



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 10:31 pm GMT

PDB ID : 2EAA
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

<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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

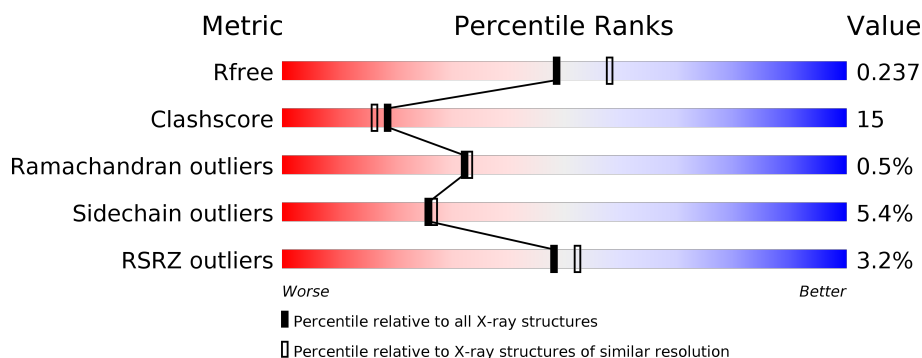
1 Overall quality at a glance

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}	100719	1062 (2.26-2.26)
Clashscore	112137	1178 (2.26-2.26)
Ramachandran outliers	110173	1145 (2.26-2.26)
Sidechain outliers	110143	1146 (2.26-2.26)
RSRZ outliers	101464	1066 (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 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	433	<div> <div>3%</div> <div> <div></div> <div>58%</div> <div>25%</div> <div>•</div> <div>13%</div> </div> </div>
1	B	433	<div> <div>3%</div> <div> <div></div> <div>64%</div> <div>21%</div> <div>•</div> <div>12%</div> </div> </div>
1	C	433	<div> <div>3%</div> <div> <div></div> <div>65%</div> <div>20%</div> <div>•</div> <div>13%</div> </div> </div>

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
3	CIT	C	1283	-	-	-	X
4	ACY	A	460	-	-	-	X
4	ACY	B	461	-	-	-	X
4	ACY	C	462	-	-	-	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
1	A	375	Total	C	N	O	S	0	0	0
			3030	1921	525	579	5			
1	B	380	Total	C	N	O	S	0	0	0
			3073	1947	534	587	5			
1	C	377	Total	C	N	O	S	0	0	0
			3045	1929	527	584	5			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

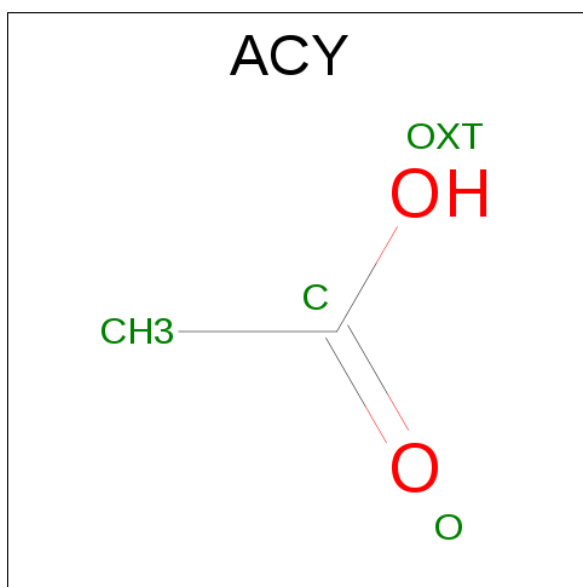
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		
2	A	1	Total	Ca	0	0
			1	1		
2	C	1	Total	Ca	0	0
			1	1		

- Molecule 3 is CITRIC ACID (three-letter code: 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 (three-letter code: ACY) (formula: C₂H₄O₂).



