Full wwPDB X-ray Structure Validation Report (i)

Dec 19, 2023 – 06:33 PM EST

PDB ID	:	1UIK
Title	:	Crystal structure of soybean beta-conglycinin alpha prime homotrimer
Authors	:	Maruyama, Y.; Maruyama, N.; Mikami, B.; Utsumi, S.
Deposited on	:	2003-07-16
Resolution	:	2.30 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 (1)) were used in the production of this report:

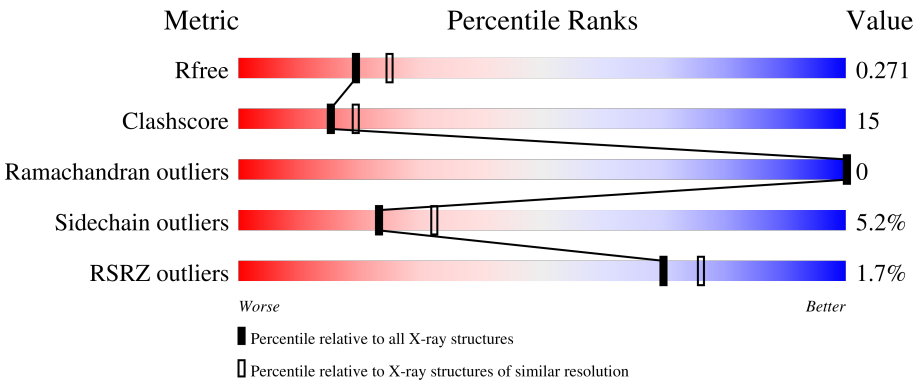
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	418	2% 64% 21% • 13%
1	B	418	% 63% 21% • 13%
1	C	418	% 65% 19% • 13%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 9348 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 alpha prime subunit of beta-conglycinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	364	2921	1857	504	558	2	0	0	0
1	B	363	2919	1855	503	559	2	0	1	0
1	C	364	2921	1857	504	558	2	0	0	0

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is water.

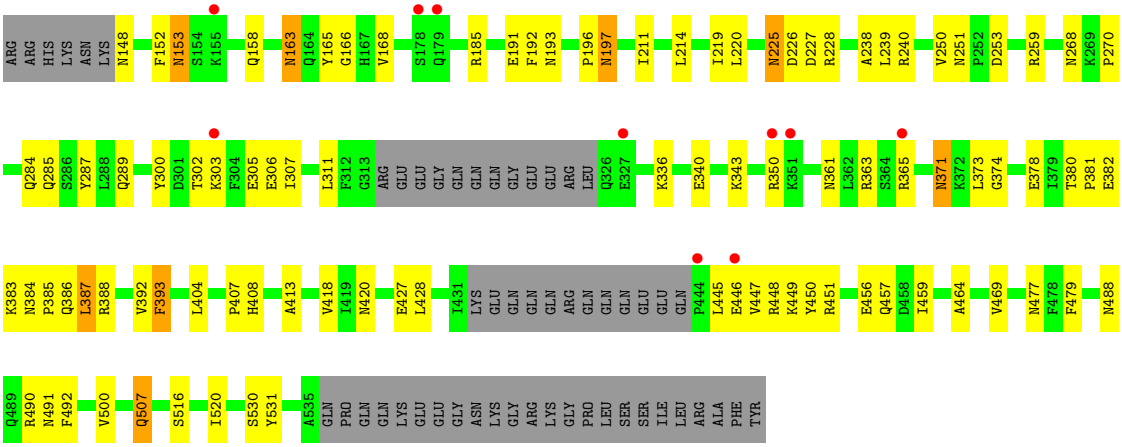
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	188	188	188	0	0
3	B	196	196	196	0	0
3	C	200	200	200	0	0

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.

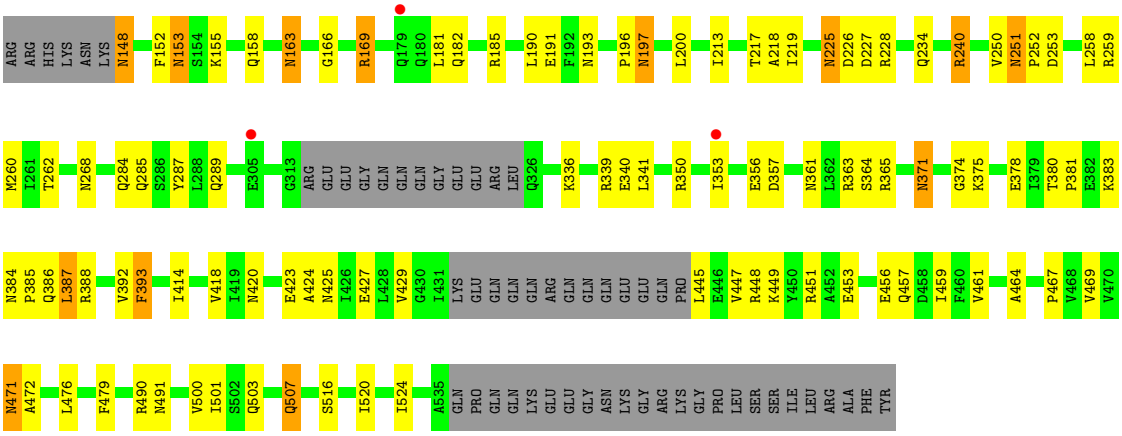
• Molecule 1: alpha prime subunit of beta-conglycinin

