Full wwPDB X-ray Structure Validation Report (i)

Mar 9, 2026 – 04:56 AM UTC

PDB ID	:	6AGM / pdb_00006agm
Title	:	Molecular basis for feedback inhibition of tyrosine-regulated 3-deoxy-d-arabino-heptulosonate-7-phosphate synthase from Escherichia coli
Authors	:	Cui, D.; Qi, J.; Wen, T.
Deposited on	:	2018-08-13
Resolution	:	2.00 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:

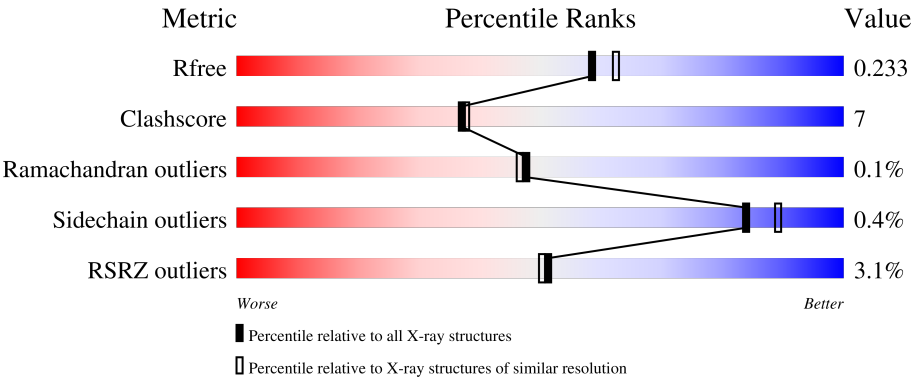
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	355	2% 79% 15% 6%
1	B	355	4% 81% 13% 6%
1	C	355	4% 79% 15% • 6%
1	D	355	3% 80% 14% 6%

2 Entry composition

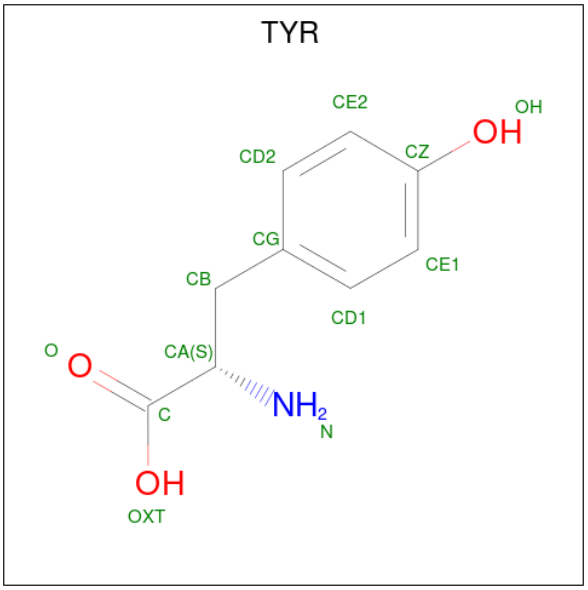
There are 3 unique types of molecules in this entry. The entry contains 10514 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Phospho-2-dehydro-3-deoxyheptonate aldolase, Tyr-sensitive.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	0	0
			2545	1579	457	493	16			
1	B	334	Total	C	N	O	S	0	0	0
			2545	1579	457	493	16			
1	C	334	Total	C	N	O	S	0	0	0
			2545	1579	457	493	16			
1	D	334	Total	C	N	O	S	0	0	0
			2545	1579	457	493	16			

- Molecule 2 is TYROSINE (CCD ID: TYR) (formula: $C_9H_{11}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			13	9	1	3		
2	B	1	Total	C	N	O	0	0
			13	9	1	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C N O 13 9 1 3	0	0
2	D	1	Total C N O 13 9 1 3	0	0

- Molecule 3 is water.

