Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 09:02 PM GMT

PDB ID	:	3A2N
Title	:	Crystal structure of DBJA (Wild Type Type II P21)
Authors	:	Sato, Y.; Senda, T.
Deposited on	:	2009-05-23
Resolution	:	1.89 Å(reported)

1   Overall quality at a glance ⓘ

The reported resolution of this entry is 1.89 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		0.227
Clashscore		6
Ramachandran outliers		0.8%
Sidechain outliers		3.0%
RSRZ outliers		20.2%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
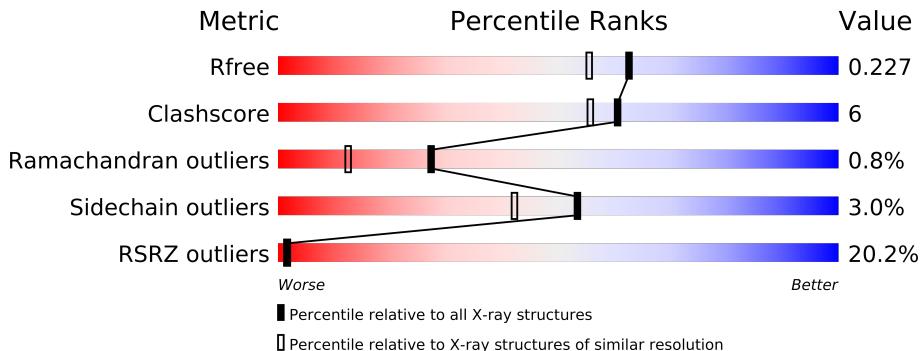
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	66092	3684 (1.90-1.90)
Clashscore	79885	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (1.90-1.90)
RSRZ outliers	66119	3686 (1.90-1.90)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	312	
1	B	312	
1	E	312	
1	F	312	

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 9801 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Haloalkane dehalogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	298	Total 2320	C 1485	N 415	O 413	S 7	0	0	0
1	B	298	Total 2330	C 1491	N 418	O 414	S 7	0	1	0
1	E	298	Total 2320	C 1485	N 415	O 413	S 7	0	0	0
1	F	299	Total 2338	C 1497	N 419	O 415	S 7	0	1	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	311	VAL	-	SEE REMARK 999	UNP P59337
A	312	ASP	-	SEE REMARK 999	UNP P59337
B	311	VAL	-	SEE REMARK 999	UNP P59337
B	312	ASP	-	SEE REMARK 999	UNP P59337
E	311	VAL	-	SEE REMARK 999	UNP P59337
E	312	ASP	-	SEE REMARK 999	UNP P59337
F	311	VAL	-	SEE REMARK 999	UNP P59337
F	312	ASP	-	SEE REMARK 999	UNP P59337

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total 1	Cl 1	0	0
2	A	1	Total 1	Cl 1	0	0
2	F	1	Total 1	Cl 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	110	Total 110	O 110	0	0
3	B	162	Total 162	O 162	0	0
3	E	45	Total 45	O 45	0	0
3	F	172	Total 173	O 173	0	1

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Haloalkane dehalogenase

Chain A:
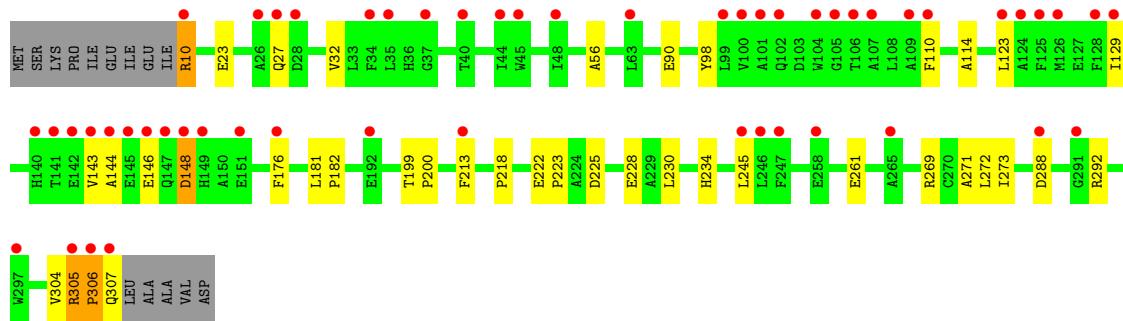
• Molecule 1: Haloalkane dehalogenase

