



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:41 AM UTC

PDB ID : 2EAA / pdb_00002eaa
Title : Crystal Structure of Adzuki Bean 7S Globulin-3
Authors : Fukuda, T.; Mikami, B.; Utsumi, S.
Deposited on : 2007-01-31
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

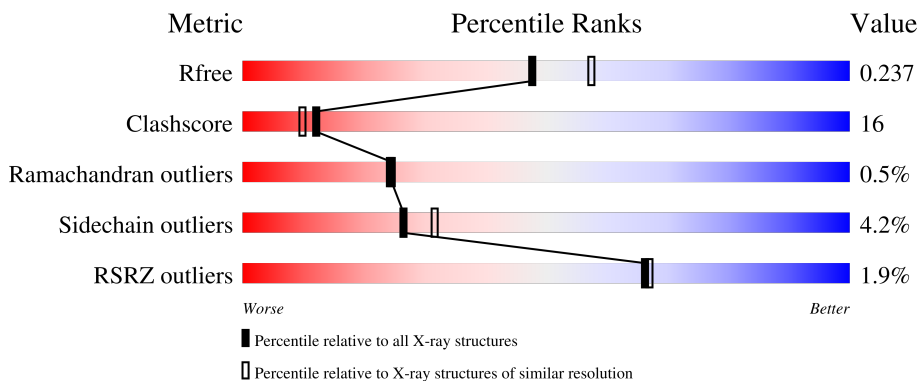
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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}	180053	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	433	
1	B	433	
1	C	433	

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	CIT	A	1285	-	X	-	-
3	CIT	B	1284	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9683 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 7S globulin-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	375	Total 3030	C 1921	N 525	O 579	S 5	0	0	0
1	B	380	Total 3073	C 1947	N 534	O 587	S 5	0	0	0
1	C	377	Total 3045	C 1929	N 527	O 584	S 5	0	0	0

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

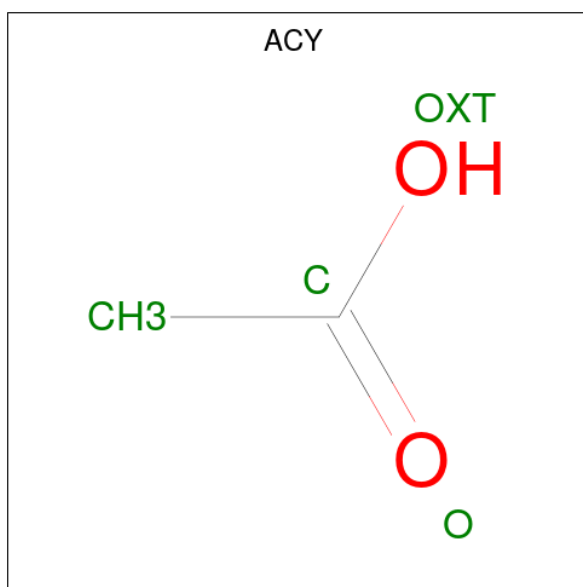
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Ca 1	0	0
2	B	1	Total 1	Ca 1	0	0
2	C	1	Total 1	Ca 1	0	0

- Molecule 3 is CITRIC ACID (CCD ID: CIT) (formula: C₆H₈O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	6	7		
3	B	1	Total	C	O	0	0
			13	6	7		
3	C	1	Total	C	O	0	0
			13	6	7		

- Molecule 4 is ACETIC ACID (CCD ID: ACY) (formula: C₂H₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	143	Total	O	0	0
			143	143		
5	B	163	Total	O	0	0
			163	163		
5	C	175	Total	O	0	0
			175	175		

GLY
SER
LEU
TYR

• Molecule 1: 7S globulin-3

Chain C:  2% 62% 23% 13%

ILE VAL HIS ARG GLU HIS GLN GLU
S13 F24 S25 S26 D27 R28 R29 F30 R42 R43 I44 L44 K52 Q53 I54 Q55 N56 L57 K66 S67 K68 P69 N70 L74 D81 F82 L83 L84 M88 G89 R90 A91 I92 D99 S100 I105 L106 E107 H110

A111 Q112 L122 V123 S228 M124 P125 M130 R132 L131 I133 I134 K135 V140 N141 E155 A156 Q157 G163 F164 S165 I168 L169 V183 E187 E188 ARG GLN GLN GLN GLN GLN E196 S197 R198 E199 E200 R208 I211 Q212 E213 L214 M215 K216 H217 A218 K219 S220 S221 S222

ARG LYS GLU SER S227 S228 Q229 D230 E231 P232 F233 N234 I235 R236 M237 P240 Y250 E251 M252 T253 P254 E255 K256 M257 P258 Q259 L260 F266 V270 D271 L278 Y282 N283 S284 K285 A286 L287 V288 M293 A297 L301 L304 S305 D306 GLN GLN GLN LYS ARG GLN

GLN E314 GLU SER L317 Y322 E325 E328 D329 A336 A337 N347 L348 N349 A357 N360 Q361 R362 M373 E379 F385 P386 A387 S388 K391 V392 E393 K394 L395 K398 Q399 S400 Q408 P409 GLU GLN GLN ARG GLU GLU GLY HIS LYS GLY ARG LYS