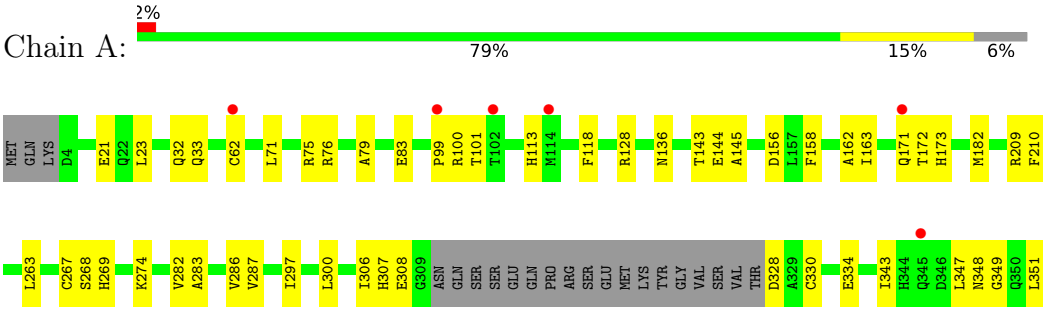
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	98	Total O 98 98	0	0
3	B	67	Total O 67 67	0	0
3	C	64	Total O 64 64	0	0
3	D	53	Total O 53 53	0	0

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.

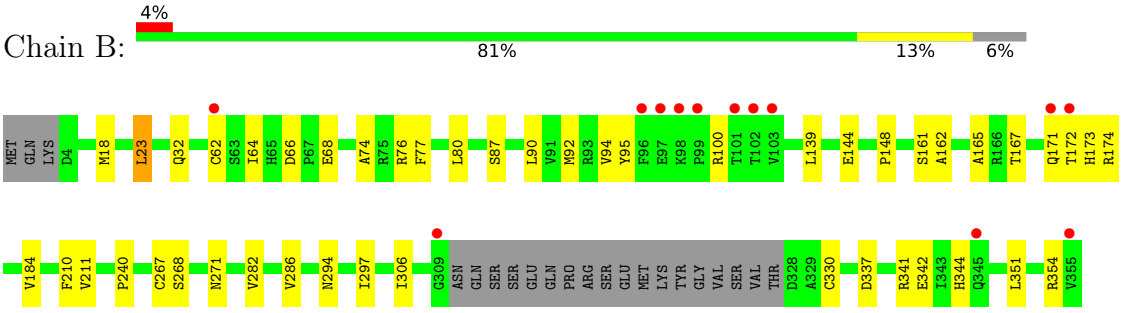
• Molecule 1: Phospho-2-dehydro-3-deoxyheptonate aldolase, Tyr-sensitive

Chain A:



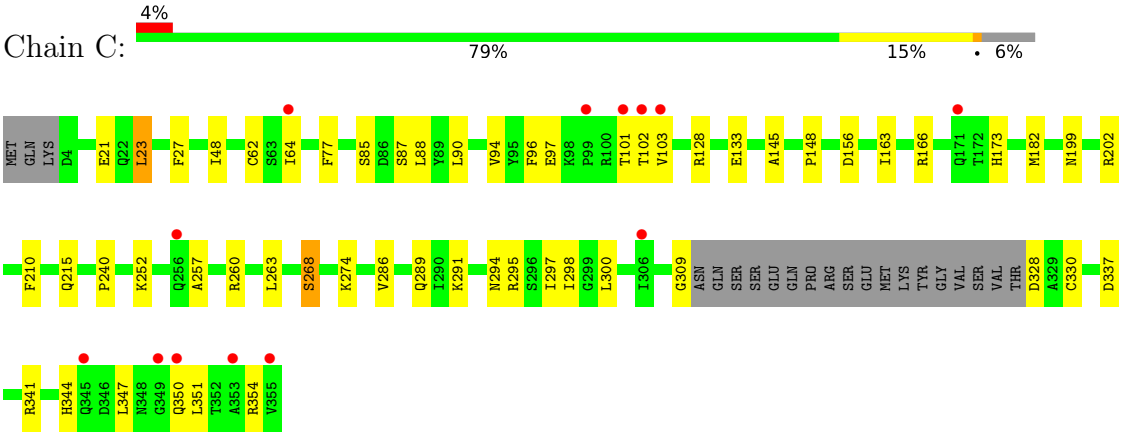
• Molecule 1: Phospho-2-dehydro-3-deoxyheptonate aldolase, Tyr-sensitive

Chain B:



