



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:28 AM UTC

PDB ID : 6F8Y / pdb_00006f8y
Title : Crystal structure of P. abyssi Sua5 complexed with L-threonine
Authors : Pichard-Kostuch, A.; Zhang, W.; Liger, D.; Daugeron, M.C.; Letoquart, J.; Li de la Sierra-Gallay, I.; Forterre, P.; Collinet, B.; van Tilbeurgh, H.; Basta, T.
Deposited on : 2017-12-13
Resolution : 2.86 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

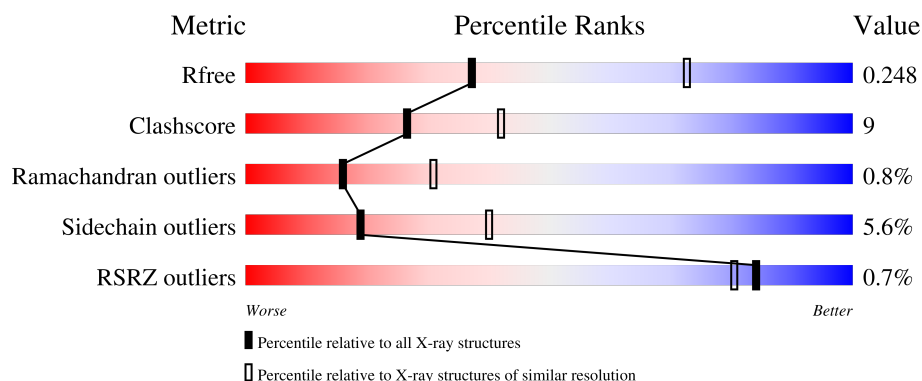
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

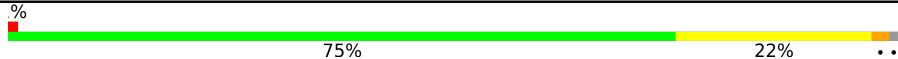
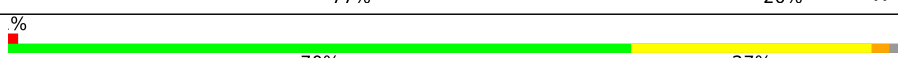
The reported resolution of this entry is 2.86 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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

Mol	Chain	Length	Quality of chain
1	A	345	
1	B	345	
1	C	345	
1	D	345	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10631 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 Threonylcarbamoyl-AMP synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	0	0	0
			2640	1690	460	484	6			
1	B	340	Total	C	N	O	S	0	0	0
			2640	1690	460	484	6			
1	C	341	Total	C	N	O	S	0	0	0
			2650	1696	463	485	6			
1	D	340	Total	C	N	O	S	0	0	0
			2640	1690	460	484	6			

There are 24 discrepancies between the modelled and reference sequences:

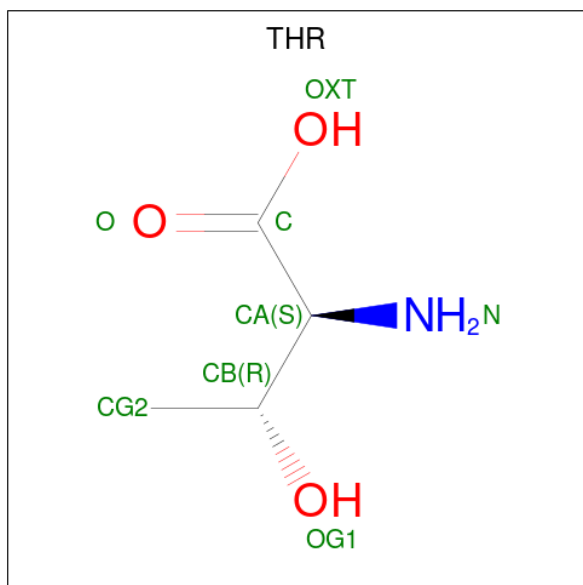
Chain	Residue	Modelled	Actual	Comment	Reference
A	341	HIS	-	expression tag	UNP Q9UYB2
A	342	HIS	-	expression tag	UNP Q9UYB2
A	343	HIS	-	expression tag	UNP Q9UYB2
A	344	HIS	-	expression tag	UNP Q9UYB2
A	345	HIS	-	expression tag	UNP Q9UYB2
A	346	HIS	-	expression tag	UNP Q9UYB2
B	341	HIS	-	expression tag	UNP Q9UYB2
B	342	HIS	-	expression tag	UNP Q9UYB2
B	343	HIS	-	expression tag	UNP Q9UYB2
B	344	HIS	-	expression tag	UNP Q9UYB2
B	345	HIS	-	expression tag	UNP Q9UYB2
B	346	HIS	-	expression tag	UNP Q9UYB2
C	341	HIS	-	expression tag	UNP Q9UYB2
C	342	HIS	-	expression tag	UNP Q9UYB2
C	343	HIS	-	expression tag	UNP Q9UYB2
C	344	HIS	-	expression tag	UNP Q9UYB2
C	345	HIS	-	expression tag	UNP Q9UYB2
C	346	HIS	-	expression tag	UNP Q9UYB2
D	341	HIS	-	expression tag	UNP Q9UYB2
D	342	HIS	-	expression tag	UNP Q9UYB2
D	343	HIS	-	expression tag	UNP Q9UYB2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	344	HIS	-	expression tag	UNP Q9UYB2
D	345	HIS	-	expression tag	UNP Q9UYB2
D	346	HIS	-	expression tag	UNP Q9UYB2

