



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:15 PM UTC

PDB ID : 7I08 / pdb_00007i08
Title : PanDDA analysis group deposition – Crystal structure of Enterococcus faecium VatD in complex with ZINC000004976927
Authors : Asthana, P.; Fraser, J.S.
Deposited on : 2025-01-25
Resolution : 2.28 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

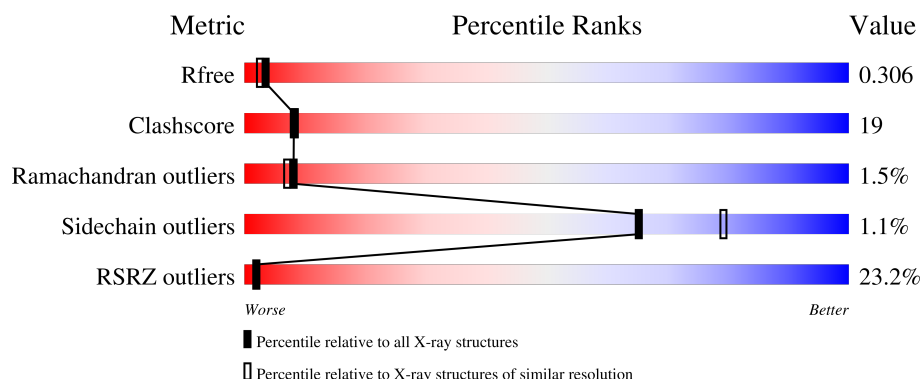
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.28 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	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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	209	<div> <div>24%</div> <div>61%</div> <div>33%</div> <div>..</div> </div>
1	B	209	<div> <div>17%</div> <div>68%</div> <div>27%</div> <div>..</div> </div>
1	C	209	<div> <div>26%</div> <div>76%</div> <div>18%</div> <div>..</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	04R	A	301[B]	-	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 11514 atoms, of which 5753 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.

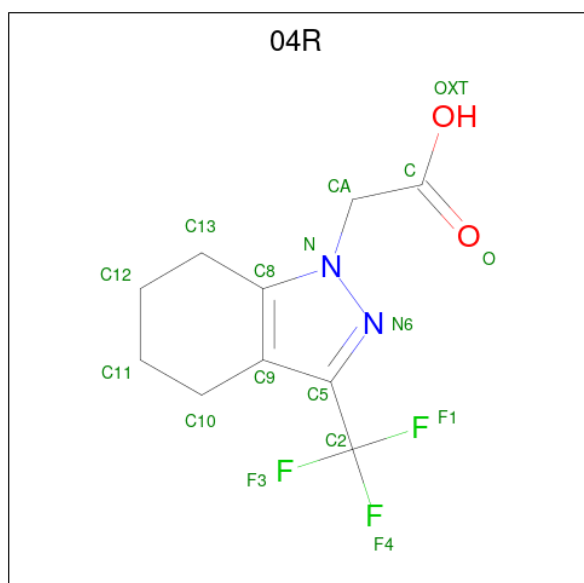
- Molecule 1 is a protein called Streptogramin A acetyltransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	203	Total	C	H	N	O	S	0	74	0
			4344	1398	2179	358	397	12			
1	B	203	Total	C	H	N	O	S	0	43	0
			3790	1214	1902	312	352	10			
1	C	202	Total	C	H	N	O	S	0	9	0
			3290	1059	1652	270	301	8			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP P50870
B	1	GLY	-	expression tag	UNP P50870
C	1	GLY	-	expression tag	UNP P50870

- Molecule 2 is [3-(trifluoromethyl)-4,5,6,7-tetrahydro-1H-indazol-1-yl]acetic acid (CCD ID: 04R) (formula: C₁₀H₁₁F₃N₂O₂).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	H	N	O	0	1
			27	10	3	10	2	2		
2	C	1	Total	C	F	H	N	O	0	1
			27	10	3	10	2	2		

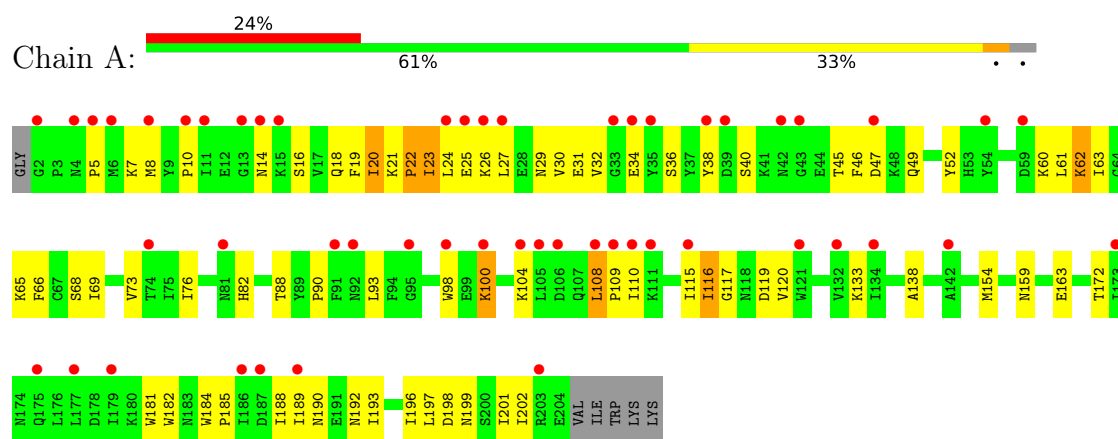
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	13	Total	O	0	13
			13	13		
3	B	16	Total	O	0	16
			16	16		
3	C	7	Total	O	0	7
			7	7		