Chain B:
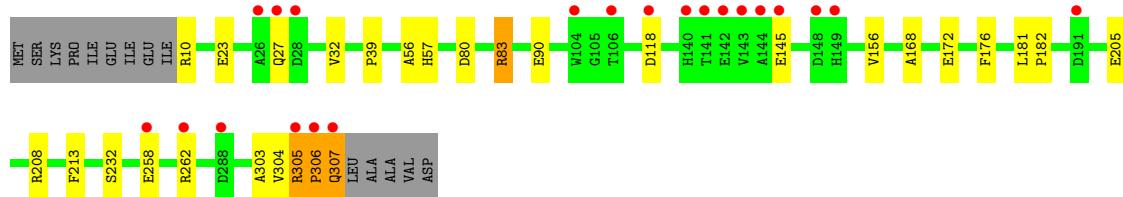
• Molecule 1: Haloalkane dehalogenase

Chain E:
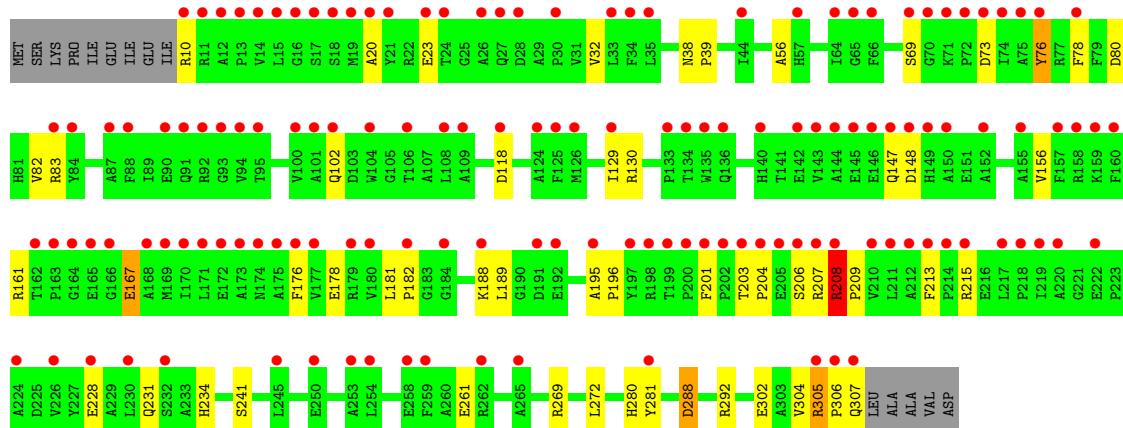
• Molecule 1: Haloalkane dehalogenase

Chain F:
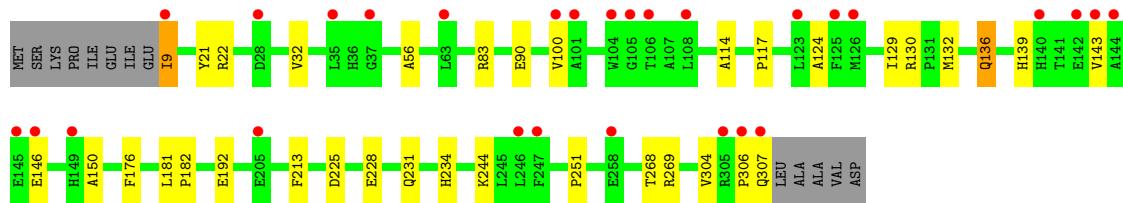
4   Data and refinement statistics   ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	125.53Å 47.77Å 99.41Å 90.00° 93.61° 90.00°	Depositor
Resolution (Å)	32.81 – 1.89 31.49 – 1.89	Depositor EDS
% Data completeness (in resolution range)	99.3 (32.81-1.89) 99.3 (31.49-1.89)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.17 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.192 , 0.228 0.192 , 0.227	Depositor DCC
R_{free} test set	4719 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	24.4	Xtriage
Anisotropy	0.082	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.43 , 45.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$< |L| > = 0.46, < L^2 > = 0.29$	Xtriage
Outliers	0 of 94027 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	9801	wwPDB-VP
Average B, all atoms (Å^2)	28.0	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 46.79 % 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 1.0884e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