GLY
SER
LEU
TYR

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	66.87Å 99.32Å 216.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.25 15.00 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.6 (15.00-2.25) 99.3 (15.00-2.25)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.17 (at 2.25Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.194 , 0.237 0.194 , 0.237	Depositor DCC
R_{free} test set	6954 reflections (10.08%)	wwPDB-VP
Wilson B-factor (Å ²)	34.4	Xtrriage
Anisotropy	0.566	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 50.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9683	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.36	0/3092	0.92	8/4173 (0.2%)
1	B	0.38	0/3136	0.93	9/4232 (0.2%)
1	C	0.38	0/3106	0.94	13/4190 (0.3%)
All	All	0.38	0/9334	0.93	30/12595 (0.2%)

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	357	ALA	N-CA-C	10.37	122.66	111.36
1	C	357	ALA	N-CA-C	10.22	122.50	111.36
1	A	357	ALA	N-CA-C	9.06	121.24	111.36
1	C	288	VAL	N-CA-C	7.16	118.59	108.36
1	B	288	VAL	N-CA-C	6.89	118.22	108.36
1	A	288	VAL	N-CA-C	6.83	118.12	108.36
1	B	27	ASP	N-CA-C	6.38	118.31	111.36
1	C	140	VAL	N-CA-C	6.38	117.73	111.67
1	C	183	VAL	N-CA-C	5.94	117.48	111.00
1	A	348	LEU	N-CA-C	5.90	118.25	108.99
1	C	74	LEU	N-CA-C	5.72	117.79	109.84
1	A	347	ASN	N-CA-C	-5.57	102.78	110.35
1	B	347	ASN	N-CA-C	-5.53	102.45	110.24
1	C	347	ASN	N-CA-C	-5.51	102.24	110.23
1	A	284	SER	N-CA-C	5.32	116.77	111.07
1	C	57	LEU	N-CA-C	-5.32	106.17	113.30
1	A	402	SER	N-CA-C	5.31	117.46	109.23
1	A	270	VAL	N-CA-C	5.30	115.53	108.11
1	C	74	LEU	CA-C-N	5.27	125.57	119.93
1	C	74	LEU	C-N-CA	5.27	125.57	119.93
1	B	270	VAL	N-CA-C	5.24	115.44	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	57	LEU	N-CA-C	-5.23	106.58	113.17
1	C	348	LEU	N-CA-C	5.14	117.06	108.99
1	C	278	LEU	N-CA-C	-5.12	100.17	108.41
1	C	157	GLN	N-CA-C	5.09	116.97	108.99
1	C	26	SER	N-CA-C	-5.07	106.35	112.54
1	B	138	ILE	CA-C-N	5.07	125.00	119.78
1	B	138	ILE	C-N-CA	5.07	125.00	119.78
1	B	29	ARG	N-CA-C	5.03	118.45	112.72
1	B	140	VAL	N-CA-C	5.02	116.44	111.67

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	3030	0	2969	122	0
1	B	3073	0	3018	91	0
1	C	3045	0	2979	89	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	13	0	5	0	0
3	B	13	0	5	0	0
3	C	13	0	5	0	0
4	A	4	0	3	0	0
4	B	4	0	3	1	0
4	C	4	0	3	0	0
5	A	143	0	0	8	0
5	B	163	0	0	6	0
5	C	175	0	0	6	0
All	All	9683	0	8990	283	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 16.

