Full wwPDB X-ray Structure Validation Report (i)

Mar 23, 2024 – 08:47 PM EDT

PDB ID	:	1SXH
Title	:	apo structure of B. megaterium transcription regulator
Authors	:	Schumacher, M.A.; Allen, G.S.; Diel, M.; Seidel, G.; Hillen, W.; Brennan, R.G.
Deposited on	:	2004-03-30
Resolution	:	2.75 Å(reported)

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

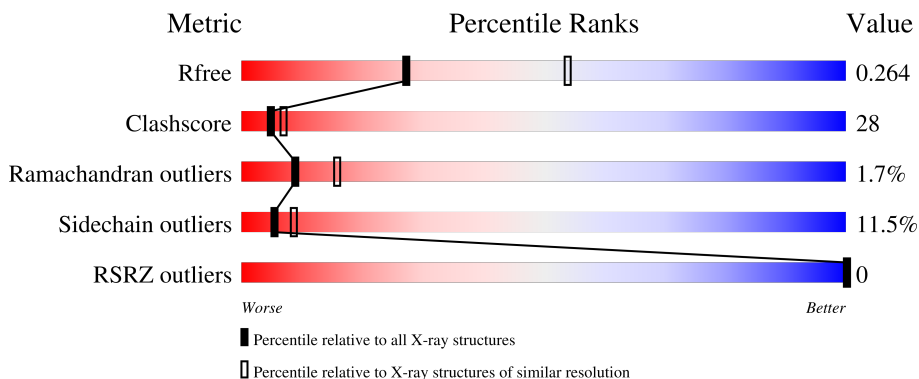|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.1

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 2.75 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		0.264
Clashscore		28
Ramachandran outliers		1.7%
Sidechain outliers		11.5%
RSRZ outliers		0

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$_{free}$	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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	280	49% 40% 8% •
1	D	280	52% 39% 6% •

WORLDWIDE
wwPDB
PROTEIN DATA BANK

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 4287 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 Glucose-resistance amylase regulator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	Se	0	0	0
			2123	1337	352	426	8			
1	D	273	Total	C	N	O	Se	0	0	0
			2123	1337	352	426	8			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	88	MSE	MET	modified residue	UNP P46828
A	112	MSE	MET	modified residue	UNP P46828
A	123	MSE	MET	modified residue	UNP P46828
A	250	MSE	MET	modified residue	UNP P46828
A	282	MSE	MET	modified residue	UNP P46828
A	294	MSE	MET	modified residue	UNP P46828
A	302	MSE	MET	modified residue	UNP P46828
A	309	MSE	MET	modified residue	UNP P46828
D	88	MSE	MET	modified residue	UNP P46828
D	112	MSE	MET	modified residue	UNP P46828
D	123	MSE	MET	modified residue	UNP P46828
D	250	MSE	MET	modified residue	UNP P46828
D	282	MSE	MET	modified residue	UNP P46828
D	294	MSE	MET	modified residue	UNP P46828
D	302	MSE	MET	modified residue	UNP P46828
D	309	MSE	MET	modified residue	UNP P46828

- Molecule 2 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	22	Total	O	0	0
			22	22		
2	D	19	Total	O	0	0
			19	19		

