Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 07:40 PM UTC

PDB ID	:	5YKB / pdb_00005ykb
Title	:	The N253F mutant structure of trehalose synthase from Deinococcus radiodurans reveals an open active-site conformation
Authors	:	Chow, S.Y.; Hsieh, Y.C.; Liaw, S.H.
Deposited on	:	2017-10-13
Resolution	:	2.76 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:

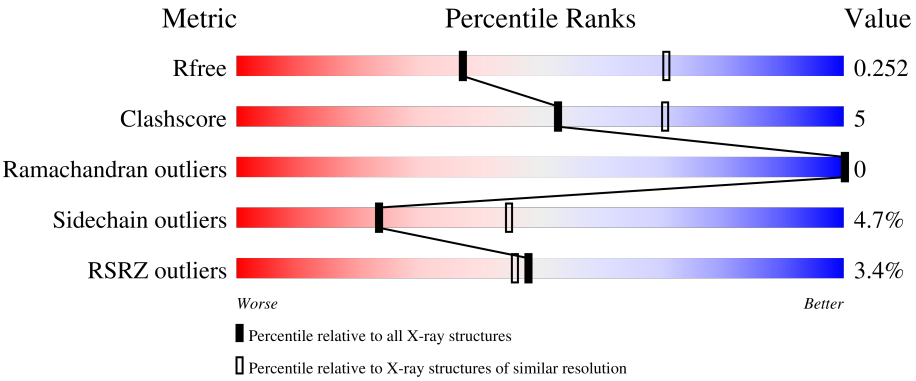
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.76 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	571	2% 81% 11% 7%
1	B	571	4% 80% 11% • 9%
1	C	571	3% 79% 12% • 7%
1	D	571	4% 80% 10% • 8%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 17196 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 Trehalose synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	529	Total	C	N	O	S	0	0	0
			4256	2730	727	783	16			
1	B	522	Total	C	N	O	S	0	0	0
			4214	2704	720	774	16			
1	C	530	Total	C	N	O	S	0	0	0
			4265	2735	728	786	16			
1	D	523	Total	C	N	O	S	0	0	0
			4216	2707	721	772	16			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	expression tag	UNP I3NX86
A	0	VAL	-	expression tag	UNP I3NX86
A	1	PRO	-	expression tag	UNP I3NX86
A	97	TRP	ARG	engineered mutation	UNP I3NX86
A	253	PHE	ASN	engineered mutation	UNP I3NX86
A	313	ILE	THR	engineered mutation	UNP I3NX86
A	380	VAL	ILE	engineered mutation	UNP I3NX86
A	553	SER	-	expression tag	UNP I3NX86
A	554	ARG	-	expression tag	UNP I3NX86
A	555	VAL	-	expression tag	UNP I3NX86
A	556	ASP	-	expression tag	UNP I3NX86
A	557	LYS	-	expression tag	UNP I3NX86
A	558	LEU	-	expression tag	UNP I3NX86
A	559	ALA	-	expression tag	UNP I3NX86
A	560	ALA	-	expression tag	UNP I3NX86
A	561	ALA	-	expression tag	UNP I3NX86
A	562	LEU	-	expression tag	UNP I3NX86
A	563	GLU	-	expression tag	UNP I3NX86
A	564	HIS	-	expression tag	UNP I3NX86
A	565	HIS	-	expression tag	UNP I3NX86
A	566	HIS	-	expression tag	UNP I3NX86

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	567	HIS	-	expression tag	UNP I3NX86
A	568	HIS	-	expression tag	UNP I3NX86
A	569	HIS	-	expression tag	UNP I3NX86
B	-1	MET	-	expression tag	UNP I3NX86
B	0	VAL	-	expression tag	UNP I3NX86
B	1	PRO	-	expression tag	UNP I3NX86
B	97	TRP	ARG	engineered mutation	UNP I3NX86
B	253	PHE	ASN	engineered mutation	UNP I3NX86
B	313	ILE	THR	engineered mutation	UNP I3NX86
B	380	VAL	ILE	engineered mutation	UNP I3NX86
B	553	SER	-	expression tag	UNP I3NX86
B	554	ARG	-	expression tag	UNP I3NX86
B	555	VAL	-	expression tag	UNP I3NX86
B	556	ASP	-	expression tag	UNP I3NX86
B	557	LYS	-	expression tag	UNP I3NX86
B	558	LEU	-	expression tag	UNP I3NX86
B	559	ALA	-	expression tag	UNP I3NX86
B	560	ALA	-	expression tag	UNP I3NX86
B	561	ALA	-	expression tag	UNP I3NX86
B	562	LEU	-	expression tag	UNP I3NX86
B	563	GLU	-	expression tag	UNP I3NX86
B	564	HIS	-	expression tag	UNP I3NX86
B	565	HIS	-	expression tag	UNP I3NX86
B	566	HIS	-	expression tag	UNP I3NX86
B	567	HIS	-	expression tag	UNP I3NX86
B	568	HIS	-	expression tag	UNP I3NX86
B	569	HIS	-	expression tag	UNP I3NX86
C	-1	MET	-	expression tag	UNP I3NX86
C	0	VAL	-	expression tag	UNP I3NX86
C	1	PRO	-	expression tag	UNP I3NX86
C	97	TRP	ARG	engineered mutation	UNP I3NX86
C	253	PHE	ASN	engineered mutation	UNP I3NX86
C	313	ILE	THR	engineered mutation	UNP I3NX86
C	380	VAL	ILE	engineered mutation	UNP I3NX86
C	553	SER	-	expression tag	UNP I3NX86
C	554	ARG	-	expression tag	UNP I3NX86
C	555	VAL	-	expression tag	UNP I3NX86
C	556	ASP	-	expression tag	UNP I3NX86
C	557	LYS	-	expression tag	UNP I3NX86
C	558	LEU	-	expression tag	UNP I3NX86
C	559	ALA	-	expression tag	UNP I3NX86
C	560	ALA	-	expression tag	UNP I3NX86