Chain A:



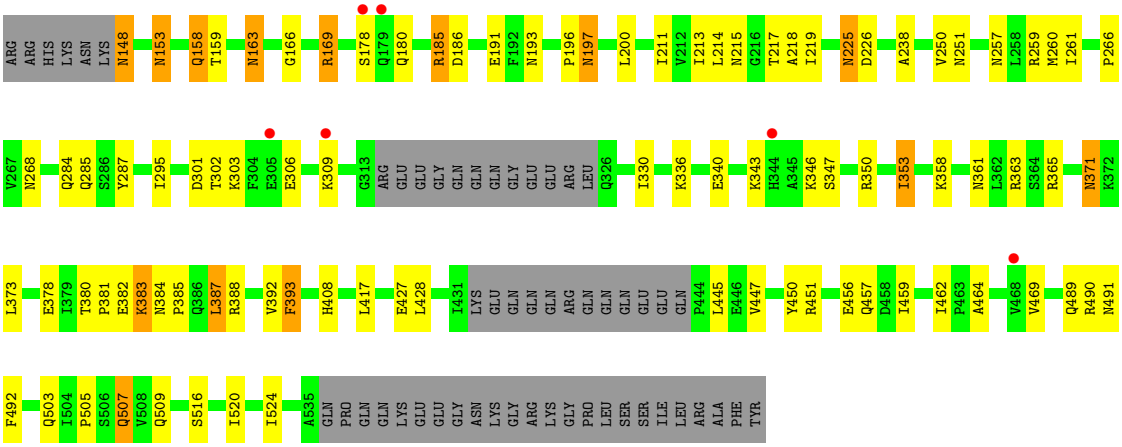
• Molecule 1: alpha prime subunit of beta-conglycinin

Chain B:



• Molecule 1: alpha prime subunit of beta-conglycinin

Chain C:


ARG ARG HIS LYS ASN LYS N148 N153 Q158 T159 N163 G166 R169 S178 Q179 Q180 R185 D186 E191 F192 N193 P196 N197 L200 I211 V212 I213 L214 N215 G216 T217 A218 I219 N225 D226 A238 V250 N251 N257 L258 R259 M260 I261 P266
V267 N268 Q284 Q285 S286 Y287 I295 D301 T302 K303 F304 E305 E306 K309 G313 ARG GLU GLU GLY GLN GLN GLN GLY GLU GLU ARG LEU Q326 I330 K336 E340 K343 H344 A345 K346 S347 R350 I353 K358 N361 L362 R363 S364 R365 N371 K372
L373 E378 I379 T380 P381 E382 K383 N384 P385 Q386 L387 R388 V392 F393 H408 L417 E427 L428 I431 LYS GLU GLN GLN GLN GLN ARG GLN GLN GLN GLN GLU GLU GLN P444 L445 E446 V447 Y450 R451 E456 Q457 D458 I459 I462 P463 A464 V468 V469 Q489 R490 N491
F492 Q503 I504 P505 S506 Q507 V508 Q509 S516 I520 I524 A535 GLN PRO GLN GLN LYS GLU GLU GLY ASN LYS GLY ARG LYS GLY PRO LEU SER SER ILE LEU ARG ALA PHE TYR

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	164.96Å 164.96Å 110.05Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	6.00 – 2.30 29.99 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (6.00-2.30) 88.5 (29.99-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	2.21 (at 2.00Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.221 , 0.269 0.223 , 0.271	Depositor DCC
R_{free} test set	5192 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	26.6	Xtriage
Anisotropy	0.605	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 55.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.54$, $< L^2 > = 0.38$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9348	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 33.62 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.7719e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: MG

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	0/2977	0.61	0/4026
1	B	0.38	0/2978	0.63	0/4027
1	C	0.36	0/2977	0.61	0/4026
All	All	0.37	0/8932	0.62	0/12079

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	2921	0	2901	87	0
1	B	2919	0	2895	105	0
1	C	2921	0	2901	87	0
2	A	1	0	0	0	1
2	B	1	0	0	0	1
2	C	1	0	0	0	0
3	A	188	0	0	6	0
3	B	196	0	0	7	0
3	C	200	0	0	3	0
All	All	9348	0	8697	261	1