- Molecule 2 is THREONINE (CCD ID: THR) (formula: $C_4H_9NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			8	4	1	3		
2	B	1	Total	C	N	O	0	0
			8	4	1	3		
2	C	1	Total	C	N	O	0	0
			8	4	1	3		
2	D	1	Total	C	N	O	0	0
			8	4	1	3		

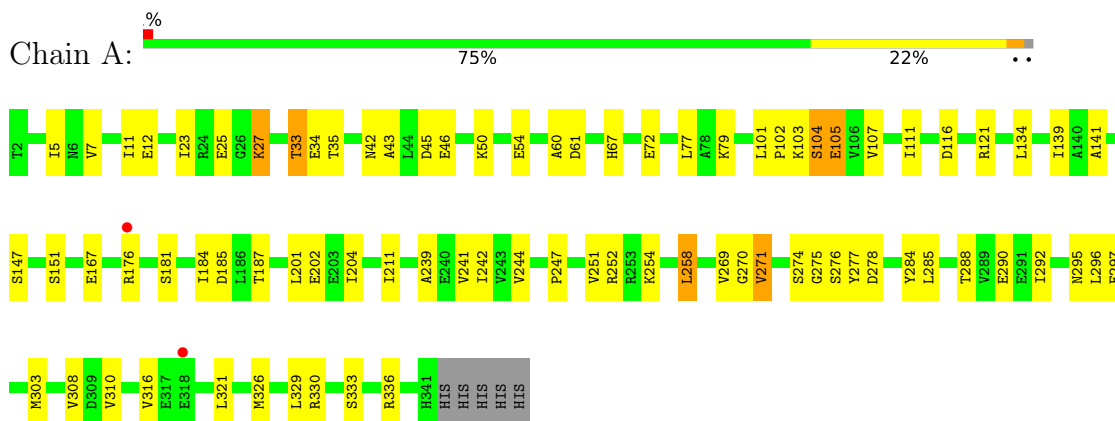
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	9	Total	O	0	0
			9	9		
3	B	7	Total	O	0	0
			7	7		
3	C	9	Total	O	0	0
			9	9		
3	D	4	Total	O	0	0
			4	4		

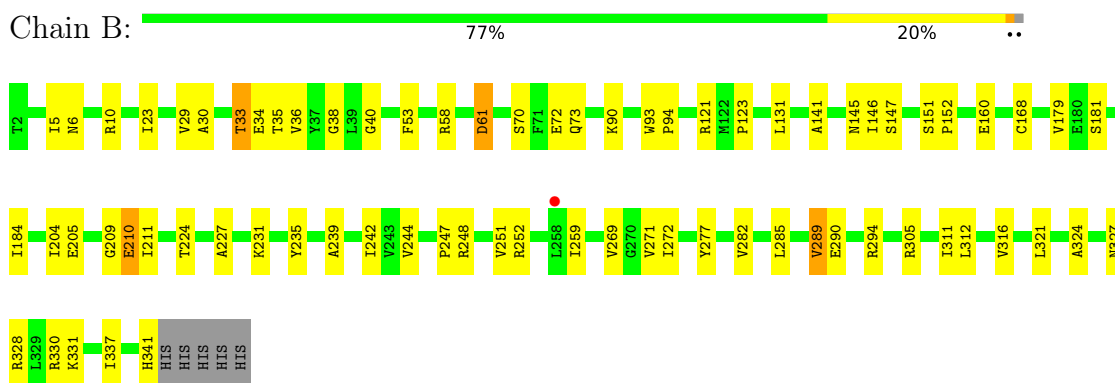
3 Residue-property plots [i](#)

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.

