Full wwPDB X-ray Structure Validation Report (i)

Oct 19, 2023 – 09:12 AM EDT

PDB ID	:	2QUH
Title	:	Crystal structures of human tryptophanyl-tRNA synthetase in complex with Trp
Authors	:	Shen, N.; Ding, J.P.
Deposited on	:	2007-08-05
Resolution	:	2.40 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:

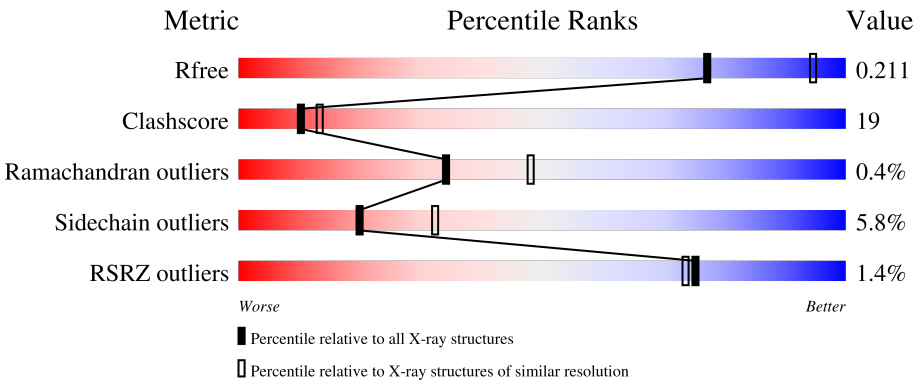
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	477	% 51% 27% • 21%
1	B	477	% 53% 24% • 20%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6394 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.

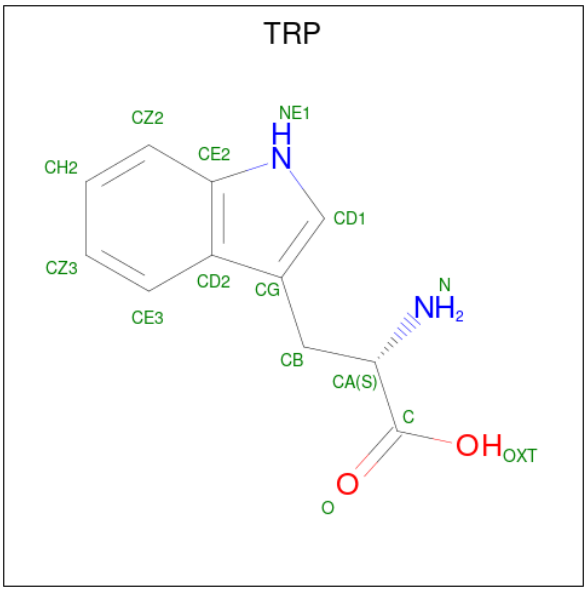
- Molecule 1 is a protein called Tryptophanyl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	379	3049	1954	517	563	15	0	0	0
1	B	381	3037	1946	512	564	15	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	472	HIS	-	expression tag	UNP P23381
A	473	HIS	-	expression tag	UNP P23381
A	474	HIS	-	expression tag	UNP P23381
A	475	HIS	-	expression tag	UNP P23381
A	476	HIS	-	expression tag	UNP P23381
A	477	HIS	-	expression tag	UNP P23381
B	472	HIS	-	expression tag	UNP P23381
B	473	HIS	-	expression tag	UNP P23381
B	474	HIS	-	expression tag	UNP P23381
B	475	HIS	-	expression tag	UNP P23381
B	476	HIS	-	expression tag	UNP P23381
B	477	HIS	-	expression tag	UNP P23381

- Molecule 2 is TRYPTOPHAN (three-letter code: TRP) (formula: $C_{11}H_{12}N_2O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	B	1	15	11	2	2	0	0
			Total	C	N	O		
2	B	1	15	11	2	2	0	0

- Molecule 3 is water.

