



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:47 AM GMT

PDB ID : 2YBU
Title : CRYSTAL STRUCTURE OF HUMAN ACIDIC CHITINASE IN COMPLEX WITH BISDIONIN F
Authors : Sutherland, T.E.; Andersen, O.A.; Betou, M.; Eggleston, I.M.; Maizels, R.M.; Van Aalten, D.; Allen, J.E.
Deposited on : 2011-03-10
Resolution : 2.25 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

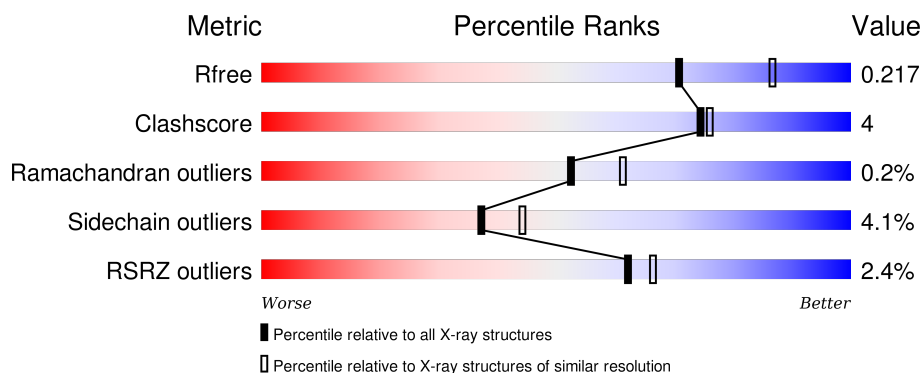
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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}	91344	1640 (2.28-2.24)
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)
RSRZ outliers	91569	1647 (2.28-2.24)

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. 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	381	<div> <div>2%</div> <div>85%</div> <div>13%</div> <div>..</div> </div>
1	B	381	<div> <div>%</div> <div>86%</div> <div>12%</div> <div>..</div> </div>
1	C	381	<div> <div>2%</div> <div>87%</div> <div>12%</div> <div>.</div> </div>
1	D	381	<div> <div>3%</div> <div>87%</div> <div>11%</div> <div>..</div> </div>
1	E	381	<div> <div>3%</div> <div>86%</div> <div>11%</div> <div>..</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	381	

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
3	CX9	A	1399	-	-	-	X
3	CX9	C	1399	-	-	-	X
3	CX9	D	1399	-	-	-	X
3	CX9	E	1399	-	-	-	X
3	CX9	F	1399	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 19347 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 ACIDIC MAMMALIAN CHITINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	376	Total	C	N	O	S	0	0	0
			2976	1919	484	559	14			
1	B	376	Total	C	N	O	S	0	0	0
			2976	1919	484	559	14			
1	C	376	Total	C	N	O	S	0	0	0
			2976	1919	484	559	14			
1	D	376	Total	C	N	O	S	0	0	0
			2976	1919	484	559	14			
1	E	376	Total	C	N	O	S	0	0	0
			2976	1919	484	559	14			
1	F	376	Total	C	N	O	S	0	0	0
			2976	1919	484	559	14			

There are 36 discrepancies between the modelled and reference sequences:

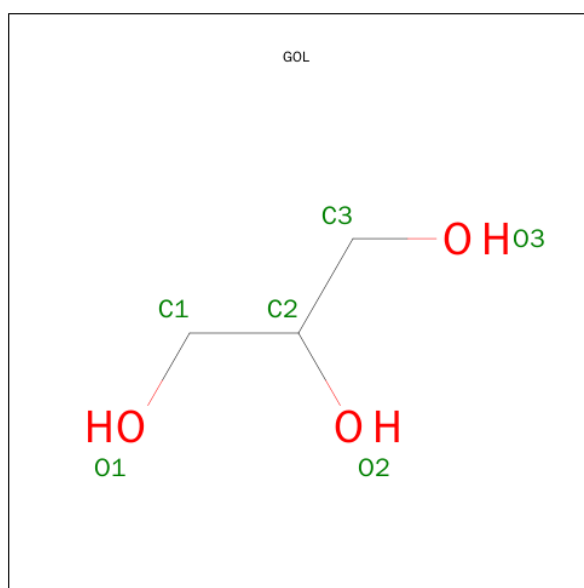
Chain	Residue	Modelled	Actual	Comment	Reference
A	18	GLU	-	EXPRESSION TAG	UNP Q9BZP6
A	19	ALA	-	EXPRESSION TAG	UNP Q9BZP6
A	20	GLU	-	EXPRESSION TAG	UNP Q9BZP6
A	45	ASP	ASN	VARIANT	UNP Q9BZP6
A	47	ASN	ASP	VARIANT	UNP Q9BZP6
A	61	MET	ARG	VARIANT	UNP Q9BZP6
B	18	GLU	-	EXPRESSION TAG	UNP Q9BZP6
B	19	ALA	-	EXPRESSION TAG	UNP Q9BZP6
B	20	GLU	-	EXPRESSION TAG	UNP Q9BZP6
B	45	ASP	ASN	VARIANT	UNP Q9BZP6
B	47	ASN	ASP	VARIANT	UNP Q9BZP6
B	61	MET	ARG	VARIANT	UNP Q9BZP6
C	18	GLU	-	EXPRESSION TAG	UNP Q9BZP6
C	19	ALA	-	EXPRESSION TAG	UNP Q9BZP6
C	20	GLU	-	EXPRESSION TAG	UNP Q9BZP6
C	45	ASP	ASN	VARIANT	UNP Q9BZP6
C	47	ASN	ASP	VARIANT	UNP Q9BZP6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	61	MET	ARG	VARIANT	UNP Q9BZP6
D	18	GLU	-	EXPRESSION TAG	UNP Q9BZP6
D	19	ALA	-	EXPRESSION TAG	UNP Q9BZP6
D	20	GLU	-	EXPRESSION TAG	UNP Q9BZP6
D	45	ASP	ASN	VARIANT	UNP Q9BZP6
D	47	ASN	ASP	VARIANT	UNP Q9BZP6
D	61	MET	ARG	VARIANT	UNP Q9BZP6
E	18	GLU	-	EXPRESSION TAG	UNP Q9BZP6
E	19	ALA	-	EXPRESSION TAG	UNP Q9BZP6
E	20	GLU	-	EXPRESSION TAG	UNP Q9BZP6
E	45	ASP	ASN	VARIANT	UNP Q9BZP6
E	47	ASN	ASP	VARIANT	UNP Q9BZP6
E	61	MET	ARG	VARIANT	UNP Q9BZP6
F	18	GLU	-	EXPRESSION TAG	UNP Q9BZP6
F	19	ALA	-	EXPRESSION TAG	UNP Q9BZP6
F	20	GLU	-	EXPRESSION TAG	UNP Q9BZP6
F	45	ASP	ASN	VARIANT	UNP Q9BZP6
F	47	ASN	ASP	VARIANT	UNP Q9BZP6
F	61	MET	ARG	VARIANT	UNP Q9BZP6