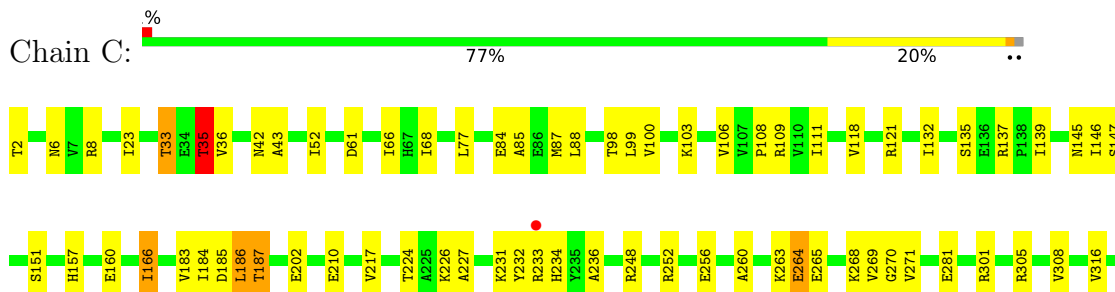
• Molecule 1: Threonylcarbamoyl-AMP synthase

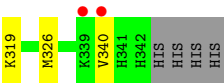


• Molecule 1: Threonylcarbamoyl-AMP synthase

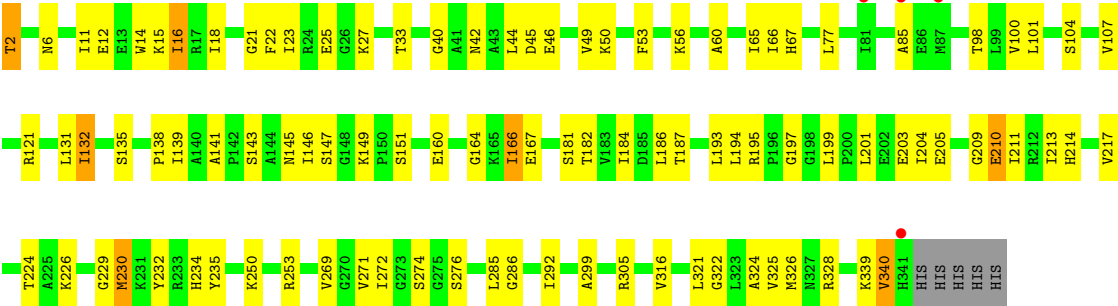


• Molecule 1: Threonylcarbamoyl-AMP synthase





● Molecule 1: Threonylcarbamoyl-AMP synthase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	152.23Å 142.38Å 103.86Å 90.00° 101.80° 90.00°	Depositor
Resolution (Å)	48.78 – 2.86 48.78 – 2.86	Depositor EDS
% Data completeness (in resolution range)	99.3 (48.78-2.86) 99.6 (48.78-2.86)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.188 , 0.252 0.192 , 0.248	Depositor DCC
R_{free} test set	2497 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	75.4	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 54.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10631	wwPDB-VP
Average B, all atoms (Å ²)	79.0	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 47.30 % 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 1.0120e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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](#)

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	0.90	0/2691	1.11	6/3642 (0.2%)
1	B	0.93	1/2691 (0.0%)	1.11	4/3642 (0.1%)
1	C	0.94	2/2702 (0.1%)	1.11	5/3657 (0.1%)
1	D	0.86	1/2691 (0.0%)	1.13	4/3642 (0.1%)
All	All	0.91	4/10775 (0.0%)	1.12	19/14583 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	61	ASP	CA-C	5.33	1.59	1.52
1	C	166	ILE	C-O	-5.26	1.17	1.23
1	D	166	ILE	C-O	-5.06	1.17	1.23
1	C	186	LEU	N-CA	5.02	1.52	1.46

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	61	ASP	N-CA-C	8.23	120.25	111.28
1	C	340	VAL	N-CA-C	6.41	117.11	107.75
1	D	340	VAL	N-CA-C	6.38	117.28	107.78
1	C	61	ASP	N-CA-C	6.24	121.67	111.37
1	B	210	GLU	N-CA-C	-6.13	101.20	110.28
1	D	40	GLY	N-CA-C	5.97	119.84	112.14
1	C	227	ALA	N-CA-C	5.88	115.07	108.25
1	A	60	ALA	CA-C-N	5.86	128.13	120.28
1	A	60	ALA	C-N-CA	5.86	128.13	120.28
1	B	227	ALA	N-CA-C	5.70	113.35	108.22
1	C	35	THR	CB-CA-C	5.69	121.75	110.42
1	A	176	ARG	N-CA-C	5.59	117.37	111.28
1	C	52	ILE	CB-CA-C	-5.53	104.63	111.70
1	B	61	ASP	N-CA-CB	-5.46	101.87	110.06
1	A	101	LEU	CA-C-N	-5.45	114.31	119.76
1	A	101	LEU	C-N-CA	-5.45	114.31	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	259	ILE	N-CA-CB	5.36	116.46	110.62
1	D	274	SER	N-CA-C	5.20	117.03	111.36
1	D	286	GLY	N-CA-C	5.15	117.55	111.63

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2640	0	2729	41	0
1	B	2640	0	2729	41	0
1	C	2650	0	2736	52	0
1	D	2640	0	2729	68	0
2	A	8	0	6	2	0
2	B	8	0	6	1	0
2	C	8	0	6	3	0
2	D	8	0	6	1	0
3	A	9	0	0	0	0
3	B	7	0	0	0	0
3	C	9	0	0	0	0
3	D	4	0	0	0	0
All	All	10631	0	10947	200	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 9.