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 (261) 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:A:507:GLN:H	1:A:507:GLN:HE21	1.02	0.99
1:A:507:GLN:H	1:A:507:GLN:NE2	1.66	0.94
1:B:507:GLN:H	1:B:507:GLN:HE21	1.05	0.93
1:C:193:ASN:HD21	1:C:259:ARG:HE	1.20	0.88
1:B:507:GLN:H	1:B:507:GLN:NE2	1.71	0.88
1:C:225:ASN:HD22	1:C:226:ASP:N	1.73	0.84
1:B:225:ASN:HD22	1:B:226:ASP:N	1.76	0.84
1:A:193:ASN:HD21	1:A:259:ARG:HE	1.28	0.81
1:C:507:GLN:H	1:C:507:GLN:HE21	1.31	0.77
1:A:381:PRO:HB3	1:A:388:ARG:HA	1.68	0.76
1:A:507:GLN:HE21	1:A:507:GLN:N	1.82	0.76
1:C:427:GLU:HG2	1:C:451:ARG:CD	2.16	0.76
1:C:158:GLN:HE21	1:C:159:THR:N	1.84	0.75
1:A:268:ASN:HD21	1:B:464:ALA:H	1.35	0.74
1:C:353:ILE:HD13	1:C:353:ILE:O	1.88	0.74
1:B:449:LYS:HB3	1:B:451:ARG:NH1	2.06	0.71
1:B:507:GLN:HE21	1:B:507:GLN:N	1.85	0.70
1:C:507:GLN:H	1:C:507:GLN:NE2	1.88	0.70
1:A:225:ASN:HD22	1:A:226:ASP:N	1.88	0.70
1:C:381:PRO:HB3	1:C:388:ARG:HA	1.74	0.68
1:C:158:GLN:HE21	1:C:158:GLN:C	1.97	0.68
1:B:350:ARG:HA	1:B:364:SER:OG	1.94	0.68
1:B:225:ASN:HD22	1:B:225:ASN:C	1.98	0.68
1:A:365:ARG:HH22	1:A:383:LYS:HE3	1.59	0.67
1:A:418:VAL:HG12	1:A:459:ILE:HD12	1.77	0.67
1:B:427:GLU:HG2	1:B:451:ARG:CD	2.25	0.67
1:B:225:ASN:HB3	1:C:491:ASN:HD22	1.61	0.66
1:B:336:LYS:HE3	1:B:340:GLU:OE2	1.96	0.66
1:A:371:ASN:C	1:A:371:ASN:HD22	1.98	0.66
1:B:169:ARG:HD3	1:B:191:GLU:OE1	1.96	0.66
1:A:491:ASN:HD22	1:C:225:ASN:HB3	1.61	0.65
1:C:382:GLU:HG2	1:C:383:LYS:HD2	1.79	0.64
1:B:268:ASN:HD21	1:C:464:ALA:H	1.45	0.64
1:A:336:LYS:O	1:A:340:GLU:HG3	1.99	0.63
1:C:445:LEU:HD22	3:C:1143:HOH:O	1.99	0.63
1:C:428:LEU:HB3	1:C:450:TYR:HB2	1.79	0.63
1:B:427:GLU:HG2	1:B:451:ARG:NE	2.13	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:ASN:ND2	1:A:373:LEU:H	1.97	0.62
1:A:153:ASN:HD22	1:A:153:ASN:C	2.02	0.61
1:B:364:SER:HB3	3:B:1178:HOH:O	1.99	0.61
1:B:427:GLU:HG2	1:B:451:ARG:HD2	1.82	0.61
1:C:193:ASN:ND2	1:C:259:ARG:HE	1.95	0.61
1:A:300:TYR:O	1:A:302:THR:HG23	2.01	0.61
1:B:153:ASN:C	1:B:153:ASN:HD22	2.05	0.60
1:B:227:ASP:HA	1:C:503:GLN:NE2	2.17	0.60
1:C:336:LYS:O	1:C:340:GLU:HG3	2.02	0.60
1:A:464:ALA:H	1:C:268:ASN:HD21	1.48	0.60
1:A:163:ASN:C	1:A:163:ASN:HD22	2.05	0.59
1:B:371:ASN:C	1:B:371:ASN:HD22	2.06	0.59
1:B:448:ARG:HD2	3:B:1090:HOH:O	2.02	0.59
1:B:429:VAL:CG1	1:B:467:PRO:HB2	2.33	0.59
1:C:427:GLU:HG2	1:C:451:ARG:HD3	1.85	0.59
1:B:350:ARG:O	1:B:353:ILE:HG23	2.03	0.59
1:C:213:ILE:HD13	1:C:260:MET:HG2	1.84	0.59
1:A:420:ASN:HB3	1:A:477:ASN:HD22	1.67	0.58
1:A:427:GLU:HG2	1:A:451:ARG:CD	2.33	0.58
1:B:427:GLU:HG2	1:B:451:ARG:HE	1.69	0.58
1:C:361:ASN:HD22	1:C:363:ARG:H	1.52	0.58
1:A:225:ASN:HB3	1:B:491:ASN:HD22	1.70	0.57
1:B:491:ASN:HB3	1:B:500:VAL:HG11	1.86	0.57
1:A:163:ASN:ND2	1:A:166:GLY:H	2.02	0.56
1:B:418:VAL:HG12	1:B:459:ILE:HD12	1.86	0.56
1:C:158:GLN:HE21	1:C:158:GLN:CA	2.17	0.56
1:C:163:ASN:C	1:C:163:ASN:HD22	2.08	0.56