All (283) 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:223:ARG:H	1:B:223:ARG:HD3	1.23	1.01
1:B:92:ILE:HB	1:B:123:VAL:HG13	1.48	0.95
1:B:236:ARG:HH21	1:B:236:ARG:HB3	1.33	0.94
1:A:229:GLN:HB3	1:A:258:PRO:HG3	1.51	0.92
1:B:223:ARG:HD3	1:B:223:ARG:N	1.88	0.86
1:B:254:PRO:HG2	1:B:255:GLU:OE1	1.78	0.84
1:C:234:ASN:OD1	1:C:236:ARG:HB2	1.78	0.84
1:C:394:LYS:HE3	1:C:394:LYS:HA	1.59	0.84
1:B:208:ARG:O	1:B:212:GLN:HG2	1.80	0.82
1:B:229:GLN:HB3	1:B:258:PRO:HG3	1.62	0.81
1:A:29:ARG:HD3	5:A:1286:HOH:O	1.80	0.80
1:C:408:GLN:HB2	1:C:409:PRO:HA	1.61	0.80
1:A:178:LYS:H	1:A:178:LYS:HZ2	1.29	0.80
1:C:112:GLN:HE21	1:C:112:GLN:HA	1.46	0.79
1:C:68:LYS:HB3	1:C:69:PRO:HD2	1.65	0.78
1:C:26:SER:HB2	1:C:42:ARG:HH12	1.49	0.78
1:A:211:ILE:O	1:A:215:MET:HB2	1.84	0.77
1:A:105:ILE:HD12	1:A:215:MET:HE1	1.67	0.77
1:B:49:GLN:HG3	5:B:1419:HOH:O	1.85	0.77
1:A:38:TYR:HA	1:A:68:LYS:HD2	1.67	0.76
1:A:214:LEU:HD23	1:A:214:LEU:H	1.49	0.76
1:A:112:GLN:HE21	1:A:112:GLN:HA	1.50	0.75
1:A:175:SER:OG	1:B:398:LYS:HD2	1.87	0.73
1:A:216:LYS:HA	1:A:216:LYS:HE2	1.71	0.73
1:B:234:ASN:HD22	1:B:236:ARG:H	1.39	0.71
1:A:24:PHE:HB3	1:A:44:LEU:HD11	1.73	0.70
1:A:52:LYS:HD3	1:A:55:GLN:NE2	2.08	0.69
1:B:379:GLU:H	1:B:379:GLU:CD	2.00	0.68
1:C:408:GLN:HB2	1:C:409:PRO:CA	2.23	0.68
1:B:24:PHE:HB3	1:B:44:LEU:HD11	1.76	0.67
1:C:283:ASN:HD21	1:C:362:ARG:HE	1.41	0.67
1:C:253:THR:H	1:C:256:LYS:HD2	1.58	0.67
1:B:283:ASN:HD21	1:B:362:ARG:HH11	1.40	0.67
1:C:24:PHE:HB3	1:C:44:LEU:HD11	1.76	0.67
1:A:37:GLN:H	1:A:37:GLN:CD	2.03	0.67
1:A:343:ASN:OD1	1:C:168:ILE:HD11	1.95	0.66
1:B:147:GLN:HB3	1:C:304:LEU:HD12	1.78	0.66
1:A:251:GLU:CD	1:A:362:ARG:HH22	2.02	0.66
1:A:277:LEU:HD13	1:A:343:ASN:ND2	2.11	0.66
1:A:213:GLU:HG2	1:B:379:GLU:OE1	1.94	0.66
1:A:178:LYS:H	1:A:178:LYS:NZ	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:LEU:HD13	1:A:343:ASN:HD21	1.61	0.65
1:C:283:ASN:HB3	1:C:360:ASN:HD21	1.62	0.65
1:B:70:ASN:HD21	1:B:208:ARG:NH2	1.94	0.65
1:C:400:SER:HB3	5:C:1457:HOH:O	1.97	0.65
1:A:293:ASN:HB3	1:A:349:ASN:HD22	1.61	0.65
1:A:240:PRO:HG3	1:A:250:TYR:CE2	2.32	0.64
1:C:387:ALA:HB1	1:C:391:LYS:HD3	1.80	0.63
1:A:206:LEU:HB2	1:A:211:ILE:HD11	1.79	0.63
1:C:395:LEU:C	1:C:395:LEU:HD23	2.25	0.62
1:B:113:LYS:HE3	1:B:262:ASP:OD2	2.00	0.62
1:B:234:ASN:ND2	1:B:236:ARG:H	1.97	0.62
1:C:385:PHE:HB3	1:C:386:PRO:HD2	1.81	0.61
1:C:398:LYS:HE2	1:C:398:LYS:HA	1.82	0.61
1:B:216:LYS:HG3	1:B:217:HIS:ND1	2.16	0.61
1:A:84:LEU:HD23	1:A:84:LEU:C	2.25	0.61
1:B:236:ARG:HH21	1:B:236:ARG:CB	2.12	0.61
1:A:69:PRO:HD3	1:A:130:ASN:ND2	2.16	0.61
1:A:147:GLN:HB2	5:A:1358:HOH:O	2.00	0.60
1:B:283:ASN:HB3	1:B:360:ASN:HD21	1.66	0.60
1:B:288:VAL:HG11	4:B:461:ACY:H3	1.83	0.60
1:B:162:ARG:HE	1:B:162:ARG:HA	1.66	0.59
1:A:231:GLU:HB3	1:A:232:PRO:HD2	1.84	0.59
1:A:253:THR:OG1	1:A:255:GLU:HG2	2.03	0.59
1:A:206:LEU:HB2	1:A:211:ILE:CD1	2.33	0.59
1:B:176:ASP:OD2	1:B:178:LYS:HB3	2.03	0.58
1:B:300:GLU:HG2	1:B:323:ARG:HD2	1.85	0.58
1:B:401:GLU:HB2	1:B:405:VAL:HG12	1.84	0.58
1:C:395:LEU:HD23	1:C:395:LEU:O	2.03	0.58
1:A:69:PRO:HD3	1:A:130:ASN:HD22	1.68	0.58
1:A:92:ILE:HD11	1:A:215:MET:HE2	1.85	0.58
1:C:165:SER:OG	1:C:168:ILE:HG12	2.03	0.58
1:A:176:ASP:HB2	1:A:178:LYS:NZ	2.19	0.58
1:A:293:ASN:CB	1:A:349:ASN:HD22	2.16	0.58
1:A:255:GLU:HB2	5:A:1413:HOH:O	2.04	0.58
1:A:196:GLU:OE1	1:B:387:ALA:HA	2.02	0.58
1:A:58:GLU:OE2	1:A:144:HIS:HE1	1.86	0.58
1:B:240:PRO:HG3	1:B:250:TYR:CE2	2.39	0.57
1:C:112:GLN:HA	1:C:112:GLN:NE2	2.18	0.57
1:A:166:LYS:O	1:A:170:GLU:HG3	2.05	0.57
1:C:52:LYS:NZ	1:C:55:GLN:HE22	2.02	0.57
1:A:16:ARG:HA	1:A:323:ARG:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:236:ARG:NH2	1:C:271:ASP:OD2	2.36	0.56
1:B:29:ARG:NH1	1:B:50:ARG:NH2	2.54	0.56
1:C:52:LYS:HE3	1:C:55:GLN:NE2	2.19	0.56
1:C:388:SER:OG	1:C:391:LYS:HB2	2.06	0.56
1:B:251:GLU:CD	1:B:362:ARG:HH22	2.13	0.56
1:A:235:LEU:HA	1:A:252:MET:CE	2.36	0.56
1:B:300:GLU:HG2	1:B:323:ARG:HH21	1.69	0.56
1:B:300:GLU:HG2	1:B:323:ARG:CD	2.36	0.56
1:A:101:ARG:CZ	1:B:377:PRO:HG3	2.37	0.55
1:B:50:ARG:HG2	5:B:1340:HOH:O	2.05	0.55
1:B:300:GLU:CG	1:B:323:ARG:HH21	2.20	0.55
1:A:219:LYS:HB3	1:A:219:LYS:NZ	2.22	0.55
1:B:401:GLU:CB	1:B:405:VAL:HG12	2.37	0.55
