Full wwPDB X-ray Structure Validation Report (i)

Oct 16, 2023 – 06:42 AM EDT

PDB ID	:	2EA7
Title	:	Crystal Structure of Adzuki Bean 7S Globulin-1
Authors	:	Fukuda, T.; Mikami, B.; Utsumi, S.
Deposited on	:	2007-01-30
Resolution	:	1.80 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 (i) 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 (i)) were used in the production of this report:

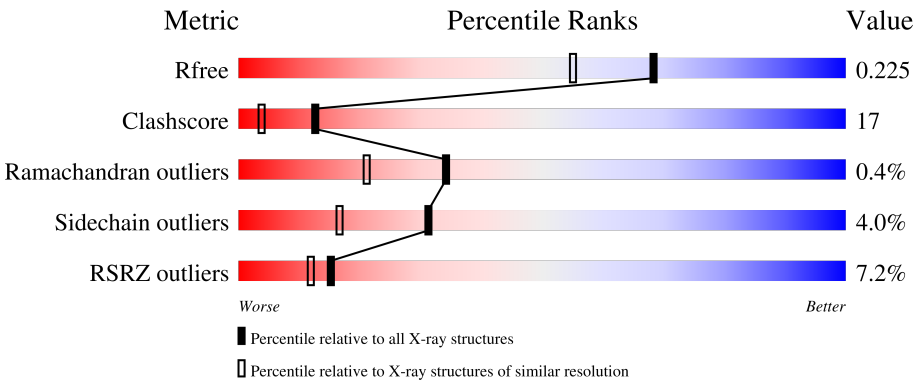
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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

Mol	Chain	Length	Quality of chain
1	A	434	9% 65% 23% • 10%
1	B	434	6% 66% 20% • 12%
1	C	434	4% 66% 19% • 13%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 10203 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.

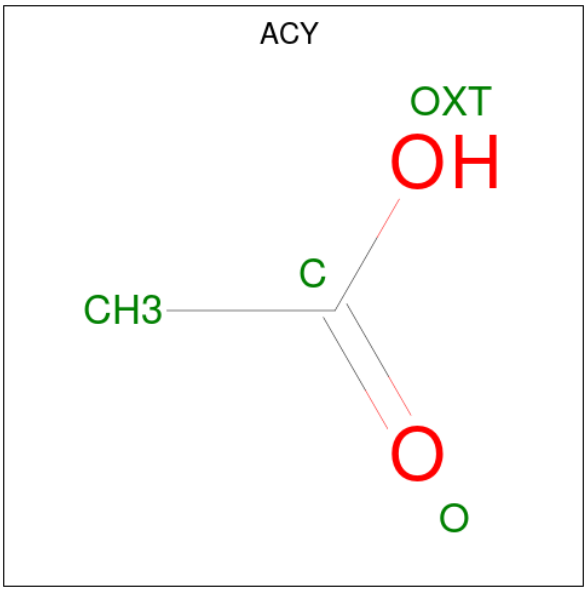
- Molecule 1 is a protein called 7S globulin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	390	3187	2015	554	612	6	0	6	0
1	B	382	3127	1980	547	594	6	0	7	0
1	C	379	3116	1978	540	591	7	0	11	0

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

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

- Molecule 3 is ACETIC ACID (three-letter code: ACY) (formula: $C_2H_4O_2$).



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

- Molecule 4 is water.

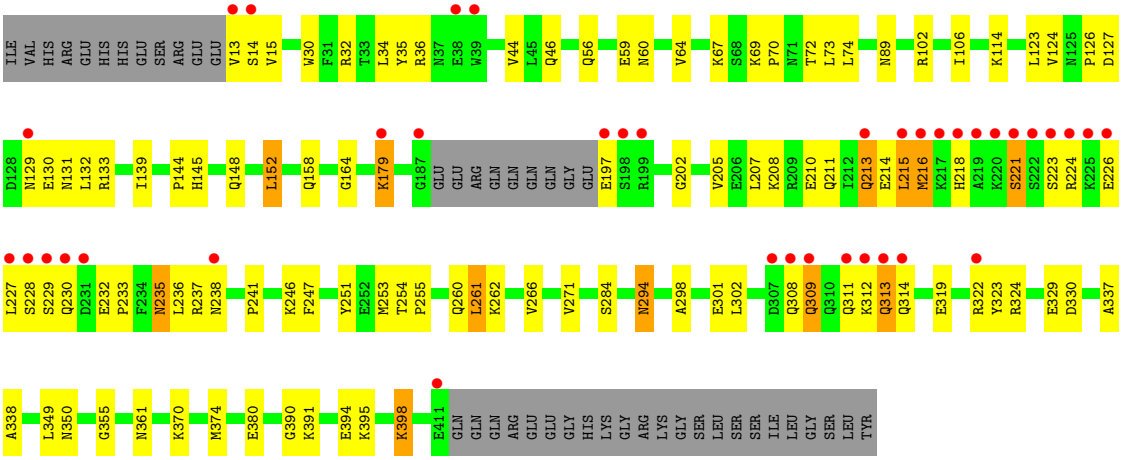
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	214	214	214	0	0
			Total	O		
4	B	247	247	247	0	0
			Total	O		
4	C	296	296	296	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