---

[1]Intensities estimated from amplitudes.

5   Model quality ⓘ

5.1   Standard geometry ⓘ

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

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	0.59	0/2388	0.61	1/3252 (0.0%)
1	B	0.65	0/2399	0.66	1/3267 (0.0%)
1	E	0.77	6/2388 (0.3%)	0.69	5/3252 (0.2%)
1	F	0.68	0/2407	0.69	2/3278 (0.1%)
All	All	0.68	6/9582 (0.1%)	0.66	9/13049 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	73	ASP	CG-OD2	12.28	1.53	1.25
1	E	76	TYR	C-O	12.03	1.46	1.23
1	E	73	ASP	CG-OD1	10.18	1.48	1.25
1	E	167	GLU	CD-OE1	8.03	1.34	1.25
1	E	208	ARG	CZ-NH1	6.38	1.41	1.33
1	E	76	TYR	CG-CD1	5.92	1.46	1.39

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	73	ASP	CB-CG-OD1	-11.52	107.94	118.30
1	E	76	TYR	CB-CG-CD2	-8.35	115.99	121.00
1	E	80	ASP	CB-CG-OD1	7.92	125.42	118.30
1	E	208	ARG	NE-CZ-NH2	-6.67	116.97	120.30
1	E	76	TYR	CG-CD2-CE2	-6.24	116.31	121.30
1	F	83	ARG	NE-CZ-NH2	-5.91	117.34	120.30
1	A	225	ASP	CB-CG-OD1	5.54	123.29	118.30
1	B	83	ARG	NE-CZ-NH2	-5.25	117.68	120.30
1	F	225	ASP	CB-CG-OD1	5.10	122.89	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2320	0	2268	28	0
1	B	2330	0	2274	32	0
1	E	2320	0	2268	38	0
1	F	2338	0	2285	31	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	F	1	0	0	0	0
3	A	110	0	0	1	0
3	B	162	0	0	3	0
3	E	45	0	0	3	0
3	F	173	0	0	2	0
All	All	9801	0	9095	109	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