1:B:20:ASN:C	1:B:20:ASN:HD22	2.14	0.54
1:A:92:ILE:HD11	1:A:215:MET:HG2	1.88	0.54
1:A:181:ASN:ND2	1:A:181:ASN:O	2.40	0.54
1:C:240:PRO:HG3	1:C:250:TYR:CE2	2.42	0.54
1:A:214:LEU:H	1:A:214:LEU:CD2	2.20	0.54
1:A:52:LYS:HD3	1:A:55:GLN:HE21	1.71	0.54
1:B:234:ASN:HD22	1:B:234:ASN:C	2.16	0.54
1:B:59:ASN:ND2	1:B:143:PRO:HB2	2.22	0.54
1:B:70:ASN:ND2	1:B:208:ARG:HH21	2.05	0.54
1:B:255:GLU:OE1	1:B:255:GLU:N	2.41	0.54
1:C:187:GLU:O	1:C:187:GLU:HG2	2.07	0.53
1:A:112:GLN:HA	1:A:112:GLN:NE2	2.21	0.53
1:A:110:HIS:CE1	1:A:234:ASN:HD22	2.26	0.53
1:B:389:GLY:O	1:B:393:GLU:HG3	2.09	0.53
1:A:255:GLU:CD	1:A:255:GLU:H	2.16	0.53
1:A:21:PRO:HB2	1:A:51:SER:HB2	1.91	0.53
1:B:229:GLN:HB3	1:B:258:PRO:CG	2.35	0.53
1:B:253:THR:HB	1:B:254:PRO:HD2	1.91	0.53
1:C:99:ASP:O	1:C:100:SER:HB3	2.09	0.53
1:A:138:ILE:HD12	1:A:138:ILE:N	2.24	0.53
1:B:252:MET:HE1	1:B:257:ASN:HD22	1.74	0.52
1:A:178:LYS:HZ2	1:A:178:LYS:N	2.02	0.52
1:B:300:GLU:CD	1:B:323:ARG:NH2	2.67	0.52
1:C:112:GLN:HB2	1:C:232:PRO:HB3	1.91	0.52
1:C:388:SER:O	1:C:392:VAL:HG23	2.09	0.52
1:A:53:GLN:O	1:C:141:ASN:HB3	2.11	0.51
1:B:283:ASN:ND2	1:B:362:ARG:HH11	2.07	0.51
1:A:210:GLN:O	1:A:213:GLU:HB3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:266:PHE:C	1:C:266:PHE:CD2	2.88	0.51
1:A:151:LEU:HD11	1:B:373:MET:HG2	1.92	0.51
1:A:65:PHE:CZ	1:A:67:SER:HB3	2.46	0.50
1:C:68:LYS:HA	1:C:130:ASN:ND2	2.26	0.50
1:C:293:ASN:CB	1:C:349:ASN:HD22	2.25	0.50
1:C:208:ARG:O	1:C:212:GLN:HG2	2.12	0.50
1:A:74:LEU:HD12	1:A:202:VAL:HA	1.91	0.50
1:C:107:GLU:HG3	5:C:1423:HOH:O	2.10	0.50
1:A:178:LYS:HZ2	1:A:178:LYS:HB2	1.75	0.50
1:C:213:GLU:OE2	1:C:216:LYS:HE2	2.12	0.50
1:B:70:ASN:ND2	1:B:208:ARG:NH2	2.59	0.50
1:C:237:ASN:C	1:C:237:ASN:HD22	2.20	0.50
1:A:390:LYS:HG3	5:A:1305:HOH:O	2.12	0.50
1:C:325:GLU:HB3	5:C:1320:HOH:O	2.11	0.50
1:A:254:PRO:HB3	1:A:261:LYS:HA	1.92	0.49
1:B:266:PHE:C	1:B:266:PHE:CD2	2.90	0.49
1:B:302:VAL:HG13	1:B:319:VAL:CG2	2.42	0.49
1:C:110:HIS:NE2	1:C:221:SER:HB3	2.27	0.49
1:A:86:VAL:HG21	1:A:106:LEU:HB3	1.92	0.49
1:C:155:GLU:OE1	1:C:200:GLU:HG2	2.12	0.49
1:C:253:THR:HB	1:C:254:PRO:HD2	1.93	0.49
1:A:147:GLN:CG	1:B:304:LEU:HD12	2.42	0.49
1:C:328:GLU:O	1:C:329:ASP:HB2	2.12	0.49
1:B:223:ARG:H	1:B:223:ARG:CD	2.08	0.49
1:B:390:LYS:HE2	5:B:1395:HOH:O	2.12	0.49
1:A:214:LEU:HD23	1:A:214:LEU:N	2.24	0.49
1:A:245:LYS:HG2	5:A:1380:HOH:O	2.12	0.48
5:B:1397:HOH:O	1:C:391:LYS:HE2	2.11	0.48
1:B:92:ILE:HD11	1:B:215:MET:HG2	1.95	0.48
1:B:122:LEU:HD21	1:B:133:ILE:CD1	2.43	0.48
1:C:28:ARG:O	1:C:28:ARG:HG3	2.13	0.48
1:A:181:ASN:HD22	1:A:185:PHE:HB2	1.77	0.48
1:A:266:PHE:C	1:A:266:PHE:CD2	2.91	0.48
1:C:90:ARG:NH1	1:C:107:GLU:OE1	2.44	0.48
1:A:235:LEU:HA	1:A:252:MET:HE3	1.95	0.48
1:B:213:GLU:O	1:B:216:LYS:HG2	2.13	0.48
1:A:163:GLY:O	1:B:321:ARG:HG2	2.14	0.48
1:C:92:ILE:HG12	1:C:105:ILE:CD1	2.44	0.48
1:C:293:ASN:HB3	1:C:349:ASN:HD22	1.78	0.48
1:B:376:ILE:HB	1:B:381:LEU:HD21	1.95	0.47
1:A:105:ILE:HB	1:A:220:SER:HA	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:ASP:C	1:A:408:GLN:H	2.23	0.47
1:A:23:TYR:CZ	1:A:25:SER:HB3	2.50	0.47
1:A:210:GLN:O	1:A:214:LEU:HD23	2.14	0.47
1:B:141:ASN:HB3	1:C:53:GLN:O	2.14	0.47
1:A:38:TYR:CE2	1:A:205:GLU:HB2	2.49	0.47
1:A:85:VAL:HG21	1:A:351:PHE:CZ	2.49	0.47
1:A:236:ARG:NH1	1:A:250:TYR:CE1	2.83	0.47
1:A:270:VAL:O	1:A:349:ASN:HA	2.15	0.47
1:C:135:LYS:NZ	5:C:1298:HOH:O	2.47	0.47
1:A:122:LEU:HD21	1:A:133:ILE:HD12	1.96	0.47
1:C:234:ASN:O	1:C:237:ASN:ND2	2.48	0.47
1:C:257:ASN:HB3	1:C:260:LEU:HD22	1.96	0.47
1:A:147:GLN:HG3	1:B:304:LEU:HD12	1.96	0.47
1:B:105:ILE:HG13	1:B:218:ALA:HB1	1.97	0.47
1:B:336:ALA:O	1:B:337:ALA:HB3	2.15	0.47
1:B:21:PRO:HB2	1:B:51:SER:HB2	1.98	0.46
1:C:30:PHE:CZ	1:C:44:LEU:HD13	2.50	0.46
1:C:270:VAL:O	1:C:349:ASN:HA	2.15	0.46
1:A:90:ARG:HD3	5:A:1352:HOH:O	2.15	0.46
1:A:127:ASP:OD2	1:A:208:ARG:HD3	2.16	0.46
1:C:198:ARG:NH1	5:C:1428:HOH:O	2.48	0.46
1:A:335:PRO:HB2	1:A:338:TYR:CD1	2.50	0.46
1:B:166:LYS:O	1:B:170:GLU:HG3	2.16	0.46
1:B:134:ILE:CD1	1:B:291:VAL:HG11	2.47	0.45
1:A:178:LYS:N	1:A:178:LYS:HD3	2.31	0.45
1:A:253:THR:HB	1:A:254:PRO:CD	2.47	0.45
1:C:110:HIS:HD1	1:C:234:ASN:HD22	1.64	0.45
1:A:298:LYS:HZ2	1:A:325:GLU:HG2	1.81	0.45