All (200) 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:C:2:THR:HG22	1:C:166:ILE:O	1.27	1.28
1:C:2:THR:CG2	1:C:166:ILE:O	2.16	0.93
1:C:248:ARG:NH1	1:C:252:ARG:HD2	1.87	0.89
1:A:270:GLY:HA3	1:A:303:MET:HE1	1.55	0.89
1:C:121:ARG:NH2	2:C:401:THR:OG1	2.06	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2:THR:HG22	1:D:166:ILE:O	1.74	0.87
1:D:77:LEU:HD22	1:D:107:VAL:HG22	1.60	0.83
1:D:272:ILE:HG22	1:D:285:LEU:HD11	1.62	0.81
1:D:182:THR:HG21	1:D:199:LEU:O	1.80	0.81
1:D:121:ARG:NH2	2:D:401:THR:OG1	2.17	0.78
1:A:33:THR:HG22	1:A:35:THR:H	1.51	0.76
1:D:145:ASN:HD22	1:D:151:SER:HA	1.51	0.75
1:A:103:LYS:HG2	1:A:104:SER:O	1.87	0.74
1:B:252:ARG:HG2	1:B:277:TYR:OH	1.88	0.74
1:D:316:VAL:H	1:D:326:MET:HE3	1.53	0.73
1:B:145:ASN:HD22	1:B:151:SER:HA	1.52	0.73
1:A:121:ARG:NH2	2:A:401:THR:OG1	2.24	0.70
1:A:27:LYS:HG2	1:A:167:GLU:HG2	1.73	0.70
1:B:33:THR:HG22	1:B:35:THR:H	1.56	0.70
1:C:85:ALA:HB2	1:C:186:LEU:HD23	1.74	0.69
1:B:327:ASN:ND2	1:B:331:LYS:HE2	2.08	0.68
1:D:187:THR:OG1	1:D:226:LYS:NZ	2.26	0.68
1:A:185:ASP:OD1	1:A:187:THR:HG22	1.94	0.67
1:C:316:VAL:HG22	1:C:326:MET:HE3	1.78	0.66
1:C:23:ILE:HG21	1:C:135:SER:OG	1.95	0.65
1:D:229:GLY:HA2	1:D:234:HIS:CD2	2.33	0.64
1:C:268:LYS:HG3	1:C:308:VAL:HA	1.80	0.64
1:D:285:LEU:HD13	1:D:292:ILE:HG23	1.80	0.64
1:A:254:LYS:O	1:A:258:LEU:HD12	1.97	0.64
1:D:182:THR:HG22	1:D:197:GLY:N	2.13	0.64
1:D:77:LEU:HD22	1:D:107:VAL:CG2	2.27	0.64
1:B:242:ILE:HB	1:B:312:LEU:HD23	1.81	0.62
1:C:33:THR:HG22	1:C:35:THR:H	1.62	0.62
1:C:160:GLU:OE1	1:C:305:ARG:NE	2.29	0.62
1:B:330:ARG:HG2	1:B:337:ILE:HD11	1.82	0.61
1:C:87:MET:HG3	1:C:88:LEU:N	2.15	0.61
1:D:67:HIS:CE1	1:D:141:ALA:HB3	2.34	0.61
1:C:252:ARG:NH1	1:C:252:ARG:HB3	2.15	0.61
1:C:43:ALA:O	1:C:111:ILE:HD11	2.01	0.60
1:D:56:LYS:NZ	1:D:143:SER:O	2.33	0.60
1:B:184:ILE:HD11	1:B:204:ILE:HD13	1.82	0.60
1:C:35:THR:HG21	2:C:401:THR:O	2.02	0.60
1:B:239:ALA:HB3	1:B:311:ILE:HD11	1.83	0.60
1:D:145:ASN:ND2	1:D:151:SER:HA	2.16	0.60
1:D:253:ARG:HH11	1:D:253:ARG:HG2	1.67	0.60
1:D:2:THR:CG2	1:D:166:ILE:O	2.50	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:184:ILE:HD11	1:D:204:ILE:HG21	1.83	0.59
1:D:33:THR:HG21	1:D:121:ARG:HH22	1.68	0.59
1:A:247:PRO:O	1:A:251:VAL:HG23	2.03	0.59
1:C:85:ALA:CB	1:C:186:LEU:HD23	2.33	0.58
1:C:233:ARG:NH1	1:C:236:ALA:HB3	2.18	0.58
1:D:272:ILE:CG2	1:D:285:LEU:HD11	2.34	0.58
1:B:160:GLU:OE2	1:B:305:ARG:HD3	2.03	0.57
1:D:324:ALA:O	1:D:328:ARG:HG2	2.05	0.57
1:A:316:VAL:HG22	1:A:326:MET:HE3	1.87	0.57
1:B:93:TRP:O	1:D:339:LYS:HD2	2.05	0.56
1:D:214:HIS:O	1:D:217:VAL:HG12	2.05	0.56
1:C:33:THR:HG21	1:C:121:ARG:HH22	1.70	0.56
1:D:193:LEU:HB2	1:D:211:ILE:CD1	2.35	0.56
1:B:272:ILE:HG22	1:B:285:LEU:HD11	1.88	0.56
1:D:184:ILE:HD11	1:D:204:ILE:HD13	1.88	0.55
1:A:43:ALA:O	1:A:111:ILE:HD11	2.07	0.55
1:C:132:ILE:HG12	1:C:139:ILE:HD12	1.87	0.55
1:D:193:LEU:HB2	1:D:211:ILE:HD11	1.88	0.55
1:B:160:GLU:OE1	1:B:305:ARG:NH1	2.37	0.55
1:D:100:VAL:O	1:D:101:LEU:HD12	2.06	0.54
1:D:213:ILE:HG23	1:D:217:VAL:HG11	1.88	0.54
