



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 26, 2026 – 11:29 PM UTC

PDB ID : 3O52 / pdb_00003o52
Title : Structure of the E.coli GDP-mannose hydrolase (yffh) in complex with tartrate
Authors : Amzel, L.M.; Gabelli, S.B.; Boto, A.N.
Deposited on : 2010-07-27
Resolution : 2.50 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

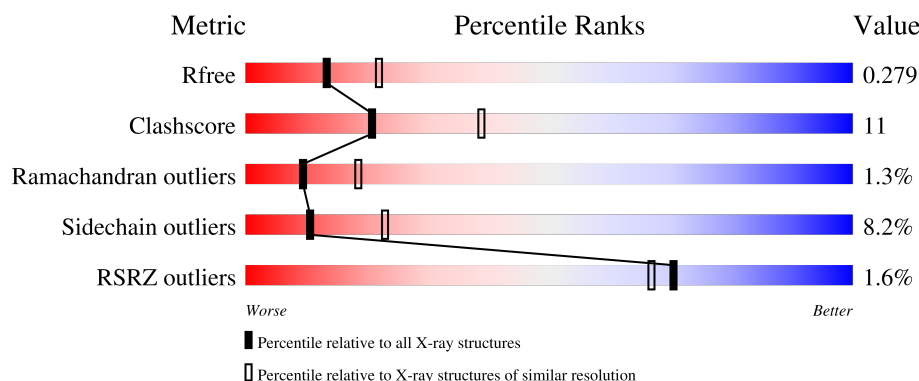
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	191	2% 68% 22% 8%
1	B	191	2% 70% 19% 8%
1	C	191	71% 17% 5% 7%
1	D	191	0% 69% 24% 6%
1	E	191	3% 63% 21% 8% 7%

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	TAR	B	7110	-	-	X	-

2 Entry composition [i](#)

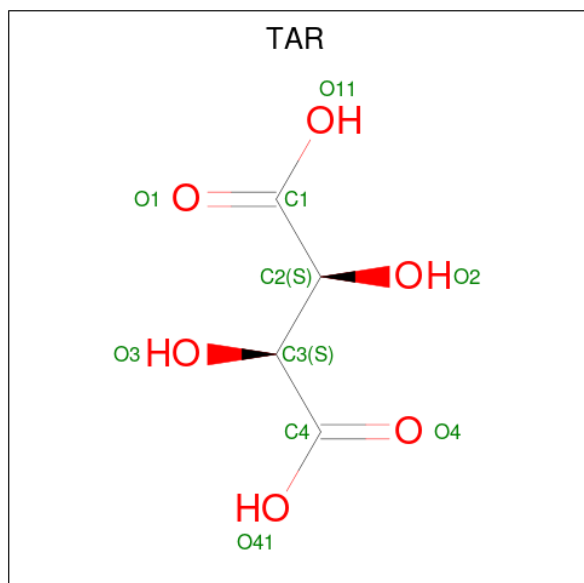
There are 5 unique types of molecules in this entry. The entry contains 7421 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 GDP-mannose pyrophosphatase nudK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	175	Total	C	N	O	S	0	1	0
			1420	904	237	274	5			
1	B	176	Total	C	N	O	S	0	0	0
			1420	902	236	277	5			
1	C	177	Total	C	N	O	S	0	0	0
			1430	908	239	278	5			
1	D	180	Total	C	N	O	S	0	0	0
			1455	922	245	283	5			
1	E	177	Total	C	N	O	S	0	0	0
			1429	908	238	278	5			

- Molecule 2 is D(-)-TARTARIC ACID (CCD ID: TAR) (formula: C₄H₆O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	4	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	4	6		
2	B	1	Total	C	O	0	0
			10	4	6		
2	C	1	Total	C	O	0	0
			10	4	6		
2	D	1	Total	C	O	0	0
			10	4	6		
2	E	1	Total	C	O	0	0
			10	4	6		

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Na	0	0
			2	2		
3	B	1	Total	Na	0	0
			1	1		
3	D	2	Total	Na	0	0
			2	2		
3	E	1	Total	Na	0	0
			1	1		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total	Cl	0	0
			1	1		
4	D	2	Total	Cl	0	0
			2	2		
4	E	1	Total	Cl	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	40	Total	O	0	0
			40	40		
5	B	53	Total	O	0	0
			53	53		
5	C	38	Total	O	0	0
			38	38		