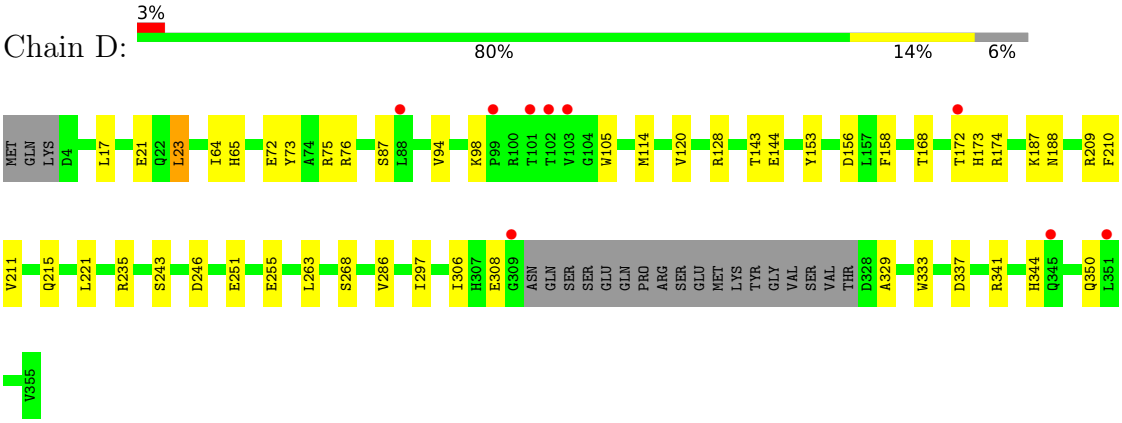
• Molecule 1: Phospho-2-dehydro-3-deoxyheptonate aldolase, Tyr-sensitive

Chain C:



• Molecule 1: Phospho-2-dehydro-3-deoxyheptonate aldolase, Tyr-sensitive

Chain D:


3%
80%
14%
6%
MET GLN LYS D4 L17 E21 Q22 L23 I64 H65 E72 Y73 A74 R75 R76 S87 L88 V94 K98 P99 R100 T101 T102 V103 G104 W105 M114 V120 R128 T143 E144 Y153 D156 L157 F158 T168 T172 H173 R174 K187 N188 R209 F210
V211 Q215 L221 R235 S243 D246 E251 E255 L263 S268 V286 I297 I306 H307 E308 G309 ASN GLN SER SER GLU GLN PRO ARG SER GLU MET LYS TYR GLY VAL SER VAL THR D328 A329 W333 D337 R341 H344 Q345 Q350 L351
V355

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	54.19Å 133.86Å 87.67Å 90.00° 91.23° 90.00°	Depositor
Resolution (Å)	38.21 – 2.00 38.21 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.9 (38.21-2.00) 97.2 (38.21-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	1.58 (at 2.00Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.193 , 0.229 0.199 , 0.233	Depositor DCC
R_{free} test set	4112 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å^2)	43.6	Xtriage
Anisotropy	0.366	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 35.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	10514	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% 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

5.1 Standard geometry

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	0.18	0/2588	0.43	0/3507
1	B	0.17	0/2588	0.43	0/3507
1	C	0.16	0/2588	0.41	0/3507
1	D	0.15	0/2588	0.40	0/3507
All	All	0.17	0/10352	0.42	0/14028

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	268	SER	Peptide
1	B	268	SER	Peptide
1	C	268	SER	Peptide
1	D	268	SER	Peptide

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	2545	0	2518	36	0
1	B	2545	0	2516	39	0
1	C	2545	0	2516	39	0
1	D	2545	0	2516	30	0
2	A	13	0	8	0	0
2	B	13	0	8	0	0
2	C	13	0	8	0	0
2	D	13	0	8	0	0
3	A	98	0	0	4	0
3	B	67	0	0	1	0
3	C	64	0	0	6	0
3	D	53	0	0	1	0
All	All	10514	0	10098	143	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 7.