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: Glucose-resistance amylase regulator
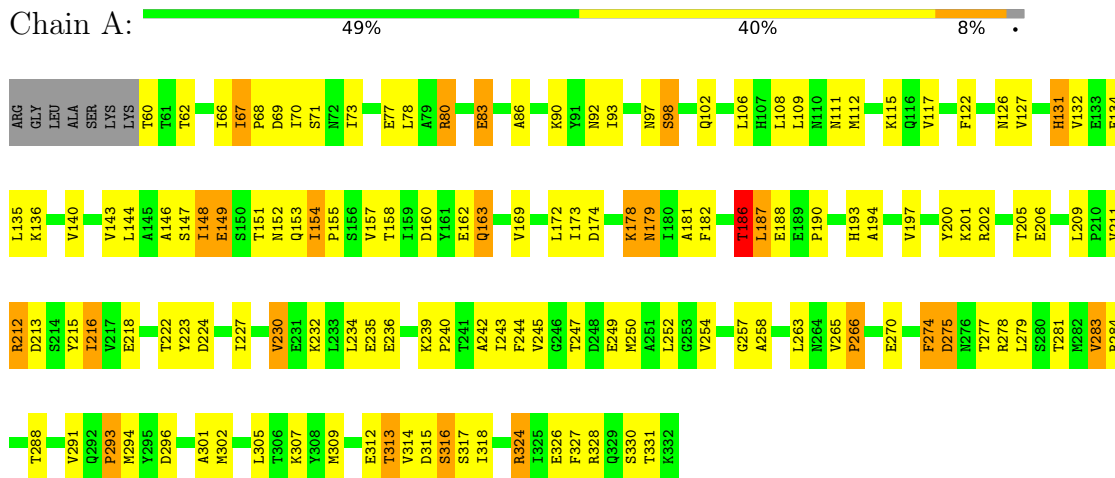
- Molecule 1: Glucose-resistance amylase regulator
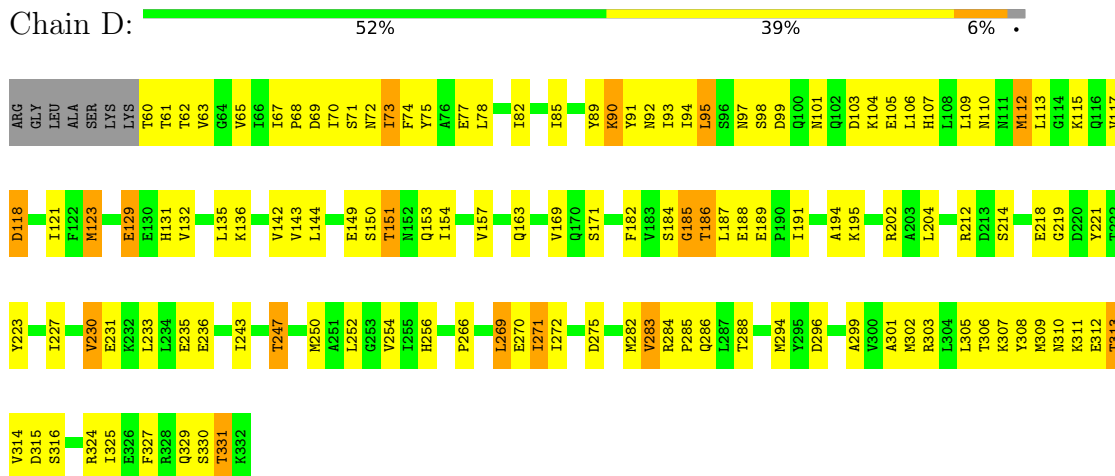
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	72.68Å 72.19Å 105.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	59.91 – 2.75 52.91 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.9 (59.91-2.75) 50.1 (52.91-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.43 (at 2.77Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.241 , 0.273 0.234 , 0.264	Depositor DCC
R_{free} test set	1195 reflections (15.87%)	wwPDB-VP
Wilson B-factor (Å^2)	64.7	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 39.9	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.047 for k,h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	4287	wwPDB-VP
Average B, all atoms (Å^2)	62.0	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 95.44 % 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 1.3599e-09.*

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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 ⓘ

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	0.54	0/2148	0.77	0/2899
1	D	0.62	0/2148	0.79	1/2899 (0.0%)
All	All	0.58	0/4296	0.78	1/5798 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	185	GLY	N-CA-C	-5.10	100.35	113.10

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	2123	0	2121	120	0
1	D	2123	0	2121	123	0
2	A	22	0	0	2	0
2	D	19	0	0	1	0
All	All	4287	0	4242	234	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 28.