1:B:491:ASN:HB3	1:B:500:VAL:CG1	2.35	0.56
1:C:371:ASN:HD22	1:C:371:ASN:C	2.07	0.56
1:C:427:GLU:HB2	1:C:469:VAL:HG12	1.86	0.56
1:C:365:ARG:HG3	1:C:365:ARG:HH11	1.68	0.56
1:B:259:ARG:HH11	1:B:420:ASN:HD22	1.54	0.55
1:A:404:LEU:HD11	1:A:469:VAL:HG13	1.87	0.55
1:C:211:ILE:O	1:C:238:ALA:HA	2.07	0.55
1:A:407:PRO:HG3	1:A:469:VAL:CG2	2.37	0.55
1:C:456:GLU:O	1:C:457:GLN:HB2	2.07	0.55
1:A:191:GLU:OE2	1:A:457:GLN:NE2	2.40	0.55
1:C:193:ASN:HD21	1:C:259:ARG:NE	2.00	0.55
1:A:361:ASN:HD22	1:A:363:ARG:H	1.55	0.54
1:C:225:ASN:HD22	1:C:225:ASN:C	2.10	0.54
1:C:353:ILE:HG12	3:C:1167:HOH:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:TYR:HA	1:C:447:VAL:HG11	1.90	0.54
1:A:448:ARG:NH2	1:A:449:LYS:O	2.40	0.54
1:A:456:GLU:O	1:A:457:GLN:HB2	2.07	0.54
1:B:336:LYS:O	1:B:340:GLU:HG3	2.08	0.54
1:A:220:LEU:HD13	1:A:239:LEU:HD23	1.90	0.54
1:B:234:GLN:HB2	3:B:1154:HOH:O	2.07	0.54
1:C:225:ASN:HD22	1:C:226:ASP:H	1.54	0.54
1:B:285:GLN:NE2	1:B:289:GLN:HE22	2.07	0.53
1:B:418:VAL:HG23	1:B:418:VAL:O	2.07	0.53
1:C:196:PRO:HD3	1:C:257:ASN:ND2	2.23	0.53
1:B:427:GLU:HB2	1:B:469:VAL:HG12	1.91	0.53
1:A:365:ARG:NH2	1:A:383:LYS:HE3	2.23	0.53
1:B:361:ASN:HD22	1:B:363:ARG:H	1.56	0.53
1:C:346:LYS:HD2	1:C:358:LYS:NZ	2.24	0.52
1:B:196:PRO:HB3	1:B:253:ASP:O	2.09	0.52
1:B:507:GLN:NE2	1:B:507:GLN:N	2.51	0.52
1:B:456:GLU:O	1:B:457:GLN:HB2	2.10	0.52
1:C:178:SER:OG	1:C:180:GLN:HB2	2.09	0.52
1:B:445:LEU:HD22	3:B:1149:HOH:O	2.08	0.52
1:B:225:ASN:HB3	1:C:491:ASN:ND2	2.25	0.52
1:C:353:ILE:HD12	1:C:383:LYS:HB3	1.91	0.52
1:A:285:GLN:NE2	1:A:289:GLN:NE2	2.58	0.52
1:B:353:ILE:HD12	1:B:383:LYS:NZ	2.25	0.52
1:A:152:PHE:HB2	1:A:459:ILE:HB	1.92	0.51
1:A:168:VAL:HG22	1:A:192:PHE:CD2	2.45	0.51
1:A:418:VAL:HG23	1:A:418:VAL:O	2.10	0.51
1:B:339:ARG:HH21	1:B:339:ARG:HG3	1.75	0.51
1:A:378:GLU:CD	1:A:490:ARG:HH22	2.12	0.51
1:B:193:ASN:HD21	1:B:259:ARG:HE	1.59	0.51
1:A:507:GLN:NE2	1:A:507:GLN:N	2.48	0.51
1:C:158:GLN:NE2	1:C:159:THR:N	2.57	0.51
1:C:350:ARG:HG2	1:C:350:ARG:HH21	1.75	0.51
1:A:384:ASN:OD1	1:A:386:GLN:HB2	2.11	0.51
1:C:371:ASN:ND2	1:C:373:LEU:H	2.08	0.51
1:A:445:LEU:HD22	3:A:1111:HOH:O	2.10	0.51
1:B:356[A]:GLU:HG2	3:B:1193:HOH:O	2.10	0.50
1:C:197:ASN:N	1:C:197:ASN:HD22	2.08	0.50
1:A:393:PHE:C	1:A:393:PHE:CD2	2.84	0.50
1:B:285:GLN:NE2	1:B:289:GLN:NE2	2.60	0.50
1:C:393:PHE:C	1:C:393:PHE:CD2	2.84	0.50
1:B:425:ASN:OD1	1:B:453:GLU:HG2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:ASN:C	1:B:163:ASN:HD22	2.15	0.50
1:B:365:ARG:HD2	1:B:383:LYS:NZ	2.27	0.50
1:A:225:ASN:HD22	1:A:225:ASN:C	2.14	0.49
1:C:169:ARG:HG2	1:C:191:GLU:HB3	1.94	0.49
1:C:456:GLU:HG2	1:C:457:GLN:HG3	1.93	0.49
1:A:380:THR:HB	1:A:381:PRO:CD	2.43	0.49
1:B:213:ILE:HD13	1:B:260:MET:HG2	1.94	0.49
1:C:378:GLU:CD	1:C:490:ARG:HH22	2.14	0.49
1:A:516:SER:O	1:A:520:ILE:HG13	2.12	0.49
1:C:153:ASN:C	1:C:153:ASN:HD22	2.14	0.49
1:A:163:ASN:C	1:A:163:ASN:ND2	2.66	0.49