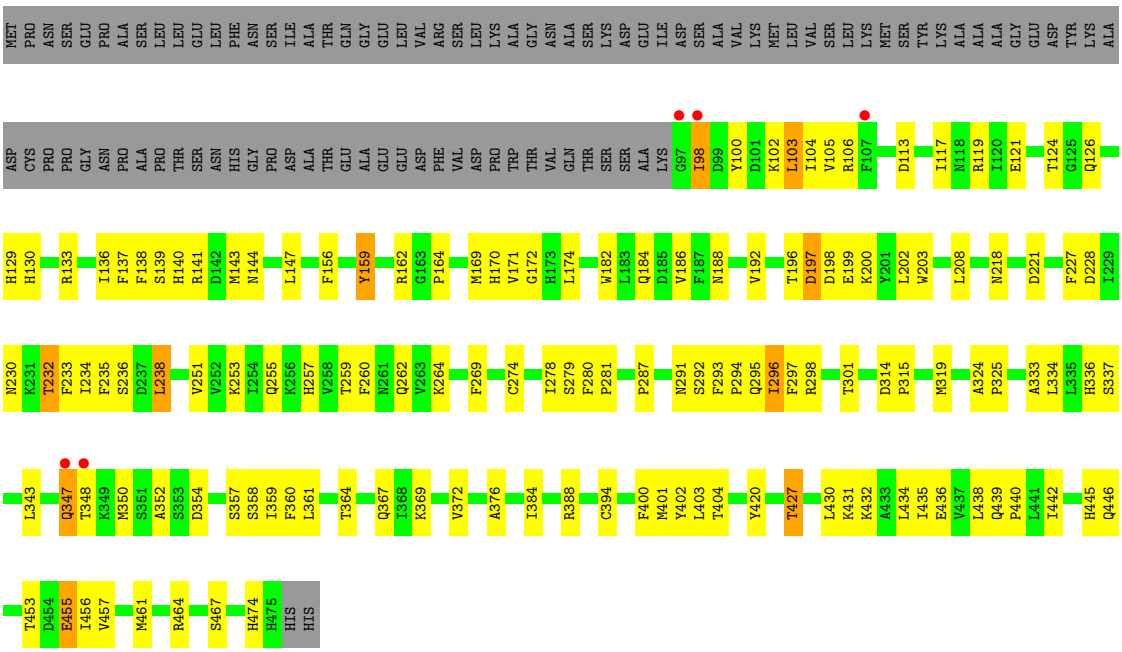
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	140	140	140	0	0
			Total	O		
3	B	138	138	138	0	0

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.

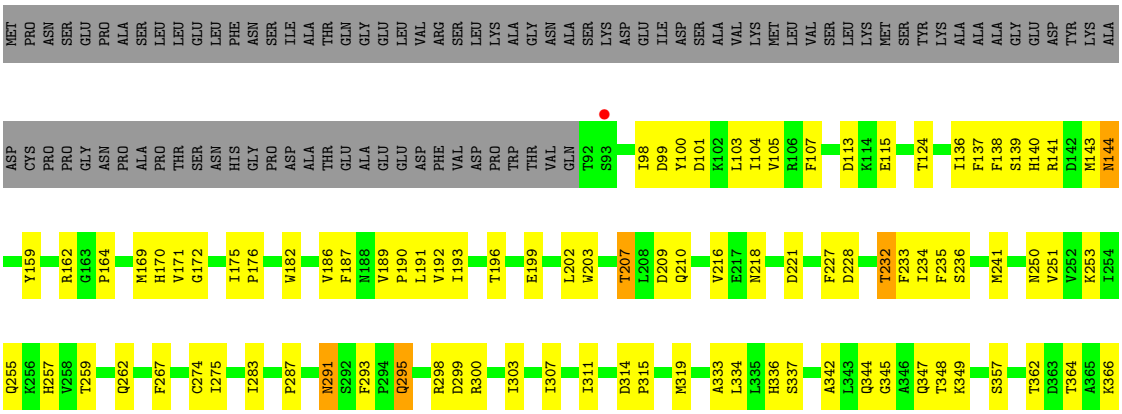
- Molecule 1: Tryptophanyl-tRNA synthetase