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	561	ALA	-	expression tag	UNP I3NX86
C	562	LEU	-	expression tag	UNP I3NX86
C	563	GLU	-	expression tag	UNP I3NX86
C	564	HIS	-	expression tag	UNP I3NX86
C	565	HIS	-	expression tag	UNP I3NX86
C	566	HIS	-	expression tag	UNP I3NX86
C	567	HIS	-	expression tag	UNP I3NX86
C	568	HIS	-	expression tag	UNP I3NX86
C	569	HIS	-	expression tag	UNP I3NX86
D	-1	MET	-	expression tag	UNP I3NX86
D	0	VAL	-	expression tag	UNP I3NX86
D	1	PRO	-	expression tag	UNP I3NX86
D	97	TRP	ARG	engineered mutation	UNP I3NX86
D	253	PHE	ASN	engineered mutation	UNP I3NX86
D	313	ILE	THR	engineered mutation	UNP I3NX86
D	380	VAL	ILE	engineered mutation	UNP I3NX86
D	553	SER	-	expression tag	UNP I3NX86
D	554	ARG	-	expression tag	UNP I3NX86
D	555	VAL	-	expression tag	UNP I3NX86
D	556	ASP	-	expression tag	UNP I3NX86
D	557	LYS	-	expression tag	UNP I3NX86
D	558	LEU	-	expression tag	UNP I3NX86
D	559	ALA	-	expression tag	UNP I3NX86
D	560	ALA	-	expression tag	UNP I3NX86
D	561	ALA	-	expression tag	UNP I3NX86
D	562	LEU	-	expression tag	UNP I3NX86
D	563	GLU	-	expression tag	UNP I3NX86
D	564	HIS	-	expression tag	UNP I3NX86
D	565	HIS	-	expression tag	UNP I3NX86
D	566	HIS	-	expression tag	UNP I3NX86
D	567	HIS	-	expression tag	UNP I3NX86
D	568	HIS	-	expression tag	UNP I3NX86
D	569	HIS	-	expression tag	UNP I3NX86

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Ca 1 1	0	0
2	B	1	Total Ca 1 1	0	0
2	C	1	Total Ca 1 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total Ca 1 1	0	0

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0

- Molecule 4 is water.

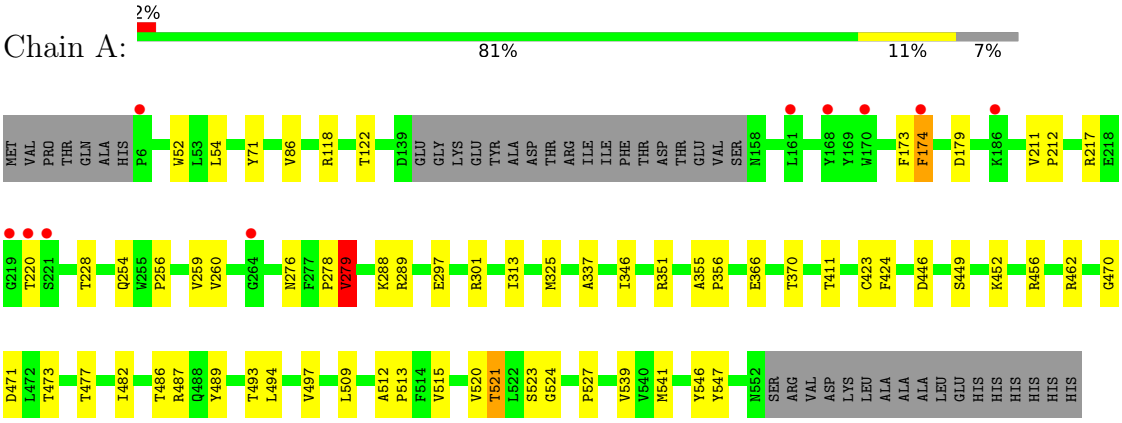
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	65	Total O 65 65	0	0
4	B	60	Total O 60 60	0	0
4	C	58	Total O 58 58	0	0
4	D	54	Total O 54 54	0	0

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.