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

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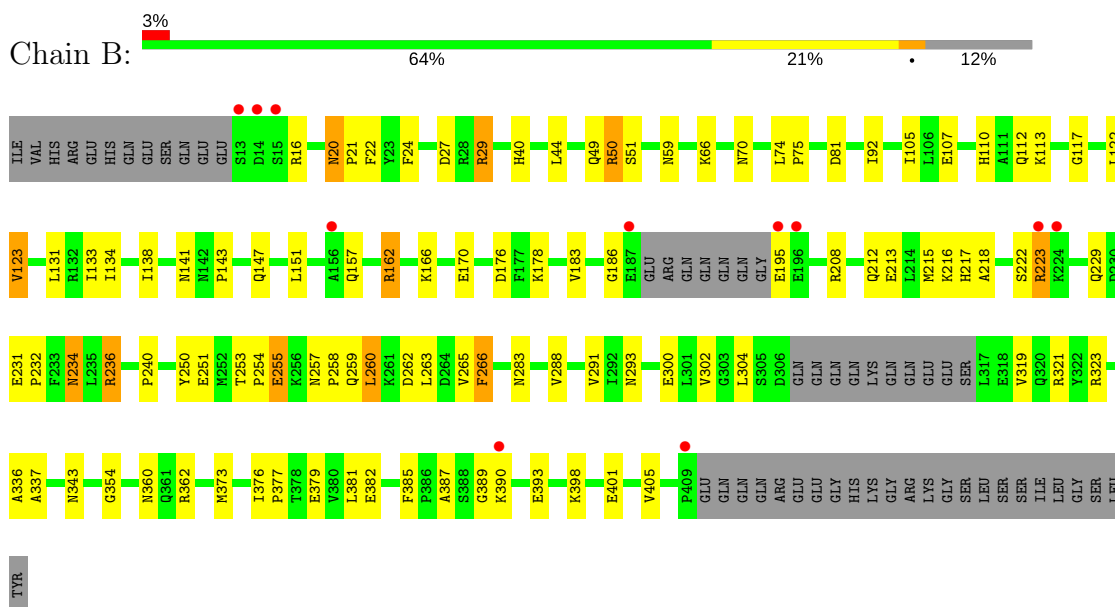
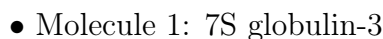
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		

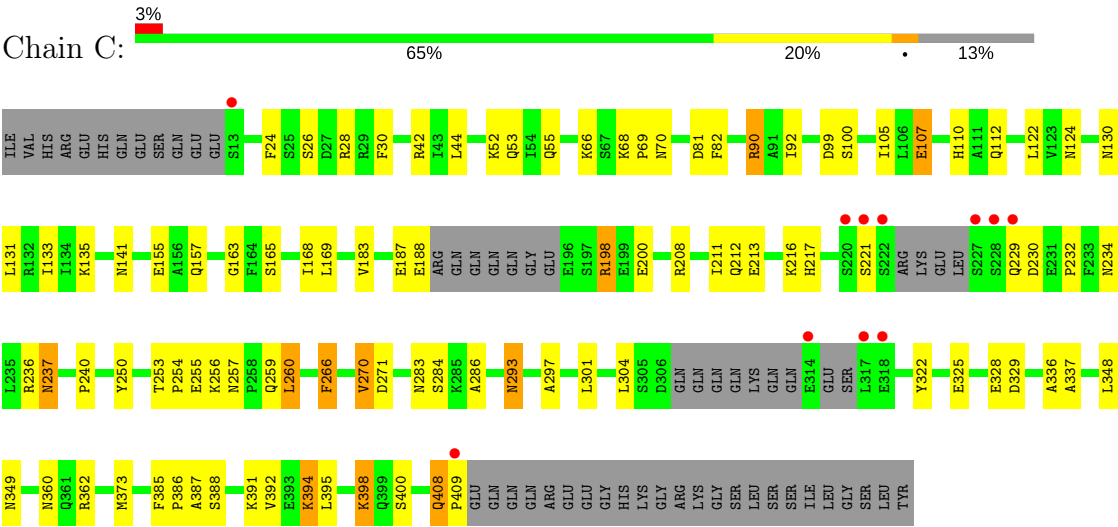
- Molecule 5 is water.

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		

- Molecule 1: 7S globulin-3



● Molecule 1: 7S globulin-3



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 49.66 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.6 (15.00-2.25) 99.7 (49.66-2.25)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.17 (at 2.25Å)	Xtriage
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 (10.12%)	DCC
Wilson B-factor (Å ²)	34.4	Xtriage
Anisotropy	0.566	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 54.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
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

Xtriage'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: CA, ACY, CIT

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	0.35	0/3092	0.63	0/4173
1	B	0.35	0/3136	0.62	0/4232
1	C	0.35	0/3106	0.63	0/4190
All	All	0.35	0/9334	0.63	0/12595