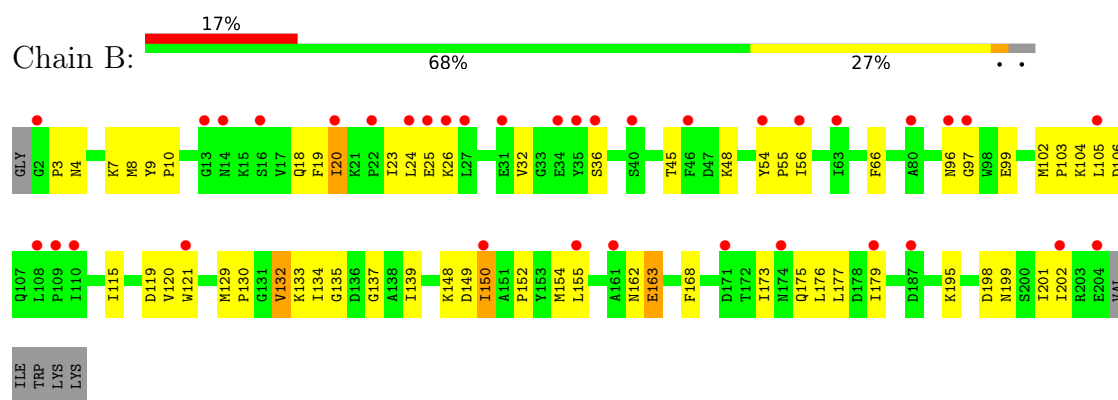
3 Residue-property plots [i](#)

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.

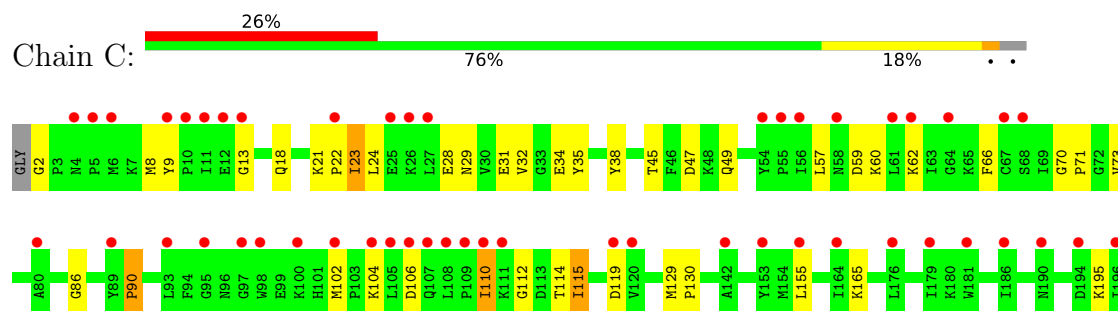
• Molecule 1: Streptogramin A acetyltransferase

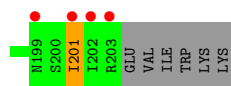


• Molecule 1: Streptogramin A acetyltransferase



• Molecule 1: Streptogramin A acetyltransferase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	44.15Å 102.33Å 146.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.30 – 2.28 48.30 – 2.28	Depositor EDS
% Data completeness (in resolution range)	98.8 (48.30-2.28) 99.2 (48.30-2.28)	Depositor EDS
R_{merge}	0.30	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.99 (at 2.27Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.237 , 0.306 0.246 , 0.306	Depositor DCC
R_{free} test set	1567 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	52.3	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 39.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	11514	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.73% of the height of the origin peak. No significant pseudotranslation is detected.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 04R

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	0.54	0/2243	0.70	0/3037
1	B	0.80	2/1961 (0.1%)	0.83	1/2659 (0.0%)
1	C	0.66	0/1691	0.78	0/2291
All	All	0.67	2/5895 (0.0%)	0.77	1/7987 (0.0%)

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	2
1	C	0	1
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	20	ILE	CG1-CD1	15.01	2.10	1.51
1	B	20	ILE	CB-CG1	-7.10	1.39	1.53

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	20	ILE	CB-CG1-CD1	-8.47	96.00	113.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	20[B]	ILE	Peptide
1	A	62[B]	LYS	Peptide
1	C	13	GLY	Peptide