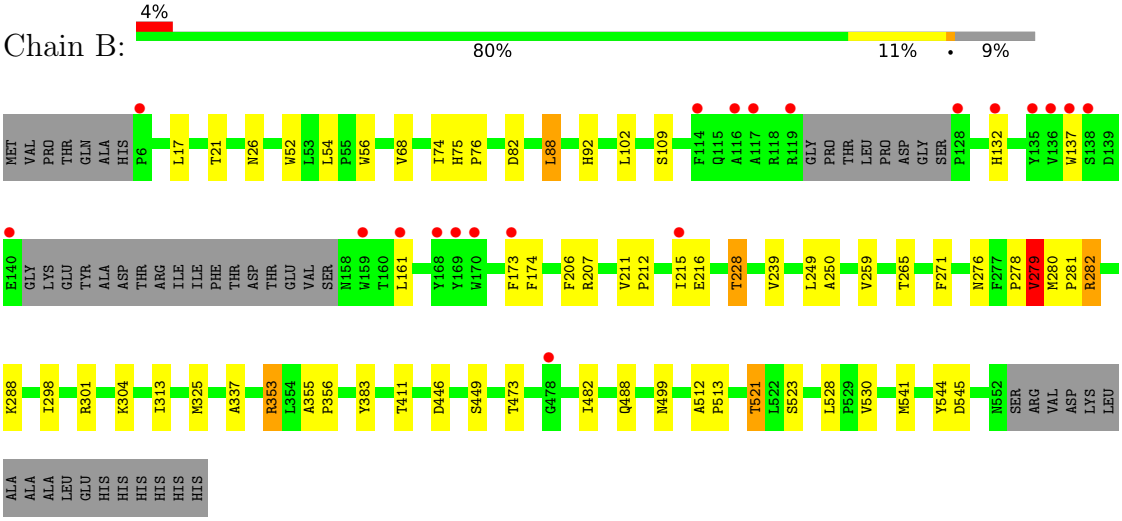
• Molecule 1: Trehalose synthase

Chain A:



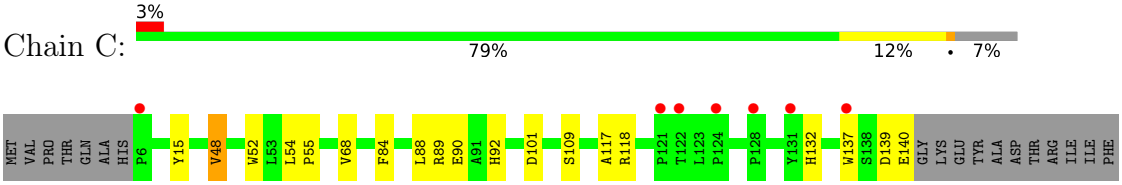
• Molecule 1: Trehalose synthase

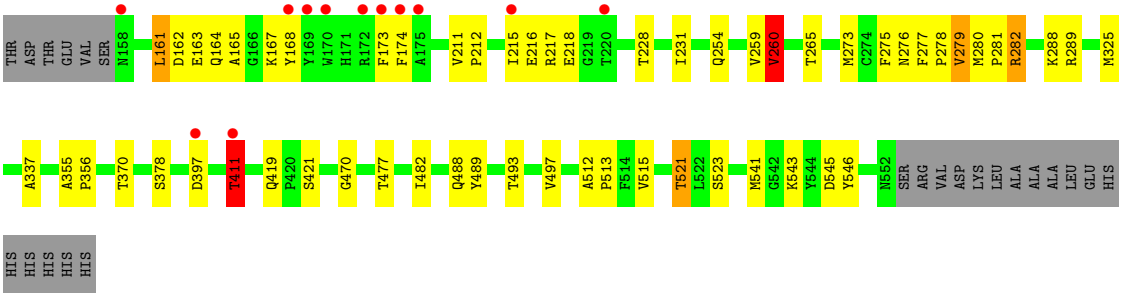
Chain B:



• Molecule 1: Trehalose synthase

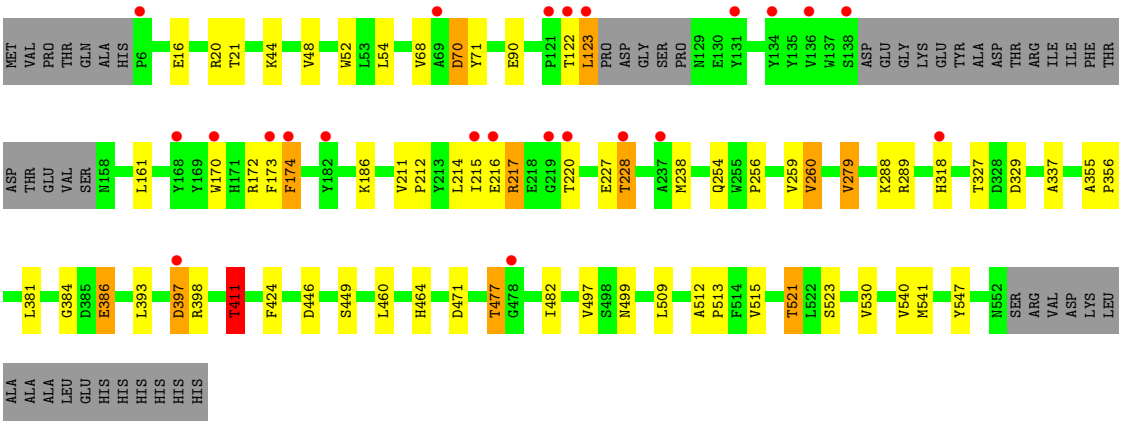
Chain C:





• Molecule 1: Trehalose synthase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	100.40Å 132.42Å 196.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.76 30.00 – 2.76	Depositor EDS
% Data completeness (in resolution range)	96.7 (30.00-2.76) 96.7 (30.00-2.76)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.21 (at 2.76Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.192 , 0.251 0.199 , 0.252	Depositor DCC
R_{free} test set	3231 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å^2)	47.8	Xtriage
Anisotropy	0.148	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 57.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	17196	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% 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

Bond lengths and bond angles in the following residue types are not validated in this section: CA, MG

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	0.65	0/4387	0.85	5/5977 (0.1%)
1	B	0.68	0/4342	0.85	4/5911 (0.1%)
1	C	0.68	0/4396	0.87	9/5989 (0.2%)
1	D	0.69	0/4344	0.89	13/5915 (0.2%)
All	All	0.67	0/17469	0.86	31/23792 (0.1%)

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	173	PHE	N-CA-C	13.12	130.38	112.93
1	D	173	PHE	N-CA-C	12.58	129.66	112.93
1	C	174	PHE	N-CA-C	-10.28	93.29	109.23
1	A	173	PHE	N-CA-C	9.94	126.15	112.93
1	B	173	PHE	N-CA-C	9.24	124.96	112.68
1	A	523	SER	N-CA-C	9.21	121.25	111.03
1	D	279	VAL	CB-CA-C	-8.59	100.54	112.14
1	D	174	PHE	N-CA-C	-8.21	96.50	109.23
1	A	174	PHE	N-CA-C	-7.67	97.42	109.07
1	D	214	LEU	N-CA-C	7.59	119.33	111.14
1	B	174	PHE	N-CA-C	-7.57	97.56	109.07
1	C	279	VAL	CB-CA-C	-7.57	101.78	112.22
1	B	279	VAL	CB-CA-C	-7.26	102.20	112.22
1	A	279	VAL	CB-CA-C	-7.20	102.42	112.14
1	B	26	ASN	N-CA-C	-7.19	99.09	109.31
1	D	477	THR	N-CA-C	-6.46	100.12	110.14
1	D	464	HIS	CA-C-N	6.24	126.14	119.28
1	D	464	HIS	C-N-CA	6.24	126.14	119.28
1	C	260	VAL	CB-CA-C	-6.21	103.91	112.04
1	D	70	ASP	N-CA-C	-5.98	98.06	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	71	TYR	N-CA-C	-5.78	106.21	113.72
1	C	411	THR	CA-C-N	-5.45	115.02	122.87
1	C	411	THR	C-N-CA	-5.45	115.02	122.87
1	C	260	VAL	N-CA-CB	5.33	117.13	110.47
1	D	397	ASP	N-CA-C	5.26	117.60	111.02
1	C	173	PHE	CB-CA-C	-5.24	101.86	110.08
1	A	71	TYR	N-CA-C	-5.18	107.13	113.50
1	D	173	PHE	CB-CA-C	-5.17	101.96	110.08
1	D	411	THR	CA-C-N	-5.13	114.11	123.34
1	D	411	THR	C-N-CA	-5.13	114.11	123.34
1	C	139	ASP	N-CA-C	-5.04	107.68	113.88

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4256	0	4063	34	0
1	B	4214	0	4022	31	0
1	C	4265	0	4069	51	0
1	D	4216	0	4032	56	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	65	0	0	1	0
4	B	60	0	0	2	0
4	C	58	0	0	1	0
4	D	54	0	0	1	0
All	All	17196	0	16186	167	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 5.