1:A:253:THR:HB	1:A:254:PRO:HD2	1.99	0.45
1:A:387:ALA:HB3	1:C:183:VAL:HG13	1.98	0.45
1:A:321:ARG:HG2	1:C:163:GLY:O	2.16	0.45
1:A:219:LYS:HB3	1:A:219:LYS:HZ3	1.82	0.45
1:C:336:ALA:O	1:C:337:ALA:HB3	2.17	0.45
1:A:97:ASN:HB3	1:A:98:PRO:CD	2.47	0.45
1:A:107:GLU:HB2	1:A:110:HIS:CE1	2.52	0.45
1:A:196:GLU:O	1:A:196:GLU:HG3	2.16	0.45
1:C:90:ARG:HH11	1:C:90:ARG:CB	2.30	0.45
1:C:112:GLN:HE22	1:C:259:GLN:HE22	1.63	0.44
1:A:387:ALA:HB2	1:C:183:VAL:HA	1.99	0.44
1:A:336:ALA:O	1:A:337:ALA:HB3	2.17	0.44
1:B:138:ILE:N	1:B:138:ILE:HD12	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:379:GLU:O	1:B:382:GLU:HB3	2.17	0.44
1:A:72:LEU:HD13	1:A:123:VAL:HG22	1.99	0.44
1:C:221:SER:HB2	5:C:1395:HOH:O	2.18	0.44
1:A:181:ASN:HA	1:A:185:PHE:HD2	1.83	0.44
1:C:84:LEU:HD23	1:C:84:LEU:C	2.43	0.44
1:A:265:VAL:HA	1:A:354:GLY:O	2.17	0.43
1:C:379:GLU:H	1:C:379:GLU:CD	2.26	0.43
1:A:92:ILE:CD1	1:A:215:MET:HE2	2.47	0.43
1:A:181:ASN:ND2	1:A:185:PHE:HB2	2.33	0.43
1:B:257:ASN:HB3	1:B:260:LEU:HD22	2.00	0.43
1:C:283:ASN:HD21	1:C:362:ARG:NE	2.13	0.43
1:A:69:PRO:HB3	1:A:126:ASP:O	2.19	0.43
1:C:82:PHE:CD1	1:C:135:LYS:HD2	2.54	0.43
1:C:125:PRO:HB2	1:C:215:MET:HE2	2.00	0.43
1:B:40:HIS:HE1	5:B:1418:HOH:O	2.01	0.43
1:C:26:SER:HA	1:C:30:PHE:CD2	2.54	0.43
1:A:76:HIS:HD2	1:A:148:ASP:OD1	2.00	0.43
1:C:68:LYS:HA	1:C:130:ASN:HD22	1.83	0.43
1:C:122:LEU:HD21	1:C:133:ILE:CD1	2.49	0.43
1:A:151:LEU:HD22	1:B:385:PHE:HZ	1.83	0.43
1:C:216:LYS:HG3	1:C:217:HIS:CD2	2.53	0.43
1:B:59:ASN:HB2	5:B:1362:HOH:O	2.19	0.43
1:A:68:LYS:H	1:A:68:LYS:HG2	1.63	0.43
1:A:181:ASN:HD22	1:A:181:ASN:C	2.27	0.43
1:A:99:ASP:O	1:A:100:SER:HB3	2.18	0.42
1:A:162:ARG:HD2	1:A:185:PHE:CD1	2.54	0.42
1:A:251:GLU:OE1	1:A:362:ARG:NH2	2.51	0.42
1:B:112:GLN:HA	1:B:112:GLN:NE2	2.34	0.42
1:B:20:ASN:ND2	1:B:22:PHE:H	2.18	0.42
1:A:45:HIS:HD2	5:A:1348:HOH:O	2.02	0.42
1:B:117:GLY:HA3	1:C:284:SER:O	2.20	0.42
1:B:107:GLU:H	1:B:110:HIS:HD1	1.67	0.42
1:A:328:GLU:O	1:A:329:ASP:HB2	2.19	0.42
1:C:293:ASN:C	1:C:293:ASN:HD22	2.27	0.42
1:B:74:LEU:HB3	1:B:75:PRO:HD2	2.02	0.42
1:B:300:GLU:OE1	1:B:323:ARG:NH2	2.53	0.42
1:A:58:GLU:HG3	1:A:59:ASN:ND2	2.35	0.42
1:A:112:GLN:HE22	1:A:259:GLN:HE22	1.67	0.42
1:B:346:SER:O	1:B:347:ASN:C	2.58	0.42
1:A:112:GLN:HB2	1:A:232:PRO:HB3	2.02	0.41
1:B:263:LEU:O	1:B:265:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:66:LYS:HA	1:C:131:LEU:O	2.20	0.41
1:C:70:ASN:HD22	1:C:211:ILE:HG13	1.85	0.41
1:C:297:ALA:HB2	1:C:348:LEU:HD22	2.02	0.41
1:A:178:LYS:HZ2	1:A:178:LYS:CB	2.33	0.41
1:C:188:GLU:O	1:C:188:GLU:HG2	2.20	0.41
1:C:252:MET:HE2	1:C:257:ASN:HB2	2.01	0.41
1:B:112:GLN:HE22	1:B:259:GLN:HE22	1.69	0.41
1:B:282:TYR:CD2	1:B:282:TYR:C	2.98	0.41
1:B:373:MET:C	1:B:375:GLU:H	2.28	0.41
1:C:286:ALA:H	1:C:360:ASN:ND2	2.18	0.41
1:A:66:LYS:HA	1:A:131:LEU:O	2.21	0.41
1:B:151:LEU:HD21	1:C:373:MET:HG2	2.02	0.41
1:A:68:LYS:HB2	1:A:69:PRO:CD	2.50	0.41
1:B:265:VAL:HA	1:B:354:GLY:O	2.21	0.41
1:A:220:SER:HB2	5:A:1364:HOH:O	2.20	0.41
1:B:183:VAL:HA	1:C:387:ALA:HB2	2.03	0.41
1:C:124:ASN:C	1:C:124:ASN:ND2	2.79	0.41
1:A:68:LYS:HB2	1:A:69:PRO:HD2	2.03	0.41
1:B:134:ILE:HD13	1:B:291:VAL:HG11	2.03	0.41
1:B:231:GLU:HB3	1:B:232:PRO:HD2	2.03	0.41
1:A:112:GLN:HE21	1:A:112:GLN:CA	2.21	0.41
1:A:397:LYS:O	1:A:397:LYS:HG2	2.21	0.41
1:B:283:ASN:HD21	1:B:362:ARG:HD3	1.84	0.41
1:A:37:GLN:H	1:A:37:GLN:NE2	2.19	0.40
1:C:257:ASN:HB3	1:C:260:LEU:HB2	2.02	0.40
1:C:112:GLN:OE1	1:C:230:ASP:O	2.39	0.40
1:C:282:TYR:CD2	1:C:282:TYR:C	2.98	0.40
1:C:408:GLN:CB	1:C:409:PRO:CA	2.94	0.40
1:A:105:ILE:HD12	1:A:215:MET:CE	2.44	0.40
1:A:219:LYS:NZ	1:A:219:LYS:CB	2.85	0.40
1:B:66:LYS:HA	1:B:131:LEU:O	2.21	0.40
1:C:301:LEU:HB3	1:C:322:TYR:HB2	2.03	0.40
1:A:82:PHE:HB2	1:A:114:ILE:HB	2.03	0.40
1:A:236:ARG:HH22	1:A:271:ASP:CG	2.29	0.40
1:A:298:LYS:HB2	1:A:343:ASN:HB2	2.03	0.40
1:B:162:ARG:HE	1:B:162:ARG:CA	2.34	0.40
1:C:169:LEU:HD23	1:C:169:LEU:HA	1.94	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	367/433 (85%)	347 (95%)	18 (5%)	2 (0%)	24	24
1	B	374/433 (86%)	357 (96%)	15 (4%)	2 (0%)	24	24
1	C	368/433 (85%)	354 (96%)	13 (4%)	1 (0%)	36	40
All	All	1109/1299 (85%)	1058 (95%)	46 (4%)	5 (0%)	24	24