All (109) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:188:LYS:HD3	3:E:327:HOH:O	1.57	1.00
1:B:305:ARG:HB2	1:B:306:PRO:HD2	1.44	1.00
1:E:304:VAL:HG21	1:F:304:VAL:HG23	1.63	0.81
1:F:9:ILE:HG23	1:F:21:TYR:O	1.80	0.81
1:B:307:GLN:HG3	1:F:117:PRO:HB3	1.65	0.79
1:E:304:VAL:CG2	1:F:304:VAL:HG23	2.14	0.78
1:B:83:ARG:HD3	3:B:407:HOH:O	1.85	0.76
1:A:269:ARG:HH22	1:B:307:GLN:NE2	1.87	0.73
1:A:304:VAL:CG2	1:B:304:VAL:HG23	2.20	0.72
1:B:258:GLU:HG2	1:B:262:ARG:NH1	2.04	0.71
1:A:304:VAL:HG21	1:B:304:VAL:HG23	1.73	0.70
1:B:208:ARG:HB2	3:B:396:HOH:O	1.92	0.70
1:F:9:ILE:HG21	1:F:22:ARG:HG3	1.75	0.69
1:B:305:ARG:CB	1:B:306:PRO:HD2	2.22	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:90:GLU:HG2	3:F:433:HOH:O	1.93	0.68
1:B:306:PRO:HA	1:F:114:ALA:O	1.94	0.67
1:A:181:LEU:HB3	1:A:182:PRO:HD3	1.77	0.66
1:B:10:ARG:CZ	1:B:23:GLU:OE1	2.44	0.66
1:E:302:GLU:O	1:E:305:ARG:HG2	1.95	0.66
1:A:304:VAL:CG2	1:B:304:VAL:CG2	2.75	0.64
1:E:304:VAL:O	1:E:305:ARG:O	2.17	0.63
1:E:305:ARG:HB2	1:E:306:PRO:CD	2.29	0.62
1:B:258:GLU:HG2	1:B:262:ARG:HH11	1.64	0.62
1:F:146:GLU:HG3	1:F:251:PRO:CB	2.31	0.60
1:B:181:LEU:HB3	1:B:182:PRO:HD3	1.82	0.60
1:A:269:ARG:NH2	1:B:307:GLN:HB2	2.16	0.60
1:E:188:LYS:HE3	1:E:189:LEU:O	2.01	0.60
1:E:83:ARG:HD2	3:E:350:HOH:O	2.02	0.58
1:F:9:ILE:HG21	1:F:22:ARG:CG	2.33	0.58
1:A:269:ARG:HD3	1:B:303:ALA:O	2.03	0.57
1:E:228:GLU:HA	1:E:231:GLN:HE21	1.68	0.57
1:B:90:GLU:HG2	3:B:362:HOH:O	2.05	0.57
1:E:201:PHE:HB3	1:E:207:ARG:HG2	1.87	0.57
1:E:304:VAL:CG2	1:F:304:VAL:CG2	2.81	0.56
1:B:307:GLN:HG3	1:F:117:PRO:CB	2.35	0.56
1:A:288:ASP:O	1:A:292:ARG:HG2	2.07	0.55
1:E:161:ARG:HA	1:E:215:ARG:HG2	1.89	0.55
1:F:139[B]:HIS:ND1	1:F:150:ALA:HA	2.21	0.55
1:B:80:ASP:OD1	1:B:83:ARG:NH2	2.39	0.54
1:A:304:VAL:HG23	1:B:304:VAL:CG2	2.38	0.54
1:A:114:ALA:O	1:E:307:GLN:N	2.41	0.54
1:F:130:ARG:NH1	3:F:414:HOH:O	2.36	0.54
1:F:268:THR:HG22	1:F:269:ARG:HD2	1.90	0.53
1:B:32:VAL:HG23	1:B:56:ALA:HB1	1.91	0.53
1:B:304:VAL:O	1:B:305:ARG:O	2.26	0.53
1:B:305:ARG:HB2	1:B:306:PRO:CD	2.29	0.53
1:A:222:GLU:HA	1:A:223:PRO:C	2.29	0.53
1:B:307:GLN:N	1:F:114:ALA:O	2.36	0.52
1:B:305:ARG:CB	1:B:306:PRO:CD	2.88	0.52
1:E:102:GLN:NE2	1:E:281:TYR:HA	2.26	0.51
1:E:305:ARG:HB2	1:E:306:PRO:HD2	1.93	0.50
1:E:203:THR:O	1:E:206:SER:N	2.42	0.50
1:A:218:PRO:HG3	1:A:230:LEU:HD12	1.92	0.50
1:E:288:ASP:O	1:E:292:ARG:HG2	2.12	0.50
1:A:305:ARG:HB2	1:A:306:PRO:HD2	1.92	0.49
1:E:38:ASN:OD1	1:E:39:PRO:HA	2.11	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:9:ILE:CG2	1:F:22:ARG:HG3	2.42	0.49