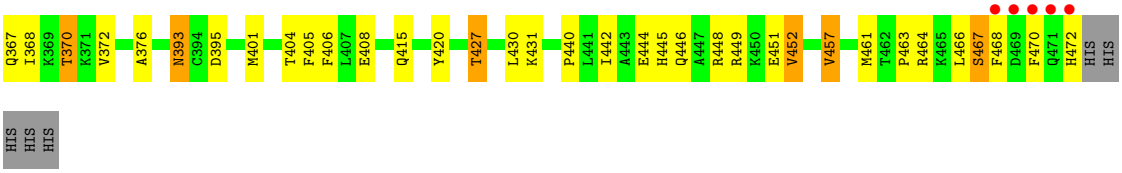
Chain A:



- Molecule 1: Tryptophanyl-tRNA synthetase

Chain B:




Q367
I368
K369
T370
K371
V372
A376
N393
C394
D395
M401
T404
F405
F406
L407
E408
Q415
Y420
T427
L430
K431
P440
L441
I442
A443
E444
H445
Q446
A447
R448
R449
K450
E451
V452
V457
M461
T462
P463
R464
K465
L466
S467
F468
D469
F470
Q471
H472
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	79.90Å 79.90Å 382.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40 49.82 – 2.40	Depositor EDS
% Data completeness (in resolution range)	86.5 (50.00-2.40) 86.6 (49.82-2.40)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.89 (at 2.39Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.207 , 0.233 0.209 , 0.211	Depositor DCC
R_{free} test set	2185 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	40.1	Xtriage
Anisotropy	0.480	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 46.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6394	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% 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)

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	0.38	0/3127	0.61	0/4227
1	B	0.37	0/3112	0.62	0/4207
All	All	0.37	0/6239	0.61	0/8434

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	3049	0	2953	122	0
1	B	3037	0	2940	108	0
2	B	30	0	18	0	0
3	A	140	0	0	3	0
3	B	138	0	0	2	0
All	All	6394	0	5911	226	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 19.