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	2165	2179	2159	110	0
1	B	1888	1902	1862	82	0
1	C	1638	1652	1619	35	0
2	A	17	10	10	12	0
2	C	17	10	10	0	0
3	A	13	0	0	14	0
3	B	16	0	0	21	0
3	C	7	0	0	4	0
All	All	5761	5753	5660	223	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 (223) 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:20:ILE:CD1	1:B:20:ILE:CG1	2.10	1.28
1:B:168:PHE:O	3:B:301[B]:HOH:O	1.57	1.20
1:B:134[B]:ILE:HA	1:B:150[B]:ILE:HD11	1.31	1.12
1:A:24[B]:LEU:HD11	1:A:27[B]:LEU:HD12	1.36	1.08
1:B:36:SER:HB2	3:B:304[B]:HOH:O	1.53	1.08
1:A:32[B]:VAL:HG12	1:A:63[B]:ILE:HD13	1.38	1.04
1:B:20:ILE:HG13	1:B:32:VAL:HG11	1.40	1.03
1:B:20:ILE:HG21	1:B:20:ILE:HD13	1.42	0.97
1:A:8:MET:SD	1:A:23[B]:ILE:HG23	2.05	0.97
1:B:20:ILE:CD1	1:B:20:ILE:HG21	1.93	0.97
1:C:71:PRO:HA	3:C:401[B]:HOH:O	1.69	0.93
1:B:56:ILE:HG23	3:B:313[B]:HOH:O	1.69	0.92
1:A:138:ALA:HB3	3:A:405[B]:HOH:O	1.69	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:ILE:CD1	1:B:20:ILE:CG2	2.49	0.91
1:A:120:VAL:HG13	3:A:405[B]:HOH:O	1.72	0.88
1:C:38:TYR:CZ	3:C:401[B]:HOH:O	2.30	0.84
1:A:24[B]:LEU:HD11	1:A:27[B]:LEU:CD1	2.11	0.80
1:C:62[B]:LYS:HD2	1:C:115:ILE:HD12	1.65	0.78
1:A:32[B]:VAL:HA	1:A:63[B]:ILE:HG23	1.66	0.77
1:A:182:TRP:HB2	3:A:409[B]:HOH:O	1.83	0.77
1:A:108[B]:LEU:HB3	1:A:109[B]:PRO:CD	2.15	0.76
1:B:20:ILE:CD1	1:B:20:ILE:CB	2.63	0.76
1:A:66[B]:PHE:CD2	3:A:409[B]:HOH:O	2.39	0.75
1:B:152[B]:PRO:CG	1:B:177:LEU:HD11	2.16	0.75
1:B:20:ILE:HD13	1:B:20:ILE:CG2	2.12	0.74
1:A:108[B]:LEU:HD22	1:A:109[B]:PRO:HD3	1.69	0.74
1:C:114:THR:C	1:C:115:ILE:HD13	2.12	0.73
1:A:108[B]:LEU:CD2	1:A:109[B]:PRO:HD3	2.19	0.73
1:B:119:ASP:O	1:B:137[B]:GLY:HA2	1.90	0.71
1:A:31[B]:GLU:O	1:A:63[B]:ILE:HG23	1.91	0.71
1:B:152[B]:PRO:HG3	1:B:177:LEU:HD11	1.70	0.71
1:C:45:THR:OG1	1:C:47:ASP:OD1	2.03	0.71
1:B:102:MET:CE	3:B:308[B]:HOH:O	2.38	0.70
1:C:195:LYS:HB3	1:C:201:ILE:HG23	1.73	0.70
1:A:62[B]:LYS:HB3	1:A:115[B]:ILE:HG13	1.74	0.69
1:A:65[B]:LYS:CB	3:A:409[B]:HOH:O	2.40	0.69
1:A:65[B]:LYS:HB2	3:A:409[B]:HOH:O	1.92	0.69
1:C:31:GLU:HA	1:C:31:GLU:OE2	1.92	0.68
1:A:8:MET:SD	1:A:23[B]:ILE:CG2	2.82	0.68
1:B:99:GLU:HB2	3:B:308[B]:HOH:O	1.93	0.67
1:B:115:ILE:HB	1:B:133[B]:LYS:HD2	1.77	0.67
1:A:8:MET:CG	1:A:23[B]:ILE:HG12	2.24	0.67
1:A:32[B]:VAL:HG12	1:A:63[B]:ILE:HG21	1.76	0.67
1:B:102:MET:HG3	1:B:103:PRO:HD2	1.76	0.67
1:A:32[B]:VAL:CG1	1:A:63[B]:ILE:HD13	2.21	0.66
1:C:38:TYR:OH	3:C:401[B]:HOH:O	2.11	0.65
1:A:63[B]:ILE:HA	2:A:301[B]:04R:H12	1.78	0.65
1:A:22:PRO:C	1:A:24[B]:LEU:H	2.02	0.64
1:B:176:LEU:CD2	3:B:314[B]:HOH:O	2.45	0.64
1:A:21[B]:LYS:NZ	1:A:32[B]:VAL:HG23	2.12	0.63
1:A:108[B]:LEU:HB3	1:A:109[B]:PRO:HD2	1.79	0.63