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	118	0
1	B	3073	0	3018	88	0
1	C	3045	0	2979	83	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	270	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (270) 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:A:178:LYS:HZ2	1:A:178:LYS:H	1.20	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:C:112:GLN:HA	1:C:112:GLN:HE21	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: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:H	1:A:214:LEU:HD23	1.49	0.76
1:A:112:GLN:HA	1:A:112:GLN:HE21	1.50	0.75
1:A:175:SER:OG	1:B:398:LYS:HD2	1.87	0.73
1:A:216:LYS:HE2	1:A:216:LYS:HA	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:C:408:GLN:HB2	1:C:409:PRO:CA	2.23	0.68
1:A:90:ARG:HH22	1:A:215:MET:HE1	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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:B:379:GLU:H	1:B:379:GLU:CD	2.00	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:A:178:LYS:NZ	1:A:178:LYS:H	1.94	0.62
1:A:251:GLU:CD	1:A:362:ARG:HH22	2.02	0.62
1:A:37:GLN:CD	1:A:37:GLN:H	2.03	0.62
1:B:113:LYS:HE3	1:B:262:ASP:OD2	2.00	0.62
1:A:176:ASP:HB2	1:A:178:LYS:HZ1	1.65	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: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:O	1:C:395:LEU:HD23	2.03	0.58
1:A:69:PRO:HD3	1:A:130:ASN:HD22	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:395:LEU:C	1:C:395:LEU:HD23	2.25	0.57
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
1:C:236:ARG:NH2	1:C:271:ASP:OD2	2.36	0.56
1:C:388:SER:OG	1:C:391:LYS:HB2	2.06	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:A:84:LEU:HD23	1:A:84:LEU:C	2.25	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:A:92:ILE:HD11	1:A:215:MET:HG2	1.88	0.54
1:A:181:ASN:O	1:A:181:ASN:ND2	2.40	0.54
1:C:240:PRO:HG3	1:C:250:TYR:CE2	2.42	0.54
1:A:214:LEU:CD2	1:A:214:LEU:H	2.20	0.54
1:A:52:LYS:HD3	1:A:55:GLN:HE21	1.71	0.54
1:B:255:GLU:OE1	1:B:255:GLU:N	2.41	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:C:187:GLU:HG2	1:C:187:GLU:O	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:ILE:N	1:A:138:ILE:HD12	2.24	0.53
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
1:A:151:LEU:HD11	1:B:373:MET:HG2	1.92	0.51
1:B:251:GLU:CD	1:B:362:ARG:HH22	2.13	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: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:B:20:ASN:HD22	1:B:20:ASN:C	2.14	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: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:B:234:ASN:C	1:B:234:ASN:HD22	2.16	0.49
1:C:328:GLU:O	1:C:329:ASP:HB2	2.12	0.49
1:B:223:ARG:CD	1:B:223:ARG:H	2.08	0.49
1:B:390:LYS:HE2	5:B:1395:HOH:O	2.12	0.49
1:A:214:LEU:N	1:A:214:LEU:HD23	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:122:LEU:HD21	1:B:133:ILE:CD1	2.43	0.48
1:B:92:ILE:HD11	1:B:215:MET:HG2	1.95	0.48
1:C:28:ARG:HG3	1:C:28:ARG:O	2.13	0.48
1:A:181:ASN:HD22	1:A:185:PHE:HB2	1.77	0.48
1:C:90:ARG:NH1	1:C:107:GLU:OE1	2.44	0.48
1:A:255:GLU:H	1:A:255:GLU:CD	2.16	0.48
1:B:213:GLU:O	1:B:216:LYS:HG2	2.13	0.48
1:A:105:ILE:HD12	1:A:215:MET:CE	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:GLY:O	1:B:321:ARG:HG2	2.14	0.48
1:A:235:LEU:HA	1:A:252:MET:HE1	1.95	0.48
1:C:293:ASN:HB3	1:C:349:ASN:HD22	1.78	0.48
1:C:92:ILE:HG12	1:C:105:ILE:CD1	2.44	0.48
1:A:178:LYS:HB2	1:A:178:LYS:HZ3	1.79	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
1:B:300:GLU:CD	1:B:323:ARG:NH2	2.67	0.47
1:A:210:GLN:O	1:A:214:LEU:HD23	2.14	0.47
1:A:23:TYR:CZ	1:A:25:SER:HB3	2.50	0.47
1:B:141:ASN:HB3	1:C:53:GLN:O	2.14	0.47
1:C:266:PHE:C	1:C:266:PHE:CD2	2.88	0.47
1:A:236:ARG:NH1	1:A:250:TYR:CE1	2.83	0.47
1:A:38:TYR:CE2	1:A:205:GLU:HB2	2.49	0.47
1:A:270:VAL:O	1:A:349:ASN:HA	2.15	0.47
1:A:85:VAL:HG21	1:A:351:PHE:CZ	2.49	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:270:VAL:O	1:C:349:ASN:HA	2.15	0.46
1:C:30:PHE:CZ	1:C:44:LEU:HD13	2.50	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:HD3	1:A:178:LYS:N	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:C:237:ASN:C	1:C:237:ASN:HD22	2.20	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:B:266:PHE:C	1:B:266:PHE:CD2	2.90	0.45
1:A:219:LYS:HB3	1:A:219:LYS:HZ3	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:336:ALA:O	1:C:337:ALA:HB3	2.17	0.45
1:A:107:GLU:HB2	1:A:110:HIS:CE1	2.52	0.45
1:A:97:ASN:HB3	1:A:98:PRO:CD	2.47	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
1:B:379:GLU:O	1:B:382:GLU:HB3	2.17	0.44
1:C:165:SER:HG	1:C:168:ILE:HG12	1.81	0.44
1:A:72:LEU:HD13	1:A:123:VAL:HG22	1.99	0.44
1:A:99:ASP:O	1:A:100:SER:HB3	2.18	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:A:265:VAL:HA	1:A:354:GLY:O	2.17	0.43
1:A:181:ASN:ND2	1:A:185:PHE:HB2	2.33	0.43
1:A:266:PHE:CD2	1:A:266:PHE:C	2.91	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: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:122:LEU:HD21	1:C:133:ILE:CD1	2.49	0.43
1:C:68:LYS:HA	1:C:130:ASN:HD22	1.83	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:HG2	1:A:68:LYS:H	1.63	0.43
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:A:406:ASP:C	1:A:408:GLN:H	2.23	0.42
1:B:112:GLN:NE2	1:B:112:GLN:HA	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:A:92:ILE:HG12	1:A:215:MET:HE2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:300:GLU:OE1	1:B:323:ARG:NH2	2.53	0.42
1:B:74:LEU:HB3	1:B:75:PRO:HD2	2.02	0.42
1:A:112:GLN:HE22	1:A:259:GLN:HE22	1.67	0.42
1:A:58:GLU:HG3	1:A:59:ASN:ND2	2.35	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
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:C:188:GLU:O	1:C:188:GLU:HG2	2.20	0.41
1:B:112:GLN:HE22	1:B:259:GLN:HE22	1.69	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: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:213:GLU:HA	1:B:213:GLU:OE2	2.21	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:HG2	1:A:397:LYS:O	2.21	0.41
1:B:283:ASN:HD21	1:B:362:ARG:HD3	1.84	0.41
1:A:298:LYS:HZ2	1:A:325:GLU:HG2	1.86	0.40
1:A:37:GLN:NE2	1:A:37:GLN:H	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:408:GLN:CB	1:C:409:PRO:CA	2.94	0.40
1:A:219:LYS:CB	1:A:219:LYS:NZ	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: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