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		

Continued on next page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total 6	C 3	O 3	0	0
2	D	1	Total 6	C 3	O 3	0	0
2	E	1	Total 6	C 3	O 3	0	0
2	F	1	Total 6	C 3	O 3	0	0

-
- The chemical structure, labeled CX9, consists of two pyrimidine rings. The left ring has atoms N7, C8, N9, C4, N3, C2, N1, and C5. It is substituted with CAA at N7, CAC at N3, and has carbonyl groups at C2 (O2) and C5 (O6). A side chain (CAK-CAL-CAO) connects N1 to the right ring. The right ring has atoms NAX, CAV, CAT, N10, and NAZ. It is substituted with NAX at N10, CAD at NAZ, and has carbonyl groups at CAV (OAF) and N10 (OAH). The label CAJ is near the NAX atom.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 28	C 16	N 8	O 4	0	0
3	A	1	Total 28	C 16	N 8	O 4	0	0
3	B	1	Total 28	C 16	N 8	O 4	0	0
3	B	1	Total 28	C 16	N 8	O 4	0	0
3	C	1	Total 28	C 16	N 8	O 4	0	0
3	C	1	Total 28	C 16	N 8	O 4	0	0
3	D	1	Total 28	C 16	N 8	O 4	0	0



Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	D	1	Total	C	N	O	0	0
			28	16	8	4		
3	E	1	Total	C	N	O	0	0
			28	16	8	4		
3	E	1	Total	C	N	O	0	0
			28	16	8	4		
3	F	1	Total	C	N	O	0	0
			28	16	8	4		
3	F	1	Total	C	N	O	0	0
			28	16	8	4		

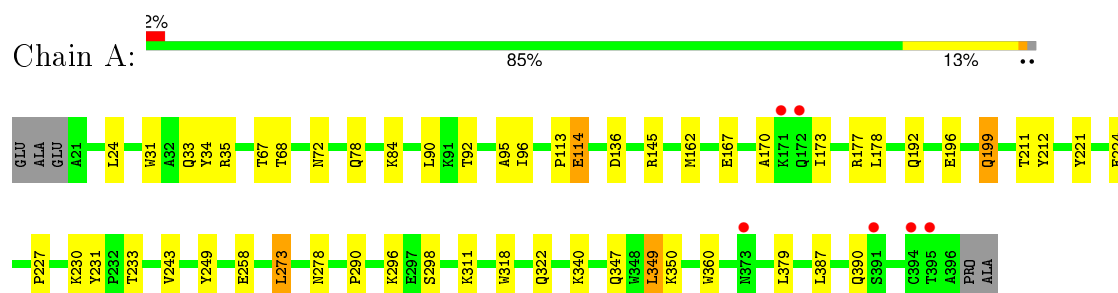
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	213	Total	O	0	0
			213	213		
4	B	220	Total	O	0	0
			220	220		
4	C	199	Total	O	0	0
			199	199		
4	D	171	Total	O	0	0
			171	171		
4	E	193	Total	O	0	0
			193	193		
4	F	123	Total	O	0	0
			123	123		

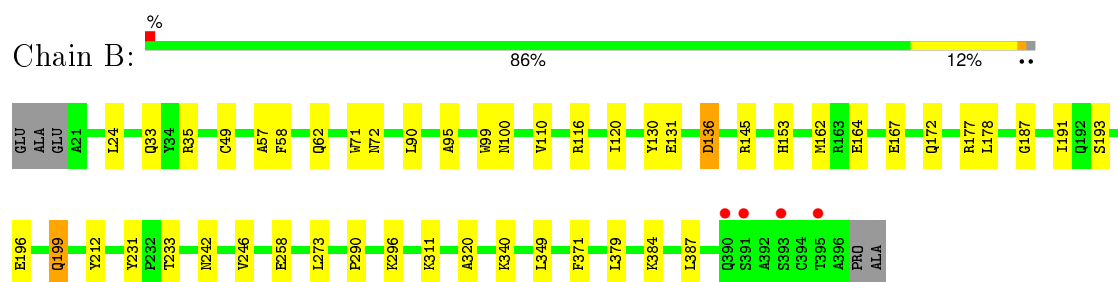
3 Residue-property plots

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.

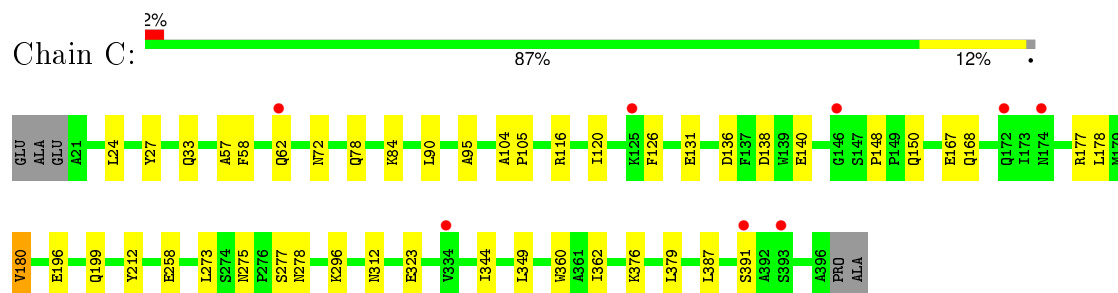
• Molecule 1: ACIDIC MAMMALIAN CHITINASE



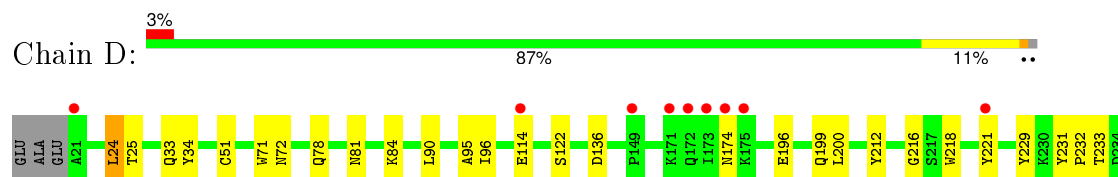
• Molecule 1: ACIDIC MAMMALIAN CHITINASE