1:B:102:MET:HE1	3:B:308[B]:HOH:O	1.99	0.62
1:C:21:LYS:HB3	1:C:22:PRO:HD3	1.81	0.62
1:B:139[B]:ILE:HB	1:B:155[B]:LEU:HD23	1.80	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63[B]:ILE:HD12	2:A:301[B]:04R:C5	2.30	0.61
1:B:4:ASN:HB3	1:B:7:LYS:HD2	1.82	0.61
1:B:149[B]:ASP:O	1:B:150[B]:ILE:HG23	2.00	0.61
1:A:20[B]:ILE:HG22	1:A:23[B]:ILE:C	2.25	0.60
1:A:63[B]:ILE:HD12	2:A:301[B]:04R:N6	2.16	0.60
1:A:66[B]:PHE:HE2	1:A:182:TRP:HA	1.67	0.59
1:B:96:ASN:O	1:C:2:GLY:HA2	2.03	0.59
1:A:31[B]:GLU:O	1:A:63[B]:ILE:CG2	2.50	0.59
1:A:116[B]:ILE:HG22	1:A:117[B]:GLY:H	1.68	0.59
1:B:115:ILE:HD12	1:B:133[B]:LYS:HD2	1.83	0.59
1:B:173:ILE:CD1	3:B:301[B]:HOH:O	2.50	0.59
1:B:152[B]:PRO:HG2	1:B:177:LEU:HD11	1.85	0.59
1:A:24[A]:LEU:HD22	1:A:27[A]:LEU:HD12	1.85	0.58
1:A:8:MET:HG2	1:A:23[B]:ILE:HG12	1.84	0.58
1:C:29:ASN:OD1	1:C:60:LYS:HE3	2.04	0.58
1:B:150[B]:ILE:C	1:B:150[B]:ILE:HD12	2.28	0.58
1:A:196:ILE:HD11	3:A:413[B]:HOH:O	2.02	0.58
1:B:154[B]:MET:HE2	1:B:163[B]:GLU:HG2	1.87	0.57
1:B:20:ILE:CG1	3:B:304[B]:HOH:O	2.53	0.57
1:B:201:ILE:HG21	3:B:314[B]:HOH:O	2.05	0.57
1:B:48:LYS:CE	3:B:312[B]:HOH:O	2.53	0.56
1:A:66[B]:PHE:CD2	1:A:181:TRP:CZ3	2.93	0.56
1:B:115:ILE:O	1:B:133[B]:LYS:HA	2.05	0.56
1:A:63[B]:ILE:CA	2:A:301[B]:04R:H12	2.36	0.56
1:A:66[B]:PHE:O	1:A:119:ASP:HA	2.06	0.56
1:A:192:ASN:HB2	3:A:413[B]:HOH:O	2.05	0.56
1:A:5:PRO:HB2	1:A:34[B]:GLU:HG2	1.88	0.55
1:A:69[B]:ILE:HD12	1:A:69[B]:ILE:N	2.21	0.55
1:B:32:VAL:CG1	3:B:304[B]:HOH:O	2.54	0.55
1:C:62[B]:LYS:HD2	1:C:115:ILE:CD1	2.36	0.55
1:A:20[B]:ILE:HD12	1:A:46:PHE:CB	2.37	0.55
1:B:135[B]:GLY:H	1:B:150[B]:ILE:CD1	2.20	0.54
1:A:63[B]:ILE:HB	2:A:301[B]:04R:C13	2.38	0.54
1:B:18:GLN:HB3	1:B:23:ILE:HD11	1.90	0.54
1:B:56:ILE:CG2	3:B:313[B]:HOH:O	2.42	0.54
1:B:121:TRP:HE3	1:B:139[B]:ILE:HD13	1.73	0.54
1:A:8:MET:CB	1:A:23[B]:ILE:HG12	2.39	0.53
1:B:175:GLN:O	1:B:179:ILE:HD13	2.08	0.53
1:A:108[B]:LEU:CB	1:A:109[B]:PRO:CD	2.86	0.53
1:A:154:MET:HE3	1:A:163:GLU:OE1	2.09	0.53
1:A:184:TRP:HZ3	3:A:413[B]:HOH:O	1.92	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:66:PHE:O	1:C:119:ASP:HA	2.09	0.52
1:A:20[B]:ILE:HD12	1:A:46:PHE:HB3	1.90	0.52
1:A:190:ASN:HA	1:A:193:ILE:HD12	1.90	0.52
1:A:20[B]:ILE:CD1	1:A:46:PHE:HB2	2.40	0.52
1:A:198:ASP:O	1:A:199:ASN:HB2	2.09	0.52
1:B:48:LYS:HE2	3:B:312[B]:HOH:O	2.09	0.52
1:B:148[B]:LYS:NZ	1:B:162[B]:ASN:OD1	2.40	0.52
1:B:18:GLN:HE22	1:B:45:THR:HA	1.74	0.52
1:B:201:ILE:CG2	3:B:314[B]:HOH:O	2.58	0.52
1:A:21[B]:LYS:N	1:A:22:PRO:HD2	2.24	0.52
1:B:25:GLU:O	1:B:26:LYS:HB2	2.11	0.51
1:A:21[B]:LYS:HZ3	1:A:32[B]:VAL:HG23	1.74	0.51
1:C:38:TYR:CE1	3:C:401[B]:HOH:O	2.55	0.51
1:A:63[B]:ILE:HB	2:A:301[B]:04R:C8	2.40	0.51