1:A:269:ARG:HH22	1:B:307:GLN:HE21	1.57	0.49
1:F:143:VAL:HG11	1:F:146:GLU:HG2	1.94	0.49
1:A:261:GLU:HA	1:A:272:LEU:HD22	1.95	0.49
1:A:90:GLU:HG2	3:A:332:HOH:O	2.13	0.49
1:A:306:PRO:O	1:A:307:GLN:HB2	2.13	0.48
1:F:146:GLU:HG3	1:F:251:PRO:HB3	1.95	0.48
1:B:27:GLN:HG2	1:B:57:HIS:CE1	2.49	0.48
1:A:110:PHE:HE1	1:A:123:LEU:HD21	1.79	0.48
1:F:32:VAL:HG23	1:F:56:ALA:HB1	1.95	0.48
1:B:10:ARG:NH1	1:B:23:GLU:OE1	2.48	0.47
1:A:129:ILE:O	1:A:234:HIS:HE1	1.97	0.47
1:A:148:ASP:N	1:A:148:ASP:OD1	2.48	0.47
1:F:143:VAL:CG1	1:F:146:GLU:HG2	2.45	0.47
1:A:32:VAL:HG22	1:A:98:TYR:HB2	1.97	0.46
1:F:244:LYS:HE2	1:F:268:THR:O	2.15	0.46
1:E:130:ARG:HA	1:E:234:HIS:CE1	2.51	0.46
1:E:102:GLN:NE2	1:E:280:HIS:O	2.48	0.45
1:F:136:GLN:CD	1:F:136:GLN:H	2.21	0.45
1:E:304:VAL:HG23	1:F:304:VAL:CG2	2.47	0.45
1:E:188:LYS:HD2	1:E:189:LEU:N	2.32	0.45
1:E:76:TYR:CE2	1:E:209:PRO:HG3	2.52	0.45
1:E:181:LEU:HB3	1:E:182:PRO:HD3	1.99	0.44
1:E:208:ARG:HB3	1:E:209:PRO:HD3	2.00	0.43
1:A:304:VAL:CG2	1:B:304:VAL:HG21	2.47	0.43
1:F:268:THR:HG22	1:F:269:ARG:CD	2.48	0.43
1:B:168:ALA:O	1:B:172:GLU:HB3	2.18	0.43
1:A:245:LEU:HD12	1:A:271:ALA:HB3	2.01	0.43
1:F:130:ARG:O	1:F:132:MET:HG3	2.19	0.43
1:A:304:VAL:HG23	1:B:304:VAL:HG21	2.00	0.43
1:A:32:VAL:HG23	1:A:56:ALA:HB1	2.01	0.43
1:E:32:VAL:HG23	1:E:56:ALA:HB1	2.01	0.43
1:F:129:ILE:O	1:F:234:HIS:HE1	2.02	0.43
1:F:228:GLU:HA	1:F:231:GLN:HE21	1.82	0.42
1:E:261:GLU:HA	1:E:272:LEU:HD22	1.99	0.42
1:E:167:GLU:CD	1:E:215:ARG:HH22	2.23	0.42
1:E:78:PHE:O	1:E:82:VAL:HG23	2.19	0.42
1:E:195:ALA:HB3	1:E:196:PRO:HD3	2.02	0.42
1:F:181:LEU:HB3	1:F:182:PRO:HD3	2.00	0.42
1:E:20:ALA:H	1:E:69:SER:HA	1.85	0.42
1:E:10:ARG:CZ	1:E:23:GLU:HB3	2.50	0.42
1:E:102:GLN:HE22	1:E:281:TYR:HA	1.83	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:305:ARG:HG3	1:B:306:PRO:N	2.35	0.41
1:F:146:GLU:HG3	1:F:251:PRO:HB2	2.03	0.41
1:E:129:ILE:O	1:E:234:HIS:HE1	2.03	0.41
1:E:269:ARG:HH21	1:F:307:GLN:HG2	1.85	0.41
1:E:178:GLU:O	1:E:182:PRO:HG2	2.20	0.41
1:F:100:VAL:HA	1:F:124:ALA:O	2.21	0.41
1:A:199:THR:N	1:A:200:PRO:CD	2.84	0.41
1:A:245:LEU:HG	1:A:273:ILE:CD1	2.50	0.41
1:E:118:ASP:HB2	3:E:316:HOH:O	2.20	0.40
1:E:241:SER:O	1:E:269:ARG:HD2	2.20	0.40
1:A:10:ARG:NH1	1:A:23:GLU:H	2.19	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	296/312 (95%)	282 (95%)	12 (4%)	2 (1%)	30	15
1	B	297/312 (95%)	287 (97%)	8 (3%)	2 (1%)	30	15
1	E	296/312 (95%)	281 (95%)	11 (4%)	4 (1%)	16	4
1	F	298/312 (96%)	289 (97%)	8 (3%)	1 (0%)	50	37
All	All	1187/1248 (95%)	1139 (96%)	39 (3%)	9 (1%)	27	12