All (226) 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:124:THR:HG21	1:B:186:VAL:HG13	1.36	1.05
1:B:207:THR:HG22	1:B:210:GLN:H	1.28	0.97
1:B:345:GLY:HA3	1:B:347:GLN:HE22	1.36	0.89
1:A:372:VAL:HG12	1:A:431:LYS:HG3	1.57	0.86
1:B:227:PHE:HB3	1:B:232:THR:HG21	1.58	0.84
1:A:174:LEU:HD21	1:A:361:LEU:HD11	1.58	0.83
1:A:350:MET:HE3	1:A:358:SER:HB2	1.60	0.82
1:A:228:ASP:O	1:A:232:THR:HG23	1.82	0.80
1:B:251:VAL:O	1:B:255:GLN:HG3	1.85	0.77
1:A:259:THR:OG1	1:A:262:GLN:HG3	1.85	0.77
1:B:250:ASN:HD21	1:B:291:ASN:ND2	1.83	0.77
1:A:227:PHE:HB3	1:A:232:THR:HG21	1.66	0.76
1:B:334:LEU:HD23	1:B:336:HIS:HE1	1.50	0.76
1:A:376:ALA:HB3	1:A:431:LYS:HE2	1.69	0.74
1:A:293:PHE:HB3	1:A:296:ILE:HG23	1.66	0.74
1:A:260:PHE:CE1	1:A:264:LYS:HD2	2.23	0.73
1:A:260:PHE:HE1	1:A:264:LYS:HD2	1.54	0.72
1:B:442:ILE:O	1:B:446:GLN:HG3	1.88	0.72
1:B:140:HIS:HD2	1:B:143:MET:H	1.38	0.71
1:A:347:GLN:H	1:A:347:GLN:NE2	1.89	0.71
1:A:359:ILE:HD13	1:A:438:LEU:HD13	1.72	0.69
1:B:345:GLY:HA3	1:B:347:GLN:NE2	2.07	0.69
1:B:334:LEU:HD23	1:B:336:HIS:CE1	2.28	0.68
1:A:169:MET:HE2	1:A:218:ASN:HA	1.76	0.68
1:A:124:THR:HB	1:A:186:VAL:HG13	1.74	0.68
1:B:228:ASP:O	1:B:232:THR:HG23	1.92	0.67
1:B:159:TYR:CZ	1:B:287:PRO:HG2	2.29	0.67
1:A:324:ALA:HB3	1:A:325:PRO:HD3	1.77	0.67
1:A:192:VAL:HG13	1:A:235:PHE:HE1	1.60	0.67
1:A:234:ILE:O	1:A:461:MET:HA	1.96	0.66
1:A:169:MET:CE	1:A:221:ASP:HB2	2.26	0.66
1:B:250:ASN:HD21	1:B:291:ASN:HD21	1.41	0.65
1:B:267:PHE:HE1	1:B:319:MET:HE3	1.61	0.65
1:A:350:MET:HE3	1:A:358:SER:CB	2.26	0.65
1:B:137:PHE:CZ	1:B:337:SER:HB3	2.31	0.65
1:A:140:HIS:HD2	1:A:143:MET:H	1.44	0.65
1:A:354:ASP:HB3	1:A:357:SER:HB2	1.79	0.65
1:A:126:GLN:HG3	1:A:186:VAL:HG22	1.76	0.65
1:B:300:ARG:HG2	1:B:303:ILE:HD11	1.79	0.64
1:A:159:TYR:CZ	1:A:287:PRO:HG2	2.32	0.63
1:B:427:THR:HG23	3:B:945:HOH:O	1.99	0.63
1:A:230:ASN:HB3	1:A:467:SER:OG	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:ILE:O	1:A:446:GLN:HG3	1.99	0.62
1:B:253:LYS:O	1:B:257:HIS:HD2	1.82	0.62
1:B:303:ILE:N	1:B:303:ILE:HD12	2.14	0.62
1:A:198:ASP:HB3	1:A:238:LEU:HD13	1.82	0.62
1:A:432:LYS:O	1:A:436:GLU:HG3	2.00	0.61
1:A:169:MET:HE1	1:A:221:ASP:HB2	1.82	0.61
1:A:174:LEU:HD21	1:A:361:LEU:HD21	1.82	0.61
1:A:260:PHE:CE2	1:A:278:ILE:HD12	2.37	0.60
1:B:124:THR:CG2	1:B:186:VAL:HG13	2.23	0.60
1:B:303:ILE:HD12	1:B:303:ILE:H	1.65	0.60
1:B:376:ALA:HB3	1:B:431:LYS:HE2	1.84	0.59
1:B:169:MET:HE1	1:B:221:ASP:HB2	1.85	0.59
1:A:144:ASN:HB2	3:A:499:HOH:O	2.02	0.59
1:A:199:GLU:HB2	1:A:280:PHE:CZ	2.38	0.58