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	367/433 (85%)	347 (95%)	18 (5%)	2 (0%)	32	33
1	B	374/433 (86%)	357 (96%)	15 (4%)	2 (0%)	32	33
1	C	368/433 (85%)	354 (96%)	13 (4%)	1 (0%)	44	50
All	All	1109/1299 (85%)	1058 (95%)	46 (4%)	5 (0%)	32	33

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

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%)	315 (94%)	22 (6%)	20	19
1	B	342/390 (88%)	324 (95%)	18 (5%)	26	28
1	C	339/390 (87%)	324 (96%)	15 (4%)	33	37
All	All	1018/1170 (87%)	963 (95%)	55 (5%)	26	27

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

Mol	Chain	Res	Type
1	A	29	ARG
1	A	37	GLN
1	A	45	HIS
1	A	81	ASP
1	A	147	GLN
1	A	148	ASP
1	A	151	LEU
1	A	157	GLN
1	A	162	ARG
1	A	178	LYS
1	A	181	ASN
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	266	PHE
1	A	293	ASN
1	A	320	GLN
1	A	348	LEU
1	A	390	LYS
1	B	16	ARG
1	B	20	ASN
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	234	ASN
1	B	236	ARG
1	B	255	GLU
1	B	260	LEU
1	B	266	PHE
1	B	293	ASN
1	B	343	ASN
1	C	81	ASP
1	C	90	ARG
1	C	107	GLU

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Mol	Chain	Res	Type
1	C	124	ASN
1	C	157	GLN
1	C	198	ARG
1	C	229	GLN
1	C	237	ASN
1	C	255	GLU
1	C	260	LEU
1	C	266	PHE
1	C	270	VAL
1	C	293	ASN
1	C	394	LYS
1	C	398	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	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	167	ASN
1	A	181	ASN
1	A	237	ASN
1	A	293	ASN
1	A	349	ASN
1	A	356	ASN
1	A	359	ASN
1	A	360	ASN
1	A	361	GLN
1	A	408	GLN
1	B	20	ASN
1	B	59	ASN
1	B	70	ASN
1	B	88	ASN
1	B	112	GLN
1	B	130	ASN
1	B	212	GLN