1:B:106:ASP:OD1	3:B:302[B]:HOH:O	2.19	0.51
3:A:412[B]:HOH:O	1:C:90:PRO:HG2	2.11	0.51
1:B:102:MET:HE2	3:B:308[B]:HOH:O	2.09	0.51
1:C:21:LYS:HB3	1:C:22:PRO:CD	2.40	0.51
1:C:24:LEU:HD12	1:C:32:VAL:HG21	1.92	0.51
1:A:65[B]:LYS:CE	1:A:182:TRP:O	2.58	0.51
1:A:20[B]:ILE:HG23	1:A:23[B]:ILE:HD12	1.92	0.51
1:B:150[B]:ILE:HG22	1:B:163[B]:GLU:OE2	2.12	0.50
1:A:52:TYR:HD2	1:A:76[B]:ILE:HG23	1.77	0.50
1:A:63[B]:ILE:HG12	1:A:63[B]:ILE:O	2.12	0.50
1:B:20:ILE:HG12	3:B:304[B]:HOH:O	2.11	0.50
1:C:104:LYS:HG3	1:C:106:ASP:OD1	2.12	0.50
1:B:173:ILE:HD11	3:B:301[B]:HOH:O	2.10	0.50
1:A:20[B]:ILE:HD11	1:A:38:TYR:HB3	1.94	0.49
1:B:129[A]:MET:HB3	1:B:130[A]:PRO:HD2	1.94	0.49
1:B:134[B]:ILE:CA	1:B:150[B]:ILE:HD11	2.22	0.49
1:A:62[B]:LYS:HB3	1:A:115[B]:ILE:CG1	2.42	0.49
1:A:68[B]:SER:C	1:A:69[B]:ILE:HD12	2.38	0.49
1:A:66[B]:PHE:CE2	1:A:181:TRP:CZ3	3.00	0.49
1:B:24:LEU:HD12	1:B:32:VAL:HG21	1.95	0.49
1:B:129[A]:MET:O	1:B:132[A]:VAL:HG13	2.12	0.49
1:B:152[B]:PRO:HG3	1:B:177:LEU:CD1	2.41	0.49
1:B:175:GLN:O	1:B:179:ILE:CD1	2.62	0.48
1:A:109[B]:PRO:O	1:A:110[B]:ILE:C	2.56	0.48
1:A:192:ASN:HB3	1:A:201:ILE:CD1	2.44	0.48
1:A:22:PRO:O	1:A:25[B]:GLU:HB2	2.14	0.48
1:B:129[B]:MET:HB3	1:B:130[B]:PRO:HD2	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:MET:HG2	1:B:9:TYR:CE2	2.49	0.47
1:B:195:LYS:HD3	3:B:311[B]:HOH:O	2.12	0.47
1:A:69[B]:ILE:CD1	2:A:301[B]:04R:H10A	2.44	0.47
1:A:20[B]:ILE:HG22	1:A:23[B]:ILE:CA	2.43	0.47
1:C:155[B]:LEU:HD13	1:C:165:LYS:HG3	1.97	0.47
1:C:115:ILE:HD13	1:C:115:ILE:N	2.29	0.47
1:B:4:ASN:HB3	1:B:7:LYS:CD	2.45	0.47
1:A:20[B]:ILE:HG23	1:A:23[B]:ILE:CG1	2.45	0.47
1:A:63[B]:ILE:HB	2:A:301[B]:04R:H13A	1.96	0.47
1:A:10:PRO:HB3	1:A:19[B]:PHE:CE2	2.50	0.47
1:A:115[A]:ILE:HD12	1:A:133:LYS:HD2	1.96	0.46
1:B:129[A]:MET:HB3	1:B:130[A]:PRO:CD	2.45	0.46
1:A:22:PRO:O	1:A:24[B]:LEU:N	2.44	0.46
1:A:98[B]:TRP:CH2	1:B:3:PRO:HD2	2.50	0.46
1:A:24[B]:LEU:HD12	1:A:24[B]:LEU:O	2.16	0.45
1:A:185:PRO:O	1:A:189:ILE:HG13	2.16	0.45
1:B:25:GLU:O	1:B:26:LYS:CB	2.65	0.45
1:B:97:GLY:N	1:B:99:GLU:OE2	2.49	0.45
1:A:66[B]:PHE:CE2	1:A:182:TRP:HA	2.48	0.45
1:A:159:ASN:OD1	1:A:159:ASN:C	2.60	0.45
1:A:62[B]:LYS:HG2	1:A:63[B]:ILE:H	1.81	0.45
1:B:48:LYS:HE3	3:B:312[B]:HOH:O	2.16	0.45
1:A:65[B]:LYS:HB3	3:A:409[B]:HOH:O	2.11	0.45
1:A:100[B]:LYS:HB3	1:A:100[B]:LYS:HE3	1.72	0.45
1:B:198:ASP:C	1:B:198:ASP:OD1	2.59	0.45
1:B:119:ASP:O	1:B:137[A]:GLY:HA2	2.16	0.44
1:A:18[B]:GLN:NE2	1:A:40:SER:HB2	2.31	0.44
1:A:20[B]:ILE:CD1	1:A:46:PHE:CB	2.95	0.44
1:A:63[B]:ILE:HD12	2:A:301[B]:04R:N	2.32	0.44
1:A:14:ASN:OD1	1:A:16:SER:HB3	2.17	0.44
1:A:45:THR:OG1	1:A:47:ASP:OD1	2.27	0.44
1:C:129:MET:HB3	1:C:130:PRO:CD	2.47	0.44