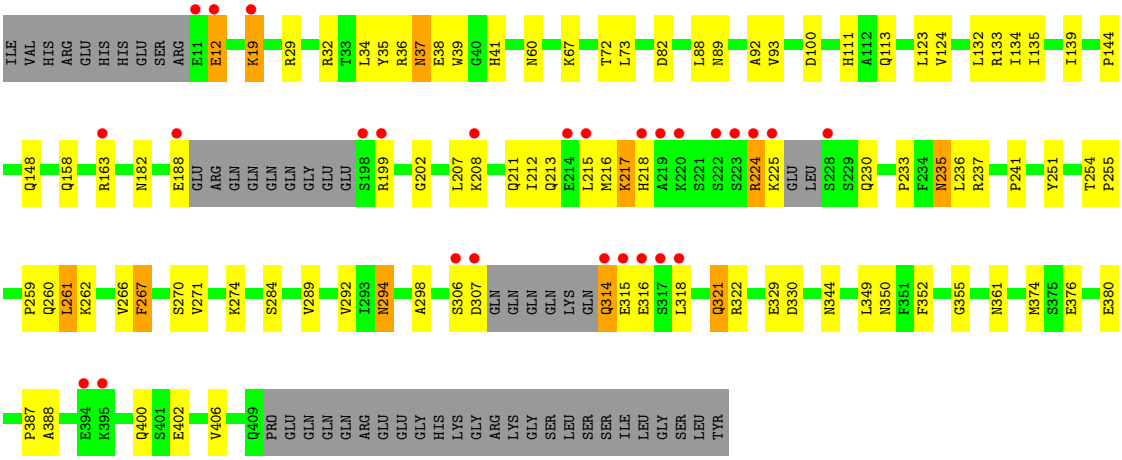
• Molecule 1: 7S globulin-1

Chain A:



• Molecule 1: 7S globulin-1

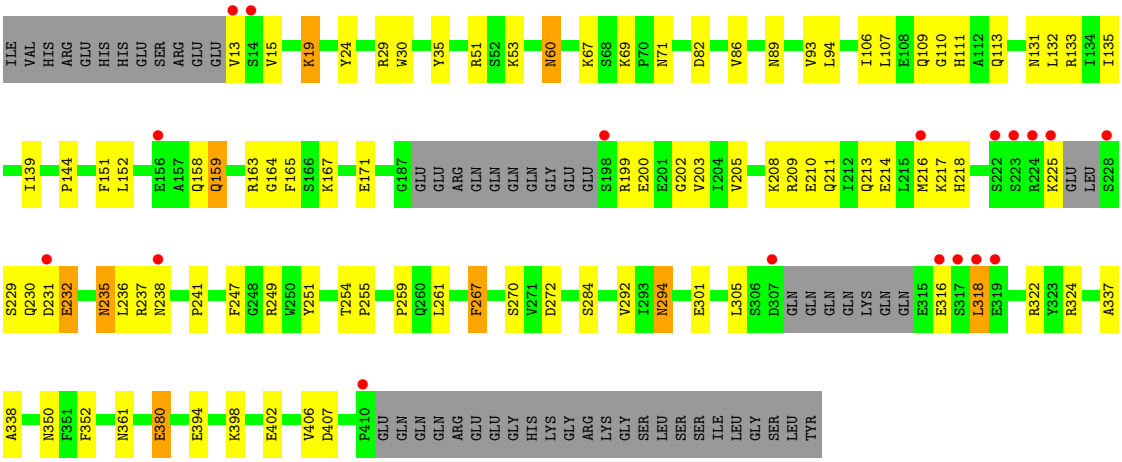
Chain B:



• Molecule 1: 7S globulin-1

Chain C:

4%
66%
19%
13%


ILE VAL HIS ARG GLU HIS HIS GLU SER ARG GLU GLU V13 S14 V15 K19 Y24 R29 W30 Y35 R51 S52 K53 N60 K67 S68 K69 P70 N71 D82 V86 N89 V93 L94 I106 L107 E108 Q109 G110 H111 A112 Q113 N131 L132 R133 I134 I135
I139 P144 F151 L152 E156 A157 Q158 Q159 R163 G164 F165 S166 K167 E171 G187 GLU GLU GLU ARG GLN GLN GLN GLN GLN GLY GLU GLU S198 R199 E200 E201 G202 V203 I204 V205 K208 R209 E210 Q211 I212 Q213 E214 L215 M216 K217 H218 S222 S223 R224 K225 GLU LEU S228
S229 Q230 D231 E232 N235 L236 R237 N238 P241 F247 G248 R249 W250 Y251 T254 P255 P259 Q260 L261 F267 S270 V271 D272 S284 V292 I293 N294 E301 L305 S306 D307 GLN GLN GLN GLN LYS GLN GLN E315 E316 S317 L318 E319 R322 Y323 R324 A337
A338 N350 F351 F352 N361 E380 E394 K398 E402 V406 D407 P410 GLU GLN GLN GLN ARG GLU GLU GLY HIS LYS GLY ARG LYS GLY SER LEU SER SER ILE LEU GLY SER LEU TYR

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	101.60Å 48.55Å 119.77Å 90.00° 97.12° 90.00°	Depositor
Resolution (Å)	14.98 – 1.80 44.94 – 1.80	Depositor EDS
% Data completeness (in resolution range)	97.4 (14.98-1.80) 97.5 (44.94-1.80)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.44 (at 1.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.193 , 0.228 0.189 , 0.225	Depositor DCC
R_{free} test set	10508 reflections (10.03%)	wwPDB-VP
Wilson B-factor (Å^2)	24.4	Xtriage
Anisotropy	0.537	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 51.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	10203	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.58% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ACY, 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	0.31	0/3276	0.59	0/4422
1	B	0.31	0/3217	0.59	0/4338
1	C	0.34	0/3224	0.62	0/4349
All	All	0.32	0/9717	0.60	0/13109

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	3187	0	3123	134	0
1	B	3127	0	3074	94	0
1	C	3116	0	3060	107	0
2	A	1	0	0	0	0
2	B	2	0	0	0	0
2	C	1	0	0	0	0
3	A	4	0	3	1	0
3	B	4	0	3	1	0
3	C	4	0	3	0	0
4	A	214	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	247	0	0	5	0
4	C	296	0	0	10	0
All	All	10203	0	9266	313	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 17.