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	213	GLU
1	B	222	SER
1	C	408	GLN
1	A	230	ASP
1	B	186	GLY

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	337/390 (86%)	320 (95%)	17 (5%)	22	24
1	B	342/390 (88%)	328 (96%)	14 (4%)	27	33
1	C	339/390 (87%)	327 (96%)	12 (4%)	32	39
All	All	1018/1170 (87%)	975 (96%)	43 (4%)	26	31

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	ARG
1	A	37	GLN
1	A	81	ASP
1	A	147	GLN
1	A	148	ASP
1	A	151	LEU
1	A	157	GLN
1	A	178	LYS
1	A	212	GLN
1	A	214	LEU
1	A	215	MET
1	A	216	LYS
1	A	255	GLU
1	A	260	LEU
1	A	320	GLN
1	A	348	LEU
1	A	390	LYS
1	B	16	ARG
1	B	27	ASP
1	B	29	ARG
1	B	50	ARG
1	B	81	ASP
1	B	123	VAL
1	B	157	GLN
1	B	162	ARG
1	B	195	GLU
1	B	223	ARG
1	B	236	ARG
1	B	255	GLU
1	B	260	LEU
1	B	379	GLU
1	C	81	ASP
1	C	88	ASN
1	C	107	GLU
1	C	124	ASN
1	C	157	GLN
1	C	229	GLN
1	C	237	ASN
1	C	255	GLU
1	C	260	LEU
1	C	270	VAL
1	C	394	LYS
1	C	398	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	49	GLN
1	A	53	GLN
1	A	55	GLN
1	A	59	ASN
1	A	76	HIS
1	A	108	GLN
1	A	112	GLN
1	A	130	ASN
1	A	144	HIS
1	A	147	GLN
1	A	157	GLN
1	A	167	ASN
1	A	181	ASN
1	A	237	ASN
1	A	293	ASN
1	A	320	GLN
1	A	349	ASN
1	A	356	ASN
1	A	359	ASN
1	A	360	ASN
1	A	361	GLN
1	A	363	ASN
1	B	20	ASN
1	B	40	HIS
1	B	59	ASN
1	B	70	ASN
1	B	112	GLN
1	B	130	ASN
1	B	147	GLN
1	B	212	GLN
1	B	229	GLN
1	B	234	ASN
1	B	283	ASN
1	B	293	ASN
1	B	356	ASN
1	B	359	ASN
1	B	360	ASN
1	B	361	GLN
1	C	37	GLN
1	C	45	HIS