All (143) 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:172:THR:HB	1:B:211:VAL:HB	1.57	0.85
1:D:172:THR:HB	1:D:211:VAL:HB	1.60	0.84
1:A:307:HIS:N	3:A:701:HOH:O	2.07	0.82
1:B:294:ASN:O	1:B:354:ARG:NE	2.12	0.81
1:B:144:GLU:HG2	1:B:162:ALA:HB3	1.63	0.79
1:B:294:ASN:HB3	1:B:354:ARG:HH21	1.48	0.78
1:B:64:ILE:HD12	1:B:94:VAL:HG13	1.70	0.74
1:C:289:GLN:OE1	3:C:701:HOH:O	2.05	0.73
1:D:21:GLU:HG3	1:D:215:GLN:HB3	1.70	0.72
1:C:102:THR:HG23	1:C:103:VAL:HG23	1.71	0.72
1:C:240:PRO:O	3:C:702:HOH:O	2.07	0.72
1:A:100:ARG:O	1:A:101:THR:HG23	1.91	0.69
1:C:133:GLU:OE2	3:C:703:HOH:O	2.12	0.68
1:D:173:HIS:HA	1:D:210:PHE:HB2	1.75	0.68
1:C:101:THR:OG1	1:C:103:VAL:O	2.12	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:350:GLN:CD	1:D:350:GLN:H	2.02	0.67
1:B:294:ASN:HB3	1:B:354:ARG:NH2	2.09	0.67
1:B:173:HIS:HA	1:B:210:PHE:HB2	1.78	0.66
1:D:251:GLU:O	1:D:255:GLU:HG3	1.96	0.65
1:D:329:ALA:HA	3:D:702:HOH:O	1.95	0.65
1:B:95:TYR:CZ	1:B:144:GLU:HG3	2.32	0.64
1:C:96:PHE:O	3:C:704:HOH:O	2.15	0.64
1:B:294:ASN:CB	1:B:354:ARG:HH21	2.11	0.62
1:A:113:HIS:ND1	3:A:704:HOH:O	2.31	0.61
1:D:72:GLU:OE2	1:D:75:ARG:NH1	2.33	0.60
1:A:21:GLU:HG3	1:A:215:GLN:HB3	1.82	0.60
1:C:337:ASP:OD2	1:C:341:ARG:NH1	2.34	0.60
1:B:294:ASN:OD1	1:B:354:ARG:NH2	2.36	0.58
1:C:48:ILE:O	1:C:260:ARG:NH1	2.37	0.58
1:C:173:HIS:HA	1:C:210:PHE:HB2	1.86	0.58
1:A:118:PHE:N	3:A:702:HOH:O	2.17	0.57
1:A:173:HIS:HA	1:A:210:PHE:HB2	1.86	0.57
1:A:83:GLU:OE2	1:C:295:ARG:NE	2.38	0.56
1:D:128:ARG:NH2	1:D:156:ASP:OD1	2.38	0.56
1:B:100:ARG:HH22	1:B:165:ALA:HB3	1.70	0.56
1:A:263:LEU:HD11	1:A:297:ILE:HG12	1.88	0.56
1:A:33:GLN:HE21	1:A:136:ASN:CG	2.14	0.55
1:D:308:GLU:N	1:D:308:GLU:OE1	2.40	0.55
1:B:87:SER:HB2	1:B:344:HIS:HD2	1.70	0.55
1:D:23:LEU:HD22	1:D:128:ARG:HD2	1.89	0.55
1:A:308:GLU:N	1:A:308:GLU:OE1	2.41	0.54
1:D:209:ARG:HH11	1:D:221:LEU:HD13	1.73	0.54
1:D:23:LEU:HD12	1:D:153:TYR:HD2	1.71	0.54
1:A:267:CYS:HA	1:A:282:VAL:HG11	1.90	0.54
1:A:71:LEU:O	1:A:75:ARG:HG3	2.08	0.54
1:D:17:LEU:HD11	1:D:120:VAL:CG2	2.39	0.53
1:A:128:ARG:NH2	1:A:156:ASP:OD1	2.41	0.53
1:B:171:GLN:CD	1:B:171:GLN:H	2.16	0.53
1:B:74:ALA:HB2	1:B:92:MET:HE1	1.89	0.53
1:B:294:ASN:CB	1:B:354:ARG:NH2	2.70	0.53