All (167) 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:170:TRP:CH2	1:D:216:GLU:HG2	1.52	1.42
1:C:161:LEU:HD23	1:C:168:TYR:CE1	1.72	1.24
1:D:170:TRP:CZ3	1:D:216:GLU:HG2	1.73	1.21
1:D:170:TRP:CH2	1:D:216:GLU:CG	2.39	1.05
1:B:353:ARG:NH2	1:B:383:TYR:O	1.92	1.02
1:C:161:LEU:CD2	1:C:168:TYR:CZ	2.43	1.00
1:C:161:LEU:HD23	1:C:168:TYR:CZ	1.96	1.00
1:C:118:ARG:O	1:C:165:ALA:HB2	1.60	0.98
1:C:161:LEU:CD2	1:C:168:TYR:CE1	2.52	0.90
1:D:170:TRP:HH2	1:D:216:GLU:HG2	1.28	0.87
1:C:477:THR:HG21	1:C:482:ILE:HB	1.58	0.86
1:D:170:TRP:HH2	1:D:216:GLU:CG	1.84	0.82
1:B:279:VAL:HG21	1:B:313:ILE:HD11	1.62	0.82
1:C:411:THR:HG21	1:D:90:GLU:OE2	1.82	0.80
1:D:170:TRP:CZ3	1:D:216:GLU:CG	2.60	0.78
4:B:760:HOH:O	1:C:543:LYS:HE2	1.86	0.74
1:B:482:ILE:HG23	1:B:541:MET:HE1	1.72	0.72
1:D:288:LYS:HG2	1:D:337:ALA:HB1	1.72	0.71
1:A:482:ILE:HG23	1:A:541:MET:HE1	1.73	0.71
1:D:216:GLU:OE2	2:D:600:CA:CA	1.69	0.70
1:C:161:LEU:HD21	1:C:168:TYR:CZ	2.26	0.70
1:C:254:GLN:HB2	1:C:259:VAL:HG13	1.74	0.69
1:D:254:GLN:HB2	1:D:259:VAL:HG13	1.75	0.69
1:C:482:ILE:HG23	1:C:541:MET:HE1	1.77	0.67
1:B:282:ARG:NH2	1:B:325:MET:O	2.28	0.66
1:D:216:GLU:N	1:D:216:GLU:OE1	2.28	0.66
1:D:215:ILE:HB	1:D:228:THR:HG22	1.78	0.63
1:C:288:LYS:HG2	1:C:337:ALA:HB1	1.80	0.63
1:A:279:VAL:HG21	1:A:313:ILE:HD11	1.81	0.63
1:D:482:ILE:HG23	1:D:541:MET:HE1	1.81	0.63
1:C:521:THR:CG2	1:C:523:SER:O	2.48	0.61
1:D:355:ALA:HB3	1:D:356:PRO:HD3	1.82	0.61
1:D:397:ASP:OD1	1:D:398:ARG:NH1	2.33	0.61
1:A:217:ARG:HB2	1:A:220:THR:HG21	1.83	0.60
1:D:215:ILE:CD1	1:D:227:GLU:HB3	2.32	0.60
1:C:482:ILE:HG23	1:C:541:MET:CE	2.31	0.59
1:A:276:ASN:OD1	1:A:278:PRO:HD2	2.02	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:482:ILE:HG23	1:A:541:MET:CE	2.32	0.59
1:C:282:ARG:NH2	1:C:325:MET:O	2.36	0.59
1:C:289:ARG:NH2	4:C:701:HOH:O	2.37	0.57
1:C:411:THR:CG2	1:D:90:GLU:OE2	2.54	0.56
1:A:470:GLY:HA2	1:A:489:TYR:HB2	1.88	0.55
1:D:327:THR:HG22	1:D:329:ASP:H	1.71	0.55
1:C:278:PRO:HD3	1:C:325:MET:HE1	1.88	0.55
1:D:521:THR:CG2	1:D:523:SER:O	2.55	0.55
1:B:355:ALA:HB3	1:B:356:PRO:HD3	1.89	0.55
1:A:462:ARG:HD2	4:A:746:HOH:O	2.07	0.54
1:B:545:ASP:OD2	1:C:545:ASP:OD2	2.26	0.53
1:C:118:ARG:HG3	1:C:162:ASP:OD2	2.08	0.53
1:D:123:LEU:H	1:D:123:LEU:HD13	1.73	0.53
1:A:355:ALA:HB3	1:A:356:PRO:HD3	1.89	0.53
1:D:217:ARG:HB2	1:D:220:THR:HG21	1.90	0.53
1:A:471:ASP:O	1:A:487:ARG:HA	2.09	0.53
1:C:118:ARG:CG	1:C:162:ASP:OD2	2.57	0.52
1:C:90:GLU:OE2	1:D:411:THR:HG21	2.10	0.52
1:B:88:LEU:C	1:B:88:LEU:HD12	2.35	0.52
1:C:118:ARG:NH1	1:C:162:ASP:OD1	2.43	0.52
1:D:327:THR:HG22	1:D:329:ASP:N	2.24	0.52
1:B:353:ARG:HG2	4:B:706:HOH:O	2.09	0.51