All (234) 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:179:ASN:HD22	1:A:179:ASN:H	1.06	1.02
1:D:68:PRO:HA	1:D:98:SER:HB3	1.56	0.88
1:A:62:THR:HG22	1:A:92:ASN:HB3	1.58	0.86
1:A:288:THR:HG22	1:A:328:ARG:H	1.43	0.84
1:A:148:ILE:HG13	1:A:190:PRO:HB2	1.57	0.84
1:D:70:ILE:H	1:D:97:ASN:ND2	1.76	0.84
1:D:75:TYR:HD1	1:D:123:MSE:HE3	1.44	0.83
1:A:266:PRO:HB2	1:A:270:GLU:HG2	1.59	0.82
1:A:157:VAL:HG11	1:A:301:ALA:HB2	1.59	0.82
1:A:179:ASN:H	1:A:179:ASN:ND2	1.78	0.81
1:A:179:ASN:HB2	1:A:215:TYR:HE2	1.46	0.80
1:D:70:ILE:H	1:D:97:ASN:HD21	1.29	0.80
1:A:66:ILE:HD11	1:A:122:PHE:CD2	2.17	0.79
1:A:66:ILE:HD11	1:A:122:PHE:HD2	1.47	0.79
1:A:148:ILE:HD13	1:A:148:ILE:H	1.49	0.78
1:D:67:ILE:HG22	1:D:123:MSE:HE2	1.63	0.78
1:D:243:ILE:HG13	1:D:269:LEU:HD21	1.66	0.78
1:D:307:LYS:HG3	1:D:312:GLU:HB2	1.67	0.77
1:A:223:TYR:HB2	1:D:282:MSE:HE3	1.68	0.76
1:D:135:LEU:HD11	1:D:142:VAL:HG21	1.68	0.75
1:D:109:LEU:HD21	1:D:135:LEU:HD13	1.69	0.75
1:A:152:ASN:ND2	1:A:318:ILE:HG21	2.02	0.75
1:A:288:THR:HG23	1:A:330:SER:OG	1.86	0.75
1:A:178:LYS:HG2	1:A:209:LEU:HD22	1.70	0.74
1:D:60:THR:N	1:D:90:LYS:HZ2	1.84	0.74
1:D:149:GLU:HG3	1:D:151:THR:H	1.52	0.74
1:D:75:TYR:CD1	1:D:123:MSE:HE3	2.24	0.73
1:D:194:ALA:O	1:D:195:LYS:HD3	1.89	0.72
1:A:222:THR:HG22	1:A:224:ASP:H	1.53	0.72
1:A:274:PHE:O	1:A:275:ASP:HB2	1.88	0.72
1:A:179:ASN:HD22	1:A:179:ASN:N	1.76	0.72
1:A:172:LEU:HD13	1:A:242:ALA:HB1	1.72	0.71
1:D:63:VAL:HG21	1:D:302:MSE:HE1	1.71	0.71
1:A:277:THR:HG22	1:A:279:LEU:H	1.56	0.70
1:A:249:GLU:HG3	1:D:282:MSE:HE1	1.74	0.70
1:A:67:ILE:N	1:A:67:ILE:HD13	2.07	0.69
1:D:78:LEU:HB2	1:D:294:MSE:HE3	1.73	0.69
1:D:135:LEU:HD21	1:D:142:VAL:HG11	1.75	0.69
1:A:230:VAL:HG13	1:A:254:VAL:HG13	1.75	0.68
1:D:187:LEU:HD12	1:D:218:GLU:OE2	1.93	0.68
1:A:288:THR:HB	1:A:327:PHE:HA	1.76	0.68
1:A:318:ILE:HD12	1:A:318:ILE:N	2.10	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:ILE:HD13	1:A:67:ILE:H	1.60	0.66
1:D:95:LEU:HD12	1:D:95:LEU:N	2.09	0.66
1:D:163:GLN:NE2	1:D:202:ARG:HH22	1.93	0.66
1:D:67:ILE:CG2	1:D:123:MSE:HE2	2.25	0.66