1:C:84:GLU:HA	1:C:87:MET:HG2	1.89	0.54
1:C:184:ILE:HG22	1:C:186:LEU:HD13	1.90	0.54
1:A:242:ILE:HD11	1:A:336:ARG:HH21	1.73	0.53
1:C:316:VAL:H	1:C:326:MET:HE3	1.74	0.53
1:D:184:ILE:CD1	1:D:204:ILE:HG21	2.39	0.53
1:B:181:SER:OG	2:B:401:THR:O	2.17	0.53
1:B:235:TYR:HE2	1:B:331:LYS:HD2	1.73	0.53
1:A:244:VAL:HG12	1:A:251:VAL:HG13	1.91	0.53
1:C:6:ASN:OD1	1:C:8:ARG:HG3	2.09	0.52
1:C:233:ARG:HH11	1:C:236:ALA:HB3	1.74	0.52
1:C:88:LEU:HD12	1:C:186:LEU:HD21	1.92	0.52
1:C:103:LYS:HE2	1:C:109:ARG:HG2	1.92	0.51
1:A:285:LEU:HD13	1:A:292:ILE:HG23	1.92	0.51
1:A:7:VAL:CG1	1:A:11:ILE:HA	2.40	0.51
1:C:270:GLY:HA2	1:C:281:GLU:O	2.11	0.51
1:B:145:ASN:ND2	1:B:151:SER:HA	2.23	0.51
1:C:184:ILE:HG22	1:C:186:LEU:CD1	2.41	0.51
1:A:274:SER:HB2	1:A:284:TYR:HE1	1.75	0.51
1:A:50:LYS:O	1:A:50:LYS:HD2	2.11	0.50
1:D:77:LEU:O	1:D:104:SER:N	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:ILE:HD12	1:B:131:LEU:HD11	1.93	0.50
1:A:7:VAL:HG12	1:A:7:VAL:O	2.12	0.50
1:B:90:LYS:O	1:D:339:LYS:NZ	2.38	0.50
1:B:205:GLU:HG2	1:B:210:GLU:HA	1.94	0.50
1:A:252:ARG:CZ	1:A:275:GLY:HA2	2.42	0.49
1:D:316:VAL:N	1:D:326:MET:HE3	2.24	0.49
1:C:23:ILE:CG2	1:C:135:SER:OG	2.59	0.49
1:D:77:LEU:CD2	1:D:107:VAL:HG22	2.38	0.49
1:A:151:SER:HB2	1:A:297:PHE:CE2	2.48	0.49
1:D:65:ILE:HG12	1:D:98:THR:HG21	1.93	0.49
1:D:14:TRP:O	1:D:18:ILE:HG13	2.13	0.49
1:B:145:ASN:HB3	1:B:152:PRO:HD3	1.95	0.49
1:A:271:VAL:HG21	1:A:277:TYR:CD1	2.48	0.49
1:A:288:THR:O	1:A:292:ILE:HG13	2.13	0.49
1:A:34:GLU:CD	1:A:121:ARG:NH1	2.71	0.48
1:D:44:LEU:HD13	1:D:138:PRO:HD2	1.95	0.48
1:D:85:ALA:HB2	1:D:186:LEU:HD13	1.95	0.48
1:C:100:VAL:HB	1:C:185:ASP:HA	1.95	0.48
1:D:194:LEU:HB3	1:D:230:MET:SD	2.53	0.48
1:D:11:ILE:CG2	1:D:16:ILE:CD1	2.92	0.48
1:B:327:ASN:HD21	1:B:331:LYS:HE2	1.78	0.48
1:C:231:LYS:O	1:C:234:HIS:HE1	1.96	0.48
1:D:53:PHE:CE2	1:D:60:ALA:HA	2.49	0.48
1:A:201:LEU:CD1	1:A:211:ILE:HD11	2.43	0.47
1:B:242:ILE:HB	1:B:312:LEU:CD2	2.44	0.47
1:D:101:LEU:HD11	1:D:186:LEU:HD12	1.96	0.47
1:D:213:ILE:HG23	1:D:217:VAL:CG1	2.44	0.47
1:A:105:GLU:H	1:A:105:GLU:CD	2.23	0.47
1:B:239:ALA:HB3	1:B:311:ILE:CD1	2.45	0.47
1:B:34:GLU:HG2	1:B:35:THR:HG23	1.97	0.47
1:B:272:ILE:CG2	1:B:285:LEU:HD11	2.44	0.47
1:C:145:ASN:ND2	1:C:151:SER:HA	2.30	0.47
1:C:33:THR:HG22	1:C:35:THR:N	2.29	0.46
1:C:252:ARG:O	1:C:256:GLU:HG3	2.15	0.46
1:D:100:VAL:C	1:D:101:LEU:HD12	2.41	0.46
1:C:252:ARG:HB3	1:C:252:ARG:HH11	1.79	0.46
1:B:29:VAL:HG22	1:B:168:CYS:HB3	1.97	0.46
1:C:35:THR:CG2	1:C:36:VAL:H	2.27	0.46
1:D:6:ASN:OD1	1:D:6:ASN:C	2.58	0.46
1:D:205:GLU:HG2	1:D:210:GLU:HA	1.97	0.46
1:B:33:THR:HB	1:B:36:VAL:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:ASN:HD22	1:A:45:ASP:HB3	1.81	0.46
1:D:131:LEU:O	1:D:135:SER:HB2	2.16	0.46
1:C:185:ASP:OD1	1:C:187:THR:HB	2.16	0.45
1:B:247:PRO:O	1:B:251:VAL:HG23	2.15	0.45
1:D:253:ARG:HG2	1:D:253:ARG:NH1	2.29	0.45
1:C:263:LYS:C	1:C:265:GLU:H	2.24	0.45
1:D:132:ILE:HD13	1:D:139:ILE:HD12	1.97	0.45
1:C:35:THR:CG2	2:C:401:THR:O	2.65	0.45