1:D:477:THR:HG22	1:D:509:LEU:CD2	2.41	0.51
1:A:254:GLN:HB2	1:A:259:VAL:HG13	1.92	0.51
1:C:488:GLN:HG3	1:C:493:THR:HG23	1.93	0.50
1:D:170:TRP:HZ3	1:D:216:GLU:CD	2.19	0.50
1:D:68:VAL:HG13	1:D:70:ASP:O	2.11	0.50
1:D:482:ILE:HD13	1:D:541:MET:HE2	1.93	0.50
1:C:482:ILE:HG12	1:C:541:MET:CE	2.42	0.50
1:A:346:ILE:HB	1:A:351:ARG:HD3	1.94	0.49
1:A:520:VAL:HG12	1:A:527:PRO:HA	1.94	0.49
1:B:482:ILE:HG23	1:B:541:MET:CE	2.41	0.49
1:C:276:ASN:OD1	1:C:278:PRO:HD2	2.12	0.49
1:C:355:ALA:HB3	1:C:356:PRO:HD3	1.95	0.49
1:C:280:MET:HB3	1:C:281:PRO:HD3	1.95	0.49
1:D:68:VAL:CG1	1:D:70:ASP:O	2.61	0.48
1:C:482:ILE:HG12	1:C:541:MET:HE3	1.95	0.48
1:C:118:ARG:NH2	1:C:164:GLN:HG3	2.29	0.48
1:D:170:TRP:HH2	1:D:216:GLU:HG3	1.71	0.48
1:D:215:ILE:HD13	1:D:227:GLU:HB3	1.96	0.48
1:A:512:ALA:O	1:A:515:VAL:HG23	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:215:ILE:HG22	1:D:216:GLU:N	2.29	0.48
1:A:52:TRP:CD1	1:A:52:TRP:C	2.92	0.47
1:A:256:PRO:HA	1:A:259:VAL:HG22	1.96	0.47
1:A:370:THR:HG21	1:A:546:TYR:CD2	2.48	0.47
1:B:276:ASN:OD1	1:B:278:PRO:HD2	2.13	0.47
1:D:20:ARG:HD2	1:D:424:PHE:CE2	2.49	0.47
1:B:211:VAL:N	1:B:212:PRO:CD	2.77	0.47
1:C:275:PHE:HB2	1:C:277:PHE:CE2	2.50	0.47
1:A:541:MET:HG2	1:A:547:TYR:CE2	2.50	0.47
1:D:256:PRO:O	1:D:260:VAL:HG23	2.15	0.47
1:B:512:ALA:HB3	1:B:513:PRO:HD3	1.96	0.47
1:D:482:ILE:HG12	1:D:541:MET:CE	2.45	0.47
1:C:482:ILE:HD13	1:C:541:MET:HE2	1.97	0.47
1:D:216:GLU:N	1:D:216:GLU:CD	2.73	0.47
1:D:397:ASP:O	1:D:397:ASP:CG	2.58	0.47
1:A:477:THR:HG22	1:A:509:LEU:CD2	2.45	0.47
1:C:117:ALA:HB1	1:C:137:TRP:HH2	1.79	0.47
1:B:279:VAL:HG21	1:B:313:ILE:CD1	2.39	0.46
1:B:88:LEU:HD13	1:B:92:HIS:CE1	2.51	0.46
1:C:215:ILE:HD11	1:C:231:ILE:HD11	1.98	0.46
1:A:211:VAL:N	1:A:212:PRO:CD	2.78	0.46
1:D:512:ALA:HB3	1:D:513:PRO:HD3	1.97	0.46
1:C:211:VAL:N	1:C:212:PRO:CD	2.79	0.46
1:A:512:ALA:HB3	1:A:513:PRO:HD3	1.98	0.46
1:A:288:LYS:HG2	1:A:337:ALA:HB1	1.98	0.46
1:A:423:CYS:O	1:A:424:PHE:C	2.58	0.46
1:D:499:ASN:HB2	1:D:541:MET:HE3	1.97	0.46
1:B:282:ARG:HD2	1:B:298:ILE:HG13	1.98	0.45
1:B:301:ARG:O	1:B:301:ARG:HG3	2.16	0.45
1:D:44:LYS:NZ	4:D:702:HOH:O	2.41	0.45
1:B:278:PRO:HD3	1:B:325:MET:HE1	1.97	0.45
1:C:15:TYR:HB2	1:C:48:VAL:HG21	1.97	0.45
1:B:17:LEU:C	1:B:17:LEU:HD12	2.42	0.45
1:C:273:MET:HE1	1:C:378:SER:HB2	1.99	0.45
1:A:539:VAL:HG12	1:D:540:VAL:HG21	1.99	0.45
1:D:52:TRP:C	1:D:52:TRP:CD1	2.95	0.45
1:D:217:ARG:CB	1:D:220:THR:HG21	2.47	0.45
1:D:541:MET:HG2	1:D:547:TYR:CE2	2.52	0.45
1:C:370:THR:HG21	1:C:546:TYR:CD2	2.52	0.44
1:C:512:ALA:O	1:C:515:VAL:HG23	2.18	0.44
1:D:211:VAL:N	1:D:212:PRO:CD	2.81	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:215:ILE:HD12	1:D:227:GLU:C	2.43	0.44