1:D:70:ILE:HG22	1:D:97:ASN:HD21	1.60	0.66
1:D:132:VAL:O	1:D:136:LYS:HG3	1.94	0.66
1:A:205:THR:HA	2:A:777:HOH:O	1.95	0.65
1:A:293:PRO:HB2	1:A:296:ASP:HB2	1.79	0.65
1:D:82:ILE:HG23	1:D:302:MSE:HG2	1.79	0.65
1:D:230:VAL:HG13	1:D:254:VAL:HG13	1.76	0.65
1:D:149:GLU:HG3	1:D:150:SER:N	2.12	0.64
1:A:247:THR:HG22	1:A:250:MSE:H	1.62	0.64
1:D:182:PHE:CE1	1:D:184:SER:HB2	2.32	0.64
1:D:219:GLY:HA3	1:D:250:MSE:CE	2.28	0.64
1:D:247:THR:HG22	1:D:250:MSE:H	1.62	0.64
1:D:306:THR:HA	1:D:309:MSE:HE2	1.81	0.63
1:D:135:LEU:CD1	1:D:142:VAL:HG21	2.29	0.62
1:D:230:VAL:HG22	1:D:254:VAL:HA	1.80	0.62
1:A:152:ASN:HD22	1:A:318:ILE:HG21	1.65	0.62
1:D:149:GLU:O	1:D:150:SER:HB2	1.99	0.62
1:A:190:PRO:O	1:A:194:ALA:HB3	2.01	0.61
1:D:252:LEU:HG	1:D:283:VAL:CG1	2.30	0.60
1:A:108:LEU:HA	1:A:111:ASN:HB2	1.84	0.60
1:D:271:ILE:HD11	1:D:330:SER:HB2	1.82	0.60
1:A:70:ILE:CD1	1:D:70:ILE:HD11	2.32	0.59
1:A:160:ASP:OD2	1:A:163:GLN:HB2	2.02	0.59
1:A:148:ILE:H	1:A:148:ILE:CD1	2.14	0.59
1:D:74:PHE:CD2	1:D:294:MSE:HE2	2.37	0.59
1:D:230:VAL:CG2	1:D:254:VAL:HA	2.32	0.59
1:D:252:LEU:HG	1:D:283:VAL:HG11	1.84	0.59
1:A:274:PHE:O	1:A:275:ASP:CB	2.50	0.59
1:A:205:THR:HG22	2:A:777:HOH:O	2.02	0.59
1:D:129:GLU:CD	1:D:129:GLU:H	2.06	0.59
1:D:271:ILE:CD1	1:D:330:SER:HB2	2.33	0.59
1:A:73:ILE:HD12	1:A:279:LEU:HD11	1.85	0.58
1:D:219:GLY:HA3	1:D:250:MSE:HE1	1.85	0.58
1:D:110:ASN:HA	1:D:113:LEU:HG	1.84	0.58
1:A:222:THR:HG22	1:A:224:ASP:N	2.19	0.57
1:D:194:ALA:C	1:D:195:LYS:HD3	2.24	0.57
1:D:157:VAL:HG11	1:D:301:ALA:HB2	1.86	0.57
1:A:143:VAL:HG12	1:A:305:LEU:HD13	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:89:TYR:O	1:D:90:LYS:HG3	2.04	0.57
1:A:305:LEU:O	1:A:309:MSE:HG3	2.04	0.57
1:D:288:THR:OG1	1:D:331:THR:HB	2.04	0.57
1:D:112:MSE:HE3	1:D:115:LYS:HZ1	1.71	0.56
1:A:83:GLU:HA	1:A:93:ILE:HD12	1.87	0.56
1:A:73:ILE:O	1:A:77:GLU:HG3	2.06	0.55
1:A:230:VAL:HG21	1:A:257:GLY:HA3	1.89	0.55
1:D:144:LEU:HD11	1:D:154:ILE:HD11	1.89	0.55
1:A:227:ILE:O	1:A:230:VAL:HG23	2.07	0.54
1:A:288:THR:CG2	1:A:328:ARG:H	2.19	0.54
1:A:152:ASN:HB3	1:A:318:ILE:HG12	1.90	0.54