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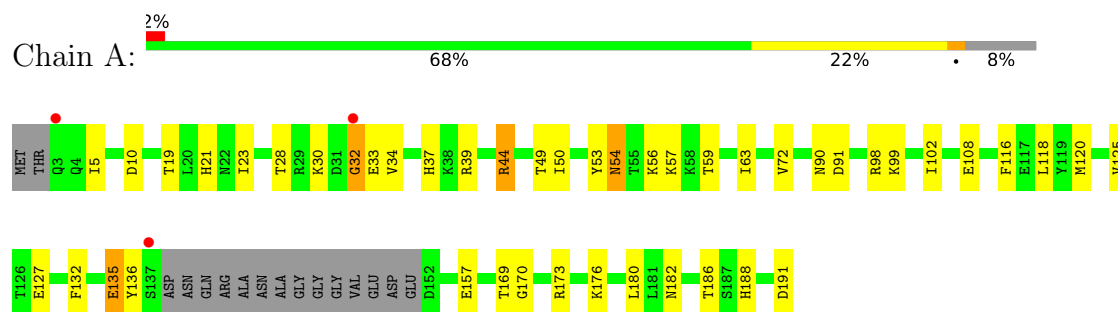
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	33	Total	O	0	0
			33	33		
5	E	33	Total	O	0	0
			33	33		

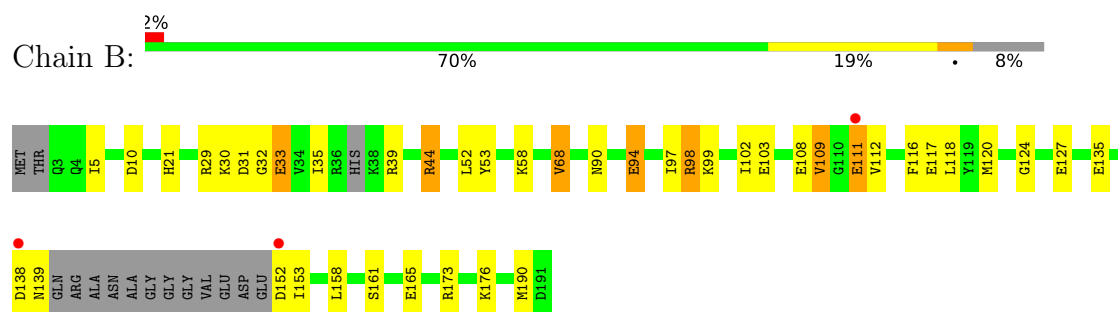
3 Residue-property plots [i](#)

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.

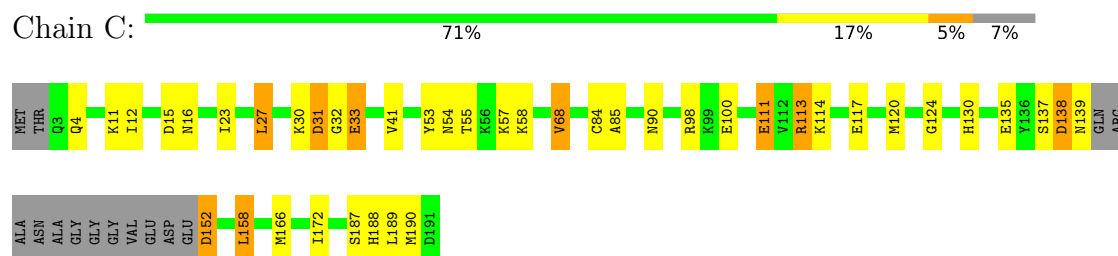
- Molecule 1: GDP-mannose pyrophosphatase nudK



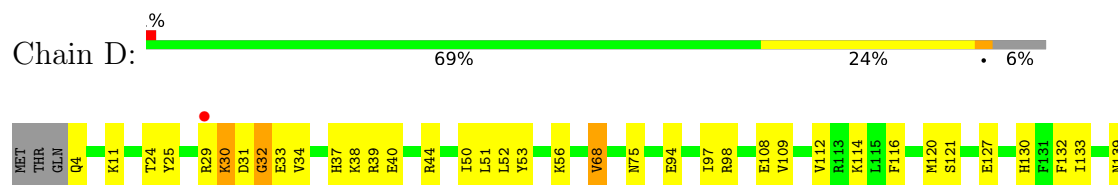
- Molecule 1: GDP-mannose pyrophosphatase nudK

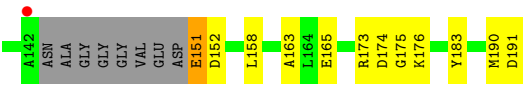


- Molecule 1: GDP-mannose pyrophosphatase nudK

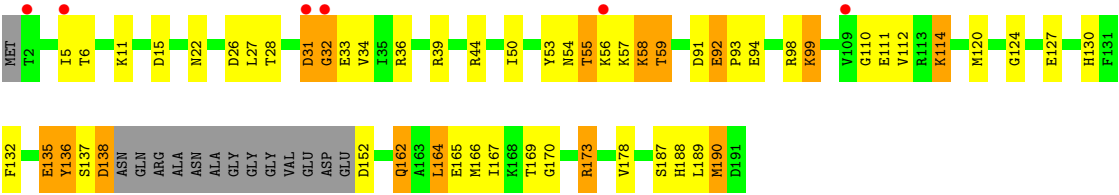


- Molecule 1: GDP-mannose pyrophosphatase nudK





● Molecule 1: GDP-mannose pyrophosphatase nudK



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	75.34Å 103.22Å 254.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.73 – 2.50 29.73 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.2 (29.73-2.50) 96.2 (29.73-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.25 (at 2.51Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.211 , 0.288 0.203 , 0.279	Depositor DCC
R_{free} test set	1684 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	47.0	Xtriage
Anisotropy	0.425	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7421	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.07% 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: TAR, CL, NA