1:A:211:ILE:O	1:A:238:ALA:HA	2.12	0.49
1:A:336:LYS:HE2	1:A:340:GLU:OE2	2.12	0.49
1:A:446:GLU:HA	1:C:285:GLN:OE1	2.13	0.49
1:A:197:ASN:HD22	1:A:197:ASN:N	2.11	0.48
1:A:343:LYS:HB2	1:A:343:LYS:NZ	2.28	0.48
1:A:371:ASN:ND2	1:A:374:GLY:H	2.11	0.48
1:C:196:PRO:HD3	1:C:257:ASN:HD22	1.78	0.48
1:C:169:ARG:HD3	1:C:191:GLU:OE2	2.13	0.48
1:C:163:ASN:ND2	1:C:166:GLY:H	2.11	0.48
1:B:451:ARG:HG2	1:B:451:ARG:HH11	1.78	0.48
1:B:356[A]:GLU:HG3	1:B:357:ASP:N	2.28	0.48
1:B:197:ASN:N	1:B:197:ASN:HD22	2.11	0.48
1:A:214:LEU:HD22	1:A:479:PHE:CD2	2.49	0.48
1:C:330:ILE:HD12	1:C:330:ILE:N	2.29	0.48
1:B:181:LEU:HD22	1:B:461:VAL:HG11	1.96	0.47
1:B:381:PRO:HB3	1:B:388:ARG:HA	1.96	0.47
1:A:196:PRO:HB3	1:A:253:ASP:O	2.14	0.47
1:C:507:GLN:HE21	1:C:507:GLN:N	2.07	0.47
1:B:471:ASN:C	1:B:471:ASN:HD22	2.17	0.47
1:B:153:ASN:HD21	1:B:155:LYS:HB2	1.79	0.47
1:B:228:ARG:HD3	1:C:505:PRO:HD3	1.97	0.47
1:B:387:LEU:HG	1:B:392:VAL:O	2.15	0.47
1:B:193:ASN:HA	1:B:258:LEU:O	2.14	0.47
1:A:193:ASN:ND2	1:A:259:ARG:HE	2.06	0.47
1:A:228:ARG:HD3	1:B:503:GLN:O	2.14	0.47
1:B:219:ILE:HB	1:B:250:VAL:HB	1.97	0.47
1:C:427:GLU:HG2	1:C:451:ARG:NE	2.30	0.47
1:A:380:THR:HB	1:A:381:PRO:HD2	1.97	0.46
1:B:418:VAL:O	1:B:418:VAL:CG2	2.62	0.46
1:C:302:THR:HG22	1:C:303:LYS:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:520:ILE:O	1:B:524:ILE:HG12	2.14	0.46
1:C:365:ARG:HG3	1:C:365:ARG:NH1	2.31	0.46
1:B:152:PHE:HB2	1:B:459:ILE:HB	1.97	0.46
1:A:491:ASN:HB3	1:A:500:VAL:HG11	1.97	0.46
1:B:380:THR:HB	1:B:381:PRO:HD2	1.98	0.46
1:C:384:ASN:HA	1:C:385:PRO:HD3	1.76	0.46
1:A:383:LYS:HD3	3:A:1125:HOH:O	2.16	0.46
1:B:163:ASN:ND2	1:B:166:GLY:H	2.14	0.46
1:B:418:VAL:HG12	1:B:459:ILE:CD1	2.45	0.46
1:B:456:GLU:HG2	1:B:457:GLN:HG3	1.98	0.46
1:C:163:ASN:C	1:C:163:ASN:ND2	2.69	0.46
1:A:413:ALA:H	1:A:488:ASN:ND2	2.14	0.45
1:C:213:ILE:CD1	1:C:260:MET:HG2	2.46	0.45
1:B:423:GLU:HB3	3:B:1137:HOH:O	2.16	0.45
1:B:393:PHE:C	1:B:393:PHE:CD2	2.90	0.45
1:B:471:ASN:HD22	1:B:472:ALA:N	2.14	0.45
1:A:225:ASN:HB3	1:B:491:ASN:ND2	2.32	0.45
1:B:353:ILE:HD12	1:B:383:LYS:HZ1	1.81	0.45
1:B:448:ARG:NH2	1:B:449:LYS:O	2.50	0.45
1:C:371:ASN:C	1:C:371:ASN:ND2	2.70	0.45
1:A:287:TYR:HA	1:B:447:VAL:HG11	1.99	0.45
1:B:217:THR:HG22	1:B:218:ALA:N	2.32	0.45
1:C:214:LEU:HD11	1:C:261:ILE:HG13	1.98	0.44
1:A:387:LEU:HG	1:A:392:VAL:O	2.17	0.44
1:A:408:HIS:HB3	1:A:492:PHE:CD1	2.53	0.44
1:B:225:ASN:C	1:B:225:ASN:ND2	2.68	0.44
1:C:427:GLU:HB2	1:C:469:VAL:CG1	2.46	0.44
1:A:418:VAL:HG12	1:A:459:ILE:CD1	2.46	0.44
1:C:169:ARG:CG	1:C:191:GLU:HB3	2.47	0.44
1:B:365:ARG:HG2	1:B:365:ARG:HH21	1.82	0.44
1:A:382:GLU:HG2	1:A:383:LYS:HD2	1.98	0.44
1:A:427:GLU:OE2	1:C:295:ILE:HG13	2.18	0.44
1:B:365:ARG:HG2	1:B:365:ARG:NH2	2.33	0.43
1:A:306:GLU:HG3	3:A:1117:HOH:O	2.18	0.43
1:B:169:ARG:HG2	1:B:191:GLU:HB3	2.01	0.43
1:B:339:ARG:HG3	1:B:339:ARG:NH2	2.34	0.43
1:A:407:PRO:HG3	1:A:469:VAL:HG21	1.99	0.43