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Mol	Chain	Res	Type
1	B	234	ASN
1	B	283	ASN
1	B	293	ASN
1	B	343	ASN
1	B	356	ASN
1	B	359	ASN
1	B	360	ASN
1	B	361	GLN
1	C	45	HIS
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	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	343	ASN
1	C	349	ASN
1	C	356	ASN
1	C	360	ASN
1	C	361	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

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
3	CIT	A	1285	-	3,12,12	1.72	1 (33%)	3,17,17	1.68	1 (33%)
4	ACY	A	460	-	1,3,3	1.77	0	0,3,3	0.00	-
3	CIT	B	1284	-	3,12,12	1.73	1 (33%)	3,17,17	1.56	1 (33%)
4	ACY	B	461	-	1,3,3	1.41	0	0,3,3	0.00	-
3	CIT	C	1283	-	3,12,12	2.00	1 (33%)	3,17,17	1.53	1 (33%)
4	ACY	C	462	-	1,3,3	1.18	0	0,3,3	0.00	-

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	-	-	0/6/16/16	0/0/0/0
4	ACY	A	460	-	-	0/0/0/0	0/0/0/0
3	CIT	B	1284	-	-	0/6/16/16	0/0/0/0
4	ACY	B	461	-	-	0/0/0/0	0/0/0/0
3	CIT	C	1283	-	-	0/6/16/16	0/0/0/0
4	ACY	C	462	-	-	0/0/0/0	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1284	CIT	C4-C3	2.53	1.58	1.54
3	A	1285	CIT	C4-C3	2.56	1.58	1.54
3	C	1283	CIT	C4-C3	3.14	1.59	1.54

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1285	CIT	C3-C4-C5	-2.66	110.80	114.95
3	B	1284	CIT	C3-C4-C5	-2.44	111.13	114.95
3	C	1283	CIT	C3-C4-C5	-2.09	111.69	114.95

There are no chirality outliers.

There are no torsion outliers.

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%)	-0.16	14 (3%) 42 45	21, 37, 70, 107	0
1	B	380/433 (87%)	-0.18	11 (2%) 52 56	21, 35, 63, 86	0
1	C	377/433 (87%)	-0.15	11 (2%) 52 56	21, 35, 68, 99	0
All	All	1132/1299 (87%)	-0.16	36 (3%) 48 52	21, 35, 67, 107	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	227	SER	7.2
1	B	13	SER	6.6
1	B	195	GLU	5.7
1	C	317	LEU	5.3
1	C	221	SER	5.3
1	A	196	GLU	5.2
1	C	229	GLN	5.2
1	B	223	ARG	4.9
1	C	222	SER	4.2
1	A	306	ASP	4.1
1	C	220	SER	3.8
1	B	14	ASP	3.6
1	C	409	PRO	3.5
1	A	220	SER	3.5
1	B	187	GLU	3.5
1	A	228	SER	3.3
1	B	196	GLU	3.2
1	A	186	GLY	3.1
1	B	224	LYS	3.1
1	B	390	LYS	3.0
1	C	314	GLU	2.8
1	C	13	SER	2.7
1	A	221	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	315	GLU	2.7
1	A	177	PHE	2.7
1	C	227	SER	2.5
1	B	409	PRO	2.5
1	B	15	SER	2.5
1	A	214	LEU	2.5
1	A	219	LYS	2.4
1	C	318	GLU	2.4
1	A	14	ASP	2.3
1	C	228	SER	2.3
1	A	187	GLU	2.2
1	A	213	GLU	2.1
1	B	156	ALA	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 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
4	ACY	C	462	4/4	0.95	0.23	7.00	35,37,37,40	0
3	CIT	A	1285	13/13	0.67	0.29	5.65	84,85,86,87	0
3	CIT	B	1284	13/13	0.61	0.28	5.11	90,92,94,94	0
4	ACY	B	461	4/4	0.97	0.17	3.66	38,39,40,42	0
3	CIT	C	1283	13/13	0.67	0.23	3.51	82,83,85,85	0
4	ACY	A	460	4/4	0.96	0.14	2.20	38,39,40,41	0
2	CA	A	906	1/1	0.97	0.13	0.93	66,66,66,66	0
2	CA	B	905	1/1	0.92	0.17	-0.19	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	CA	C	904	1/1	0.86	0.08	-1.19	79,79,79,79	0

6.5 Other polymers [i](#)

There are no such residues in this entry.