1:C:231:LYS:HE2	1:C:232:TYR:CZ	2.52	0.45
1:D:2:THR:HG23	1:D:164:GLY:HA2	1.98	0.44
1:C:260:ALA:O	1:C:264:GLU:HB3	2.18	0.44
1:A:5:ILE:HG22	1:A:7:VAL:HG23	1.99	0.44
1:A:79:LYS:O	1:A:102:PRO:HG2	2.16	0.44
1:B:40:GLY:HA2	1:B:141:ALA:HB2	1.99	0.44
1:D:181:SER:O	1:D:195:ARG:NH2	2.48	0.44
1:C:98:THR:HB	1:C:183:VAL:HG22	1.99	0.44
1:C:106:VAL:O	1:C:108:PRO:HD3	2.17	0.44
1:D:235:TYR:CZ	1:D:328:ARG:HD2	2.53	0.44
1:B:327:ASN:CG	1:B:331:LYS:HE2	2.42	0.44
1:D:18:ILE:HG22	1:D:22:PHE:HE2	1.82	0.44
1:B:53:PHE:CE2	1:B:58:ARG:HD3	2.52	0.44
1:D:322:GLY:O	1:D:325:VAL:HG22	2.17	0.44
1:C:248:ARG:NH1	1:C:252:ARG:CD	2.70	0.44
1:D:42:ASN:HB3	1:D:45:ASP:HB3	2.00	0.44
1:D:66:ILE:HG21	1:D:77:LEU:CD1	2.48	0.44
1:A:290:GLU:HA	1:A:321:LEU:HD12	2.00	0.43
1:C:157:HIS:ND1	1:C:301:ARG:HD2	2.33	0.43
1:A:185:ASP:CG	1:A:187:THR:HG22	2.44	0.43
1:B:93:TRP:HA	1:B:94:PRO:C	2.42	0.43
1:A:34:GLU:CD	1:A:121:ARG:HH11	2.27	0.43
1:A:67:HIS:CE1	1:A:141:ALA:HB3	2.54	0.43
1:D:27:LYS:HB3	1:D:167:GLU:HG2	2.00	0.43
1:C:99:LEU:HD22	1:C:186:LEU:HD22	2.01	0.42
1:B:61:ASP:OD2	1:B:231:LYS:NZ	2.41	0.42
1:B:121:ARG:NH2	1:B:123:PRO:HB3	2.35	0.42
1:A:77:LEU:HD22	1:A:107:VAL:HG22	2.00	0.42
1:B:30:ALA:HA	1:B:38:GLY:O	2.18	0.42
1:C:84:GLU:O	1:C:87:MET:HG3	2.19	0.42
1:D:42:ASN:HD22	1:D:45:ASP:HB2	1.83	0.42
1:B:244:VAL:HG12	1:B:251:VAL:HG13	2.01	0.42
1:B:289:VAL:CG1	1:B:321:LEU:HB2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:160:GLU:OE1	1:D:305:ARG:NH1	2.48	0.42
1:D:272:ILE:HD12	1:D:299:ALA:HB1	2.00	0.42
1:A:326:MET:HE2	1:A:329:LEU:HD12	2.00	0.42
1:C:66:ILE:HD12	1:C:118:VAL:HG21	2.02	0.42
1:A:241:VAL:O	1:A:333:SER:HB2	2.20	0.42
1:A:326:MET:O	1:A:330:ARG:HG3	2.20	0.42
1:C:33:THR:HG21	1:C:35:THR:HG22	2.01	0.42
1:C:33:THR:HB	1:C:36:VAL:O	2.19	0.42
1:D:12:GLU:O	1:D:15:LYS:HB2	2.19	0.42
1:D:209:GLY:O	1:D:210:GLU:C	2.63	0.42
1:D:321:LEU:HD22	1:D:321:LEU:N	2.36	0.41
1:B:6:ASN:OD1	1:B:6:ASN:C	2.63	0.41
1:B:70:SER:HB2	1:B:72:GLU:OE2	2.21	0.41
1:A:184:ILE:HD11	1:A:204:ILE:HD13	2.03	0.41
1:D:21:GLY:O	1:D:25:GLU:HG3	2.20	0.41
1:D:44:LEU:HD13	1:D:138:PRO:CD	2.50	0.41
1:A:295:ASN:O	1:A:296:LEU:C	2.63	0.41
1:C:33:THR:CG2	1:C:35:THR:HG22	2.51	0.41
1:C:42:ASN:HD21	1:C:137:ARG:HE	1.69	0.41
1:D:11:ILE:HG23	1:D:16:ILE:CD1	2.51	0.41
1:D:77:LEU:CD2	1:D:107:VAL:CG2	2.97	0.41
1:D:229:GLY:HA2	1:D:234:HIS:NE2	2.36	0.41
1:A:11:ILE:HD12	1:A:11:ILE:N	2.36	0.41
1:B:35:THR:HB	1:B:179:VAL:O	2.21	0.41
1:B:290:GLU:HG2	1:B:294:ARG:HH11	1.86	0.40
1:C:35:THR:CG2	1:C:36:VAL:N	2.84	0.40
1:A:151:SER:HB2	1:A:297:PHE:CD2	2.57	0.40
1:A:181:SER:OG	2:A:401:THR:OXT	2.32	0.40
1:B:324:ALA:O	1:B:328:ARG:HG2	2.20	0.40
1:D:250:LYS:HB3	1:D:340:VAL:HG11	2.03	0.40
1:A:326:MET:HE2	1:A:326:MET:HA	2.03	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	338/345 (98%)	316 (94%)	18 (5%)	4 (1%)	10	22
1	B	338/345 (98%)	316 (94%)	19 (6%)	3 (1%)	14	28
1	C	339/345 (98%)	320 (94%)	18 (5%)	1 (0%)	36	54
1	D	338/345 (98%)	314 (93%)	21 (6%)	3 (1%)	14	28
All	All	1353/1380 (98%)	1266 (94%)	76 (6%)	11 (1%)	16	31