All (313) 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:19:LYS:HE2	1:B:19:LYS:H	0.99	1.12
1:C:322:ARG:HB3	1:C:324:ARG:HH22	1.19	1.05
1:C:322:ARG:HB3	1:C:324:ARG:NH2	1.75	1.00
1:B:306:SER:HB2	1:B:321:GLN:HE22	1.28	0.98
1:C:35[B]:TYR:OH	1:C:202:GLY:HA3	1.65	0.96
1:B:19:LYS:HE2	1:B:19:LYS:N	1.81	0.95
1:A:322[A]:ARG:HD2	1:A:324:ARG:HG3	1.49	0.94
1:B:19:LYS:H	1:B:19:LYS:CE	1.81	0.93
1:A:223:SER:HB2	1:A:226:GLU:HG2	1.51	0.93
1:C:135:ILE:CD1	1:C:292:VAL:HG21	2.00	0.92
1:A:311:GLN:HG2	1:A:314:GLN:HE21	1.36	0.90
1:B:89[B]:ASN:HD21	1:B:294:ASN:ND2	1.69	0.90
1:A:322[A]:ARG:HH21	1:C:165:PHE:HA	1.39	0.87
1:C:208:LYS:HB2	1:C:211:GLN:HE21	1.39	0.87
1:B:32:ARG:HH22	1:C:316:GLU:HB2	1.39	0.86
1:B:89[B]:ASN:HD21	1:B:294:ASN:HD21	1.27	0.81
1:C:318:LEU:HD13	1:C:318:LEU:H	1.45	0.81
1:A:226:GLU:HB3	1:A:233:PRO:O	1.79	0.81
1:C:208:LYS:H	1:C:211:GLN:NE2	1.79	0.81
1:A:235:ASN:HD21	1:A:237:ARG:HB2	1.46	0.80
1:A:301:GLU:HG2	1:A:324:ARG:HG2	1.65	0.79
1:B:217:LYS:HG2	1:B:218:HIS:ND1	1.97	0.78
1:A:308:GLN:HG3	1:A:319:GLU:OE2	1.82	0.78
1:B:93:VAL:HB	1:B:124[A]:VAL:CG1	2.14	0.78
1:B:199:ARG:HA	4:C:745:HOH:O	1.82	0.77
1:C:71:ASN:HD21	1:C:209:ARG:HH11	1.34	0.74
1:C:208:LYS:H	1:C:211:GLN:HE21	1.35	0.74
1:C:19:LYS:H	1:C:19:LYS:HD2	1.53	0.73
1:B:89[B]:ASN:ND2	1:B:294:ASN:HD21	1.85	0.73
1:C:135:ILE:HD13	1:C:292:VAL:HG21	1.70	0.73
1:A:302:LEU:N	1:A:322[A]:ARG:NH1	2.38	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:380:GLU:CD	1:C:380:GLU:H	1.94	0.70
1:A:322[A]:ARG:CD	1:A:324:ARG:HE	2.05	0.69
1:C:324:ARG:NH2	4:C:657:HOH:O	2.25	0.69
1:C:29:ARG:HH11	1:C:29:ARG:HG2	1.58	0.69
1:C:93:VAL:HG22	1:C:106:ILE:HD13	1.74	0.68
1:B:89[B]:ASN:ND2	1:B:133:ARG:NH1	2.43	0.66
1:C:13:VAL:HA	1:C:322:ARG:NH2	2.10	0.66
1:B:35:TYR:OH	1:B:202:GLY:HA3	1.96	0.66
1:A:235:ASN:ND2	1:A:237:ARG:H	1.93	0.65
1:A:164:GLY:O	1:B:322:ARG:HD3	1.96	0.65
1:A:301:GLU:HB3	1:A:322[A]:ARG:CZ	2.25	0.65
1:C:24:TYR:O	1:C:51:ARG:NH2	2.30	0.65
1:C:301:GLU:HG2	1:C:324:ARG:CD	2.25	0.65
1:A:241:PRO:HG3	1:A:251:TYR:CE2	2.32	0.64
1:B:254:THR:HB	1:B:255:PRO:HD2	1.79	0.64
1:A:74:LEU:HB3	1:A:123:LEU:HD23	1.80	0.64
1:A:322[A]:ARG:NH2	1:C:165:PHE:HA	2.12	0.63
1:B:306:SER:CB	1:B:321:GLN:HE22	2.06	0.63
1:C:301:GLU:HG2	1:C:324:ARG:HD3	1.80	0.63
1:B:224:ARG:N	1:B:224:ARG:HD2	2.13	0.63
1:A:322[A]:ARG:HD2	1:A:324:ARG:HE	1.62	0.62
1:A:322[A]:ARG:HD3	1:A:323:TYR:N	2.15	0.62
1:A:322[A]:ARG:HD2	1:A:324:ARG:CG	2.28	0.62
1:A:215:LEU:HD12	1:A:216:MET:N	2.14	0.62
1:C:53:LYS:HD3	4:C:731:HOH:O	1.99	0.62
1:A:322[A]:ARG:CD	1:A:324:ARG:NE	2.63	0.61
1:A:60[B]:ASN:ND2	1:A:139:ILE:HG23	2.15	0.61
1:A:322[A]:ARG:HD2	1:A:324:ARG:NE	2.16	0.61
1:C:230:GLN:OE1	1:C:259:PRO:HB2	2.01	0.61
1:B:92:ALA:HB1	1:B:123:LEU:HD11	1.82	0.61
1:C:133:ARG:NH2	1:C:294:ASN:ND2	2.49	0.61
1:B:37:ASN:ND2	1:B:39:TRP:H	2.00	0.60
1:B:380:GLU:H	1:B:380:GLU:CD	2.02	0.60
1:A:322[A]:ARG:HE	1:A:324:ARG:HH21	1.48	0.60
1:A:197:GLU:HG2	1:B:388:ALA:HA	1.83	0.60
1:B:36:ARG:HG3	1:B:41:HIS:HB3	1.82	0.60
1:A:226:GLU:HB2	4:A:658:HOH:O	2.01	0.60
1:A:391:LYS:HB3	1:A:391:LYS:NZ	2.17	0.60
1:A:14:SER:O	1:A:322[A]:ARG:HB3	2.02	0.60
1:A:197:GLU:HG3	1:B:387:PRO:O	2.01	0.59
1:A:390:GLY:O	1:A:394:GLU:HG3	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:209:ARG:CZ	1:C:213:GLN:NE2	2.65	0.59
1:C:133:ARG:HH22	1:C:294:ASN:HD22	1.50	0.59
1:A:32:ARG:HG3	1:B:315:GLU:HG2	1.85	0.58