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	0.75	0/1444	0.89	0/1948
1	B	0.78	0/1439	0.96	1/1940 (0.1%)
1	C	0.71	0/1451	0.93	2/1958 (0.1%)
1	D	0.92	5/1476 (0.3%)	1.13	7/1991 (0.4%)
1	E	1.44	19/1450 (1.3%)	1.16	16/1957 (0.8%)
All	All	0.96	24/7260 (0.3%)	1.02	26/9794 (0.3%)

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	E	0	1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	138	ASP	CG-OD2	23.73	1.70	1.25
1	E	31	ASP	CG-OD2	17.93	1.59	1.25
1	D	121	SER	C-N	16.69	1.53	1.33
1	E	138	ASP	C-O	13.56	1.50	1.23
1	E	190	MET	CG-SD	13.47	2.14	1.80
1	E	56	LYS	C-O	9.85	1.36	1.24
1	D	30	LYS	CD-CE	9.28	1.80	1.52
1	E	55	THR	C-O	8.39	1.35	1.24
1	E	54	ASN	CG-ND2	8.02	1.50	1.33
1	E	32	GLY	C-O	7.42	1.32	1.23
1	D	121	SER	C-O	-7.14	1.16	1.24
1	E	56	LYS	C-N	6.63	1.43	1.33
1	D	30	LYS	CE-NZ	6.55	1.69	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	59	THR	CB-CG2	6.49	1.74	1.52
1	E	138	ASP	CB-CG	6.43	1.68	1.52
1	E	135	GLU	C-N	6.42	1.41	1.33
1	E	58	LYS	CE-NZ	6.34	1.68	1.49
1	D	30	LYS	CG-CD	6.20	1.71	1.52
1	E	54	ASN	CB-CG	5.87	1.66	1.52
1	E	32	GLY	C-N	5.65	1.41	1.33
1	E	31	ASP	C-O	5.34	1.30	1.23
1	E	136	TYR	CE2-CZ	5.32	1.51	1.38
1	E	54	ASN	CG-OD1	5.11	1.33	1.23
1	E	190	MET	SD-CE	5.09	1.92	1.79

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	121	SER	O-C-N	-16.79	108.02	121.12
1	E	138	ASP	CA-C-O	-15.34	94.72	120.80
1	D	120	MET	CA-C-N	-13.93	110.02	122.28
1	D	120	MET	C-N-CA	-13.93	110.02	122.28
1	E	138	ASP	CB-CG-OD2	-9.10	97.47	118.40
1	E	32	GLY	O-C-N	7.62	132.69	122.48
1	B	68	VAL	CB-CA-C	-7.00	102.92	111.88
1	E	137	SER	N-CA-C	6.84	117.61	108.38
1	E	56	LYS	O-C-N	6.75	132.20	122.28
1	E	31	ASP	CB-CG-OD1	6.65	133.70	118.40
1	C	68	VAL	CB-CA-C	-6.52	103.49	112.04
1	D	30	LYS	CG-CD-CE	-6.10	97.28	111.30
1	D	120	MET	O-C-N	6.01	130.70	122.46
1	E	190	MET	CG-SD-CE	-5.80	88.15	100.90
1	C	27	LEU	CA-CB-CG	5.76	136.46	116.30
1	E	138	ASP	OD1-CG-OD2	5.65	136.46	122.90
1	E	92	GLU	CA-C-N	5.51	124.97	119.24
1	E	92	GLU	C-N-CA	5.51	124.97	119.24
1	D	32	GLY	N-CA-C	5.49	120.43	113.24
1	E	32	GLY	N-CA-C	5.38	121.99	115.31
1	E	27	LEU	N-CA-C	5.32	117.07	108.34
1	E	190	MET	CB-CG-SD	-5.31	96.77	112.70
1	D	68	VAL	CB-CA-C	-5.20	105.23	112.04
1	E	135	GLU	O-C-N	5.14	128.92	122.65
1	E	56	LYS	CA-C-O	-5.14	113.73	120.00
1	E	31	ASP	OD1-CG-OD2	-5.06	110.75	122.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	32	GLY	Mainchain

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	1420	0	1426	30	0
1	B	1420	0	1421	33	0
1	C	1430	0	1430	38	0
1	D	1455	0	1452	39	0
1	E	1429	0	1431	36	0
2	A	20	0	8	2	0
2	B	10	0	4	4	0
2	C	10	0	4	0	0
2	D	10	0	3	0	0
2	E	10	0	4	1	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
3	D	2	0	0	0	0
3	E	1	0	0	0	0
4	C	1	0	0	0	0
4	D	2	0	0	0	0
4	E	1	0	0	0	0
5	A	40	0	0	3	0
5	B	53	0	0	5	0
5	C	38	0	0	4	0
5	D	33	0	0	3	0
5	E	33	0	0	5	0
All	All	7421	0	7183	160	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 11.