1:B:337:ASP:OD2	1:B:341:ARG:NH1	2.41	0.53
1:C:128:ARG:NH2	1:C:156:ASP:OD1	2.43	0.52
1:B:294:ASN:C	1:B:354:ARG:NH2	2.68	0.51
1:B:148:PRO:HG3	1:B:173:HIS:CG	2.45	0.51
1:A:145:ALA:O	3:A:703:HOH:O	2.19	0.50
1:A:347:LEU:HD23	1:A:351:LEU:HD11	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:263:LEU:HD11	1:C:297:ILE:HG12	1.94	0.50
1:A:328:ASP:OD2	1:A:328:ASP:N	2.45	0.49
1:C:309:GLY:O	1:C:328:ASP:N	2.45	0.49
1:B:294:ASN:C	1:B:354:ARG:HH21	2.21	0.49
1:D:76:ARG:HB3	1:D:333:TRP:CZ2	2.48	0.49
1:A:269:HIS:HB3	1:A:274:LYS:HZ2	1.78	0.48
1:A:99:PRO:HB2	1:A:100:ARG:HG3	1.95	0.48
1:A:287:VAL:HG21	1:A:343:ILE:HG12	1.96	0.48
1:C:87:SER:HB2	1:C:344:HIS:HD2	1.77	0.48
1:A:76:ARG:NH1	1:A:306:ILE:HG23	2.27	0.48
1:C:64:ILE:HG13	1:C:94:VAL:HG13	1.95	0.47
1:A:286:VAL:HG11	1:A:300:LEU:HD21	1.96	0.47
1:B:95:TYR:CE2	1:B:144:GLU:HG3	2.49	0.47
1:C:48:ILE:HA	1:C:298:ILE:HG12	1.97	0.47
1:C:77:PHE:CZ	1:C:90:LEU:HB3	2.50	0.47
1:D:243:SER:OG	1:D:246:ASP:OD1	2.29	0.47
1:C:199:ASN:OD1	1:C:202:ARG:NH1	2.49	0.46
1:C:294:ASN:O	1:C:354:ARG:NH1	2.38	0.46
1:C:27:PHE:HB2	1:C:128:ARG:HD3	1.97	0.46
1:B:161:SER:O	1:B:184:VAL:HA	2.16	0.46
1:B:351:LEU:HD23	1:B:351:LEU:HA	1.78	0.46
1:C:291:LYS:O	1:C:350:GLN:NE2	2.47	0.45
1:A:62:CYS:CB	1:A:330:CYS:HG	2.30	0.45
1:D:263:LEU:HD11	1:D:297:ILE:HG12	1.98	0.45
1:C:252:LYS:HB2	1:C:252:LYS:HE3	1.73	0.45
1:D:144:GLU:OE2	1:D:187:LYS:NZ	2.38	0.45
1:B:76:ARG:HH21	1:B:306:ILE:HD12	1.81	0.45
1:D:65:HIS:ND1	1:D:105:TRP:HZ3	2.15	0.45
1:C:23:LEU:HD22	1:C:128:ARG:HD2	1.99	0.45
1:C:347:LEU:HD23	1:C:347:LEU:HA	1.78	0.45
1:B:80:LEU:HD13	1:B:341:ARG:NH1	2.32	0.44
1:B:92:MET:HE2	1:B:139:LEU:HD13	1.99	0.44
1:B:76:ARG:NH2	1:B:306:ILE:HD12	2.32	0.44
1:C:96:PHE:C	1:C:97:GLU:HG3	2.42	0.44
1:A:334:GLU:H	1:A:334:GLU:CD	2.23	0.44
1:A:348:ASN:OD1	1:A:349:GLY:N	2.50	0.44
1:B:294:ASN:O	1:B:354:ARG:CZ	2.65	0.44
1:D:114:MET:HE2	1:D:114:MET:HB3	1.75	0.44
1:C:274:LYS:HA	1:C:274:LYS:HE2	1.99	0.43
1:D:73:TYR:HB2	1:D:306:ILE:HD11	1.99	0.43
1:A:171:GLN:NE2	1:A:172:THR:HG23	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:CYS:N	1:B:330:CYS:SG	2.90	0.43
1:C:148:PRO:HG3	1:C:173:HIS:CG	2.54	0.43
1:C:62:CYS:N	1:C:330:CYS:SG	2.90	0.43