1:B:393:ASN:ND2	1:B:395:ASP:H	2.01	0.58
1:B:207:THR:HG22	1:B:210:GLN:N	2.10	0.58
1:B:344:GLN:HE21	1:B:357:SER:HA	1.69	0.58
1:A:347:GLN:HG2	1:A:348:THR:N	2.19	0.58
1:A:260:PHE:HE2	1:A:278:ILE:HD12	1.68	0.57
1:A:169:MET:CE	1:A:218:ASN:HA	2.34	0.56
1:B:364:THR:OG1	1:B:367:GLN:HG3	2.04	0.56
1:B:344:GLN:NE2	1:B:357:SER:HA	2.20	0.56
1:A:199:GLU:HB2	1:A:280:PHE:CE1	2.40	0.56
1:B:216:VAL:HG13	1:B:461:MET:HE1	1.88	0.56
1:B:182:TRP:CZ2	1:B:186:VAL:HG21	2.41	0.56
1:B:393:ASN:HD22	1:B:393:ASN:C	2.08	0.56
1:B:139:SER:OG	1:B:336:HIS:HD2	1.89	0.55
1:B:216:VAL:HA	1:B:461:MET:HE1	1.88	0.55
1:A:359:ILE:HD12	1:A:402:TYR:CE2	2.41	0.55
1:A:401:MET:O	1:A:404:THR:HB	2.06	0.55
1:B:100:TYR:O	1:B:104:ILE:HG13	2.07	0.55
1:B:452:VAL:HG22	1:B:452:VAL:O	2.06	0.54
1:B:470:PHE:HB2	1:B:472:HIS:CE1	2.43	0.54
1:A:359:ILE:HD12	1:A:402:TYR:HE2	1.71	0.54
1:B:140:HIS:CD2	1:B:143:MET:H	2.22	0.54
1:A:259:THR:H	1:A:262:GLN:NE2	2.05	0.54
1:B:466:LEU:O	1:B:468:PHE:N	2.40	0.54
1:B:162:ARG:O	1:B:164:PRO:HD3	2.07	0.54
1:B:169:MET:CE	1:B:221:ASP:HB2	2.38	0.54
1:A:296:ILE:O	1:A:296:ILE:HD12	2.08	0.53
1:B:170:HIS:HD2	1:B:172:GLY:N	2.05	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:ALA:HB1	1:B:357:SER:HB2	1.89	0.53
1:B:144:ASN:HB3	3:B:821:HOH:O	2.07	0.53
1:B:192:VAL:HG13	1:B:235:PHE:HE1	1.74	0.53
1:B:221:ASP:OD1	1:B:445:HIS:HE1	1.92	0.53
1:B:303:ILE:H	1:B:303:ILE:CD1	2.20	0.53
1:A:136:ILE:HD11	1:A:404:THR:HG22	1.91	0.53
1:B:401:MET:O	1:B:404:THR:HB	2.08	0.53
1:A:174:LEU:CD2	1:A:361:LEU:HD21	2.39	0.53
1:A:140:HIS:CD2	1:A:143:MET:H	2.25	0.53
1:A:274:CYS:HA	1:B:259:THR:HA	1.91	0.53
1:A:141:ARG:HG3	1:A:334:LEU:HB2	1.91	0.52
1:A:113:ASP:O	1:A:117:ILE:HG13	2.08	0.52
1:A:253:LYS:O	1:A:257:HIS:HD2	1.93	0.52
1:A:259:THR:HA	1:B:274:CYS:HA	1.91	0.52
1:B:207:THR:HB	1:B:210:GLN:HG3	1.92	0.52
1:A:350:MET:HA	1:A:357:SER:OG	2.09	0.52
1:A:453:THR:OG1	1:A:456:ILE:HG13	2.10	0.51
1:B:234:ILE:O	1:B:461:MET:HG2	2.11	0.51
1:B:345:GLY:CA	1:B:347:GLN:HE22	2.17	0.51
1:B:189:VAL:HB	1:B:190:PRO:HD2	1.92	0.51
1:A:174:LEU:HD21	1:A:361:LEU:CD1	2.36	0.51
1:A:292:SER:C	1:A:294:PRO:HD3	2.31	0.51
1:B:372:VAL:HG12	1:B:431:LYS:HG3	1.92	0.51
1:B:345:GLY:CA	1:B:347:GLN:NE2	2.74	0.51
1:A:169:MET:HE3	1:A:221:ASP:HB2	1.92	0.51
1:A:184:GLN:OE1	1:A:232:THR:HG22	2.11	0.51
1:B:466:LEU:O	1:B:467:SER:C	2.50	0.50
1:A:361:LEU:HD13	1:A:445:HIS:CE1	2.46	0.50
1:A:455:GLU:OE1	1:A:455:GLU:N	2.39	0.50
1:B:141:ARG:NH1	1:B:314:ASP:OD1	2.45	0.50
1:A:137:PHE:CZ	1:A:337:SER:HB3	2.47	0.50
1:A:354:ASP:HB3	1:A:357:SER:CB	2.41	0.50