1:B:66:PHE:O	1:B:119:ASP:HA	2.18	0.44
1:C:8:MET:HG2	1:C:23:ILE:HG12	2.00	0.44
1:A:21[B]:LYS:N	1:A:22:PRO:CD	2.81	0.44
1:A:192:ASN:HB3	1:A:201:ILE:HD11	2.00	0.44
1:A:172:THR:HG23	1:A:202:ILE:HD13	2.00	0.43
1:B:150[B]:ILE:HD12	1:B:150[B]:ILE:O	2.17	0.43
1:A:82[A]:HIS:HB2	1:B:121:TRP:CZ3	2.54	0.43
1:A:90[B]:PRO:HB2	1:A:93[B]:LEU:HD22	2.00	0.43
1:C:114:THR:O	1:C:115:ILE:HD13	2.17	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:ILE:CG1	1:B:32:VAL:HG11	2.28	0.43
1:A:69[B]:ILE:HD11	2:A:301[B]:04R:H11A	2.01	0.43
1:B:133[B]:LYS:HG2	1:B:149[B]:ASP:OD2	2.18	0.43
1:B:199:ASN:O	1:B:202:ILE:HG12	2.19	0.43
1:A:49:GLN:HB3	1:A:73[B]:VAL:O	2.18	0.43
1:A:21[B]:LYS:HZ2	1:A:32[B]:VAL:HG23	1.83	0.43
1:A:188:ILE:O	1:A:192:ASN:ND2	2.48	0.43
1:A:196:ILE:CD1	3:A:413[B]:HOH:O	2.62	0.43
1:B:134[B]:ILE:HA	1:B:150[B]:ILE:CD1	2.23	0.43
1:C:110:ILE:HG23	1:C:112:GLY:H	1.84	0.43
1:A:7:LYS:HE3	1:A:10:PRO:HA	2.01	0.42
1:A:30[B]:VAL:HA	1:A:61[B]:LEU:O	2.19	0.42
1:B:102:MET:HE2	1:B:102:MET:HB2	1.76	0.42
1:A:24[B]:LEU:CD1	1:A:27[B]:LEU:HG	2.49	0.42
1:A:88[B]:THR:HG21	1:B:139[B]:ILE:HD11	2.00	0.42
1:A:109[B]:PRO:O	1:A:109[B]:PRO:HG2	2.19	0.42
1:C:59:ASP:OD1	1:C:59:ASP:N	2.50	0.42
1:B:54:TYR:O	1:B:55:PRO:C	2.61	0.42
1:A:32[B]:VAL:CG1	1:A:63[B]:ILE:HG21	2.48	0.42
1:B:115:ILE:HD12	1:B:133[B]:LYS:HE3	2.01	0.42
1:C:62[A]:LYS:HE3	1:C:115:ILE:HG23	2.01	0.42
1:C:70:GLY:O	1:C:73:VAL:HG23	2.20	0.42
1:B:104:LYS:O	1:B:105:LEU:C	2.63	0.42
1:B:8:MET:HG2	1:B:9:TYR:CD2	2.54	0.41
1:A:197:LEU:O	1:C:86:GLY:HA3	2.20	0.41
1:A:30[B]:VAL:HG21	2:A:301[B]:04R:O	2.20	0.41
1:A:20[B]:ILE:HG23	1:A:23[B]:ILE:CD1	2.51	0.41
1:A:24[B]:LEU:CD1	1:A:27[B]:LEU:CG	2.99	0.41
1:A:36:SER:HB3	2:A:301[B]:04R:H10	2.02	0.41
1:C:49:GLN:HB3	1:C:73:VAL:O	2.21	0.41
1:C:9:TYR:CE2	1:C:18:GLN:HG2	2.55	0.41
1:C:102:MET:HE3	1:C:102:MET:HB2	1.91	0.41
1:A:199:ASN:O	1:A:202:ILE:HG12	2.21	0.41
1:C:18:GLN:OE1	1:C:23:ILE:HD12	2.21	0.41
1:C:28:GLU:O	1:C:29:ASN:HB2	2.21	0.41
1:C:34:GLU:O	1:C:35:TYR:HB2	2.21	0.41
1:A:196:ILE:HG13	3:A:413[B]:HOH:O	2.21	0.41
1:A:32[B]:VAL:HA	1:A:63[B]:ILE:CG2	2.45	0.40
1:A:104[A]:LYS:O	1:A:108[A]:LEU:HG	2.20	0.40
1:A:29[B]:ASN:OD1	1:A:60:LYS:HE3	2.20	0.40
1:A:31[B]:GLU:HG2	1:A:62[B]:LYS:HG3	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:PRO:HG3	1:B:19:PHE:CE2	2.57	0.40
1:B:115:ILE:HB	1:B:133[B]:LYS:CD	2.49	0.40
1:C:57:LEU:HD22	1:C:110:ILE:HD11	2.03	0.40
1:B:121:TRP:CE3	1:B:139[B]:ILE:HD13	2.56	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	275/209 (132%)	234 (85%)	30 (11%)	11 (4%)	2	1
1	B	244/209 (117%)	227 (93%)	13 (5%)	4 (2%)	7	6
1	C	207/209 (99%)	197 (95%)	9 (4%)	1 (0%)	24	29
All	All	726/627 (116%)	658 (91%)	52 (7%)	16 (2%)	8	3