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Mol	Chain	Res	Type
1	C	53	GLN
1	C	55	GLN
1	C	70	ASN
1	C	88	ASN
1	C	108	GLN
1	C	112	GLN
1	C	124	ASN
1	C	130	ASN
1	C	147	GLN
1	C	157	GLN
1	C	212	GLN
1	C	217	HIS
1	C	229	GLN
1	C	237	ASN
1	C	283	ASN
1	C	293	ASN
1	C	320	GLN
1	C	349	ASN
1	C	356	ASN
1	C	359	ASN
1	C	360	ASN
1	C	361	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 for Mogul analysis.

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
4	ACY	C	462	-	3,3,3	0.82	0	3,3,3	0.93	0
3	CIT	A	1285	-	12,12,12	2.29	4 (33%)	17,17,17	3.01	8 (47%)
3	CIT	B	1284	-	12,12,12	2.38	4 (33%)	17,17,17	3.06	8 (47%)
3	CIT	C	1283	-	12,12,12	2.43	4 (33%)	17,17,17	2.97	6 (35%)
4	ACY	A	460	-	3,3,3	0.82	0	3,3,3	1.00	0
4	ACY	B	461	-	3,3,3	0.89	0	3,3,3	0.96	0

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
3	CIT	A	1285	-	-	9/16/16/16	-
3	CIT	B	1284	-	-	9/16/16/16	-
3	CIT	C	1283	-	-	5/16/16/16	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1284	CIT	C3-C6	6.00	1.59	1.53
3	C	1283	CIT	C3-C6	5.82	1.59	1.53
3	A	1285	CIT	C3-C6	5.58	1.59	1.53
3	C	1283	CIT	C4-C3	4.41	1.59	1.54
3	A	1285	CIT	C4-C3	3.71	1.58	1.54
3	B	1284	CIT	C4-C3	3.67	1.58	1.54
3	C	1283	CIT	C4-C5	2.49	1.58	1.50
3	A	1285	CIT	C4-C5	2.48	1.58	1.50
3	B	1284	CIT	C4-C5	2.46	1.58	1.50
3	B	1284	CIT	C2-C3	2.31	1.56	1.54
3	A	1285	CIT	C2-C3	2.20	1.56	1.54
3	C	1283	CIT	C2-C3	2.05	1.56	1.54