1:A:160:ASP:OD1	1:A:162:GLU:HB3	2.08	0.54
1:D:266:PRO:HB2	1:D:270:GLU:HG2	1.90	0.54
1:D:103:ASP:O	1:D:107:HIS:HB2	2.09	0.53
1:D:186:THR:HG22	1:D:188:GLU:HG2	1.89	0.53
1:D:149:GLU:O	1:D:150:SER:CB	2.57	0.53
1:A:281:THR:HG23	1:A:328:ARG:HH21	1.74	0.52
1:D:288:THR:HG23	1:D:327:PHE:HA	1.91	0.52
1:D:131:HIS:O	1:D:135:LEU:HB2	2.09	0.52
1:D:189:GLU:HB3	1:D:191:ILE:HG22	1.90	0.52
1:A:149:GLU:HG3	1:A:154:ILE:HG23	1.92	0.52
1:A:288:THR:HG22	1:A:328:ARG:N	2.20	0.52
1:D:65:VAL:CG2	1:D:95:LEU:HG	2.39	0.52
1:A:245:VAL:HG12	1:A:247:THR:H	1.75	0.52
1:D:231:GLU:O	1:D:235:GLU:HG3	2.09	0.52
1:D:74:PHE:CE2	1:D:294:MSE:SE	3.13	0.52
1:A:86:ALA:HB2	1:A:302:MSE:CE	2.40	0.51
1:D:286:GLN:HG3	2:D:761:HOH:O	2.10	0.51
1:A:131:HIS:O	1:A:135:LEU:HB2	2.11	0.51
1:D:73:ILE:O	1:D:77:GLU:HG3	2.10	0.51
1:D:98:SER:O	1:D:99:ASP:HB2	2.11	0.51
1:A:92:ASN:HD21	1:D:115:LYS:NZ	2.08	0.51
1:D:65:VAL:HG22	1:D:95:LEU:HG	1.93	0.51
1:D:227:ILE:O	1:D:230:VAL:HG23	2.11	0.50
1:D:271:ILE:HD13	1:D:271:ILE:H	1.75	0.50
1:A:258:ALA:O	1:A:263:LEU:HB2	2.11	0.50
1:D:68:PRO:HD3	1:D:123:MSE:O	2.12	0.50
1:D:121:ILE:HD11	1:D:302:MSE:CE	2.41	0.50
1:D:185:GLY:HA3	1:D:221:TYR:CE2	2.47	0.50
1:D:90:LYS:O	1:D:90:LYS:HD3	2.12	0.49
1:D:93:ILE:HG23	1:D:93:ILE:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:ARG:O	1:A:206:GLU:HB2	2.13	0.49
1:A:157:VAL:HG11	1:A:301:ALA:CB	2.37	0.49
1:A:80:ARG:HH12	1:D:97:ASN:HB3	1.78	0.49
1:A:187:LEU:O	1:A:193:HIS:HB3	2.13	0.49
1:D:112:MSE:O	1:D:117:VAL:HG22	2.11	0.49
1:D:212:ARG:HG3	1:D:212:ARG:HH11	1.77	0.49
1:D:85:ILE:HG13	1:D:299:ALA:HA	1.94	0.48
1:A:117:VAL:O	1:A:140:VAL:HG11	2.13	0.48
1:D:82:ILE:HD13	1:D:121:ILE:HD12	1.95	0.48
1:D:129:GLU:CD	1:D:129:GLU:N	2.66	0.48
1:A:108:LEU:O	1:A:112:MSE:HG2	2.14	0.48
1:D:310:ASN:C	1:D:311:LYS:HG2	2.34	0.48
1:A:80:ARG:HH22	1:D:99:ASP:HA	1.78	0.48
1:D:223:TYR:OH	1:D:256:HIS:HD2	1.96	0.48
1:A:97:ASN:O	1:A:108:LEU:HD11	2.13	0.48
1:A:122:PHE:HB3	1:A:144:LEU:HD23	1.95	0.48
1:A:181:ALA:HB3	1:A:243:ILE:HG12	1.95	0.48
1:A:252:LEU:HG	1:A:283:VAL:HG11	1.95	0.48