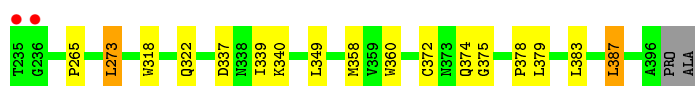


• Molecule 1: ACIDIC MAMMALIAN CHITINASE

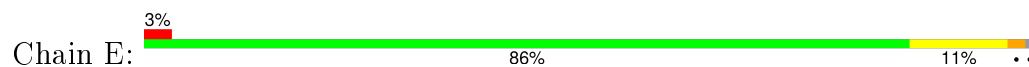


• Molecule 1: ACIDIC MAMMALIAN CHITINASE

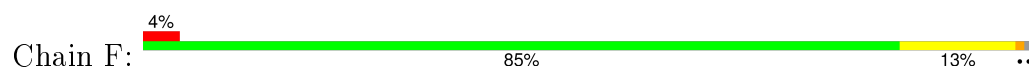




• Molecule 1: ACIDIC MAMMALIAN CHITINASE



• Molecule 1: ACIDIC MAMMALIAN CHITINASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	144.78Å 149.19Å 151.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.97 – 2.25 19.97 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.6 (19.97-2.25) 99.6 (19.97-2.25)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.42 (at 2.26Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.173 , 0.219 0.171 , 0.217	Depositor DCC
R_{free} test set	1544 reflections (1.01%)	DCC
Wilson B-factor (Å ²)	27.7	Xtriage
Anisotropy	0.257	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 45.6	EDS
Estimated twinning fraction	0.017 for -h,l,k 0.049 for -l,-k,-h 0.016 for k,h,-l 0.006 for k,l,h 0.006 for l,h,k	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 154444 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	19347	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, CX9

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	1.17	10/3068 (0.3%)	0.93	5/4182 (0.1%)
1	B	1.17	5/3068 (0.2%)	0.93	3/4182 (0.1%)
1	C	1.14	3/3068 (0.1%)	0.92	1/4182 (0.0%)
1	D	1.09	2/3068 (0.1%)	0.90	1/4182 (0.0%)
1	E	1.08	0/3068	0.94	5/4182 (0.1%)
1	F	0.93	2/3068 (0.1%)	0.82	1/4182 (0.0%)
All	All	1.10	22/18408 (0.1%)	0.91	16/25092 (0.1%)

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	258	GLU	CG-CD	8.97	1.65	1.51
1	C	278	ASN	CB-CG	7.93	1.69	1.51
1	A	249	TYR	CD2-CE2	7.49	1.50	1.39
1	A	278	ASN	CB-CG	6.67	1.66	1.51
1	A	199	GLN	CG-CD	6.16	1.65	1.51
1	A	114	GLU	CG-CD	6.14	1.61	1.51
1	D	221	TYR	CD2-CE2	6.04	1.48	1.39
1	A	34	TYR	CD2-CE2	-5.98	1.30	1.39
1	C	126	PHE	CE1-CZ	5.87	1.48	1.37
1	B	258	GLU	CD-OE1	5.71	1.31	1.25
1	A	298	SER	CB-OG	-5.61	1.34	1.42
1	A	221	TYR	CE2-CZ	5.48	1.45	1.38
1	B	199	GLN	CG-CD	5.46	1.63	1.51
1	D	114	GLU	CG-CD	5.44	1.60	1.51
1	B	258	GLU	CG-CD	5.43	1.60	1.51
1	F	278	ASN	CB-CG	5.37	1.63	1.51
1	B	164	GLU	CG-CD	5.34	1.59	1.51
1	A	258	GLU	CD-OE1	5.17	1.31	1.25
1	A	224	GLU	CG-CD	5.16	1.59	1.51
1	B	320	ALA	CA-CB	5.13	1.63	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	258	GLU	CD-OE1	5.04	1.31	1.25
1	F	221	TYR	CD2-CE2	5.02	1.46	1.39

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	145	ARG	NE-CZ-NH1	8.23	124.41	120.30
1	E	230	LYS	CD-CE-NZ	-7.53	94.39	111.70
1	D	273	LEU	CB-CG-CD1	6.75	122.47	111.00
1	A	349	LEU	CA-CB-CG	6.56	130.39	115.30
1	E	180	VAL	CB-CA-C	-6.50	99.05	111.40
1	C	180	VAL	CB-CA-C	-6.28	99.48	111.40
1	E	379	LEU	CB-CG-CD2	6.11	121.39	111.00
1	B	35	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	A	35	ARG	NE-CZ-NH2	-5.97	117.31	120.30
1	E	273	LEU	CA-CB-CG	5.87	128.79	115.30
1	B	145	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	E	379	LEU	CB-CG-CD1	5.65	120.60	111.00
1	F	349	LEU	CA-CB-CG	5.53	128.02	115.30
1	B	136	ASP	CB-CG-OD1	5.06	122.86	118.30
1	A	349	LEU	CB-CG-CD1	5.04	119.56	111.00
1	A	273	LEU	CA-CB-CG	5.01	126.83	115.30

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	2976	0	2821	23	0
1	B	2976	0	2821	26	0
1	C	2976	0	2821	24	0
1	D	2976	0	2821	22	0
1	E	2976	0	2821	27	0
1	F	2976	0	2821	26	0
2	A	6	0	8	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	6	0	8	0	0
2	C	6	0	8	0	0
2	D	6	0	8	0	0
2	E	6	0	8	0	0
2	F	6	0	8	0	0
3	A	56	0	36	4	0
3	B	56	0	36	1	0
3	C	56	0	36	1	0
3	D	56	0	36	3	0
3	E	56	0	36	2	0
3	F	56	0	36	3	0
4	A	213	0	0	1	0
4	B	220	0	0	2	0
4	C	199	0	0	2	0
4	D	171	0	0	2	0
4	E	193	0	0	1	0
4	F	123	0	0	0	0
All	All	19347	0	17190	143	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 4.