1:A:286:VAL:HG13	1:A:297:ILE:HG21	1.99	0.43
1:B:32:GLN:NE2	1:B:32:GLN:H	2.16	0.43
1:B:77:PHE:CZ	1:B:90:LEU:HB3	2.54	0.43
1:C:85:SER:HA	1:C:88:LEU:O	2.19	0.43
1:C:347:LEU:HB3	1:C:351:LEU:CD1	2.49	0.43
1:B:342:GLU:OE1	3:B:701:HOH:O	2.21	0.43
1:A:32:GLN:HE22	1:A:136:ASN:HD22	1.67	0.43
1:C:145:ALA:HB3	1:C:163:ILE:HD13	2.01	0.43
1:A:143:THR:HB	1:A:158:PHE:CE1	2.54	0.42
1:B:171:GLN:HG2	1:B:172:THR:H	1.85	0.42
1:B:267:CYS:HA	1:B:282:VAL:HG11	2.02	0.42
1:D:87:SER:HB3	1:D:344:HIS:CD2	2.54	0.42
1:D:128:ARG:HH22	1:D:156:ASP:CG	2.27	0.42
1:C:21:GLU:HG3	1:C:215:GLN:HB3	2.01	0.42
1:C:347:LEU:HB3	1:C:351:LEU:HD13	2.02	0.42
1:A:209:ARG:HH21	1:A:221:LEU:HD23	1.85	0.42
1:C:295:ARG:HA	1:C:354:ARG:NH1	2.35	0.42
1:D:168:THR:O	1:D:174:ARG:HG3	2.19	0.42
1:C:286:VAL:HG11	1:C:300:LEU:HD21	2.02	0.42
1:A:182:MET:HE3	1:A:182:MET:HB3	1.95	0.41
1:D:337:ASP:OD1	1:D:341:ARG:HD2	2.19	0.41
1:A:283:ALA:HB1	1:A:343:ILE:HD11	2.02	0.41
1:B:18:MET:HE3	1:B:23:LEU:HG	2.01	0.41
1:D:143:THR:HB	1:D:158:PHE:CE1	2.54	0.41
1:D:98:LYS:HB2	1:D:98:LYS:HE3	1.72	0.41
1:B:66:ASP:OD1	1:B:68:GLU:N	2.53	0.41
1:C:182:MET:HE2	1:C:182:MET:HB3	1.95	0.41
1:D:64:ILE:HG13	1:D:94:VAL:HG13	2.03	0.41
1:A:347:LEU:HD12	1:A:347:LEU:HA	1.78	0.41
1:A:145:ALA:HB3	1:A:163:ILE:HD13	2.03	0.41
1:C:298:ILE:HD11	3:C:720:HOH:O	2.20	0.41
1:D:350:GLN:CD	1:D:350:GLN:N	2.77	0.41
1:B:286:VAL:HG13	1:B:297:ILE:HG21	2.03	0.40
1:C:257:ALA:O	3:C:705:HOH:O	2.22	0.40
1:A:79:ALA:O	1:A:83:GLU:HG3	2.22	0.40
1:B:167:THR:O	1:B:174:ARG:HA	2.21	0.40
1:C:166:ARG:HE	1:C:166:ARG:HB3	1.74	0.40
1:A:144:GLU:HG3	1:A:162:ALA:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:188:ASN:O	1:D:235:ARG:NH2	2.50	0.40
1:A:76:ARG:HH12	1:A:306:ILE:HG23	1.84	0.40
1:B:240:PRO:HB3	1:B:271:ASN:HA	2.03	0.40
1:D:286:VAL:HG13	1:D:297:ILE:HG21	2.02	0.40
1:B:171:GLN:CD	1:B:171:GLN:N	2.80	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	330/355 (93%)	324 (98%)	6 (2%)	0	100	100
1	B	330/355 (93%)	322 (98%)	8 (2%)	0	100	100
1	C	330/355 (93%)	321 (97%)	8 (2%)	1 (0%)	36	35
1	D	330/355 (93%)	325 (98%)	5 (2%)	0	100	100
All	All	1320/1420 (93%)	1292 (98%)	27 (2%)	1 (0%)	48	46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	268	SER