1:A:288:THR:HG21	1:A:331:THR:OG1	2.14	0.48
1:D:78:LEU:HD22	1:D:123:MSE:HE1	1.96	0.48
1:D:233:LEU:O	1:D:236:GLU:HB3	2.14	0.48
1:A:122:PHE:HD1	1:A:144:LEU:HD22	1.79	0.47
1:D:219:GLY:HA3	1:D:250:MSE:HE3	1.95	0.47
1:A:106:LEU:CD2	1:A:134:GLU:HG2	2.45	0.47
1:A:252:LEU:HG	1:A:283:VAL:CG1	2.44	0.47
1:A:111:ASN:HB3	1:A:115:LYS:NZ	2.30	0.47
1:A:186:THR:HA	1:A:218:GLU:OE1	2.14	0.47
1:D:272:ILE:HG23	1:D:288:THR:HG22	1.96	0.47
1:D:299:ALA:O	1:D:303:ARG:HG3	2.14	0.47
1:A:80:ARG:NH1	1:D:97:ASN:HB3	2.29	0.46
1:A:211:VAL:HG12	1:A:211:VAL:O	2.15	0.46
1:A:80:ARG:NH1	1:D:99:ASP:OD2	2.49	0.46
1:A:201:LYS:O	1:A:205:THR:HG23	2.15	0.46
1:D:305:LEU:O	1:D:309:MSE:HG3	2.14	0.46
1:A:67:ILE:O	1:A:98:SER:HB2	2.15	0.46
1:D:182:PHE:CZ	1:D:184:SER:HB2	2.50	0.46
1:D:266:PRO:HA	1:D:269:LEU:O	2.14	0.46
1:D:73:ILE:HD13	1:D:73:ILE:N	2.31	0.46
1:A:179:ASN:ND2	1:A:179:ASN:N	2.44	0.46
1:D:89:TYR:O	1:D:90:LYS:CG	2.64	0.46
1:A:317:SER:C	1:A:318:ILE:HD12	2.36	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:ILE:HD13	1:A:148:ILE:N	2.22	0.45
1:D:284:ARG:HA	1:D:284:ARG:HD3	1.70	0.45
1:A:174:ASP:OD1	1:A:174:ASP:N	2.50	0.45
1:A:288:THR:HA	1:A:326:GLU:O	2.17	0.45
1:D:94:ILE:C	1:D:95:LEU:HD12	2.36	0.45
1:A:135:LEU:HG	1:A:154:ILE:HD13	1.99	0.45
1:A:212:ARG:HG3	1:A:212:ARG:HH11	1.81	0.45
1:D:73:ILE:HD13	1:D:74:PHE:H	1.81	0.45
1:D:82:ILE:HG23	1:D:302:MSE:CG	2.45	0.45
1:D:89:TYR:HB3	1:D:91:TYR:CE2	2.52	0.45
1:D:307:LYS:HE2	1:D:313:THR:O	2.16	0.45
1:D:118:ASP:OD1	1:D:118:ASP:N	2.50	0.45
1:D:310:ASN:O	1:D:311:LYS:HG2	2.17	0.44
1:A:305:LEU:HG	1:A:309:MSE:HE2	2.00	0.44
1:A:132:VAL:O	1:A:136:LYS:HB2	2.17	0.44
1:D:252:LEU:HG	1:D:283:VAL:HG13	1.99	0.44
1:A:66:ILE:HG13	1:A:66:ILE:O	2.17	0.44
1:A:111:ASN:HB3	1:A:115:LYS:HZ1	1.83	0.44
1:A:234:LEU:O	1:A:239:LYS:HE3	2.18	0.44
1:A:69:ASP:OD2	1:A:71:SER:HB3	2.18	0.44
1:A:307:LYS:HA	1:A:312:GLU:HG3	2.00	0.43
1:D:121:ILE:HD11	1:D:302:MSE:HE2	1.99	0.43
1:A:232:LYS:O	1:A:235:GLU:HB2	2.18	0.43
1:D:266:PRO:HD3	1:D:329:GLN:O	2.18	0.43
1:A:143:VAL:HA	1:A:155:PRO:HB2	1.99	0.43
1:A:178:LYS:O	1:A:209:LEU:HD13	2.18	0.43