All (143) 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:B:196:GLU:HB3	1:B:199:GLN:HE21	1.40	0.86
1:C:196:GLU:HB3	1:C:199:GLN:HE21	1.42	0.84
1:C:33:GLN:HE22	1:C:72:ASN:HD21	1.22	0.84
1:A:231:TYR:HD2	1:A:233:THR:HG22	1.43	0.84
3:E:1399:CX9:OAF	3:E:1399:CX9:HAL	1.78	0.83
1:B:231:TYR:HD2	1:B:233:THR:HG22	1.41	0.82
1:E:196:GLU:HB3	1:E:199:GLN:HE21	1.46	0.81
1:B:33:GLN:HE22	1:B:72:ASN:HD21	1.29	0.78
1:D:196:GLU:HB3	1:D:199:GLN:HE21	1.47	0.77
1:B:120:ILE:HG12	1:B:162:MET:HE3	1.68	0.75
1:F:339:ILE:HD12	1:F:374:GLN:NE2	2.02	0.73
1:A:318:TRP:CH2	1:A:340:LYS:HD2	2.25	0.71
1:A:33:GLN:HE22	1:A:72:ASN:HD21	1.39	0.71
1:E:33:GLN:HE22	1:E:72:ASN:HD21	1.37	0.69
1:C:323:GLU:OE1	4:C:2163:HOH:O	2.10	0.69
1:F:167:GLU:HG3	1:F:177:ARG:HD3	1.73	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:339:ILE:HD12	1:D:374:GLN:NE2	2.08	0.67
1:F:33:GLN:HE22	1:F:72:ASN:HD21	1.43	0.63
1:B:231:TYR:CD2	1:B:233:THR:HG22	2.30	0.63
1:A:113:PRO:HG2	1:A:114:GLU:OE2	1.99	0.62
1:A:390:GLN:HB2	4:A:2211:HOH:O	2.01	0.60
1:A:296:LYS:HD3	1:D:34:TYR:HB3	1.84	0.59
1:B:33:GLN:NE2	1:B:72:ASN:HD21	1.97	0.58
1:D:33:GLN:HE22	1:D:72:ASN:HD21	1.49	0.58
1:F:33:GLN:NE2	1:F:72:ASN:HD21	2.02	0.58
1:E:127:LEU:HD12	1:E:178:LEU:HD13	1.86	0.58
1:B:153:HIS:HB3	4:B:2096:HOH:O	2.04	0.56
1:A:196:GLU:HB3	1:A:199:GLN:HE21	1.72	0.55
1:C:148:PRO:HB2	1:C:150:GLN:OE1	2.08	0.54
1:E:115:ASN:N	1:E:115:ASN:HD22	2.05	0.54
1:F:225:ASN:OD1	1:F:269:HIS:HD2	1.92	0.53
1:D:231:TYR:CG	1:D:232:PRO:HD2	2.44	0.52
1:B:371:PHE:CE2	1:C:376:LYS:HD3	2.44	0.52
1:F:360:TRP:CD1	3:F:1398:CX9:HADB	2.45	0.52
1:E:196:GLU:HB3	1:E:199:GLN:NE2	2.20	0.52
1:A:167:GLU:HG3	1:A:177:ARG:HD3	1.90	0.52
1:B:296:LYS:HD3	1:F:34:TYR:HB3	1.91	0.51
1:C:391:SER:HB2	4:C:2196:HOH:O	2.09	0.51
1:B:340:LYS:HE3	4:B:2204:HOH:O	2.08	0.51
1:E:61:MET:HE2	1:E:119:PHE:CD1	2.46	0.51
1:C:312:ASN:HD21	1:E:235:THR:HB	1.76	0.51
1:C:360:TRP:CD1	3:C:1398:CX9:HADB	2.46	0.51
1:F:347:GLN:HA	1:F:347:GLN:NE2	2.25	0.51
1:C:296:LYS:HE2	1:E:244:ASP:CG	2.31	0.51
1:E:319:ASP:OD2	1:E:322:GLN:NE2	2.35	0.51
1:A:33:GLN:NE2	1:A:72:ASN:HD21	2.07	0.50
1:E:177:ARG:HG2	1:E:178:LEU:O	2.12	0.49
1:B:167:GLU:HG3	1:B:177:ARG:HD3	1.94	0.49
1:A:360:TRP:CD1	3:A:1398:CX9:HADB	2.47	0.49
1:D:372:CYS:HB2	4:D:2159:HOH:O	2.11	0.49
1:E:172:GLN:O	1:E:173:ILE:HG23	2.13	0.49
1:E:216:GLY:HA3	1:E:218:TRP:CZ3	2.48	0.49
1:A:170:ALA:HB2	1:A:177:ARG:HA	1.95	0.48
1:B:196:GLU:HB3	1:B:199:GLN:NE2	2.21	0.48
1:C:275:ASN:OD1	1:C:277:SER:HB2	2.14	0.48
1:D:24:LEU:O	1:D:51:CYS:HB3	2.13	0.48
1:F:33:GLN:HE22	1:F:72:ASN:ND2	2.12	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:33:GLN:NE2	1:D:72:ASN:HD21	2.12	0.47
1:D:229:TYR:O	1:D:322:GLN:HG2	2.14	0.47
1:D:196:GLU:HB3	1:D:199:GLN:NE2	2.23	0.47
1:F:225:ASN:OD1	1:F:269:HIS:CD2	2.68	0.47
1:C:344:ILE:HG13	1:F:38:LEU:HD21	1.95	0.47
1:F:31:TRP:CD1	3:F:1398:CX9:HACB	2.49	0.47
1:A:290:PRO:HA	1:D:71:TRP:CD2	2.49	0.47
1:A:33:GLN:HE22	1:A:72:ASN:ND2	2.10	0.47
1:B:110:VAL:HA	1:B:116:ARG:HG2	1.97	0.47
1:E:269:HIS:HA	1:E:299:GLY:O	2.15	0.47
1:D:360:TRP:CD1	3:D:1398:CX9:HADB	2.50	0.47
1:F:216:GLY:HA3	1:F:218:TRP:CZ3	2.49	0.47
3:A:1399:CX9:C6	3:A:1399:CX9:CAP	2.93	0.47
1:B:130:TYR:O	1:B:131:GLU:HB2	2.14	0.47
3:F:1399:CX9:C6	3:F:1399:CX9:CAP	2.92	0.46
1:D:383:LEU:O	1:D:387:LEU:HB2	2.15	0.46
1:A:84:LYS:HD2	1:A:92:THR:HG23	1.97	0.46