1:A:309:GLN:HE22	1:A:311:GLN:C	2.06	0.58
1:C:318:LEU:H	1:C:318:LEU:CD1	2.16	0.58
1:C:318:LEU:HD22	1:C:318:LEU:O	2.03	0.58
1:A:32:ARG:CG	1:B:315:GLU:HG2	2.33	0.58
1:A:35:TYR:OH	1:A:202:GLY:HA3	2.03	0.58
1:B:93:VAL:HB	1:B:124[A]:VAL:HG12	1.84	0.58
1:B:135:ILE:HD13	1:B:292:VAL:HG11	1.85	0.58
1:B:306:SER:HB2	1:B:321:GLN:NE2	2.10	0.58
1:A:106:ILE:HB	1:A:221:SER:HA	1.85	0.58
1:A:395:LYS:O	1:A:398:LYS:HD3	2.03	0.58
1:B:139:ILE:HD12	1:B:139:ILE:N	2.19	0.58
1:C:199:ARG:HA	4:C:668:HOH:O	2.03	0.57
1:A:322[A]:ARG:HG2	1:A:324:ARG:CZ	2.35	0.57
1:A:284:SER:HB3	1:A:361:ASN:HD21	1.69	0.57
1:B:307:ASP:O	1:B:316:GLU:HB2	2.04	0.57
1:C:209:ARG:HG2	4:C:748:HOH:O	2.04	0.57
1:A:302:LEU:N	1:A:322[A]:ARG:HH12	2.02	0.57
1:B:224:ARG:HA	4:B:681:HOH:O	2.04	0.57
1:C:167:LYS:O	1:C:171:GLU:HG3	2.04	0.57
1:C:237[B]:ARG:NH2	1:C:272:ASP:OD2	2.35	0.57
1:A:230:GLN:HA	1:A:260:GLN:HG3	1.86	0.57
1:B:402:GLU:HB3	1:B:406:VAL:HG12	1.87	0.57
1:C:241:PRO:HG3	1:C:251:TYR:CE2	2.39	0.57
1:B:37:ASN:C	1:B:37:ASN:HD22	2.07	0.56
1:A:179:LYS:HE2	4:A:654:HOH:O	2.04	0.56
1:A:208:LYS:NZ	1:A:208:LYS:HB3	2.20	0.56
1:A:301:GLU:HB3	1:A:322[A]:ARG:NH1	2.19	0.56
1:A:133:ARG:HH12	1:A:294:ASN:HD22	1.53	0.56
1:A:133:ARG:HH12	1:A:294:ASN:ND2	2.02	0.56
1:A:322[A]:ARG:HH21	1:C:165:PHE:CA	2.15	0.56
1:A:210:GLU:CD	1:A:210:GLU:H	2.10	0.55
1:B:93:VAL:HB	1:B:124[A]:VAL:HG13	1.89	0.55
1:C:139:ILE:N	1:C:139:ILE:HD12	2.22	0.55
1:A:370:LYS:HD2	4:C:665:HOH:O	2.07	0.55
1:B:93:VAL:O	1:B:123:LEU:HD12	2.07	0.55
1:B:241:PRO:HG3	1:B:251:TYR:CE2	2.42	0.54
1:C:159[A]:GLN:NE2	1:C:163:ARG:HB2	2.23	0.54
1:C:394:GLU:O	1:C:398:LYS:HG2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:GLU:C	1:A:322[A]:ARG:HH12	2.10	0.54
1:A:374:MET:HG2	1:C:152:LEU:HD21	1.89	0.54
1:A:322[A]:ARG:NH2	1:C:164:GLY:O	2.41	0.54
1:A:309:GLN:NE2	1:A:311:GLN:O	2.41	0.54
1:B:111:HIS:HD2	4:B:615:HOH:O	1.91	0.54
1:C:19:LYS:HD2	1:C:19:LYS:N	2.23	0.54
1:C:93:VAL:HG22	1:C:106:ILE:CD1	2.38	0.54
1:B:208:LYS:H	1:B:211:GLN:NE2	2.05	0.54
1:A:261:LEU:HG	1:A:266:VAL:O	2.07	0.53
1:C:30:TRP:CH2	1:C:51:ARG:HD3	2.43	0.53
1:A:322[A]:ARG:NE	1:A:324:ARG:HE	2.07	0.53
1:B:230:GLN:HA	1:B:260:GLN:HG3	1.90	0.53
1:B:236:LEU:HD11	1:B:270:SER:HB2	1.91	0.53
1:A:235:ASN:ND2	1:A:237:ARG:HB2	2.20	0.53
1:C:135:ILE:HD11	1:C:292:VAL:HG21	1.85	0.53
1:C:133:ARG:HH22	1:C:294:ASN:ND2	2.05	0.53
1:C:254:THR:HB	1:C:255:PRO:HD2	1.90	0.53
1:C:229:SER:HB3	1:C:232:GLU:HB2	1.89	0.53
1:C:19:LYS:H	1:C:19:LYS:CD	2.13	0.53
1:A:322[A]:ARG:NE	1:C:164:GLY:O	2.42	0.53
1:B:284:SER:HB3	1:B:361:ASN:HD21	1.74	0.53
1:A:230:GLN:HE21	1:A:260:GLN:HA	1.74	0.52
1:B:182:ASN:ND2	1:B:188:GLU:HG2	2.24	0.52
1:A:301:GLU:C	1:A:322[A]:ARG:NH1	2.62	0.52
1:A:73:LEU:HD13	1:A:124:VAL:HG22	1.91	0.52
1:A:210:GLU:O	1:A:214:GLU:HG3	2.08	0.52
1:A:44:VAL:HG22	1:A:64:VAL:HG22	1.91	0.52
1:C:217:LYS:HE3	1:C:218:HIS:CE1	2.45	0.52
1:A:215:LEU:HD23	1:B:380:GLU:HG2	1.93	0.51
1:B:208:LYS:H	1:B:211:GLN:HE21	1.58	0.51
1:A:36:ARG:HH11	1:A:36:ARG:HG3	1.75	0.51
1:A:309:GLN:NE2	1:A:314:GLN:HB2	2.25	0.51
1:B:148[A]:GLN:OE1	1:C:305:LEU:HB2	2.11	0.51
1:A:227:LEU:O	1:A:227:LEU:HD12	2.11	0.51
1:A:59:GLU:OE1	1:A:145:HIS:HE1	1.93	0.51
1:C:69:LYS:HA	1:C:131[A]:ASN:HD22	1.75	0.50
1:B:34:LEU:HD22	1:C:316:GLU:OE1	2.11	0.50
1:B:314:GLN:NE2	1:B:314:GLN:N	2.60	0.50
1:A:72:THR:O	1:A:124:VAL:HG13	2.12	0.50
1:A:380[A]:GLU:HG2	4:A:635:HOH:O	2.11	0.49