1:D:215:ILE:C	1:D:216:GLU:CD	2.86	0.43
1:C:470:GLY:HA2	1:C:489:TYR:HB2	2.00	0.43
1:C:89:ARG:NH1	1:C:90:GLU:OE2	2.51	0.43
1:A:297:GLU:O	1:A:301:ARG:HG2	2.18	0.43
1:D:482:ILE:HG23	1:D:541:MET:CE	2.46	0.43
1:A:521:THR:CG2	1:A:524:GLY:H	2.31	0.43
1:A:254:GLN:HB2	1:A:259:VAL:CG1	2.49	0.43
1:C:162:ASP:C	1:C:164:GLN:H	2.25	0.43
1:D:512:ALA:O	1:D:515:VAL:HG23	2.18	0.43
1:A:452:LYS:O	1:A:456:ARG:HG2	2.18	0.43
1:A:278:PRO:HD3	1:A:325:MET:HE1	1.99	0.43
1:A:366:GLU:O	1:A:370:THR:HG23	2.18	0.43
1:C:88:LEU:HD22	1:C:92:HIS:CE1	2.54	0.43
1:B:56:TRP:CD1	1:B:56:TRP:C	2.97	0.42
1:B:132:HIS:O	1:B:137:TRP:CZ3	2.72	0.42
1:B:250:ALA:HB2	1:B:271:PHE:CG	2.54	0.42
1:B:280:MET:HB3	1:B:281:PRO:HD3	2.00	0.42
1:A:486:THR:HA	1:A:494:LEU:O	2.19	0.42
1:B:102:LEU:HB2	1:B:206:PHE:CD1	2.54	0.42
1:C:132:HIS:O	1:C:137:TRP:HZ3	2.02	0.42
1:B:521:THR:CG2	1:B:523:SER:O	2.67	0.42
1:C:161:LEU:CD2	1:C:168:TYR:CE2	3.00	0.42
1:B:499:ASN:O	1:B:544:TYR:HA	2.19	0.42
1:D:384:GLY:N	1:D:386:GLU:OE2	2.51	0.42
1:D:477:THR:HG22	1:D:509:LEU:HD23	2.02	0.42
1:D:446:ASP:HB3	1:D:449:SER:HB3	2.02	0.42
1:B:288:LYS:HG2	1:B:337:ALA:HB1	2.02	0.42
1:B:446:ASP:HB3	1:B:449:SER:HB3	2.01	0.42
1:A:446:ASP:HB3	1:A:449:SER:HB3	2.01	0.42
1:C:55:PRO:HD3	1:C:101:ASP:OD2	2.20	0.41
1:B:215:ILE:HB	1:B:228:THR:HG22	2.02	0.41
1:C:512:ALA:HB3	1:C:513:PRO:HD3	2.02	0.41
1:A:370:THR:HG21	1:A:546:TYR:CE2	2.54	0.41
1:C:259:VAL:O	1:C:260:VAL:C	2.62	0.41
1:D:215:ILE:CD1	1:D:227:GLU:CB	2.98	0.41
1:C:52:TRP:CD1	1:C:52:TRP:C	2.98	0.41
1:D:238:MET:C	1:D:238:MET:SD	3.04	0.41
1:A:482:ILE:HG12	1:A:541:MET:HE3	2.02	0.41
1:D:16:GLU:OE2	1:D:318:HIS:ND1	2.50	0.41
1:C:162:ASP:C	1:C:164:GLN:N	2.79	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:170:TRP:CZ3	1:D:216:GLU:CD	2.96	0.41
1:B:52:TRP:CZ2	1:B:207:ARG:HD3	2.56	0.41
1:B:75:HIS:CG	1:B:76:PRO:HD2	2.56	0.41
1:C:84:PHE:CE1	1:C:88:LEU:HD12	2.56	0.41
1:B:52:TRP:CD1	1:B:52:TRP:C	2.99	0.40
1:A:278:PRO:CD	1:A:325:MET:HE1	2.50	0.40
1:D:471:ASP:OD1	1:D:471:ASP:C	2.64	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	525/571 (92%)	500 (95%)	25 (5%)	0	100	100
1	B	516/571 (90%)	498 (96%)	18 (4%)	0	100	100
1	C	526/571 (92%)	505 (96%)	21 (4%)	0	100	100
1	D	517/571 (90%)	499 (96%)	18 (4%)	0	100	100
All	All	2084/2284 (91%)	2002 (96%)	82 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	448/484 (93%)	433 (97%)	15 (3%)	33	57
1	B	443/484 (92%)	419 (95%)	24 (5%)	20	38
1	C	449/484 (93%)	427 (95%)	22 (5%)	22	43
1	D	443/484 (92%)	421 (95%)	22 (5%)	22	42
All	All	1783/1936 (92%)	1700 (95%)	83 (5%)	23	45