1:B:295:GLN:HG3	1:B:463:PRO:HB2	1.93	0.50
1:A:403:LEU:HD21	1:A:434:LEU:HA	1.93	0.50
1:B:449:ARG:O	1:B:452:VAL:HG13	2.12	0.50
1:A:251:VAL:O	1:A:255:GLN:HG3	2.12	0.50
1:B:457:VAL:HG12	1:B:461:MET:HE2	1.94	0.50
1:A:369:LYS:HA	1:A:435:ILE:HD13	1.94	0.49
1:A:404:THR:HG21	3:A:565:HOH:O	2.12	0.49
1:A:420:TYR:OH	1:A:427:THR:HB	2.12	0.49
1:A:314:ASP:N	1:A:315:PRO:HD2	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:GLN:HG2	1:A:296:ILE:N	2.27	0.49
1:B:448:ARG:O	1:B:451:GLU:HB2	2.12	0.49
1:A:394:CYS:HB3	1:A:400:PHE:CD2	2.48	0.49
1:A:221:ASP:OD2	1:A:445:HIS:HE1	1.95	0.49
1:A:259:THR:H	1:A:262:GLN:HE21	1.61	0.49
1:A:278:ILE:HG22	1:B:275:ILE:HG22	1.94	0.49
1:A:105:VAL:HG13	1:A:106:ARG:N	2.27	0.49
1:A:139:SER:OG	1:A:336:HIS:HD2	1.95	0.48
1:A:197:ASP:CG	1:A:238:LEU:HD22	2.33	0.48
1:A:255:GLN:HE21	1:A:279:SER:HB2	1.78	0.48
1:A:364:THR:OG1	1:A:367:GLN:HG3	2.14	0.48
1:B:103:LEU:O	1:B:107:PHE:HB2	2.13	0.48
1:A:280:PHE:N	1:A:281:PRO:CD	2.77	0.48
1:A:295:GLN:HG2	1:A:296:ILE:HG22	1.95	0.48
1:B:169:MET:HE1	1:B:218:ASN:HA	1.96	0.48
1:A:435:ILE:O	1:A:439:GLN:HG3	2.14	0.48
1:B:393:ASN:HD21	1:B:395:ASP:HB2	1.78	0.48
1:A:124:THR:CB	1:A:186:VAL:HG13	2.42	0.48
1:A:296:ILE:HG13	1:A:297:PHE:CD1	2.49	0.47
1:B:348:THR:HG22	1:B:349:LYS:O	2.14	0.47
1:B:100:TYR:HB3	1:B:138:PHE:CE2	2.49	0.47
1:B:136:ILE:HD13	1:B:405:PHE:CD2	2.49	0.47
1:B:170:HIS:HD2	1:B:172:GLY:H	1.62	0.47
1:B:344:GLN:HE21	1:B:357:SER:CA	2.28	0.47
1:B:169:MET:CE	1:B:218:ASN:HA	2.44	0.47
1:B:393:ASN:ND2	1:B:393:ASN:C	2.67	0.47
1:A:162:ARG:O	1:A:164:PRO:HD3	2.14	0.46
1:A:293:PHE:N	1:A:294:PRO:HD3	2.30	0.46
1:A:352:ALA:HA	1:A:360:PHE:CZ	2.50	0.46
1:B:440:PRO:O	1:B:444:GLU:HB2	2.15	0.46
1:A:169:MET:HE3	1:A:221:ASP:CB	2.46	0.46
1:B:101:ASP:O	1:B:105:VAL:HG23	2.16	0.46
1:A:347:GLN:NE2	1:A:347:GLN:N	2.60	0.46
1:A:350:MET:CE	1:A:358:SER:HB2	2.39	0.46
1:A:333:ALA:C	1:A:334:LEU:HD12	2.37	0.45
1:A:347:GLN:N	1:A:347:GLN:HE21	2.14	0.45
1:B:366:LYS:O	1:B:370:THR:CG2	2.65	0.45
1:A:121:GLU:HG3	1:A:126:GLN:O	2.16	0.45
1:B:171:VAL:HG13	1:B:406:PHE:CZ	2.51	0.45
1:B:207:THR:HG23	1:B:209:ASP:H	1.81	0.45
1:A:182:TRP:CZ2	1:A:186:VAL:HG21	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:ASN:HB3	1:A:301:THR:HG22	1.98	0.45
1:A:457:VAL:HG12	1:A:461:MET:CE	2.47	0.45
1:B:259:THR:HG23	1:B:262:GLN:HE21	1.80	0.45
1:A:170:HIS:HA	1:A:360:PHE:HA	1.97	0.45
1:A:281:PRO:HB3	1:A:319:MET:HE3	1.98	0.45
1:A:198:ASP:HB3	1:A:238:LEU:CD1	2.47	0.44
1:A:453:THR:OG1	1:A:455:GLU:HG2	2.16	0.44