All (160) 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:D:30:LYS:CD	1:D:30:LYS:CE	1.80	1.60
1:D:30:LYS:CE	1:D:30:LYS:NZ	1.69	1.54
1:E:58:LYS:CE	1:E:58:LYS:NZ	1.68	1.53
1:E:190:MET:CG	1:E:190:MET:SD	2.14	1.36
1:E:138:ASP:OD2	1:E:138:ASP:CG	1.70	1.33
1:B:44:ARG:NH1	2:B:7110:TAR:O41	1.67	1.26
1:C:120:MET:CE	1:D:175:GLY:HA3	2.03	0.88
1:C:120:MET:HE1	1:D:175:GLY:HA3	1.55	0.87
1:B:21:HIS:HE1	5:B:208:HOH:O	1.60	0.84
1:D:31:ASP:OD1	1:D:32:GLY:N	2.13	0.82
1:D:158:LEU:HD11	1:D:163:ALA:HB2	1.63	0.81
1:D:25:TYR:OH	1:D:39:ARG:NH1	2.14	0.80
1:C:120:MET:HE1	1:D:175:GLY:CA	2.11	0.80
1:A:37:HIS:HD2	1:E:91:ASP:OD2	1.65	0.80
1:B:94:GLU:O	1:B:98:ARG:HG2	1.82	0.79
1:D:30:LYS:CE	1:D:30:LYS:CG	2.63	0.77
1:A:10:ASP:OD1	1:A:21:HIS:HD2	1.68	0.76
1:B:138:ASP:HA	1:B:139:ASN:C	2.10	0.76
1:A:90:ASN:HD21	1:D:40:GLU:H	1.34	0.75
1:C:113:ARG:CG	1:C:113:ARG:HH11	1.99	0.75
1:C:54:ASN:HD22	1:C:57:LYS:H	1.33	0.74
1:E:111:GLU:HB2	5:E:303:HOH:O	1.88	0.73
1:C:54:ASN:ND2	1:C:57:LYS:H	1.87	0.71
1:E:120:MET:HA	1:E:120:MET:HE2	1.72	0.71
1:E:58:LYS:NZ	1:E:58:LYS:CD	2.54	0.71
1:A:32:GLY:HA2	1:A:33:GLU:C	2.16	0.70
1:E:55:THR:HA	1:E:190:MET:HE2	1.74	0.70
1:D:53:TYR:HB2	1:D:190:MET:HE3	1.73	0.70
1:E:190:MET:HB2	5:E:209:HOH:O	1.92	0.70
1:E:190:MET:SD	1:E:190:MET:CB	2.80	0.69
1:C:120:MET:HA	1:C:120:MET:HE2	1.74	0.69
1:B:10:ASP:OD1	1:B:21:HIS:HD2	1.75	0.69
1:D:151:GLU:N	1:D:151:GLU:CD	2.51	0.69
1:B:99:LYS:O	1:B:103:GLU:HG3	1.94	0.67
1:B:44:ARG:NH1	2:B:7110:TAR:C4	2.56	0.67
1:D:4:GLN:N	5:D:300:HOH:O	2.27	0.67
1:D:30:LYS:CD	1:D:30:LYS:NZ	2.59	0.66
1:C:113:ARG:HH11	1:C:113:ARG:HG3	1.59	0.66
1:A:125:VAL:HG12	1:A:127:GLU:H	1.60	0.66
1:C:117:GLU:HG3	5:C:201:HOH:O	1.96	0.65
1:D:151:GLU:HG2	1:D:152:ASP:H	1.61	0.65
1:A:44:ARG:NH2	5:A:195:HOH:O	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:94:GLU:HB2	5:D:192:HOH:O	1.98	0.63
1:A:176:LYS:HE3	2:A:7110:TAR:O11	1.98	0.63
1:C:98:ARG:HH22	1:C:111:GLU:HA	1.62	0.63
1:C:117:GLU:CG	5:C:201:HOH:O	2.46	0.63
1:C:120:MET:HE2	1:D:175:GLY:HA3	1.80	0.62
1:B:21:HIS:CE1	5:B:208:HOH:O	2.41	0.62
1:E:53:TYR:O	1:E:135:GLU:HA	1.99	0.62
1:A:54:ASN:HD21	1:A:56:LYS:HB3	1.65	0.61
1:D:52:LEU:HD21	1:D:109:VAL:HG11	1.83	0.61
1:A:37:HIS:CD2	1:E:91:ASP:OD2	2.52	0.60
1:A:91:ASP:OD2	1:D:37:HIS:HD2	1.84	0.60
1:E:15:ASP:HB3	5:E:199:HOH:O	1.99	0.60
1:C:120:MET:CE	1:D:175:GLY:CA	2.73	0.60