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	273/293 (93%)	272 (100%)	1 (0%)	84	89
1	B	273/293 (93%)	272 (100%)	1 (0%)	84	89
1	C	273/293 (93%)	272 (100%)	1 (0%)	84	89
1	D	273/293 (93%)	272 (100%)	1 (0%)	84	89
All	All	1092/1172 (93%)	1088 (100%)	4 (0%)	84	89

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	B	23	LEU
1	C	23	LEU
1	D	23	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	33	GLN
1	A	65	HIS
1	A	225	GLN
1	A	273	ASN
1	B	32	GLN
1	B	125	GLN
1	B	206	GLN
1	B	208	HIS
1	C	15	GLN
1	C	348	ASN
1	D	125	GLN
1	D	206	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 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	TYR	D	601	-	12,13,13	0.72	1 (8%)	13,17,17	0.72	1 (7%)
2	TYR	B	601	-	12,13,13	0.71	1 (8%)	13,17,17	0.74	1 (7%)
2	TYR	A	601	-	12,13,13	0.71	1 (8%)	13,17,17	0.75	1 (7%)
2	TYR	C	601	-	12,13,13	0.68	1 (8%)	13,17,17	0.76	1 (7%)

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	TYR	D	601	-	-	0/8/8/8	0/1/1/1
2	TYR	B	601	-	-	0/8/8/8	0/1/1/1
2	TYR	A	601	-	-	0/8/8/8	0/1/1/1
2	TYR	C	601	-	-	0/8/8/8	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	TYR	OXT-C	-2.25	1.23	1.30
2	D	601	TYR	OXT-C	-2.22	1.23	1.30
2	A	601	TYR	OXT-C	-2.20	1.23	1.30
2	C	601	TYR	OXT-C	-2.12	1.23	1.30

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	601	TYR	OXT-C-O	-2.61	118.15	124.08
2	A	601	TYR	OXT-C-O	-2.58	118.24	124.08
2	B	601	TYR	OXT-C-O	-2.54	118.31	124.08
2	D	601	TYR	OXT-C-O	-2.52	118.36	124.08

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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	334/355 (94%)	0.06	6 (1%)	67	67	31, 47, 76, 139	0
1	B	334/355 (94%)	0.17	13 (3%)	43	42	34, 50, 98, 152	0
1	C	334/355 (94%)	0.17	13 (3%)	43	42	32, 51, 103, 142	0
1	D	334/355 (94%)	0.23	9 (2%)	56	55	34, 53, 89, 161	0
All	All	1336/1420 (94%)	0.16	41 (3%)	51	50	31, 50, 94, 161	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	345	GLN	3.9
1	C	102	THR	3.8
1	B	172	THR	3.6
1	C	99	PRO	3.6
1	B	99	PRO	3.5
1	B	355	VAL	3.5
1	A	102	THR	3.4
1	D	102	THR	3.4
1	D	99	PRO	3.4
1	D	172	THR	3.4
1	C	353	ALA	3.2
1	D	103	VAL	3.2
1	C	171	GLN	3.0
1	A	99	PRO	2.9
1	B	102	THR	2.8
1	B	309	GLY	2.8
1	A	345	GLN	2.7
1	C	345	GLN	2.7
1	B	171	GLN	2.7
1	C	64	ILE	2.6
1	A	171	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	97	GLU	2.6
1	C	101	THR	2.5
1	A	114	MET	2.5
1	C	355	VAL	2.4
1	A	62	CYS	2.4
1	C	256	GLN	2.3
1	B	98	LYS	2.3
1	C	306	ILE	2.3
1	B	62	CYS	2.3
1	D	309	GLY	2.3
1	B	101	THR	2.3
1	D	88	LEU	2.2
1	C	349	GLY	2.1
1	D	345	GLN	2.1
1	D	101	THR	2.1
1	B	96	PHE	2.1
1	B	103	VAL	2.1
1	C	103	VAL	2.1
1	D	351	LEU	2.0
1	C	350	GLN	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, 95^{th} 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	TYR	B	601	13/13	0.93	0.08	32,36,39,39	0
2	TYR	A	601	13/13	0.96	0.06	34,37,41,42	0
2	TYR	C	601	13/13	0.96	0.06	35,38,39,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	TYR	D	601	13/13	0.96	0.06	36,38,40,40	0

6.5 Other polymers (i)

There are no such residues in this entry.