1:D:231:TYR:CD1	1:D:232:PRO:HD2	2.50	0.46
1:B:95:ALA:HA	1:B:136:ASP:O	2.15	0.46
1:C:95:ALA:HA	1:C:136:ASP:O	2.15	0.46
1:D:216:GLY:HA3	1:D:218:TRP:CH2	2.51	0.46
3:D:1399:CX9:O6	3:D:1399:CX9:HAL	2.15	0.46
1:D:375:GLY:O	1:D:378:PRO:HD3	2.16	0.46
1:A:211:THR:HB	1:A:243:VAL:HG22	1.97	0.45
1:D:122:SER:HB2	4:D:2023:HOH:O	2.15	0.45
1:E:157:VAL:O	1:E:161:GLU:HG3	2.16	0.45
1:A:192:GLN:NE2	1:B:193:SER:HB3	2.32	0.45
1:B:49:CYS:O	1:B:384:LYS:HE2	2.16	0.45
1:E:54:LEU:HB3	1:E:80:PHE:CZ	2.52	0.45
1:D:95:ALA:HA	1:D:136:ASP:O	2.17	0.45
1:F:95:ALA:HA	1:F:136:ASP:O	2.16	0.44
1:C:167:GLU:HG3	1:C:177:ARG:HD3	1.98	0.44
1:F:187:GLY:O	1:F:191:ILE:HG13	2.18	0.44
1:B:187:GLY:O	1:B:191:ILE:HG13	2.18	0.44
1:B:71:TRP:CD2	1:F:290:PRO:HA	2.53	0.44
1:D:318:TRP:CH2	1:D:340:LYS:HD2	2.52	0.44
1:E:61:MET:HE2	1:E:119:PHE:CE1	2.53	0.43
1:E:270:ASN:OD1	1:E:299:GLY:HA2	2.18	0.43
1:A:347:GLN:HE22	1:A:350:LYS:NZ	2.16	0.43
1:C:104:ALA:HB3	1:C:105:PRO:HD3	1.99	0.43
1:E:275:ASN:HA	1:E:276:PRO:HD2	1.85	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:GLN:HE22	1:B:72:ASN:ND2	2.05	0.43
3:B:1399:CX9:CAP	3:B:1399:CX9:C6	2.97	0.43
1:B:57:ALA:HA	1:B:58:PHE:HA	1.85	0.43
1:F:177:ARG:HG2	1:F:178:LEU:O	2.19	0.43
1:A:177:ARG:HG2	1:A:178:LEU:O	2.19	0.43
1:C:138:ASP:OD1	1:C:140:GLU:OE2	2.37	0.43
1:E:116:ARG:HE	1:E:161:GLU:CD	2.23	0.43
1:B:242:ASN:O	1:B:246:VAL:HG23	2.19	0.43
1:C:33:GLN:NE2	1:C:72:ASN:HD21	2.03	0.42
3:D:1399:CX9:CAP	3:D:1399:CX9:C6	2.97	0.42
1:C:177:ARG:HG2	1:C:178:LEU:O	2.19	0.42
1:D:96:ILE:O	1:D:96:ILE:HG23	2.20	0.42
1:A:67:THR:HG23	1:A:68:THR:O	2.19	0.42
1:F:157:VAL:O	1:F:161:GLU:HG3	2.19	0.42
1:C:312:ASN:HD21	1:E:235:THR:CB	2.33	0.42
3:A:1399:CX9:OAF	3:A:1399:CX9:HAL	2.19	0.42
1:F:196:GLU:HB3	1:F:199:GLN:HE21	1.85	0.42
1:F:57:ALA:HA	1:F:58:PHE:HA	1.85	0.42
1:A:31:TRP:CD1	3:A:1398:CX9:HACB	2.55	0.41
1:F:271:PHE:CD1	1:F:271:PHE:N	2.87	0.41
1:D:25:THR:O	1:D:358:MET:HA	2.20	0.41
1:B:99:TRP:HD1	1:B:100:ASN:HD22	1.68	0.41
1:C:84:LYS:NZ	1:C:131:GLU:O	2.53	0.41
1:A:95:ALA:HA	1:A:136:ASP:O	2.21	0.41
1:A:231:TYR:CD2	1:A:233:THR:HG22	2.36	0.41
1:E:172:GLN:O	1:E:173:ILE:CG2	2.68	0.41
1:C:344:ILE:CG1	1:F:38:LEU:HD21	2.49	0.41
1:C:116:ARG:O	1:C:120:ILE:HG13	2.20	0.41
1:E:115:ASN:N	1:E:115:ASN:ND2	2.69	0.41
1:F:347:GLN:HE22	1:F:350:LYS:NZ	2.18	0.41
1:E:57:ALA:HA	1:E:58:PHE:HA	1.83	0.41
1:E:360:TRP:CD1	3:E:1398:CX9:HADB	2.56	0.41
1:B:290:PRO:HA	1:F:71:TRP:CD2	2.55	0.41
1:C:27:TYR:O	1:C:362:ILE:HG22	2.20	0.41
1:B:177:ARG:HG2	1:B:178:LEU:O	2.21	0.41
1:C:167:GLU:HG3	1:C:177:ARG:CD	2.51	0.40
1:B:311:LYS:HE3	1:B:311:LYS:HB2	1.87	0.40
1:D:81:ASN:O	1:D:84:LYS:HB2	2.21	0.40
1:E:61:MET:CE	1:E:119:PHE:CE1	3.05	0.40
1:C:57:ALA:HA	1:C:58:PHE:HA	1.86	0.40
1:E:216:GLY:HA3	1:E:218:TRP:CH2	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:211:THR:HB	1:F:243:VAL:HG22	2.04	0.40
1:A:227:PRO:HB2	1:A:322:GLN:HB3	2.02	0.40
1:E:390:GLN:HB2	4:E:2188:HOH:O	2.20	0.40
1:F:215:HIS:HB2	1:F:224:GLU:O	2.22	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	374/381 (98%)	363 (97%)	10 (3%)	1 (0%)	46	52
1	B	374/381 (98%)	365 (98%)	9 (2%)	0	100	100
1	C	374/381 (98%)	365 (98%)	9 (2%)	0	100	100
1	D	374/381 (98%)	366 (98%)	7 (2%)	1 (0%)	46	52
1	E	374/381 (98%)	362 (97%)	11 (3%)	1 (0%)	46	52
1	F	374/381 (98%)	362 (97%)	11 (3%)	1 (0%)	46	52
All	All	2244/2286 (98%)	2183 (97%)	57 (2%)	4 (0%)	52	61