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	116[A]	ILE
1	A	116[B]	ILE
1	A	26[A]	LYS
1	A	26[B]	LYS
1	B	150[A]	ILE
1	B	150[B]	ILE
1	B	163[A]	GLU
1	B	163[B]	GLU
1	A	22	PRO
1	A	23[A]	ILE
1	A	23[B]	ILE
1	A	100[A]	LYS
1	A	100[B]	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	90	PRO
1	A	108[A]	LEU
1	A	108[B]	LEU

5.3.2 Protein sidechains ⓘ

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	240/182 (132%)	240 (100%)	0	100	100
1	B	209/182 (115%)	206 (99%)	3 (1%)	59	74
1	C	181/182 (100%)	177 (98%)	4 (2%)	45	62
All	All	630/546 (115%)	623 (99%)	7 (1%)	65	79

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	120	VAL
1	B	132[A]	VAL
1	B	132[B]	VAL
1	C	23	ILE
1	C	110	ILE
1	C	115	ILE
1	C	201	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	174	ASN
1	B	42	ASN
1	B	96	ASN
1	B	192	ASN
1	C	166	GLN
1	C	183	ASN
1	C	190	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 oligosaccharides 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	04R	C	301[B]	-	18,18,18	1.46	3 (16%)	23,27,27	2.85	10 (43%)
2	04R	A	301[B]	-	18,18,18	0.99	1 (5%)	23,27,27	3.85	9 (39%)

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	04R	C	301[B]	-	-	4/10/17/17	0/2/2/2
2	04R	A	301[B]	-	-	2/10/17/17	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301[B]	04R	C10-C9	2.69	1.55	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301[B]	04R	CA-C	2.18	1.55	1.51
2	C	301[B]	04R	F4-C2	2.06	1.40	1.32
2	A	301[B]	04R	C10-C9	2.06	1.54	1.51

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301[B]	04R	C2-C5-N6	10.62	131.07	118.50
2	A	301[B]	04R	C13-C8-C9	-9.00	115.42	125.54
2	C	301[B]	04R	C9-C5-N6	-6.59	108.12	111.24
2	A	301[B]	04R	C9-C5-N6	-6.05	108.37	111.24
2	A	301[B]	04R	F4-C2-C5	-5.26	104.90	112.39
2	C	301[B]	04R	C2-C5-N6	5.07	124.51	118.50
2	C	301[B]	04R	C-CA-N	-4.87	104.45	112.48
2	C	301[B]	04R	F1-C2-C5	-4.77	105.59	112.39
2	A	301[B]	04R	CA-N-N6	4.43	125.04	118.99
2	C	301[B]	04R	C13-C8-C9	-4.19	120.83	125.54
2	A	301[B]	04R	C8-N-N6	-4.17	109.52	113.85
2	C	301[B]	04R	F3-C2-C5	-4.17	106.45	112.39
2	A	301[B]	04R	CA-N-C8	-3.85	125.44	129.10
2	C	301[B]	04R	F4-C2-C5	-2.64	108.63	112.39
2	A	301[B]	04R	F1-C2-C5	-2.46	108.89	112.39
2	C	301[B]	04R	OXT-C-O	-2.38	117.22	123.33
2	A	301[B]	04R	OXT-C-CA	2.34	122.60	113.38
2	C	301[B]	04R	C12-C13-C8	2.18	115.17	110.42
2	C	301[B]	04R	F4-C2-F1	2.05	115.06	106.20

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301[B]	04R	C-CA-N-N6
2	A	301[B]	04R	C-CA-N-C8
2	C	301[B]	04R	C-CA-N-N6
2	C	301[B]	04R	C-CA-N-C8
2	C	301[B]	04R	O-C-CA-N
2	C	301[B]	04R	OXT-C-CA-N

There are no ring outliers.