1:C:186:ASP:O	1:C:266:PRO:HD2	2.18	0.43
1:C:340:GLU:O	1:C:343:LYS:HE2	2.18	0.43
1:C:516:SER:O	1:C:520:ILE:HG13	2.18	0.43
1:B:259:ARG:HH11	1:B:420:ASN:ND2	2.15	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:371:ASN:ND2	1:B:374:GLY:H	2.16	0.43
1:C:361:ASN:ND2	1:C:363:ARG:H	2.14	0.43
1:A:259:ARG:HH11	1:A:420:ASN:HD22	1.66	0.43
1:A:384:ASN:HA	1:A:385:PRO:HD3	1.76	0.43
1:C:417:LEU:HD11	1:C:462:ILE:HD11	2.01	0.42
1:B:190:LEU:HB3	1:B:262:THR:HB	2.01	0.42
1:B:424:ALA:HB2	1:B:476:LEU:HD22	2.01	0.42
1:C:185:ARG:HH21	1:C:185:ARG:HB2	1.84	0.42
1:C:214:LEU:O	1:C:215:ASN:ND2	2.52	0.42
1:C:387:LEU:HG	1:C:392:VAL:O	2.19	0.42
1:A:448:ARG:HD2	3:A:1100:HOH:O	2.19	0.42
1:B:516:SER:O	1:B:520:ILE:HG13	2.20	0.42
1:A:270:PRO:HG2	1:B:182:GLN:NE2	2.35	0.42
1:C:417:LEU:O	1:C:459:ILE:HA	2.20	0.42
1:B:418:VAL:HG22	1:B:479:PHE:HB2	2.01	0.42
1:C:148:ASN:C	1:C:148:ASN:HD22	2.22	0.42
1:C:302:THR:CG2	1:C:306:GLU:HB3	2.50	0.42
1:B:378:GLU:CD	1:B:490:ARG:HH12	2.23	0.42
1:B:500:VAL:HG23	1:B:501:ILE:N	2.33	0.42
1:C:380:THR:HB	1:C:381:PRO:CD	2.50	0.42
1:A:303:LYS:NZ	1:A:305:GLU:CD	2.72	0.42
1:B:250:VAL:O	1:B:252:PRO:HD3	2.20	0.42
1:B:418:VAL:HA	1:B:459:ILE:HD13	2.01	0.42
1:A:219:ILE:HB	1:A:250:VAL:HB	2.02	0.41
1:A:226:ASP:O	1:A:227:ASP:HB3	2.21	0.41
1:C:520:ILE:O	1:C:524:ILE:HG12	2.20	0.41
1:A:185:ARG:HD2	3:A:1108:HOH:O	2.19	0.41
1:A:365:ARG:HH22	1:A:383:LYS:CE	2.29	0.41
1:B:353:ILE:HG22	3:B:1177:HOH:O	2.20	0.41
1:C:309:LYS:HB2	1:C:309:LYS:HE3	1.89	0.41
1:C:505:PRO:O	1:C:509:GLN:HG3	2.20	0.41
1:A:448:ARG:HH21	1:A:448:ARG:HG3	1.85	0.41
1:B:163:ASN:C	1:B:163:ASN:ND2	2.74	0.41
1:B:371:ASN:C	1:B:371:ASN:ND2	2.72	0.41
1:A:371:ASN:C	1:A:371:ASN:ND2	2.67	0.41
1:A:530:SER:O	1:A:531:TYR:HB2	2.20	0.41
1:C:347:SER:HB2	3:C:1071:HOH:O	2.19	0.41
1:A:259:ARG:HH11	1:A:420:ASN:ND2	2.19	0.41
1:A:163:ASN:ND2	1:A:165:TYR:H	2.19	0.41
1:B:153:ASN:C	1:B:153:ASN:ND2	2.73	0.41
1:B:451:ARG:HH11	1:B:451:ARG:CG	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:VAL:HG11	1:C:287:TYR:HA	2.03	0.41
1:B:251:ASN:C	1:B:251:ASN:HD22	2.24	0.41
1:B:356[A]:GLU:HG3	1:B:357:ASP:OD1	2.20	0.41
1:B:384:ASN:HA	1:B:385:PRO:HD3	1.75	0.41
1:C:191:GLU:OE1	1:C:457:GLN:NE2	2.53	0.41
1:C:408:HIS:HB3	1:C:492:PHE:CD1	2.56	0.41
1:A:268:ASN:ND2	1:B:414:ILE:HG12	2.36	0.41
1:B:240:ARG:H	1:B:386:GLN:NE2	2.19	0.40
1:B:471:ASN:C	1:B:471:ASN:ND2	2.75	0.40
1:C:219:ILE:HB	1:C:250:VAL:HB	2.02	0.40
1:A:214:LEU:HD22	1:A:479:PHE:CE2	2.56	0.40
1:A:307:ILE:HG23	1:A:311:LEU:HD12	2.03	0.40
1:A:418:VAL:O	1:A:418:VAL:CG2	2.68	0.40
1:A:428:LEU:HB3	1:A:450:TYR:HB2	2.02	0.40
1:B:380:THR:HB	1:B:381:PRO:CD	2.50	0.40
1:C:217:THR:HG22	1:C:218:ALA:N	2.37	0.40
1:A:153:ASN:C	1:A:153:ASN:ND2	2.72	0.40
1:A:350:ARG:HG3	3:A:1179:HOH:O	2.22	0.40
1:B:148:ASN:C	1:B:148:ASN:HD22	2.24	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1001:MG:MG	2:B:1002:MG:MG[6_666]	0.06	2.14