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	173	ILE
1	A	173	ILE
1	F	131	GLU
1	D	265	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	311/314 (99%)	299 (96%)	12 (4%)	39	48
1	B	311/314 (99%)	302 (97%)	9 (3%)	50	60
1	C	311/314 (99%)	300 (96%)	11 (4%)	43	53
1	D	311/314 (99%)	299 (96%)	12 (4%)	39	48
1	E	311/314 (99%)	295 (95%)	16 (5%)	29	32
1	F	311/314 (99%)	295 (95%)	16 (5%)	29	32
All	All	1866/1884 (99%)	1790 (96%)	76 (4%)	37	44

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LEU
1	A	78	GLN
1	A	90	LEU
1	A	96	ILE
1	A	162	MET
1	A	212	TYR
1	A	230	LYS
1	A	273	LEU
1	A	311	LYS
1	A	349	LEU
1	A	379	LEU
1	A	387	LEU
1	B	24	LEU
1	B	62	GLN
1	B	90	LEU
1	B	172	GLN
1	B	212	TYR
1	B	273	LEU
1	B	349	LEU
1	B	379	LEU
1	B	387	LEU
1	C	24	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	62	GLN
1	C	78	GLN
1	C	90	LEU
1	C	168	GLN
1	C	180	VAL
1	C	212	TYR
1	C	273	LEU
1	C	349	LEU
1	C	379	LEU
1	C	387	LEU
1	D	24	LEU
1	D	78	GLN
1	D	90	LEU
1	D	174	ASN
1	D	200	LEU
1	D	212	TYR
1	D	233	THR
1	D	273	LEU
1	D	337	ASP
1	D	349	LEU
1	D	379	LEU
1	D	387	LEU
1	E	24	LEU
1	E	90	LEU
1	E	114	GLU
1	E	172	GLN
1	E	174	ASN
1	E	180	VAL
1	E	200	LEU
1	E	212	TYR
1	E	230	LYS
1	E	233	THR
1	E	273	LEU
1	E	349	LEU
1	E	353	LYS
1	E	379	LEU
1	E	385	LYS
1	E	387	LEU
1	F	24	LEU
1	F	90	LEU
1	F	144	SER
1	F	147	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	160	GLN
1	F	172	GLN
1	F	200	LEU
1	F	201	SER
1	F	230	LYS
1	F	233	THR
1	F	271	PHE
1	F	273	LEU
1	F	337	ASP
1	F	349	LEU
1	F	379	LEU
1	F	387	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	64	ASN
1	A	85	ASN
1	A	100	ASN
1	A	115	ASN
1	A	129	GLN
1	A	160	GLN
1	A	192	GLN
1	A	199	GLN
1	A	312	ASN
1	A	347	GLN
1	B	33	GLN
1	B	64	ASN
1	B	78	GLN
1	B	85	ASN
1	B	100	ASN
1	B	115	ASN
1	B	129	GLN
1	B	160	GLN
1	B	172	GLN
1	B	192	GLN
1	B	312	ASN
1	C	33	GLN
1	C	64	ASN
1	C	100	ASN
1	C	115	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	160	GLN
1	C	192	GLN
1	C	199	GLN
1	C	312	ASN
1	D	33	GLN
1	D	64	ASN
1	D	85	ASN
1	D	100	ASN
1	D	115	ASN
1	D	129	GLN
1	D	192	GLN
1	D	199	GLN
1	D	347	GLN
1	E	33	GLN
1	E	64	ASN
1	E	85	ASN
1	E	100	ASN
1	E	115	ASN
1	E	192	GLN
1	E	199	GLN
1	E	351	HIS
1	F	33	GLN
1	F	64	ASN
1	F	100	ASN
1	F	115	ASN
1	F	129	GLN
1	F	160	GLN
1	F	192	GLN
1	F	199	GLN
1	F	347	GLN
1	F	390	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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

18 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	GOL	A	1397	-	5,5,5	0.30	0	5,5,5	1.15	0
3	CX9	A	1398	-	17,31,31	1.78	4 (23%)	17,47,47	2.80	9 (52%)
3	CX9	A	1399	-	17,31,31	1.74	4 (23%)	17,47,47	2.01	5 (29%)
2	GOL	B	1397	-	5,5,5	0.33	0	5,5,5	1.04	0
3	CX9	B	1398	-	17,31,31	1.46	3 (17%)	17,47,47	2.24	7 (41%)
3	CX9	B	1399	-	17,31,31	1.77	3 (17%)	17,47,47	2.08	5 (29%)
2	GOL	C	1397	-	5,5,5	0.28	0	5,5,5	1.36	1 (20%)
3	CX9	C	1398	-	17,31,31	0.96	1 (5%)	17,47,47	2.73	5 (29%)
3	CX9	C	1399	-	17,31,31	1.76	2 (11%)	17,47,47	2.55	6 (35%)
2	GOL	D	1397	-	5,5,5	0.44	0	5,5,5	0.93	0
3	CX9	D	1398	-	17,31,31	1.52	5 (29%)	17,47,47	3.19	8 (47%)
3	CX9	D	1399	-	17,31,31	1.78	3 (17%)	17,47,47	1.93	5 (29%)
2	GOL	E	1397	-	5,5,5	0.43	0	5,5,5	1.09	1 (20%)
3	CX9	E	1398	-	17,31,31	1.44	3 (17%)	17,47,47	2.29	6 (35%)
3	CX9	E	1399	-	17,31,31	1.78	4 (23%)	17,47,47	2.86	6 (35%)
2	GOL	F	1397	-	5,5,5	0.26	0	5,5,5	0.94	0
3	CX9	F	1398	-	17,31,31	1.47	3 (17%)	17,47,47	4.42	9 (52%)
3	CX9	F	1399	-	17,31,31	1.87	4 (23%)	17,47,47	1.73	6 (35%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	A	1397	-	-	0/4/4/4	0/0/0/0
3	CX9	A	1398	-	-	0/6/6/6	0/4/4/4
3	CX9	A	1399	-	-	0/6/6/6	0/4/4/4
2	GOL	B	1397	-	-	0/4/4/4	0/0/0/0
3	CX9	B	1398	-	-	0/6/6/6	0/4/4/4
3	CX9	B	1399	-	-	0/6/6/6	0/4/4/4
2	GOL	C	1397	-	-	0/4/4/4	0/0/0/0
3	CX9	C	1398	-	-	0/6/6/6	0/4/4/4
3	CX9	C	1399	-	-	0/6/6/6	0/4/4/4
2	GOL	D	1397	-	-	0/4/4/4	0/0/0/0
3	CX9	D	1398	-	-	0/6/6/6	0/4/4/4
3	CX9	D	1399	-	-	0/6/6/6	0/4/4/4
2	GOL	E	1397	-	-	0/4/4/4	0/0/0/0
3	CX9	E	1398	-	-	0/6/6/6	0/4/4/4
3	CX9	E	1399	-	-	0/6/6/6	0/4/4/4
2	GOL	F	1397	-	-	0/4/4/4	0/0/0/0
3	CX9	F	1398	-	-	0/6/6/6	0/4/4/4
3	CX9	F	1399	-	-	0/6/6/6	0/4/4/4