1:C:133:ARG:NH2	1:C:294:ASN:HD22	2.08	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:GLU:HG3	1:A:233:PRO:HD2	1.94	0.49
1:B:67:LYS:HA	1:B:132:LEU:O	2.12	0.49
1:A:60[B]:ASN:HD21	1:A:139:ILE:HG23	1.76	0.49
1:C:208:LYS:HB2	1:C:211:GLN:NE2	2.19	0.49
1:C:322:ARG:CB	1:C:324:ARG:HH22	2.07	0.49
1:A:34:LEU:HG	1:A:44:VAL:HG23	1.94	0.49
1:C:229:SER:CB	1:C:232:GLU:HB2	2.42	0.49
1:B:89[B]:ASN:ND2	1:B:294:ASN:ND2	2.46	0.49
1:B:163[A]:ARG:NH2	1:C:322:ARG:NH1	2.60	0.49
1:C:402:GLU:HB2	1:C:406:VAL:HG12	1.95	0.49
1:A:309:GLN:HE22	1:A:311:GLN:CA	2.26	0.49
1:C:135:ILE:HD12	1:C:292:VAL:HG11	1.94	0.48
1:C:60[B]:ASN:OD1	1:C:144:PRO:HB2	2.12	0.48
1:C:71:ASN:HD21	1:C:209:ARG:NH1	2.06	0.48
1:A:294:ASN:CB	1:A:350:ASN:HD22	2.27	0.48
1:A:60[B]:ASN:HD21	1:A:139:ILE:CG2	2.27	0.48
1:A:148:GLN:NE2	1:B:318:LEU:HD22	2.28	0.48
1:A:73:LEU:HB3	1:A:207:LEU:HD11	1.95	0.48
1:B:36:ARG:HG2	1:B:37:ASN:N	2.29	0.48
1:C:110:GLY:HA3	1:C:237[A]:ARG:NH1	2.29	0.48
1:A:271:VAL:O	1:A:350:ASN:HA	2.13	0.48
1:C:151:PHE:CE2	1:C:203:VAL:HB	2.49	0.48
1:C:13:VAL:O	1:C:13:VAL:HG13	2.14	0.48
1:C:109:GLN:NE2	4:C:733:HOH:O	2.47	0.47
1:A:207:LEU:HD12	1:A:207:LEU:N	2.28	0.47
1:A:230:GLN:NE2	1:A:260:GLN:HG2	2.29	0.47
1:B:163[A]:ARG:NH2	1:C:322:ARG:HH12	2.12	0.47
1:A:34:LEU:HD11	1:A:44:VAL:CG2	2.44	0.47
1:A:67:LYS:HA	1:A:132:LEU:O	2.15	0.47
1:B:213:GLN:HA	1:B:213:GLN:HE21	1.79	0.47
1:A:255:PRO:HB3	1:A:262:LYS:HA	1.95	0.47
1:B:274:LYS:HE3	4:B:678:HOH:O	2.14	0.47
1:A:298:ALA:HB2	1:A:349:LEU:HD22	1.97	0.47
1:C:231:ASP:HB2	4:C:755:HOH:O	2.14	0.46
1:A:294:ASN:HB3	1:A:350:ASN:HD22	1.80	0.46
1:A:311:GLN:O	1:A:314:GLN:HB2	2.14	0.46
1:B:289:VAL:HG11	3:B:461:ACY:H2	1.97	0.46
1:C:15:VAL:HG12	1:C:322:ARG:HB2	1.97	0.46
1:A:32:ARG:HB2	1:A:46[A]:GLN:NE2	2.30	0.46
1:B:215:LEU:HD21	1:C:380:GLU:HG2	1.96	0.46
1:C:249:ARG:HD2	1:C:251:TYR:OH	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:294:ASN:HB3	1:C:350:ASN:HD22	1.80	0.46
1:B:60:ASN:ND2	1:B:144:PRO:HB2	2.31	0.46
1:C:284:SER:HB3	1:C:361:ASN:HD21	1.81	0.46
1:B:213:GLN:HA	1:B:213:GLN:NE2	2.31	0.45
1:A:56:GLN:NE2	4:A:574:HOH:O	2.49	0.45
1:A:127:ASP:OD2	1:A:130:GLU:HB2	2.16	0.45
1:C:29:ARG:HG2	1:C:29:ARG:NH1	2.29	0.45
1:A:152:LEU:HD11	1:B:374:MET:HG2	1.99	0.45
1:B:123:LEU:HD21	1:B:134:ILE:CD1	2.45	0.45
1:B:294:ASN:C	1:B:294:ASN:HD22	2.20	0.45
1:A:114:LYS:HD3	1:A:230:GLN:HE22	1.82	0.45
1:B:225:LYS:HD2	1:B:225:LYS:N	2.32	0.45
1:B:329:GLU:O	1:B:330:ASP:HB2	2.17	0.45
1:A:322[A]:ARG:HH21	1:C:164:GLY:C	2.20	0.45
1:B:230:GLN:HG2	1:B:259:PRO:HB2	1.98	0.45
1:B:261:LEU:HG	1:B:266:VAL:O	2.16	0.45
1:C:71:ASN:ND2	1:C:209:ARG:HH11	2.10	0.45
1:A:70:PRO:HD3	1:A:131:ASN:ND2	2.32	0.45
1:B:12:GLU:N	1:B:12:GLU:OE1	2.50	0.45
1:B:271:VAL:O	1:B:350:ASN:HA	2.17	0.45
1:C:107:LEU:HA	4:C:650:HOH:O	2.17	0.45
1:A:34:LEU:HD11	1:A:44:VAL:HG21	1.99	0.44
1:A:309:GLN:NE2	1:A:311:GLN:H	2.15	0.44
1:B:89[B]:ASN:CG	1:B:294:ASN:HD21	2.19	0.44
1:A:32:ARG:HB2	1:A:46[A]:GLN:HE22	1.82	0.44
1:A:309:GLN:HE22	1:A:311:GLN:N	2.15	0.44
1:C:200:GLU:HG3	1:C:205:VAL:HG11	2.00	0.44
1:A:302:LEU:O	1:A:322[A]:ARG:NH1	2.51	0.44
1:B:182:ASN:HD21	1:B:188:GLU:HG2	1.82	0.44
1:B:267:PHE:C	1:B:267:PHE:CD2	2.90	0.44
1:C:208:LYS:N	1:C:211:GLN:HE21	2.11	0.44
1:C:322:ARG:HD3	1:C:324:ARG:HH12	1.83	0.44
1:A:311:GLN:CG	1:A:314:GLN:HG3	2.47	0.44
3:A:460:ACY:H3	4:A:485:HOH:O	2.18	0.44
1:A:232:GLU:HG2	4:A:657:HOH:O	2.18	0.43
1:A:246:LYS:HE3	1:A:247:PHE:CE2	2.53	0.43