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	358/418 (86%)	344 (96%)	14 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	358/418 (86%)	346 (97%)	12 (3%)	0	100	100
1	C	358/418 (86%)	346 (97%)	12 (3%)	0	100	100
All	All	1074/1254 (86%)	1036 (96%)	38 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	328/376 (87%)	315 (96%)	13 (4%)	31	44
1	B	328/376 (87%)	309 (94%)	19 (6%)	20	27
1	C	328/376 (87%)	309 (94%)	19 (6%)	20	27
All	All	984/1128 (87%)	933 (95%)	51 (5%)	23	32

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	148	ASN
1	A	153	ASN
1	A	158	GLN
1	A	163	ASN
1	A	197	ASN
1	A	225	ASN
1	A	240	ARG
1	A	251	ASN
1	A	284	GLN
1	A	371	ASN
1	A	387	LEU
1	A	393	PHE
1	A	507	GLN
1	B	148	ASN
1	B	153	ASN
1	B	158	GLN

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Mol	Chain	Res	Type
1	B	163	ASN
1	B	169	ARG
1	B	185	ARG
1	B	197	ASN
1	B	200	LEU
1	B	225	ASN
1	B	240	ARG
1	B	251	ASN
1	B	284	GLN
1	B	341	LEU
1	B	371	ASN
1	B	375	LYS
1	B	387	LEU
1	B	393	PHE
1	B	471	ASN
1	B	507	GLN
1	C	148	ASN
1	C	153	ASN
1	C	158	GLN
1	C	163	ASN
1	C	169	ARG
1	C	185	ARG
1	C	197	ASN
1	C	200	LEU
1	C	225	ASN
1	C	251	ASN
1	C	284	GLN
1	C	301	ASP
1	C	353	ILE
1	C	371	ASN
1	C	383	LYS
1	C	387	LEU
1	C	393	PHE
1	C	489	GLN
1	C	507	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (92) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	148	ASN
1	A	153	ASN
1	A	163	ASN