1:B:192:VAL:HG11	1:B:293:PHE:CZ	2.52	0.44
1:B:466:LEU:O	1:B:468:PHE:HD1	1.99	0.44
1:A:98:ILE:HG23	1:A:100:TYR:CZ	2.53	0.44
1:A:384:ILE:O	1:A:388:ARG:HG2	2.17	0.44
1:B:159:TYR:O	1:B:307:ILE:HG23	2.18	0.44
1:A:119:ARG:HG2	1:A:147:LEU:HD13	2.00	0.44
1:A:129:HIS:HB2	1:A:182:TRP:CD2	2.53	0.43
1:B:366:LYS:O	1:B:370:THR:HG22	2.19	0.43
1:A:124:THR:HG21	1:A:186:VAL:CG1	2.48	0.43
1:A:170:HIS:HD2	1:A:172:GLY:N	2.16	0.43
1:A:259:THR:HG23	1:A:262:GLN:HE21	1.83	0.43
1:B:169:MET:HE3	1:B:221:ASP:CB	2.48	0.43
1:B:169:MET:HE3	1:B:221:ASP:CG	2.38	0.43
1:B:333:ALA:C	1:B:334:LEU:HD12	2.38	0.43
1:B:457:VAL:HG12	1:B:461:MET:CE	2.48	0.43
1:B:113:ASP:OD1	1:B:115:GLU:HB3	2.19	0.43
1:B:175:ILE:HB	1:B:176:PRO:CD	2.49	0.43
1:B:241:MET:CE	1:B:283:ILE:HD12	2.49	0.43
1:A:439:GLN:N	1:A:440:PRO:HD2	2.34	0.43
1:B:314:ASP:N	1:B:315:PRO:HD2	2.34	0.43
1:A:98:ILE:HD11	1:A:103:LEU:HD12	2.00	0.43
1:B:300:ARG:CG	1:B:303:ILE:HD11	2.48	0.42
1:B:347:GLN:CD	1:B:347:GLN:H	2.22	0.42
1:A:264:LYS:HG3	1:A:269:PHE:O	2.18	0.42
1:B:364:THR:O	1:B:368:ILE:HG13	2.19	0.42
1:A:100:TYR:HB3	1:A:138:PHE:CE2	2.54	0.42
1:A:102:LYS:O	1:A:105:VAL:HG12	2.20	0.42
1:A:354:ASP:CB	1:A:357:SER:HB2	2.45	0.42
1:B:190:PRO:HD3	1:B:468:PHE:CD2	2.55	0.42
1:A:100:TYR:O	1:A:104:ILE:HG13	2.20	0.42
1:A:343:LEU:HD23	1:A:343:LEU:HA	1.89	0.42
1:B:196:THR:HB	1:B:199:GLU:HB2	2.00	0.42
1:B:259:THR:H	1:B:262:GLN:NE2	2.16	0.42
1:B:186:VAL:HG12	1:B:187:PHE:N	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:LEU:HD21	1:B:193:ILE:HD11	2.01	0.41
1:A:98:ILE:CD1	1:A:103:LEU:HD12	2.50	0.41
1:B:300:ARG:CG	1:B:303:ILE:CD1	2.98	0.41
1:A:233:PHE:CZ	1:A:235:PHE:HB3	2.55	0.41
1:A:298:ARG:HD2	3:A:489:HOH:O	2.19	0.41
1:B:233:PHE:CZ	1:B:235:PHE:HB3	2.56	0.41
1:A:192:VAL:HG11	1:A:293:PHE:CZ	2.55	0.41
1:B:137:PHE:CE1	1:B:337:SER:HB3	2.55	0.41
1:A:170:HIS:HD2	1:A:172:GLY:H	1.67	0.41
1:B:345:GLY:C	1:B:347:GLN:NE2	2.74	0.41
1:B:420:TYR:HE1	1:B:427:THR:HA	1.86	0.41
1:A:130:HIS:HB3	1:A:133:ARG:NH2	2.36	0.41
1:B:98:ILE:HG22	1:B:99:ASP:N	2.34	0.41
1:A:124:THR:CG2	1:A:186:VAL:HG13	2.51	0.40
1:A:196:THR:HB	1:A:199:GLU:HB3	2.04	0.40
1:A:208:LEU:HD12	1:B:253:LYS:HE3	2.02	0.40
1:A:457:VAL:HG12	1:A:461:MET:HE2	2.03	0.40
1:A:200:LYS:HD3	1:A:200:LYS:HA	1.77	0.40
1:B:228:ASP:O	1:B:232:THR:CG2	2.67	0.40
1:B:234:ILE:O	1:B:461:MET:HA	2.21	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	377/477 (79%)	361 (96%)	16 (4%)	0	100	100
1	B	379/477 (80%)	364 (96%)	12 (3%)	3 (1%)	19	29
All	All	756/954 (79%)	725 (96%)	28 (4%)	3 (0%)	34	48