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	144	ALA
1	B	305	ARG
1	E	148	ASP
1	E	305	ARG
1	F	306	PRO
1	A	306	PRO
1	B	306	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	147	GLN
1	E	204	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	232/244 (95%)	223 (96%)	9 (4%)	43	30
1	B	233/244 (96%)	224 (96%)	9 (4%)	43	30
1	E	232/244 (95%)	227 (98%)	5 (2%)	64	57
1	F	234/244 (96%)	229 (98%)	5 (2%)	66	59
All	All	931/976 (95%)	903 (97%)	28 (3%)	53	42

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ARG
1	A	27	GLN
1	A	143	VAL
1	A	146	GLU
1	A	148	ASP
1	A	176	PHE
1	A	213	PHE
1	A	228	GLU
1	A	305	ARG
1	B	39	PRO
1	B	118	ASP
1	B	145	GLU
1	B	156	VAL
1	B	176	PHE
1	B	205	GLU
1	B	213	PHE
1	B	232	SER
1	B	307	GLN
1	E	156	VAL
1	E	176	PHE

Continued from previous page...

Mol	Chain	Res	Type
1	E	208	ARG
1	E	213	PHE
1	E	288	ASP
1	F	9	ILE
1	F	136	GLN
1	F	176	PHE
1	F	192	GLU
1	F	213	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	139	HIS
1	A	234	HIS
1	B	231	GLN
1	B	234	HIS
1	B	307	GLN
1	E	111	HIS
1	E	139	HIS
1	E	231	GLN
1	E	234	HIS
1	F	231	GLN
1	F	234	HIS

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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.

5.7 Other polymers (i)

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(Å^2)	Q<0.9
1	A	298/312 (95%)	1.00	53 (17%)	2	2	20, 26, 39, 55	0
1	B	298/312 (95%)	0.53	21 (7%)	16	16	18, 23, 33, 51	0
1	E	298/312 (95%)	2.32	140 (46%)	1	0	24, 39, 60, 64	0
1	F	299/312 (95%)	0.60	28 (9%)	9	8	15, 20, 33, 58	0
All	All	1193/1248 (95%)	1.11	242 (20%)	2	1	15, 25, 48, 64	0