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	209	GLY
1	C	264	GLU
1	B	248	ARG
1	D	46	GLU
1	D	210	GLU
1	A	25	GLU
1	A	46	GLU
1	A	276	SER
1	B	10	ARG
1	A	239	ALA
1	D	232	TYR

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	279/284 (98%)	260 (93%)	19 (7%)	14	30
1	B	279/284 (98%)	266 (95%)	13 (5%)	23	47
1	C	280/284 (99%)	265 (95%)	15 (5%)	20	42
1	D	279/284 (98%)	263 (94%)	16 (6%)	18	39
All	All	1117/1136 (98%)	1054 (94%)	63 (6%)	19	40

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	GLU
1	A	23	ILE
1	A	27	LYS
1	A	33	THR
1	A	54	GLU
1	A	72	GLU
1	A	104	SER
1	A	105	GLU
1	A	116	ASP
1	A	134	LEU
1	A	139	ILE
1	A	147	SER
1	A	202	GLU
1	A	258	LEU
1	A	269	VAL
1	A	271	VAL
1	A	278	ASP
1	A	308	VAL
1	A	310	VAL
1	B	5	ILE
1	B	33	THR
1	B	73	GLN
1	B	146	ILE
1	B	147	SER
1	B	211	ILE
1	B	224	THR
1	B	269	VAL
1	B	271	VAL
1	B	282	VAL
1	B	289	VAL
1	B	316	VAL
1	B	341	HIS
1	C	33	THR
1	C	35	THR
1	C	68	ILE
1	C	77	LEU
1	C	146	ILE
1	C	147	SER
1	C	187	THR
1	C	202	GLU
1	C	210	GLU
1	C	217	VAL