1:A:277:THR:CG2	1:A:278:ARG:N	2.81	0.43
1:A:281:THR:HG23	1:A:328:ARG:NH2	2.33	0.43
1:A:147:SER:O	1:A:158:THR:HG21	2.18	0.43
1:A:153:GLN:HE21	1:A:153:GLN:HB2	1.66	0.43
1:D:72:ASN:ND2	1:D:73:ILE:HD13	2.34	0.43
1:D:99:ASP:OD1	1:D:104:LYS:HE3	2.19	0.43
1:A:186:THR:O	1:A:188:GLU:N	2.52	0.43
1:A:146:ALA:HA	1:A:158:THR:HG22	2.00	0.42
1:A:154:ILE:HD12	1:A:155:PRO:HD2	2.01	0.42
1:D:121:ILE:CD1	1:D:302:MSE:HE3	2.48	0.42
1:D:69:ASP:OD1	1:D:71:SER:HB3	2.19	0.42
1:A:92:ASN:ND2	1:D:115:LYS:HD3	2.34	0.42
1:A:182:PHE:HD2	1:A:244:PHE:O	2.02	0.42
1:A:186:THR:C	1:A:188:GLU:H	2.22	0.42
1:D:70:ILE:HG12	1:D:70:ILE:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:223:TYR:OH	1:D:256:HIS:CD2	2.72	0.42
1:A:245:VAL:HG21	1:A:254:VAL:HG21	2.01	0.42
1:D:101:ASN:O	1:D:105:GLU:HG3	2.19	0.42
1:A:216:ILE:HD13	1:A:216:ILE:O	2.18	0.42
1:D:70:ILE:N	1:D:97:ASN:HD21	2.08	0.42
1:D:324:ARG:HG2	1:D:325:ILE:H	1.85	0.42
1:A:109:LEU:HD23	1:A:109:LEU:O	2.20	0.42
1:D:308:TYR:OH	1:D:314:VAL:HG21	2.20	0.42
1:A:169:VAL:HG21	1:A:200:TYR:HA	2.02	0.42
1:D:212:ARG:HH11	1:D:212:ARG:CG	2.33	0.42
1:A:127:VAL:HG23	1:A:148:ILE:HD13	2.02	0.41
1:A:291:VAL:HB	1:A:324:ARG:HG3	2.01	0.41
1:D:62:THR:HG22	1:D:92:ASN:HB3	2.02	0.41
1:D:78:LEU:C	1:D:78:LEU:HD23	2.41	0.41
1:D:285:PRO:O	1:D:286:GLN:C	2.56	0.41
1:A:182:PHE:HE1	1:A:197:VAL:HG22	1.85	0.41
1:D:310:ASN:O	1:D:311:LYS:CG	2.69	0.41
1:A:173:ILE:HD12	1:A:209:LEU:HD12	2.03	0.41
1:A:215:TYR:CE1	1:A:240:PRO:HG3	2.55	0.41
1:A:265:VAL:HA	1:A:266:PRO:HA	1.84	0.41
1:A:307:LYS:NZ	1:A:314:VAL:HG21	2.36	0.41
1:D:271:ILE:HD13	1:D:271:ILE:N	2.36	0.41
1:A:149:GLU:C	1:A:151:THR:H	2.24	0.41
1:A:216:ILE:O	1:A:216:ILE:HG23	2.21	0.41
1:A:314:VAL:CG1	1:A:315:ASP:N	2.84	0.40
1:D:303:ARG:O	1:D:306:THR:HB	2.21	0.40
1:A:149:GLU:OE2	1:A:151:THR:OG1	2.39	0.40
1:D:315:ASP:N	1:D:315:ASP:OD1	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	271/280 (97%)	238 (88%)	25 (9%)	8 (3%)	4	6
1	D	271/280 (97%)	240 (89%)	30 (11%)	1 (0%)	34	53
All	All	542/560 (97%)	478 (88%)	55 (10%)	9 (2%)	9	16