All (242) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	307	GLN	10.1
1	A	306	PRO	9.9
1	B	306	PRO	8.5
1	F	307	GLN	8.0
1	E	203	THR	7.9
1	E	168	ALA	7.7
1	E	16	GLY	7.7
1	E	164	GLY	7.4
1	B	307	GLN	7.4
1	A	144	ALA	7.3
1	E	73	ASP	7.1
1	E	143	VAL	7.1
1	E	205	GLU	7.1
1	F	306	PRO	6.8
1	E	84	TYR	6.7
1	E	204	PRO	6.5
1	E	201	PHE	6.3
1	E	170	ILE	6.2
1	E	14	VAL	6.1
1	A	307	GLN	6.1
1	E	171	LEU	6.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	13	PRO	6.0
1	E	70	GLY	6.0
1	E	219	ILE	6.0
1	E	144	ALA	6.0
1	E	211	LEU	5.9
1	E	197	TYR	5.9
1	E	200	PRO	5.8
1	E	208	ARG	5.8
1	E	160	PHE	5.8
1	A	145	GLU	5.8
1	E	206	SER	5.7
1	E	12	ALA	5.6
1	E	10	ARG	5.6
1	E	18	SER	5.6
1	E	142	GLU	5.5
1	E	27	GLN	5.3
1	E	169	MET	5.3
1	E	76	TYR	5.1
1	E	133	PRO	5.1
1	E	148	ASP	5.1
1	A	148	ASP	5.1
1	E	306	PRO	5.1
1	E	163	PRO	5.0
1	E	65	GLY	4.9
1	B	28	ASP	4.9
1	E	15	LEU	4.9
1	A	143	VAL	4.9
1	A	28	ASP	4.8
1	E	145	GLU	4.8
1	E	179	ARG	4.8
1	E	72	PRO	4.7
1	B	26	ALA	4.6
1	E	149	HIS	4.6
1	E	174	ASN	4.6
1	E	21	TYR	4.5
1	E	191	ASP	4.5
1	A	142	GLU	4.5
1	A	146	GLU	4.4
1	E	199	THR	4.4
1	A	26	ALA	4.4
1	A	100	VAL	4.3
1	B	144	ALA	4.2

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	202	PRO	4.2
1	E	159	LYS	4.2
1	E	173	ALA	4.2
1	E	176	PHE	4.2
1	F	144	ALA	4.1
1	A	35	LEU	4.1
1	E	146	GLU	4.1
1	E	17	SER	4.0
1	A	27	GLN	3.9
1	A	125	PHE	3.9
1	B	305	ARG	3.9
1	E	28	ASP	3.9
1	E	172	GLU	3.8
1	A	101	ALA	3.7
1	A	149	HIS	3.7
1	E	184	GLY	3.7
1	B	27	GLN	3.7
1	E	91	GLN	3.7
1	E	258	GLU	3.7
1	E	166	GLY	3.7
1	E	165	GLU	3.7
1	E	226	VAL	3.6
1	A	141	THR	3.6
1	E	177	VAL	3.6
1	E	152	ALA	3.6
1	B	142	GLU	3.6
1	E	220	ALA	3.5
1	A	106	THR	3.5
1	E	180	VAL	3.5
1	E	162	THR	3.5
1	B	149	HIS	3.4
1	E	74	ILE	3.4
1	E	136	GLN	3.4
1	E	195	ALA	3.4
1	E	101	ALA	3.4
1	A	147	GLN	3.3
1	E	95	THR	3.3
1	A	124	ALA	3.3
1	B	143	VAL	3.3
1	E	108	LEU	3.3
1	E	228	GLU	3.3
1	F	101	ALA	3.2

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	140	HIS	3.2
1	F	125	PHE	3.2
1	A	245	LEU	3.2
1	F	35	LEU	3.2
1	E	88	PHE	3.2
1	E	94	VAL	3.1
1	E	215	ARG	3.1
1	E	118	ASP	3.1
1	A	34	PHE	3.1
1	E	71	LYS	3.1
1	E	188	LYS	3.1
1	E	125	PHE	3.1
1	F	145	GLU	3.0
1	E	69	SER	3.0
1	E	126	MET	3.0
1	A	305	ARG	3.0
1	E	182	PRO	3.0
1	A	123	LEU	3.0
1	E	35	LEU	3.0
1	A	104	TRP	3.0
1	A	247	PHE	3.0
1	E	78	PHE	3.0
1	E	20	ALA	3.0
1	E	222	GLU	3.0
1	E	213	PHE	3.0
1	E	87	ALA	3.0
1	E	11	ARG	3.0
1	A	37	GLY	2.9
1	E	135	TRP	2.9
1	E	100	VAL	2.9
1	A	246	LEU	2.9
1	E	24	THR	2.9
1	F	305	ARG	2.9
1	E	90	GLU	2.9
1	E	75	ALA	2.9
1	E	217	LEU	2.9
1	E	207	ARG	2.9
1	E	124	ALA	2.9
1	F	106	THR	2.8
1	F	100	VAL	2.8
1	E	224	ALA	2.8
1	F	28	ASP	2.8

Continued on next page...