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1398	CX9	C4-N3	-3.93	1.34	1.39
3	A	1398	CX9	C4-N3	-3.87	1.34	1.39
3	F	1398	CX9	C4-N3	-3.52	1.35	1.39
3	D	1398	CX9	C4-N3	-3.00	1.35	1.39
3	E	1398	CX9	C6-C5	-2.01	1.37	1.41
3	D	1398	CX9	C8-N9	2.04	1.38	1.34
3	E	1399	CX9	CAD-NAZ	2.05	1.51	1.47
3	E	1399	CX9	CAT-NAZ	2.10	1.41	1.39
3	A	1399	CX9	C4-N3	2.13	1.41	1.39
3	A	1398	CX9	CAD-NAZ	2.16	1.52	1.47
3	B	1398	CX9	CAD-NAZ	2.18	1.52	1.47
3	F	1399	CX9	C4-N3	2.21	1.41	1.39
3	B	1398	CX9	CAC-N3	2.31	1.52	1.47
3	B	1399	CX9	CAP-N10	2.34	1.41	1.38
3	A	1399	CX9	CAC-N3	2.37	1.52	1.47
3	A	1399	CX9	CAT-NAZ	2.50	1.42	1.39
3	F	1398	CX9	CAC-N3	2.61	1.52	1.47
3	D	1398	CX9	CAD-NAZ	2.61	1.53	1.47
3	A	1398	CX9	CAT-NAZ	2.62	1.42	1.39
3	C	1398	CX9	CAC-N3	2.79	1.53	1.47
3	D	1398	CX9	CAC-N3	2.82	1.53	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	1398	CX9	CAP-N10	2.90	1.42	1.38
3	E	1398	CX9	CAD-NAZ	2.94	1.53	1.47
3	D	1398	CX9	CAT-NAZ	3.00	1.42	1.39
3	B	1399	CX9	CAT-NAZ	3.06	1.42	1.39
3	D	1399	CX9	CAP-N10	3.47	1.43	1.38
3	D	1399	CX9	CAT-NAZ	3.48	1.43	1.39
3	E	1398	CX9	CAC-N3	3.51	1.54	1.47
3	E	1399	CX9	CAP-N10	3.58	1.43	1.38
3	F	1399	CX9	CAP-N10	3.64	1.43	1.38
3	C	1399	CX9	CAP-N10	3.66	1.43	1.38
3	D	1399	CX9	C6-N1	3.71	1.43	1.38
3	F	1399	CX9	C6-N1	3.81	1.44	1.38
3	F	1399	CX9	CAT-NAZ	3.96	1.43	1.39
3	C	1399	CX9	C6-N1	4.53	1.45	1.38
3	A	1398	CX9	CAC-N3	4.57	1.57	1.47
3	E	1399	CX9	C6-N1	4.73	1.45	1.38
3	A	1399	CX9	C6-N1	5.06	1.45	1.38
3	B	1399	CX9	C6-N1	5.38	1.46	1.38

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1398	CX9	C5-C6-N1	-11.85	113.54	120.52
3	E	1399	CX9	CAL-CA0-N10	-7.85	105.66	112.29
3	D	1398	CX9	C5-C6-N1	-7.14	116.31	120.52
3	C	1399	CX9	CAL-CA0-N10	-6.33	106.95	112.29
3	A	1398	CX9	C5-C6-N1	-6.12	116.92	120.52
3	F	1398	CX9	CAL-CA0-N10	-5.64	107.53	112.29
3	D	1398	CX9	CAV-CAP-N10	-5.50	117.28	120.52
3	B	1398	CX9	C5-C6-N1	-5.48	117.29	120.52
3	E	1398	CX9	C5-C6-N1	-5.22	117.44	120.52
3	A	1398	CX9	CAV-CAP-N10	-5.02	117.56	120.52
3	C	1398	CX9	C5-C6-N1	-4.94	117.61	120.52
3	D	1398	CX9	CAL-CA0-N10	-4.52	108.48	112.29
3	A	1399	CX9	CAL-CA0-N10	-4.49	108.50	112.29
3	E	1399	CX9	CAV-CAP-N10	-3.94	118.20	120.52
3	F	1398	CX9	CAV-CAP-N10	-3.74	118.31	120.52
3	B	1398	CX9	CA0-CAL-CAK	-3.48	101.21	111.38
3	C	1398	CX9	CAT-CAV-NAX	-3.25	106.49	109.48
3	D	1398	CX9	CAT-CAV-NAX	-3.23	106.51	109.48
3	D	1398	CX9	CA0-CAL-CAK	-3.22	101.98	111.38
3	A	1398	CX9	CA0-CAL-CAK	-3.18	102.10	111.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1398	CX9	CAT-CAV-NAX	-3.07	106.66	109.48
3	B	1398	CX9	CAL-CA0-N10	-3.05	109.72	112.29
3	C	1399	CX9	CAV-CAP-N10	-3.05	118.72	120.52
3	B	1399	CX9	CAT-CAV-NAX	-3.04	106.69	109.48
3	F	1399	CX9	CAT-CAV-NAX	-3.00	106.72	109.48
3	D	1399	CX9	C5-C6-N1	-2.92	118.80	120.52
3	B	1398	CX9	CAT-CAV-NAX	-2.73	106.97	109.48
3	F	1398	CX9	CA0-CAL-CAK	-2.71	103.46	111.38
3	D	1399	CX9	CAT-CAV-NAX	-2.55	107.13	109.48
3	A	1399	CX9	C5-C6-N1	-2.54	119.02	120.52
3	A	1398	CX9	CAL-CA0-N10	-2.46	110.21	112.29
3	E	1398	CX9	CA0-CAL-CAK	-2.44	104.25	111.38
3	A	1399	CX9	CAV-CAT-NAN	-2.43	106.13	110.83
3	E	1399	CX9	CAT-CAV-NAX	-2.41	107.26	109.48
3	A	1398	CX9	CAT-CAV-NAX	-2.39	107.28	109.48
2	E	1397	GOL	C3-C2-C1	-2.35	101.89	111.12
3	F	1399	CX9	CAL-CA0-N10	-2.31	110.34	112.29
3	E	1398	CX9	CAV-CAT-NAN	-2.22	106.53	110.83
3	F	1398	CX9	CAC-N3-C4	-2.16	115.14	118.39
3	C	1399	CX9	CAV-CAT-NAN	-2.06	106.85	110.83
3	F	1399	CX9	CAV-CAT-NAN	-2.05	106.87	110.83
3	E	1399	CX9	CAV-CAT-NAN	-2.04	106.88	110.83
3	C	1398	CX9	CAV-CAP-N10	-2.02	119.33	120.52
3	B	1399	CX9	CA0-CAL-CAK	2.08	117.47	111.38
3	B	1399	CX9	CAL-CAK-N1	2.16	114.12	112.29
2	C	1397	GOL	O2-C2-C1	2.20	118.72	108.65
3	E	1398	CX9	CAC-N3-C2	2.20	124.23	119.51
3	D	1399	CX9	CA0-CAL-CAK	2.20	117.81	111.38
3	B	1398	CX9	C6-C5-C4	2.27	121.55	119.93
3	A	1398	CX9	CAL-CAK-N1	2.35	114.27	112.29
3	B	1398	CX9	CAC-N3-C2	2.41	124.69	119.51
3	F	1399	CX9	CAP-CAV-CAT	2.44	121.67	119.93
3	A	1398	CX9	CAC-N3-C2	2.47	124.81	119.51
3	F	1399	CX9	CAL-CAK-N1	2.47	114.38	112.29
3	E	1399	CX9	CAP-CAV-CAT	2.67	121.84	119.93
3	F	1399	CX9	CAK-N1-C6	2.72	121.77	119.10
3	D	1398	CX9	CAL-CAK-N1	3.04	114.86	112.29
3	A	1398	CX9	C6-C5-C4	3.05	122.11	119.93
3	A	1399	CX9	CAL-CAK-N1	3.15	114.95	112.29
3	C	1399	CX9	CAK-N1-C6	3.18	122.22	119.10
3	B	1398	CX9	CAL-CAK-N1	3.34	115.11	112.29
3	C	1399	CX9	CA0-CAL-CAK	3.43	121.40	111.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1398	CX9	CAD-NAZ-CAT	3.45	123.56	118.39
3	D	1399	CX9	CAL-CA0-N10	3.46	115.22	112.29
3	F	1398	CX9	CAC-N3-C2	3.69	127.44	119.51
3	A	1399	CX9	CAK-N1-C6	3.71	122.74	119.10
3	D	1399	CX9	CA0-N10-CAP	3.85	122.88	119.10
3	B	1399	CX9	CA0-N10-CAP	3.94	122.97	119.10
3	E	1398	CX9	C6-C5-C4	4.05	122.83	119.93
3	C	1399	CX9	CAL-CAK-N1	4.07	115.73	112.29
3	E	1398	CX9	CAL-CAK-N1	4.12	115.77	112.29
3	A	1398	CX9	CAD-NAZ-CAT	4.27	124.78	118.39
3	D	1398	CX9	C6-C5-C4	4.29	123.00	119.93
3	C	1398	CX9	C6-C5-C4	4.58	123.21	119.93
3	B	1399	CX9	CAK-N1-C6	4.92	123.93	119.10
3	E	1399	CX9	CAK-N1-C6	5.33	124.34	119.10
3	C	1398	CX9	CAL-CAK-N1	7.04	118.23	112.29
3	F	1398	CX9	CAL-CAK-N1	7.05	118.25	112.29
3	F	1398	CX9	C6-C5-C4	7.09	125.00	119.93