1 monomer is involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301[B]	04R	12	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

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, 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	203/209 (97%)	1.52	51 (25%) 1 1	21, 54, 92, 118	71 (34%)
1	B	203/209 (97%)	1.22	36 (17%) 4 4	19, 56, 93, 134	39 (19%)
1	C	202/209 (96%)	1.54	54 (26%) 1 1	26, 68, 106, 154	5 (2%)
All	All	608/627 (96%)	1.43	141 (23%) 2 2	19, 59, 97, 154	115 (18%)

All (141) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	177	LEU	7.7
1	A	110[A]	ILE	7.6
1	B	25	GLU	6.1
1	C	58	ASN	5.6
1	C	164	ILE	5.0
1	C	202[A]	ILE	4.9
1	C	201	ILE	4.8
1	A	108[A]	LEU	4.8
1	A	132	VAL	4.7
1	C	26	LYS	4.5
1	A	92[A]	ASN	4.4
1	C	56	ILE	4.3
1	B	26	LYS	4.2
1	A	95[A]	GLY	4.2
1	A	2	GLY	4.1
1	C	199	ASN	3.9
1	A	186	ILE	3.9
1	C	13	GLY	3.9
1	A	105[A]	LEU	3.9
1	A	25[A]	GLU	3.8
1	C	6	MET	3.8
1	C	186	ILE	3.8
1	B	155[A]	LEU	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	20	ILE	3.8
1	A	26[A]	LYS	3.7
1	B	46	PHE	3.7
1	C	100	LYS	3.7
1	C	105	LEU	3.7
1	B	80	ALA	3.7
1	C	102	MET	3.6
1	A	109[A]	PRO	3.6
1	A	6	MET	3.6
1	B	108	LEU	3.6
1	B	174	ASN	3.6
1	C	25	GLU	3.6
1	A	134	ILE	3.6
1	A	189	ILE	3.6
1	B	13	GLY	3.6
1	C	97	GLY	3.5
1	B	110	ILE	3.5
1	B	109	PRO	3.5
1	A	115[A]	ILE	3.5
1	C	12	GLU	3.5
1	A	5	PRO	3.3
1	C	109	PRO	3.3
1	B	179	ILE	3.3
1	A	33[A]	GLY	3.3
1	A	98[A]	TRP	3.2
1	A	104[A]	LYS	3.2
1	C	181	TRP	3.2
1	C	27	LEU	3.2
1	A	13	GLY	3.1
1	C	95	GLY	3.1
1	A	187	ASP	3.1
1	A	24[A]	LEU	3.1
1	B	56	ILE	3.0
1	C	179	ILE	3.0
1	C	110	ILE	3.0
1	C	119	ASP	3.0
1	A	38	TYR	2.9
1	C	68	SER	2.9
1	A	8	MET	2.9
1	A	81[A]	ASN	2.9
1	C	64[A]	GLY	2.9
1	C	55	PRO	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	27	LEU	2.9
1	C	142	ALA	2.9
1	B	121	TRP	2.9
1	B	97	GLY	2.8
1	C	62[A]	LYS	2.8
1	C	176	LEU	2.8
1	C	155[A]	LEU	2.8
1	C	67	CYS	2.8
1	C	108	LEU	2.8
1	A	179	ILE	2.7
1	B	31	GLU	2.7
1	B	24	LEU	2.7
1	C	80	ALA	2.7
1	A	106[A]	ASP	2.7
1	B	2	GLY	2.7
1	C	196	ILE	2.7
1	C	98	TRP	2.7
1	C	54	TYR	2.7
1	B	187	ASP	2.7
1	C	194	ASP	2.7
1	C	10	PRO	2.6
1	B	161[A]	ALA	2.6
1	C	22	PRO	2.6
1	B	150[A]	ILE	2.6
1	A	10	PRO	2.5
1	A	15	LYS	2.5
1	A	54	TYR	2.5
1	B	35	TYR	2.5
1	A	121	TRP	2.5
1	C	11	ILE	2.5
1	B	204	GLU	2.5
1	A	27[A]	LEU	2.5
1	B	16	SER	2.5
1	A	100[A]	LYS	2.4
1	A	111[A]	LYS	2.4
1	A	14	ASN	2.4
1	C	203[A]	ARG	2.4
1	C	5	PRO	2.4
1	B	96	ASN	2.4
1	B	171	ASP	2.4
1	A	11	ILE	2.4
1	A	91[A]	PHE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	40	SER	2.3
1	B	202	ILE	2.3
1	A	42	ASN	2.3
1	C	106	ASP	2.3
1	A	43	GLY	2.2
1	A	35[A]	TYR	2.2
1	B	36	SER	2.2
1	C	104	LYS	2.2
1	C	120	VAL	2.2
1	B	54	TYR	2.2
1	A	39	ASP	2.2
1	A	59	ASP	2.2
1	B	63	ILE	2.2
1	A	47	ASP	2.2
1	C	61[A]	LEU	2.1
1	C	93	LEU	2.1
1	C	111	LYS	2.1
1	B	22	PRO	2.1
1	B	34	GLU	2.1
1	C	190	ASN	2.1
1	A	142	ALA	2.1
1	B	105	LEU	2.1
1	B	14	ASN	2.1
1	C	89	TYR	2.1
1	C	153	TYR	2.1
1	A	34[A]	GLU	2.1
1	A	173	ILE	2.1
1	A	175	GLN	2.1
1	A	203	ARG	2.1
1	C	107	GLN	2.0
1	A	4	ASN	2.0
1	C	4	ASN	2.0
1	C	9	TYR	2.0
1	A	74[A]	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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	04R	C	301[B]	17/17	0.47	0.38	68,88,105,107	27
2	04R	A	301[B]	17/17	0.90	0.26	49,67,86,87	27

6.5 Other polymers [i](#)

There are no such residues in this entry.