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	467	SER
1	B	298	ARG
1	B	299	ASP

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	330/416 (79%)	311 (94%)	19 (6%)	20	32
1	B	327/416 (79%)	308 (94%)	19 (6%)	20	32
All	All	657/832 (79%)	619 (94%)	38 (6%)	20	32

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	98	ILE
1	A	103	LEU
1	A	156	PHE
1	A	159	TYR
1	A	171	VAL
1	A	188	ASN
1	A	197	ASP
1	A	202	LEU
1	A	203	TRP
1	A	232	THR
1	A	236	SER
1	A	238	LEU
1	A	296	ILE
1	A	347	GLN
1	A	427	THR
1	A	430	LEU
1	A	455	GLU
1	A	464	ARG
1	A	474	HIS
1	B	144	ASN
1	B	202	LEU

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Mol	Chain	Res	Type
1	B	203	TRP
1	B	207	THR
1	B	232	THR
1	B	236	SER
1	B	291	ASN
1	B	295	GLN
1	B	311	ILE
1	B	362	THR
1	B	370	THR
1	B	393	ASN
1	B	408	GLU
1	B	415	GLN
1	B	427	THR
1	B	430	LEU
1	B	452	VAL
1	B	457	VAL
1	B	464	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	140	HIS
1	A	170	HIS
1	A	188	ASN
1	A	255	GLN
1	A	257	HIS
1	A	262	GLN
1	A	336	HIS
1	A	347	GLN
1	A	389	GLN
1	A	445	HIS
1	A	471	GLN
1	B	140	HIS
1	B	145	GLN
1	B	170	HIS
1	B	257	HIS
1	B	262	GLN
1	B	291	ASN
1	B	295	GLN
1	B	336	HIS
1	B	344	GLN
1	B	347	GLN

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Mol	Chain	Res	Type
1	B	393	ASN
1	B	439	GLN
1	B	445	HIS

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)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	TRP	B	817	-	14,16,16	1.75	3 (21%)	16,22,22	1.01	1 (6%)
2	TRP	B	818	-	14,16,16	1.77	3 (21%)	16,22,22	1.08	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TRP	B	817	-	-	0/7/8/8	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TRP	B	818	-	-	0/7/8/8	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	818	TRP	CH2-CZ2	3.66	1.45	1.36
2	B	817	TRP	CH2-CZ2	3.62	1.45	1.36
2	B	817	TRP	CZ3-CE3	3.54	1.44	1.36
2	B	818	TRP	CZ3-CE3	3.34	1.44	1.36
2	B	818	TRP	CH2-CZ3	2.73	1.45	1.38
2	B	817	TRP	CH2-CZ3	2.39	1.44	1.38

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	818	TRP	OXT-C-O	-2.25	118.99	124.09
2	B	817	TRP	OXT-C-O	-2.16	119.18	124.09

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	379/477 (79%)	-0.25	5 (1%)	77	75	31, 44, 66, 90	0
1	B	381/477 (79%)	-0.22	6 (1%)	72	70	29, 41, 70, 136	0
All	All	760/954 (79%)	-0.23	11 (1%)	75	73	29, 43, 68, 136	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	93	SER	5.7
1	B	472	HIS	5.7
1	B	471	GLN	5.5
1	B	469	ASP	3.5
1	B	470	PHE	3.4
1	A	97	GLY	3.1
1	B	468	PHE	3.0
1	A	347	GLN	2.8
1	A	98	ILE	2.8
1	A	348	THR	2.6
1	A	107	PHE	2.3

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	TRP	B	817	15/15	0.95	0.16	38,41,45,46	0
2	TRP	B	818	15/15	0.96	0.19	35,38,41,44	0

6.5 Other polymers (i)

There are no such residues in this entry.