MSE:HB2	1.85	0.42
1:B:137:ASN:HA	1:B:140:MSE:HE2	2.02	0.41
1:B:238:TYR:CZ	1:B:242:ILE:HD13	2.55	0.41
1:D:36:GLU:HB3	1:D:37:ASP:H	1.56	0.41
1:D:181:GLU:HG3	1:D:210:MSE:HE3	2.02	0.41
1:A:34:ASN:C	1:A:36:GLU:H	2.23	0.41
1:A:78:LEU:HA	1:A:79:PRO:HD3	1.86	0.41
1:C:20[B]:LYS:NZ	3:C:320:HOH:O	2.51	0.41
1:D:136:ARG:HH21	1:D:137:ASN:ND2	2.19	0.41
1:D:194:ILE:O	1:D:197:ARG:HB2	2.19	0.41
1:A:55[A]:ARG:HG2	3:A:604:HOH:O	2.20	0.41
1:D:159:LEU:N	1:D:159:LEU:HD12	2.35	0.41
1:A:130[A]:LEU:HD13	1:A:135:ILE:CG2	2.48	0.41
1:C:74:LEU:HD13	1:C:159[B]:LEU:CD2	2.51	0.40
1:D:85:ARG:C	1:D:86:GLN:HG2	2.42	0.40
1:B:64:GLY:HA3	1:B:155:LEU:HD11	2.04	0.40
1:B:117:LEU:HA	1:B:117:LEU:HD23	1.86	0.40
1:B:223:LYS:HE3	1:B:247:GLY:O	2.22	0.40
1:B:233:MSE:O	1:B:234:SER:HB3	2.20	0.40
1:A:22:LYS:HD3	1:A:23:PHE:CE2	2.56	0.40
1:A:91:PRO:HG2	1:A:124:ALA:HB2	2.03	0.40
1:B:74:LEU:HD22	1:B:159:LEU:HD23	2.02	0.40
1:D:89:CYS:O	1:D:121:SER:HA	2.21	0.40
1:C:20[B]:LYS:NZ	3:C:324:HOH:O	2.54	0.40

There are no symmetry-related clashes.

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	256/266 (96%)	251 (98%)	5 (2%)	0	100	100
1	B	230/266 (86%)	227 (99%)	2 (1%)	1 (0%)	30	27
1	C	235/266 (88%)	230 (98%)	4 (2%)	1 (0%)	30	27
1	D	245/266 (92%)	239 (98%)	4 (2%)	2 (1%)	16	12
All	All	966/1064 (91%)	947 (98%)	15 (2%)	4 (0%)	30	27

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	234	SER
1	C	234	SER
1	D	234	SER
1	D	209	ASN

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	217/211 (103%)	204 (94%)	13 (6%)	16	13
1	B	199/211 (94%)	190 (96%)	9 (4%)	23	21
1	C	199/211 (94%)	187 (94%)	12 (6%)	16	13
1	D	208/211 (99%)	188 (90%)	20 (10%)	7	4
All	All	823/844 (98%)	769 (93%)	54 (7%)	14	10

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	35	ASP
1	A	67	TRP
1	A	103[A]	ARG
1	A	103[B]	ARG
1	A	136	ARG
1	A	164	SER
1	A	180	GLU
1	A	193	ASP
1	A	206	VAL
1	A	220	ASN
1	A	242	ILE
1	A	257	SER
1	B	13	LEU
1	B	38	GLU
1	B	67	TRP
1	B	136	ARG
1	B	174	HIS
1	B	177	TYR
1	B	197	ARG
1	B	231	ILE
1	B	264	LEU
1	C	11	GLU
1	C	37	ASP
1	C	38	GLU
1	C	39	GLU
1	C	67	TRP
1	C	86	GLN
1	C	132	ASN
1	C	193	ASP
1	C	209	ASN
1	C	233	MSE
1	C	236	GLU
1	C	256	ASN
1	D	11	GLU
1	D	15	LEU
1	D	26	LYS
1	D	56	LEU
1	D	67	TRP
1	D	69	ARG
1	D	86	GLN
1	D	100	LEU

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Mol	Chain	Res	Type
1	D	103	ARG
1	D	134	LEU
1	D	160[A]	VAL
1	D	160[B]	VAL
1	D	174	HIS
1	D	193	ASP
1	D	197	ARG
1	D	206	VAL
1	D	213	LYS
1	D	236	GLU
1	D	264	LEU
1	D	265	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	12	ASN
1	A	137	ASN
1	A	186	ASN
1	B	21	GLN
1	B	41	GLN
1	B	80	GLN
1	B	105	HIS
1	B	137	ASN
1	B	224	GLN
1	C	34	ASN
1	C	41	GLN
1	C	132	ASN
1	C	137	ASN
1	C	256	ASN
1	D	21	GLN
1	D	77	ASN
1	D	80	GLN
1	D	86	GLN
1	D	105	HIS
1	D	137	ASN
1	D	224	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 oligosaccharides in this entry.

5.6   Ligand geometry ⓘ

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	ACY	B	266	-	3,3,3	1.09	0	3,3,3	0.61	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	266	ACY	2	0

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, 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(Å²)	Q<0.9
1	A	239/266 (89%)	-0.13	3 (1%)	74	73	13, 38, 76, 108	16 (6%)
1	B	228/266 (85%)	-0.12	8 (3%)	47	45	13, 38, 71, 111	7 (3%)
1	C	225/266 (84%)	-0.01	14 (6%)	28	26	13, 38, 69, 100	16 (7%)
1	D	241/266 (90%)	0.38	20 (8%)	19	17	12, 44, 82, 153	27 (11%)
All	All	933/1064 (87%)	0.03	45 (4%)	36	35	12, 39, 77, 153	66 (7%)

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	10	ASN	8.1
1	D	185	LEU	7.8
1	C	37	ASP	7.5
1	D	187	ALA	7.4
1	D	186	ASN	7.2
1	B	38	GLU	7.0
1	D	182	SER	6.9
1	D	179	GLY	6.8
1	D	177	TYR	6.1
1	D	183	ASP	5.1
1	B	165	PRO	5.0
1	D	172	ASN	4.8
1	D	178	GLY	4.8
1	C	187	ALA	4.5
1	B	172	ASN	4.4
1	D	184	ASP	4.2
1	D	33	GLY	4.2
1	D	36	GLU	4.1
1	D	180	GLU	3.9
1	D	181	GLU	3.6
1	B	40	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	165	PRO	3.4
1	C	33	GLY	3.3
1	C	201	ILE	3.2
1	C	164	SER	3.1
1	B	175	ALA	3.0
1	C	188	ARG	2.7
1	C	12	ASN	2.7
1	A	207[A]	GLU	2.6
1	B	137	ASN	2.6
1	C	236	GLU	2.5
1	C	189	GLN	2.5
1	D	175	ALA	2.5
1	C	163	GLY	2.4
1	A	185	LEU	2.4
1	C	35	ASP	2.4
1	C	134[A]	LEU	2.4
1	A	35	ASP	2.4
1	D	40	THR	2.3
1	D	165	PRO	2.3
1	B	37	ASP	2.2
1	C	206	VAL	2.1
1	D	164	SER	2.1
1	D	258	SER	2.0
1	B	173	TRP	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3　Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4　Ligands ⓘ

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	ACY	B	266	4/4	0.77	0.15	45,56,68,69	0

6.5 Other polymers ⓘ

There are no such residues in this entry.