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1398	CX9	2	0
3	A	1399	CX9	2	0
3	B	1399	CX9	1	0
3	C	1398	CX9	1	0
3	D	1398	CX9	1	0
3	D	1399	CX9	2	0
3	E	1398	CX9	1	0
3	E	1399	CX9	1	0
3	F	1398	CX9	2	0
3	F	1399	CX9	1	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(Å ²)	Q<0.9
1	A	376/381 (98%)	-0.40	6 (1%) 74 77	13, 22, 42, 65	0
1	B	376/381 (98%)	-0.50	4 (1%) 82 84	12, 22, 37, 53	0
1	C	376/381 (98%)	-0.39	8 (2%) 67 71	12, 24, 44, 70	0
1	D	376/381 (98%)	-0.33	11 (2%) 55 60	13, 27, 50, 73	0
1	E	376/381 (98%)	-0.28	10 (2%) 58 62	11, 26, 48, 74	0
1	F	376/381 (98%)	-0.07	16 (4%) 39 43	16, 37, 62, 80	0
All	All	2256/2286 (98%)	-0.33	55 (2%) 62 66	11, 26, 51, 80	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	174	ASN	4.8
1	E	391	SER	4.6
1	A	391	SER	4.4
1	F	174	ASN	4.3
1	D	172	GLN	4.3
1	F	235	THR	4.2
1	B	391	SER	4.2
1	C	172	GLN	3.7
1	E	174	ASN	3.7
1	F	221	TYR	3.7
1	A	172	GLN	3.6
1	E	62	GLN	3.6
1	E	172	GLN	3.5
1	C	174	ASN	3.5
1	F	175	LYS	3.3
1	D	221	TYR	3.3
1	F	173	ILE	3.3
1	F	172	GLN	3.3
1	D	235	THR	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	171	LYS	3.1
1	F	21	ALA	3.0
1	F	236	GLY	3.0
1	F	395	THR	3.0
1	C	391	SER	3.0
1	A	395	THR	3.0
1	F	168	GLN	2.9
1	E	168	GLN	2.8
1	D	173	ILE	2.8
1	F	390	GLN	2.8
1	B	390	GLN	2.7
1	D	171	LYS	2.7
1	F	114	GLU	2.7
1	E	175	LYS	2.6
1	C	334	VAL	2.6
1	F	160	GLN	2.5
1	A	394	CYS	2.5
1	B	393	SER	2.4
1	A	373	ASN	2.4
1	F	171	LYS	2.4
1	D	175	LYS	2.4
1	D	236	GLY	2.3
1	C	62	GLN	2.3
1	E	171	LYS	2.3
1	E	334	VAL	2.3
1	E	393	SER	2.3
1	E	63	ASN	2.2
1	C	393	SER	2.2
1	B	395	THR	2.2
1	F	351	HIS	2.2
1	D	114	GLU	2.1
1	D	21	ALA	2.1
1	D	149	PRO	2.1
1	C	146	GLY	2.0
1	C	125	LYS	2.0
1	F	203	TYR	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 [i](#)

There are no carbohydrates 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. 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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	CX9	C	1399	28/28	0.77	0.24	7.27	40,46,50,51	28
3	CX9	E	1399	28/28	0.80	0.21	6.97	40,46,50,51	28
3	CX9	F	1399	28/28	0.77	0.28	3.74	65,69,74,75	28
3	CX9	D	1399	28/28	0.81	0.22	3.21	48,50,54,56	28
3	CX9	A	1399	28/28	0.84	0.24	2.27	50,53,57,58	28
3	CX9	B	1399	28/28	0.83	0.24	1.65	48,54,59,60	28
2	GOL	B	1397	6/6	0.96	0.10	0.88	28,34,38,41	0
2	GOL	C	1397	6/6	0.95	0.11	0.81	28,38,43,52	0
3	CX9	B	1398	28/28	0.97	0.08	0.38	9,18,29,32	0
2	GOL	E	1397	6/6	0.95	0.10	0.23	25,35,39,42	0
2	GOL	A	1397	6/6	0.97	0.09	0.12	22,31,33,38	0
2	GOL	F	1397	6/6	0.97	0.09	0.02	32,38,40,47	0
3	CX9	F	1398	28/28	0.97	0.08	0.02	21,28,31,32	0
2	GOL	D	1397	6/6	0.97	0.09	-0.08	22,31,35,41	0
3	CX9	D	1398	28/28	0.98	0.07	-0.15	14,18,22,23	0
3	CX9	A	1398	28/28	0.98	0.07	-0.61	11,16,27,28	0
3	CX9	C	1398	28/28	0.97	0.07	-0.82	13,21,33,34	0
3	CX9	E	1398	28/28	0.97	0.08	-0.92	14,24,35,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.