1:B:31:ASP:O	1:B:33:GLU:N	2.27	0.59
1:D:94:GLU:O	1:D:98:ARG:HG3	2.02	0.59
1:E:59:THR:OG1	1:E:136:TYR:OH	2.19	0.58
1:E:53:TYR:HD2	1:E:190:MET:HE3	1.69	0.58
1:B:90:ASN:ND2	5:B:207:HOH:O	2.34	0.58
1:C:152:ASP:HA	1:D:29:ARG:HH22	1.68	0.57
1:D:158:LEU:CD1	1:D:163:ALA:HB2	2.33	0.57
1:E:57:LYS:O	1:E:59:THR:HG23	2.04	0.57
1:D:114:LYS:NZ	1:D:130:HIS:HD2	2.02	0.57
1:A:59:THR:OG1	1:A:136:TYR:OH	2.21	0.57
1:E:190:MET:CG	1:E:190:MET:CE	2.83	0.57
1:B:138:ASP:CA	1:B:139:ASN:C	2.78	0.57
1:B:118:LEU:HB2	1:B:120:MET:HE1	1.88	0.56
5:A:209:HOH:O	1:B:120:MET:HG3	2.06	0.55
1:B:118:LEU:HB2	1:B:120:MET:CE	2.36	0.55
1:E:164:LEU:HA	1:E:167:ILE:HD12	1.88	0.55
1:A:21:HIS:HE1	5:A:215:HOH:O	1.90	0.55
1:B:52:LEU:HD22	1:B:109:VAL:HG11	1.88	0.55
1:C:114:LYS:NZ	1:C:130:HIS:HD2	2.05	0.54
1:D:50:ILE:HA	1:D:132:PHE:O	2.07	0.54
1:E:138:ASP:OD2	1:E:138:ASP:CB	2.54	0.54
1:B:53:TYR:O	1:B:135:GLU:HA	2.08	0.54
1:B:44:ARG:HH12	2:B:7110:TAR:C4	2.20	0.54
1:B:10:ASP:OD1	1:B:21:HIS:CD2	2.60	0.54
1:E:162:GLN:O	1:E:166:MET:HG3	2.08	0.54
1:D:52:LEU:HD21	1:D:109:VAL:CG1	2.37	0.53
1:C:23:ILE:HD12	1:C:41:VAL:HG21	1.91	0.53
1:C:166:MET:HB3	1:C:172:ILE:HG13	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:114:LYS:HZ3	1:D:130:HIS:HD2	1.58	0.52
1:E:50:ILE:HA	1:E:132:PHE:O	2.09	0.52
1:E:136:TYR:CD1	1:E:136:TYR:C	2.87	0.52
1:D:51:LEU:HB3	1:D:133:ILE:HG22	1.90	0.52
1:E:187:SER:C	1:E:189:LEU:H	2.18	0.52
1:C:120:MET:HE1	1:D:175:GLY:HA2	1.91	0.51
1:B:29:ARG:HD3	1:B:35:ILE:CD1	2.40	0.51
1:A:54:ASN:ND2	1:A:56:LYS:HB3	2.27	0.50
1:A:98:ARG:O	1:A:102:ILE:HG12	2.11	0.50
1:E:99:LYS:NZ	5:E:206:HOH:O	2.44	0.50
1:C:55:THR:HG22	5:C:216:HOH:O	2.11	0.50
1:A:49:THR:HG23	1:A:180:LEU:HD11	1.95	0.49
1:C:137:SER:C	1:C:139:ASN:H	2.21	0.49
1:E:28:THR:HG22	1:E:34:VAL:HG22	1.93	0.49
1:A:182:ASN:O	1:A:186:THR:HG23	2.13	0.48
1:A:32:GLY:HA2	1:A:33:GLU:O	2.13	0.48
1:A:120:MET:HE2	1:A:176:LYS:HB3	1.95	0.48
1:B:111:GLU:O	1:B:111:GLU:HG3	2.12	0.48
1:D:75:ASN:CG	1:D:173:ARG:NH1	2.73	0.47
1:B:127:GLU:CD	2:B:7110:TAR:H3	2.40	0.47
1:A:188:HIS:O	1:A:191:ASP:HB2	2.15	0.47
1:C:53:TYR:O	1:C:135:GLU:HA	2.14	0.47
1:C:152:ASP:OD2	1:C:152:ASP:N	2.48	0.47
1:C:124:GLY:HA3	1:D:44:ARG:NH1	2.30	0.46
1:E:170:GLY:O	1:E:173:ARG:HD2	2.15	0.46
1:D:24:THR:OG1	1:D:38:LYS:HD3	2.15	0.46
1:B:29:ARG:HD3	1:B:35:ILE:HD12	1.98	0.46
1:D:53:TYR:HB2	1:D:190:MET:CE	2.44	0.46
1:D:29:ARG:O	1:D:31:ASP:O	2.33	0.46