Full wwPDB X-ray Structure Validation Report 3A2N

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	45	TRP	2.8
1	E	129	ILE	2.8
1	A	105	GLY	2.8
1	E	150	ALA	2.8
1	A	213	PHE	2.8
1	E	218	PRO	2.7
1	E	175	ALA	2.7
1	E	253	ALA	2.7
1	A	126	MET	2.7
1	B	118	ASP	2.7
1	E	157	PHE	2.7
1	E	232	SER	2.7
1	F	146	GLU	2.7
1	E	102	GLN	2.7
1	B	262	ARG	2.7
1	E	230	LEU	2.7
1	E	92	ARG	2.6
1	F	104	TRP	2.6
1	A	109	ALA	2.6
1	E	33	LEU	2.6
1	F	258	GLU	2.6
1	E	109	ALA	2.6
1	E	147	GLN	2.6
1	E	134	THR	2.6
1	E	83	ARG	2.6
1	E	19	MET	2.5
1	A	128	PHE	2.5
1	E	23	GLU	2.5
1	F	37	GLY	2.5
1	A	10	ARG	2.5
1	F	108	LEU	2.5
1	A	63	LEU	2.5
1	E	104	TRP	2.5
1	A	129	ILE	2.5
1	A	151	GLU	2.5
1	E	192	GLU	2.5
1	F	63	LEU	2.4
1	B	288	ASP	2.4
1	A	288	ASP	2.4
1	E	210	VAL	2.4
1	E	259	PHE	2.4
1	F	126	MET	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	214	PRO	2.3
1	A	297	TRP	2.3
1	B	104	TRP	2.3
1	F	205	GLU	2.3
1	E	155	ALA	2.3
1	E	93	GLY	2.3
1	E	158	ARG	2.3
1	F	143	VAL	2.3
1	B	258	GLU	2.3
1	E	140	HIS	2.3
1	E	30	PRO	2.3
1	E	64	ILE	2.3
1	E	305	ARG	2.2
1	B	141	THR	2.2
1	E	212	ALA	2.2
1	A	99	LEU	2.2
1	F	123	LEU	2.2
1	A	140	HIS	2.2
1	A	176	PHE	2.2
1	A	258	GLU	2.2
1	A	110	PHE	2.2
1	A	265	ALA	2.2
1	E	66	PHE	2.2
1	F	140	HIS	2.2
1	A	102	GLN	2.2
1	F	247	PHE	2.2
1	E	106	THR	2.2
1	A	48	ILE	2.1
1	E	26	ALA	2.1
1	F	105	GLY	2.1
1	E	245	LEU	2.1
1	A	107	ALA	2.1
1	E	265	ALA	2.1
1	F	9	ILE	2.1
1	E	281	TYR	2.1
1	A	192	GLU	2.1
1	B	191	ASP	2.1
1	F	149	HIS	2.1
1	A	44	ILE	2.1
1	B	148	ASP	2.1
1	E	250	GLU	2.1
1	E	44	ILE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	145	GLU	2.1
1	F	142	GLU	2.1
1	A	291	GLY	2.1
1	A	40	THR	2.0
1	E	254	LEU	2.0
1	E	262	ARG	2.0
1	F	246	LEU	2.0
1	B	106	THR	2.0
1	E	34	PHE	2.0
1	E	57	HIS	2.0
1	E	198	ARG	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	CL	F	313	1/1	0.20	0.88	10,10,10,10	0
2	CL	B	313	1/1	0.14	-0.05	12,12,12,12	0
2	CL	A	313	1/1	0.15	-1.57	15,15,15,15	0

6.5 Other polymers ⓘ

There are no such residues in this entry.