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1284	CIT	O7-C3-C6	-6.57	99.64	108.96
3	C	1283	CIT	O7-C3-C6	-6.31	100.01	108.96
3	B	1284	CIT	C2-C3-C6	6.28	123.92	110.03
3	A	1285	CIT	O7-C3-C6	-6.22	100.13	108.96
3	A	1285	CIT	C2-C3-C6	6.03	123.38	110.03
3	C	1283	CIT	C2-C3-C6	5.55	122.30	110.03
3	C	1283	CIT	O6-C6-C3	-5.19	103.18	113.14
3	A	1285	CIT	O6-C6-C3	-5.11	103.32	113.14
3	B	1284	CIT	O6-C6-C3	-5.04	103.47	113.14
3	C	1283	CIT	O5-C6-C3	4.23	130.28	122.09
3	A	1285	CIT	O5-C6-C3	4.18	130.19	122.09
3	B	1284	CIT	O5-C6-C3	4.09	130.01	122.09
3	A	1285	CIT	C4-C3-C6	-2.96	103.49	110.03
3	B	1284	CIT	C4-C3-C6	-2.87	103.69	110.03
3	C	1283	CIT	C4-C3-C6	-2.67	104.12	110.03
3	A	1285	CIT	O2-C1-C2	2.60	122.57	114.35
3	B	1284	CIT	O2-C1-C2	2.58	122.51	114.35
3	C	1283	CIT	O2-C1-C2	2.57	122.49	114.35
3	A	1285	CIT	O3-C5-C4	2.09	128.87	122.95
3	A	1285	CIT	O4-C5-C4	-2.07	107.78	114.35
3	B	1284	CIT	O3-C5-C4	2.04	128.74	122.95
3	B	1284	CIT	O4-C5-C4	-2.04	107.89	114.35

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1283	CIT	C2-C3-C4-C5
3	C	1283	CIT	O7-C3-C4-C5
3	C	1283	CIT	C6-C3-C4-C5
3	A	1285	CIT	C2-C3-C6-O6
3	B	1284	CIT	C2-C3-C6-O6
3	B	1284	CIT	O1-C1-C2-C3
3	C	1283	CIT	O1-C1-C2-C3
3	A	1285	CIT	O1-C1-C2-C3
3	A	1285	CIT	O2-C1-C2-C3
3	B	1284	CIT	O2-C1-C2-C3
3	C	1283	CIT	O2-C1-C2-C3
3	B	1284	CIT	O7-C3-C6-O6
3	A	1285	CIT	C2-C3-C6-O5
3	B	1284	CIT	C2-C3-C6-O5
3	B	1284	CIT	O7-C3-C4-C5
3	A	1285	CIT	O7-C3-C6-O6

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Mol	Chain	Res	Type	Atoms
3	A	1285	CIT	C4-C3-C6-O5
3	A	1285	CIT	C4-C3-C6-O6
3	B	1284	CIT	C4-C3-C6-O5
3	B	1284	CIT	C4-C3-C6-O6
3	A	1285	CIT	O7-C3-C4-C5
3	A	1285	CIT	O7-C3-C6-O5
3	B	1284	CIT	O7-C3-C6-O5

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	461	ACY	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	375/433 (86%)	-0.15	8 (2%) 63 64	21, 37, 70, 107	0
1	B	380/433 (87%)	-0.23	7 (1%) 67 68	20, 35, 63, 86	0
1	C	377/433 (87%)	-0.26	7 (1%) 66 67	21, 35, 68, 99	0
All	All	1132/1299 (87%)	-0.21	22 (1%) 66 67	20, 35, 67, 107	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	13	SER	4.1
1	B	14	ASP	3.8
1	B	15	SER	3.4
1	C	409	PRO	3.2
1	C	227	SER	3.1
1	C	317	LEU	2.8
1	C	228	SER	2.8
1	C	229	GLN	2.7
1	A	221	SER	2.7
1	A	214	LEU	2.6
1	A	196	GLU	2.5
1	A	228	SER	2.4
1	A	227	SER	2.3
1	A	409	PRO	2.2
1	B	195	GLU	2.2
1	C	408	GLN	2.2
1	B	409	PRO	2.1
1	B	223	ARG	2.1
1	C	219	LYS	2.1
1	B	187	GLU	2.1
1	A	186	GLY	2.0
1	A	14	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	CIT	C	1283	13/13	0.62	0.17	82,83,85,85	0
3	CIT	B	1284	13/13	0.65	0.17	90,92,94,94	0
3	CIT	A	1285	13/13	0.67	0.15	84,85,86,87	0
2	CA	C	904	1/1	0.89	0.06	79,79,79,79	0
2	CA	B	905	1/1	0.90	0.10	78,78,78,78	0
4	ACY	C	462	4/4	0.93	0.09	35,37,37,40	0
4	ACY	B	461	4/4	0.94	0.08	38,39,40,42	0
4	ACY	A	460	4/4	0.94	0.07	38,39,40,41	0
2	CA	A	906	1/1	0.96	0.16	66,66,66,66	0

6.5 Other polymers [i](#)

There are no such residues in this entry.