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	149	GLU
1	A	313	THR
1	A	316	SER
1	D	275	ASP
1	A	68	PRO
1	A	186	THR
1	A	187	LEU
1	A	275	ASP
1	A	293	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	239/236 (101%)	210 (88%)	29 (12%)	5	8
1	D	239/236 (101%)	213 (89%)	26 (11%)	6	10
All	All	478/472 (101%)	423 (88%)	55 (12%)	5	9

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	THR
1	A	67	ILE
1	A	78	LEU
1	A	80	ARG
1	A	83	GLU
1	A	90	LYS
1	A	98	SER

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Mol	Chain	Res	Type
1	A	102	GLN
1	A	126	ASN
1	A	131	HIS
1	A	148	ILE
1	A	154	ILE
1	A	163	GLN
1	A	178	LYS
1	A	179	ASN
1	A	186	THR
1	A	212	ARG
1	A	213	ASP
1	A	216	ILE
1	A	230	VAL
1	A	236	GLU
1	A	266	PRO
1	A	274	PHE
1	A	283	VAL
1	A	284	ARG
1	A	294	MSE
1	A	313	THR
1	A	316	SER
1	A	324	ARG
1	D	61	THR
1	D	73	ILE
1	D	90	LYS
1	D	95	LEU
1	D	106	LEU
1	D	112	MSE
1	D	118	ASP
1	D	123	MSE
1	D	129	GLU
1	D	143	VAL
1	D	151	THR
1	D	153	GLN
1	D	169	VAL
1	D	171	SER
1	D	186	THR
1	D	204	LEU
1	D	214	SER
1	D	230	VAL
1	D	247	THR
1	D	269	LEU

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Mol	Chain	Res	Type
1	D	271	ILE
1	D	283	VAL
1	D	296	ASP
1	D	313	THR
1	D	316	SER
1	D	331	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	ASN
1	A	102	GLN
1	A	126	ASN
1	A	131	HIS
1	A	153	GLN
1	A	163	GLN
1	A	179	ASN
1	A	192	ASN
1	A	259	GLN
1	A	286	GLN
1	A	292	GLN
1	A	329	GLN
1	D	72	ASN
1	D	97	ASN
1	D	111	ASN
1	D	163	GLN
1	D	192	ASN
1	D	193	HIS
1	D	256	HIS

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, 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	265/280 (94%)	-0.34	0	100	100	29, 62, 100, 117	0
1	D	265/280 (94%)	-0.43	0	100	100	27, 51, 107, 122	0
All	All	530/560 (94%)	-0.38	0	100	100	27, 59, 105, 122	0

There are no RSRZ outliers to report.

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 ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.