1:E:167:ILE:HG12	1:E:178:VAL:HG22	1.97	0.46
1:A:170:GLY:O	1:A:173:ARG:HD3	2.16	0.46
1:C:114:LYS:NZ	1:C:130:HIS:CD2	2.83	0.46
1:B:152:ASP:OD2	1:B:152:ASP:C	2.59	0.45
1:B:153:ILE:HD12	5:E:206:HOH:O	2.16	0.45
1:B:161:SER:O	1:B:165:GLU:HG2	2.17	0.45
1:C:98:ARG:NH2	1:C:111:GLU:HA	2.28	0.45
1:E:57:LYS:HB3	1:E:59:THR:HG23	1.98	0.45
1:A:44:ARG:NH1	2:A:7110:TAR:O4	2.50	0.45
1:C:113:ARG:CG	1:C:113:ARG:NH1	2.71	0.45
1:C:114:LYS:HZ3	1:C:130:HIS:HD2	1.64	0.45
1:A:136:TYR:OH	1:A:157:GLU:OE2	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:188:HIS:C	1:C:190:MET:H	2.25	0.45
1:E:26:ASP:OD2	1:E:36:ARG:HD3	2.17	0.45
1:E:166:MET:HA	1:E:169:THR:OG1	2.17	0.44
1:B:98:ARG:HD3	1:B:112:VAL:HG11	1.99	0.44
1:A:182:ASN:ND2	5:B:201:HOH:O	2.49	0.44
1:C:58:LYS:HA	1:C:190:MET:HE3	1.99	0.44
1:A:173:ARG:HA	1:B:118:LEU:HD22	1.98	0.44
1:E:114:LYS:NZ	1:E:130:HIS:HD2	2.15	0.44
1:B:102:ILE:HG12	1:B:108:GLU:HA	2.00	0.43
1:B:39:ARG:HG2	1:C:90:ASN:O	2.17	0.43
1:B:176:LYS:HG2	5:B:200:HOH:O	2.18	0.43
1:C:31:ASP:O	1:C:33:GLU:N	2.51	0.43
1:C:85:ALA:O	1:C:100:GLU:OE1	2.37	0.43
1:E:127:GLU:OE2	2:E:7110:TAR:H3	2.18	0.42
1:C:117:GLU:HG2	5:C:201:HOH:O	2.15	0.42
1:A:50:ILE:HA	1:A:132:PHE:O	2.20	0.42
1:C:30:LYS:HD2	1:C:30:LYS:H	1.85	0.42
1:C:158:LEU:HD23	1:C:158:LEU:N	2.35	0.42
1:D:183:TYR:CD2	1:D:183:TYR:C	2.97	0.42
1:E:94:GLU:HG3	1:E:112:VAL:HG21	2.01	0.42
1:C:12:ILE:HG21	1:C:15:ASP:HB2	2.00	0.41
1:D:174:ASP:OD1	1:D:176:LYS:HG2	2.21	0.41
1:E:92:GLU:HA	1:E:93:PRO:HD3	1.90	0.41
1:A:53:TYR:O	1:A:135:GLU:HA	2.20	0.41
1:A:54:ASN:ND2	1:A:57:LYS:HG2	2.35	0.41
1:B:98:ARG:HH11	1:B:98:ARG:HB3	1.85	0.41
1:E:187:SER:O	1:E:187:SER:OG	2.37	0.41
1:D:37:HIS:HE1	5:D:206:HOH:O	2.03	0.41
1:D:139:ASN:OD1	1:D:139:ASN:N	2.52	0.41
1:A:118:LEU:HA	1:B:173:ARG:O	2.20	0.41
1:A:28:THR:HG22	1:A:34:VAL:HG22	2.03	0.40
1:B:58:LYS:HE3	1:B:190:MET:O	2.21	0.40
1:C:187:SER:C	1:C:189:LEU:H	2.28	0.40
1:E:53:TYR:HB2	1:E:190:MET:HE3	2.03	0.40
1:A:54:ASN:ND2	1:A:57:LYS:H	2.19	0.40
1:C:16:ASN:HB3	1:D:40:GLU:OE2	2.20	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	171/191 (90%)	158 (92%)	11 (6%)	2 (1%)	10	20
1	B	170/191 (89%)	163 (96%)	4 (2%)	3 (2%)	6	12
1	C	173/191 (91%)	163 (94%)	8 (5%)	2 (1%)	10	20
1	D	176/191 (92%)	166 (94%)	9 (5%)	1 (1%)	21	38
1	E	173/191 (91%)	154 (89%)	16 (9%)	3 (2%)	7	13
All	All	863/955 (90%)	804 (93%)	48 (6%)	11 (1%)	9	18