1:B:207:LEU:HD12	1:B:212:ILE:HD13	2.00	0.43
1:C:225:LYS:O	1:C:225:LYS:HG2	2.19	0.43
1:A:302:LEU:C	1:A:322[A]:ARG:NH1	2.72	0.43
1:A:380[A]:GLU:OE1	1:C:211:GLN:OE1	2.36	0.43
1:C:113[B]:GLN:NE2	1:C:231:ASP:O	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:ASP:OD2	1:A:130:GLU:N	2.51	0.43
1:A:266:VAL:HA	1:A:355:GLY:O	2.18	0.43
1:B:212:ILE:O	1:B:216:MET:HG2	2.19	0.43
1:C:35[B]:TYR:CD2	1:C:203:VAL:HG22	2.54	0.43
1:B:217:LYS:HD3	1:B:217:LYS:N	2.33	0.43
1:C:267:PHE:C	1:C:267:PHE:CD2	2.92	0.43
1:A:36:ARG:HG3	1:A:36:ARG:NH1	2.33	0.43
1:B:89[B]:ASN:HD21	1:B:133:ARG:NH1	2.15	0.43
1:B:100:ASP:OD1	1:B:100:ASP:N	2.52	0.43
1:C:13:VAL:O	1:C:13:VAL:HG22	2.18	0.43
1:A:309:GLN:CD	1:A:311:GLN:H	2.22	0.42
1:A:205:VAL:HG23	1:A:207:LEU:HD11	2.01	0.42
1:C:318:LEU:HD13	1:C:318:LEU:N	2.25	0.42
1:A:208:LYS:H	1:A:211:GLN:NE2	2.17	0.42
1:A:30:TRP:O	1:A:46[A]:GLN:HG2	2.19	0.42
1:B:217:LYS:HD3	1:B:217:LYS:H	1.84	0.42
1:B:255:PRO:CB	1:B:262:LYS:HA	2.50	0.42
1:C:111:HIS:HE1	4:C:673:HOH:O	2.03	0.42
1:B:400:GLN:OE1	1:B:402:GLU:HB2	2.20	0.42
1:C:294:ASN:CB	1:C:350:ASN:HD22	2.33	0.42
1:B:88:LEU:HD11	1:B:135:ILE:CG2	2.50	0.42
1:C:94:LEU:HD23	1:C:113[A]:GLN:OE1	2.19	0.42
1:A:102:ARG:HD3	1:B:376:GLU:O	2.20	0.42
1:A:311:GLN:HG3	1:A:314:GLN:HG3	2.02	0.42
1:B:37:ASN:ND2	1:B:37:ASN:C	2.71	0.42
1:C:86:VAL:HG21	1:C:352:PHE:CZ	2.55	0.42
1:A:210:GLU:CD	1:A:210:GLU:N	2.72	0.42
1:A:311:GLN:HE21	1:A:313:GLN:HG2	1.84	0.42
1:A:391:LYS:HB3	1:A:391:LYS:HZ2	1.83	0.42
1:C:318:LEU:HD22	1:C:318:LEU:C	2.40	0.42
1:A:218:HIS:HA	4:A:628:HOH:O	2.20	0.41
1:A:337:ALA:O	1:A:338:ALA:HB3	2.20	0.41
1:B:113:GLN:HB2	1:B:233:PRO:HB3	2.01	0.41
1:A:229:SER:HB2	1:A:232:GLU:CB	2.50	0.41
1:C:337:ALA:O	1:C:338:ALA:HB3	2.20	0.41
1:B:73:LEU:HD13	1:B:124[B]:VAL:HG22	2.02	0.41
1:A:205:VAL:HG23	1:A:207:LEU:CD1	2.50	0.41
1:A:213:GLN:OE1	1:A:213:GLN:N	2.54	0.41
1:A:329:GLU:O	1:A:330:ASP:HB2	2.21	0.41
1:A:69:LYS:HE2	1:A:69:LYS:HB3	1.83	0.41
1:C:89[B]:ASN:HD22	1:C:133:ARG:HH21	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:209:ARG:HD2	1:C:209:ARG:HA	1.88	0.41
1:C:236:LEU:HD11	1:C:270:SER:HB2	2.02	0.41
1:B:38:GLU:HG2	4:B:637:HOH:O	2.20	0.41
1:A:246:LYS:HE3	1:A:247:PHE:CZ	2.56	0.41
1:C:106:ILE:HD11	1:C:216[A]:MET:HG3	2.03	0.41
1:A:124:VAL:O	1:A:126:PRO:HD3	2.20	0.41
1:A:133:ARG:NH1	1:A:294:ASN:ND2	2.68	0.41
1:A:254:THR:HB	1:A:255:PRO:HD2	2.02	0.41
1:B:29:ARG:NH2	4:B:630:HOH:O	2.54	0.41
1:B:135:ILE:HD11	1:B:352:PHE:CD2	2.56	0.40
1:C:67:LYS:HA	1:C:132:LEU:O	2.21	0.40
1:C:159[A]:GLN:HE21	1:C:163:ARG:HG2	1.86	0.40
1:A:395:LYS:O	1:A:398:LYS:CD	2.69	0.40
1:B:298:ALA:HB2	1:B:349:LEU:HD22	2.02	0.40
1:C:69:LYS:HA	1:C:131[A]:ASN:ND2	2.36	0.40
1:C:247:PHE:CZ	1:C:407:ASP:HB2	2.57	0.40
1:A:179:LYS:HD3	1:A:179:LYS:HA	1.90	0.40
1:A:236:LEU:HA	1:A:253:MET:SD	2.61	0.40
1:A:13:VAL:C	1:A:15:VAL:H	2.24	0.40
1:B:72:THR:O	1:B:124[A]:VAL:HG23	2.21	0.40
1:B:225:LYS:HD2	1:B:225:LYS:H	1.86	0.40
1:C:35[B]:TYR:HH	1:C:202:GLY:HA3	1.79	0.40
1:A:70:PRO:HB3	1:A:127:ASP:O	2.21	0.40
1:A:398:LYS:O	1:A:398:LYS:HG2	2.21	0.40
1:B:29:ARG:HB3	1:B:29:ARG:HH21	1.86	0.40
1:B:266:VAL:HA	1:B:355:GLY: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	392/434 (90%)	370 (94%)	17 (4%)	5 (1%)	12 3
1	B	381/434 (88%)	370 (97%)	11 (3%)	0	100 100
1	C	382/434 (88%)	367 (96%)	15 (4%)	0	100 100
All	All	1155/1302 (89%)	1107 (96%)	43 (4%)	5 (0%)	34 21