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Mol	Chain	Res	Type
1	C	224	THR
1	C	226	LYS
1	C	269	VAL
1	C	271	VAL
1	C	319	LYS
1	D	2	THR
1	D	16	ILE
1	D	23	ILE
1	D	49	VAL
1	D	50	LYS
1	D	132	ILE
1	D	146	ILE
1	D	147	SER
1	D	149	LYS
1	D	201	LEU
1	D	203	GLU
1	D	224	THR
1	D	230	MET
1	D	269	VAL
1	D	271	VAL
1	D	276	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	295	ASN
1	B	157	HIS
1	B	234	HIS
1	C	234	HIS
1	D	125	HIS
1	D	145	ASN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	THR	B	401	-	7,7,7	1.01	1 (14%)	8,9,9	1.10	1 (12%)
2	THR	D	401	-	7,7,7	1.22	1 (14%)	8,9,9	1.21	1 (12%)
2	THR	A	401	-	7,7,7	0.80	1 (14%)	8,9,9	1.54	2 (25%)
2	THR	C	401	-	7,7,7	0.92	0	8,9,9	1.55	2 (25%)

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	THR	B	401	-	-	0/8/8/8	-
2	THR	D	401	-	-	0/8/8/8	-
2	THR	A	401	-	-	0/8/8/8	-
2	THR	C	401	-	-	1/8/8/8	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	THR	OXT-C	-2.36	1.23	1.30
2	B	401	THR	OXT-C	-2.15	1.23	1.30
2	A	401	THR	OXT-C	-2.06	1.24	1.30

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	THR	OXT-C-O	-3.35	116.48	124.08
2	C	401	THR	OXT-C-O	-3.22	116.78	124.08
2	B	401	THR	OXT-C-O	-2.65	118.07	124.08
2	C	401	THR	OXT-C-CA	2.59	123.09	114.15
2	A	401	THR	OXT-C-CA	2.53	122.88	114.15
2	D	401	THR	OXT-C-O	-2.51	118.38	124.08

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	401	THR	O-C-CA-N

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	THR	1	0
2	D	401	THR	1	0
2	A	401	THR	2	0
2	C	401	THR	3	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	340/345 (98%)	-0.24	2 (0%) 85 82	47, 73, 116, 136	0
1	B	340/345 (98%)	-0.25	1 (0%) 90 89	45, 70, 119, 145	0
1	C	341/345 (98%)	-0.37	3 (0%) 81 76	47, 68, 102, 158	0
1	D	340/345 (98%)	0.06	4 (1%) 76 71	55, 87, 123, 151	0
All	All	1361/1380 (98%)	-0.20	10 (0%) 84 80	45, 75, 117, 158	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	341	HIS	6.5
1	D	81	ILE	3.8
1	C	339	LYS	3.5
1	C	340	VAL	2.7
1	D	87	MET	2.7
1	B	258	LEU	2.6
1	A	176	ARG	2.3
1	D	85	ALA	2.2
1	C	233	ARG	2.1
1	A	318	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	THR	D	401	8/8	0.94	0.11	73,82,88,88	0
2	THR	C	401	8/8	0.95	0.13	64,69,75,78	0
2	THR	B	401	8/8	0.98	0.07	51,57,62,63	0
2	THR	A	401	8/8	0.99	0.06	59,64,72,72	0

6.5 Other polymers [i](#)

There are no such residues in this entry.