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	30	LYS
1	A	30	LYS
1	A	32	GLY
1	B	32	GLY
1	E	110	GLY
1	C	32	GLY
1	C	138	ASP
1	D	127	GLU
1	E	188	HIS
1	B	124	GLY
1	E	124	GLY

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	158/168 (94%)	145 (92%)	13 (8%)	10	23
1	B	158/168 (94%)	146 (92%)	12 (8%)	12	26
1	C	159/168 (95%)	147 (92%)	12 (8%)	12	26
1	D	161/168 (96%)	149 (92%)	12 (8%)	12	26
1	E	159/168 (95%)	143 (90%)	16 (10%)	7	15
All	All	795/840 (95%)	730 (92%)	65 (8%)	10	23

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	19	THR
1	A	23	ILE
1	A	39	ARG
1	A	44	ARG
1	A	54	ASN
1	A	63	ILE
1	A	72	VAL
1	A	99	LYS
1	A	108	GLU
1	A	116	PHE
1	A	135	GLU
1	A	169	THR
1	B	5	ILE
1	B	33	GLU
1	B	44	ARG
1	B	68	VAL
1	B	94	GLU
1	B	97	ILE
1	B	98	ARG
1	B	109	VAL
1	B	111	GLU
1	B	116	PHE
1	B	117	GLU
1	B	158	LEU
1	C	4	GLN
1	C	11	LYS
1	C	27	LEU
1	C	31	ASP
1	C	33	GLU
1	C	68	VAL

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Mol	Chain	Res	Type
1	C	84	CYS
1	C	111	GLU
1	C	113	ARG
1	C	138	ASP
1	C	152	ASP
1	C	158	LEU
1	D	11	LYS
1	D	33	GLU
1	D	34	VAL
1	D	56	LYS
1	D	68	VAL
1	D	97	ILE
1	D	108	GLU
1	D	112	VAL
1	D	116	PHE
1	D	151	GLU
1	D	165	GLU
1	D	191	ASP
1	E	5	ILE
1	E	6	THR
1	E	11	LYS
1	E	22	ASN
1	E	31	ASP
1	E	33	GLU
1	E	39	ARG
1	E	44	ARG
1	E	98	ARG
1	E	99	LYS
1	E	114	LYS
1	E	152	ASP
1	E	162	GLN
1	E	164	LEU
1	E	165	GLU
1	E	173	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	HIS
1	A	37	HIS
1	A	54	ASN
1	A	79	GLN

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Mol	Chain	Res	Type
1	A	90	ASN
1	B	21	HIS
1	B	182	ASN
1	B	185	GLN
1	C	54	ASN
1	C	130	HIS
1	C	185	GLN
1	D	37	HIS
1	D	130	HIS
1	D	182	ASN
1	E	130	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 10 are monoatomic - leaving 6 for Mogul analysis.

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	TAR	A	7112	-	9,9,9	1.09	0	12,12,12	1.01	1 (8%)
2	TAR	B	7110	-	9,9,9	1.10	0	12,12,12	1.54	3 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	TAR	A	7110	3	9,9,9	1.28	0	12,12,12	1.15	1 (8%)
2	TAR	C	7110	-	9,9,9	1.09	0	12,12,12	1.49	3 (25%)
2	TAR	E	7110	3	9,9,9	1.08	0	12,12,12	1.45	4 (33%)
2	TAR	D	7110	3	9,9,9	1.25	0	12,12,12	1.27	2 (16%)

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	TAR	A	7112	-	-	6/12/12/12	-
2	TAR	B	7110	-	-	10/12/12/12	-
2	TAR	A	7110	3	-	4/12/12/12	-
2	TAR	C	7110	-	-	6/12/12/12	-
2	TAR	E	7110	3	-	8/12/12/12	-
2	TAR	D	7110	3	-	11/12/12/12	-

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	7110	TAR	O41-C4-C3	2.69	120.78	113.31
2	B	7110	TAR	O11-C1-C2	2.61	120.57	113.31
2	D	7110	TAR	O11-C1-C2	2.59	120.50	113.31
2	B	7110	TAR	O1-C1-C2	-2.41	115.21	121.62
2	C	7110	TAR	O11-C1-C2	2.31	119.73	113.31
2	B	7110	TAR	C2-C3-C4	2.30	114.92	109.82
2	E	7110	TAR	O11-C1-C2	2.30	119.69	113.31
2	E	7110	TAR	C3-C2-C1	2.22	114.73	109.82
2	D	7110	TAR	O1-C1-C2	-2.17	115.84	121.62
2	A	7110	TAR	C3-C2-C1	-2.13	105.10	109.82
2	E	7110	TAR	C2-C3-C4	2.11	114.50	109.82
2	E	7110	TAR	O1-C1-C2	-2.10	116.02	121.62
2	A	7112	TAR	O41-C4-C3	2.08	119.11	113.31
2	C	7110	TAR	C2-C3-C4	2.05	114.36	109.82