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	224	ARG
1	A	228	SER
1	A	312	LYS
1	A	221	SER
1	A	313	GLN

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	358/391 (92%)	344 (96%)	14 (4%)	32 17
1	B	351/391 (90%)	337 (96%)	14 (4%)	31 16
1	C	352/391 (90%)	337 (96%)	15 (4%)	29 14
All	All	1061/1173 (90%)	1018 (96%)	43 (4%)	31 16

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

Mol	Chain	Res	Type
1	A	89	ASN
1	A	129	ASN
1	A	152	LEU
1	A	158	GLN
1	A	179	LYS
1	A	213	GLN
1	A	215	LEU
1	A	216	MET

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Mol	Chain	Res	Type
1	A	235	ASN
1	A	238	ASN
1	A	261	LEU
1	A	294	ASN
1	A	309	GLN
1	A	398	LYS
1	B	12	GLU
1	B	19	LYS
1	B	37	ASN
1	B	82	ASP
1	B	158	GLN
1	B	217	LYS
1	B	224	ARG
1	B	235	ASN
1	B	261	LEU
1	B	267	PHE
1	B	294	ASN
1	B	314	GLN
1	B	321	GLN
1	B	344	ASN
1	C	19	LYS
1	C	60[A]	ASN
1	C	60[B]	ASN
1	C	82	ASP
1	C	158	GLN
1	C	159[A]	GLN
1	C	159[B]	GLN
1	C	232	GLU
1	C	235	ASN
1	C	238	ASN
1	C	261	LEU
1	C	267	PHE
1	C	294	ASN
1	C	318	LEU
1	C	380	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	HIS
1	A	56	GLN
1	A	109	GLN