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Mol	Chain	Res	Type
1	A	164	GLN
1	A	167	HIS
1	A	179	GLN
1	A	180	GLN
1	A	193	ASN
1	A	215	ASN
1	A	225	ASN
1	A	251	ASN
1	A	254	ASN
1	A	268	ASN
1	A	284	GLN
1	A	289	GLN
1	A	294	ASN
1	A	326	GLN
1	A	337	GLN
1	A	361	ASN
1	A	371	ASN
1	A	386	GLN
1	A	400	ASN
1	A	420	ASN
1	A	477	ASN
1	A	484	ASN
1	A	487	ASN
1	A	488	ASN
1	A	491	ASN
1	A	503	GLN
1	A	507	GLN
1	A	522	ASN
1	B	148	ASN
1	B	153	ASN
1	B	163	ASN
1	B	172	GLN
1	B	179	GLN
1	B	182	GLN
1	B	193	ASN
1	B	225	ASN
1	B	251	ASN
1	B	254	ASN
1	B	257	ASN
1	B	268	ASN
1	B	289	GLN
1	B	294	ASN

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Mol	Chain	Res	Type
1	B	326	GLN
1	B	361	ASN
1	B	371	ASN
1	B	386	GLN
1	B	400	ASN
1	B	420	ASN
1	B	471	ASN
1	B	477	ASN
1	B	484	ASN
1	B	487	ASN
1	B	488	ASN
1	B	491	ASN
1	B	503	GLN
1	B	507	GLN
1	B	522	ASN
1	C	148	ASN
1	C	153	ASN
1	C	158	GLN
1	C	163	ASN
1	C	179	GLN
1	C	182	GLN
1	C	193	ASN
1	C	215	ASN
1	C	225	ASN
1	C	251	ASN
1	C	254	ASN
1	C	257	ASN
1	C	268	ASN
1	C	284	GLN
1	C	289	GLN
1	C	294	ASN
1	C	326	GLN
1	C	337	GLN
1	C	361	ASN
1	C	371	ASN
1	C	386	GLN
1	C	400	ASN
1	C	410	ASN
1	C	420	ASN
1	C	477	ASN
1	C	484	ASN
1	C	487	ASN

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Mol	Chain	Res	Type
1	C	488	ASN
1	C	491	ASN
1	C	503	GLN
1	C	507	GLN
1	C	522	ASN

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 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	364/418 (87%)	-0.15	10 (2%)	54	62	20, 32, 47, 57	0
1	B	363/418 (86%)	-0.27	3 (0%)	86	89	18, 31, 46, 55	0
1	C	364/418 (87%)	-0.23	6 (1%)	72	77	16, 31, 46, 55	0
All	All	1091/1254 (87%)	-0.22	19 (1%)	70	76	16, 31, 47, 57	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	350	ARG	3.6
1	A	444	PRO	3.5
1	B	353	ILE	3.2
1	A	155	LYS	3.0
1	C	179	GLN	3.0
1	C	344	HIS	2.9
1	A	351	LYS	2.7
1	A	178	SER	2.7
1	C	305	GLU	2.5
1	A	179	GLN	2.5
1	C	468	VAL	2.5
1	A	365	ARG	2.5
1	B	305	GLU	2.4
1	A	327	GLU	2.4
1	C	178	SER	2.4
1	B	179	GLN	2.2
1	A	446	GLU	2.2
1	A	303	LYS	2.0
1	C	309	LYS	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
2	MG	C	1003	1/1	0.96	0.15	34,34,34,34	1
2	MG	A	1001	1/1	0.98	0.06	47,47,47,47	0
2	MG	B	1002	1/1	0.99	0.06	49,49,49,49	0

6.5 Other polymers (i)

There are no such residues in this entry.