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	7112	TAR	C1-C2-C3-O3
2	A	7112	TAR	C1-C2-C3-C4
2	A	7112	TAR	O2-C2-C3-O3
2	A	7112	TAR	O2-C2-C3-C4
2	B	7110	TAR	C1-C2-C3-C4
2	B	7110	TAR	O3-C3-C4-O4
2	B	7110	TAR	O3-C3-C4-O41
2	C	7110	TAR	O1-C1-C2-O2
2	C	7110	TAR	O11-C1-C2-O2
2	E	7110	TAR	O1-C1-C2-O2
2	E	7110	TAR	O11-C1-C2-O2
2	E	7110	TAR	C1-C2-C3-C4
2	B	7110	TAR	O2-C2-C3-O3
2	E	7110	TAR	O2-C2-C3-O3
2	A	7110	TAR	O3-C3-C4-O4
2	A	7110	TAR	O3-C3-C4-O41
2	B	7110	TAR	O1-C1-C2-O2
2	B	7110	TAR	O11-C1-C2-O2
2	C	7110	TAR	O3-C3-C4-O4
2	C	7110	TAR	O3-C3-C4-O41
2	E	7110	TAR	O3-C3-C4-O4
2	E	7110	TAR	O3-C3-C4-O41
2	C	7110	TAR	O1-C1-C2-C3
2	C	7110	TAR	O11-C1-C2-C3
2	B	7110	TAR	O2-C2-C3-C4
2	E	7110	TAR	C1-C2-C3-O3
2	A	7110	TAR	O1-C1-C2-O2
2	A	7110	TAR	O11-C1-C2-O2
2	B	7110	TAR	C1-C2-C3-O3
2	E	7110	TAR	O2-C2-C3-C4
2	B	7110	TAR	O11-C1-C2-C3
2	D	7110	TAR	O1-C1-C2-O2
2	D	7110	TAR	O2-C2-C3-C4
2	D	7110	TAR	C1-C2-C3-O3
2	B	7110	TAR	O1-C1-C2-C3
2	D	7110	TAR	O11-C1-C2-O2
2	A	7112	TAR	O1-C1-C2-C3
2	D	7110	TAR	C1-C2-C3-C4
2	A	7112	TAR	O11-C1-C2-C3
2	D	7110	TAR	O1-C1-C2-C3
2	D	7110	TAR	O11-C1-C2-C3
2	D	7110	TAR	C2-C3-C4-O4
2	D	7110	TAR	C2-C3-C4-O41

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Mol	Chain	Res	Type	Atoms
2	D	7110	TAR	O2-C2-C3-O3
2	D	7110	TAR	O3-C3-C4-O41

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	7110	TAR	4	0
2	A	7110	TAR	2	0
2	E	7110	TAR	1	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	175/191 (91%)	-0.14	3 (1%) 69 65	32, 48, 75, 87	1 (0%)
1	B	176/191 (92%)	-0.26	3 (1%) 69 65	30, 44, 71, 83	0
1	C	177/191 (92%)	-0.16	0 100 100	34, 50, 74, 87	0
1	D	180/191 (94%)	-0.05	2 (1%) 78 75	37, 54, 83, 109	0
1	E	177/191 (92%)	0.17	6 (3%) 48 43	29, 58, 105, 121	0
All	All	885/955 (92%)	-0.09	14 (1%) 70 67	29, 50, 84, 121	1 (0%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	2	THR	3.0
1	A	137	SER	2.9
1	D	142	ALA	2.7
1	E	31	ASP	2.5
1	A	32	GLY	2.5
1	D	29	ARG	2.5
1	B	152	ASP	2.4
1	E	109	VAL	2.4
1	B	111	GLU	2.4
1	B	138	ASP	2.3
1	A	3[A]	GLN	2.3
1	E	32	GLY	2.3
1	E	5	ILE	2.3
1	E	56	LYS	2.2

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($\text{\AA}^2$)	Q<0.9
2	TAR	C	7110	10/10	0.61	0.14	92,93,93,93	0
2	TAR	A	7112	10/10	0.70	0.11	90,92,92,92	0
2	TAR	A	7110	10/10	0.75	0.14	49,53,55,57	0
2	TAR	B	7110	10/10	0.82	0.11	57,59,62,62	0
3	NA	A	7113	1/1	0.83	0.11	61,61,61,61	0
3	NA	D	7112	1/1	0.84	0.12	59,59,59,59	0
2	TAR	D	7110	10/10	0.85	0.10	69,73,74,74	0
2	TAR	E	7110	10/10	0.85	0.10	53,55,56,57	0
4	CL	E	7112	1/1	0.85	0.09	77,77,77,77	0
3	NA	D	7111	1/1	0.86	0.10	63,63,63,63	0
3	NA	A	7114	1/1	0.88	0.22	58,58,58,58	0
4	CL	D	7113	1/1	0.90	0.16	71,71,71,71	1
4	CL	D	7114	1/1	0.92	0.05	78,78,78,78	0
3	NA	B	7111	1/1	0.92	0.17	48,48,48,48	0
3	NA	E	7111	1/1	0.94	0.07	43,43,43,43	0
4	CL	C	192	1/1	0.96	0.15	69,69,69,69	0

6.5 Other polymers [i](#)

There are no such residues in this entry.