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Mol	Chain	Res	Type
1	A	129	ASN
1	A	131	ASN
1	A	145	HIS
1	A	158	GLN
1	A	211	GLN
1	A	230	GLN
1	A	235	ASN
1	A	238	ASN
1	A	294	ASN
1	A	311	GLN
1	A	314	GLN
1	A	350	ASN
1	A	357	ASN
1	A	360	ASN
1	A	361	ASN
1	B	37	ASN
1	B	60	ASN
1	B	109	GLN
1	B	131	ASN
1	B	159	GLN
1	B	182	ASN
1	B	211	GLN
1	B	213	GLN
1	B	230	GLN
1	B	235	ASN
1	B	238	ASN
1	B	294	ASN
1	B	321	GLN
1	B	344	ASN
1	B	357	ASN
1	B	360	ASN
1	B	361	ASN
1	C	56	GLN
1	C	71	ASN
1	C	109	GLN
1	C	211	GLN
1	C	213	GLN
1	C	218	HIS
1	C	235	ASN
1	C	238	ASN
1	C	294	ASN
1	C	321	GLN

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Mol	Chain	Res	Type
1	C	350	ASN
1	C	357	ASN
1	C	361	ASN
1	C	409	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 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	ACY	B	461	-	3,3,3	0.56	0	3,3,3	0.85	0
3	ACY	C	462	-	3,3,3	0.54	0	3,3,3	0.84	0
3	ACY	A	460	-	3,3,3	0.51	0	3,3,3	0.79	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	461	ACY	1	0
3	A	460	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 (i)

6.1 Protein, DNA and RNA chains (i)

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	390/434 (89%)	0.44	38 (9%)	7	6	17, 31, 75, 102	0
1	B	382/434 (88%)	0.14	27 (7%)	16	12	18, 30, 69, 95	0
1	C	379/434 (87%)	0.09	18 (4%)	31	25	17, 24, 55, 86	0
All	All	1151/1302 (88%)	0.23	83 (7%)	15	12	17, 29, 67, 102	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	223	SER	12.2
1	A	221	SER	10.1
1	A	222	SER	9.5
1	A	227	LEU	9.4
1	C	225	LYS	9.0
1	A	216	MET	8.6
1	A	228	SER	8.0
1	B	223	SER	8.0
1	A	224	ARG	7.4
1	B	317	SER	7.2
1	B	224	ARG	7.2
1	C	13	VAL	7.1
1	A	226	GLU	7.1
1	C	317	SER	6.1
1	A	218	HIS	6.1
1	A	13	VAL	5.9
1	A	220	LYS	5.8
1	B	12	GLU	5.3
1	C	316	GLU	5.3
1	A	225	LYS	5.0
1	C	223	SER	5.0
1	B	11	GLU	4.9
1	C	224	ARG	4.9

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Mol	Chain	Res	Type	RSRZ
1	B	316	GLU	4.9
1	C	222	SER	4.8
1	B	188	GLU	4.7
1	A	217	LYS	4.7
1	A	411	GLU	4.6
1	B	225	LYS	4.5
1	A	215	LEU	4.5
1	A	229	SER	4.5
1	A	230	GLN	4.4
1	A	14	SER	4.1
1	A	197	GLU	4.1
1	A	313	GLN	4.1
1	B	314	GLN	4.1
1	C	228	SER	4.0
1	C	410	PRO	4.0
1	B	315	GLU	4.0
1	C	319	GLU	3.8
1	B	318	LEU	3.6
1	A	312	LYS	3.4
1	B	222	SER	3.4
1	C	307	ASP	3.4
1	A	213	GLN	3.2
1	B	214	GLU	3.2
1	B	220	LYS	3.0
1	A	198	SER	3.0
1	B	306	SER	3.0
1	A	308	GLN	3.0
1	A	39	TRP	3.0
1	B	199	ARG	2.9
1	A	311	GLN	2.9
1	B	163[A]	ARG	2.8
1	B	228	SER	2.8
1	C	198	SER	2.8
1	A	322[A]	ARG	2.7
1	C	318	LEU	2.7
1	A	238	ASN	2.7
1	B	198	SER	2.7
1	B	19	LYS	2.7
1	A	129	ASN	2.6
1	A	219	ALA	2.5
1	A	307	ASP	2.5
1	A	309	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	231	ASP	2.5
1	C	156	GLU	2.5
1	B	395	LYS	2.4
1	C	216[A]	MET	2.4
1	B	219	ALA	2.3
1	B	307	ASP	2.3
1	A	314	GLN	2.2
1	A	187	GLY	2.2
1	A	38	GLU	2.2
1	B	215	LEU	2.1
1	C	238	ASN	2.1
1	C	14	SER	2.1
1	B	394	GLU	2.1
1	A	199	ARG	2.1
1	A	179	LYS	2.1
1	B	208	LYS	2.1
1	B	218	HIS	2.0
1	C	231	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 monosaccharides 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(Å^2)	Q<0.9
3	ACY	A	460	4/4	0.61	0.31	46,47,47,48	0
2	CA	B	453	1/1	0.84	0.13	65,65,65,65	0
3	ACY	C	462	4/4	0.91	0.17	39,40,40,41	0
2	CA	B	452	1/1	0.93	0.18	54,54,54,54	0
3	ACY	B	461	4/4	0.94	0.11	52,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CA	C	451	1/1	0.94	0.22	47,47,47,47	0
2	CA	A	450	1/1	0.98	0.13	42,42,42,42	0

6.5 Other polymers (i)

There are no such residues in this entry.