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	LEU
1	A	86	VAL
1	A	118	ARG
1	A	122	THR
1	A	174	PHE
1	A	179	ASP
1	A	228	THR
1	A	260	VAL
1	A	279	VAL
1	A	289	ARG
1	A	411	THR
1	A	473	THR
1	A	493	THR
1	A	497	VAL
1	A	521	THR
1	B	21	THR
1	B	54	LEU
1	B	68	VAL
1	B	74	ILE
1	B	82	ASP
1	B	88	LEU
1	B	109	SER
1	B	161	LEU
1	B	216	GLU
1	B	228	THR
1	B	239	VAL
1	B	249	LEU
1	B	259	VAL
1	B	265	THR
1	B	279	VAL
1	B	282	ARG
1	B	304	LYS
1	B	353	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	411	THR
1	B	473	THR
1	B	488	GLN
1	B	521	THR
1	B	528	LEU
1	B	530	VAL
1	C	48	VAL
1	C	54	LEU
1	C	68	VAL
1	C	109	SER
1	C	140	GLU
1	C	161	LEU
1	C	163	GLU
1	C	167	LYS
1	C	216	GLU
1	C	217	ARG
1	C	218	GLU
1	C	228	THR
1	C	260	VAL
1	C	265	THR
1	C	279	VAL
1	C	282	ARG
1	C	397	ASP
1	C	411	THR
1	C	419	GLN
1	C	421	SER
1	C	497	VAL
1	C	521	THR
1	D	21	THR
1	D	48	VAL
1	D	54	LEU
1	D	122	THR
1	D	123	LEU
1	D	161	LEU
1	D	172	ARG
1	D	174	PHE
1	D	186	LYS
1	D	217	ARG
1	D	228	THR
1	D	260	VAL
1	D	279	VAL
1	D	289	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	381	LEU
1	D	386	GLU
1	D	393	LEU
1	D	411	THR
1	D	460	LEU
1	D	497	VAL
1	D	521	THR
1	D	530	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	192	HIS
1	A	445	GLN
1	B	132	HIS
1	B	369	ASN
1	B	469	HIS
1	B	536	GLN
1	C	192	HIS
1	C	419	GLN
1	C	488	GLN
1	D	105	ASN
1	D	254	GLN
1	D	369	ASN
1	D	445	GLN
1	D	536	GLN

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

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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

There are no such residues in this entry.

5.8 Polymer linkage issues

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	529/571 (92%)	0.04	10 (1%)	66	64	23, 48, 82, 117	0
1	B	522/571 (91%)	0.06	20 (3%)	44	41	23, 45, 96, 127	0
1	C	530/571 (92%)	0.06	19 (3%)	46	44	23, 45, 95, 122	0
1	D	523/571 (91%)	0.17	23 (4%)	39	38	25, 47, 100, 117	0
All	All	2104/2284 (92%)	0.08	72 (3%)	48	46	23, 47, 93, 127	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	123	LEU	6.2
1	C	174	PHE	6.1
1	B	137	TRP	3.7
1	B	128	PRO	3.7
1	C	170	TRP	3.6
1	D	216	GLU	3.6
1	B	136	VAL	3.5
1	D	174	PHE	3.4
1	D	228	THR	3.4
1	D	138	SER	3.3
1	D	6	PRO	3.3
1	B	173	PHE	3.3
1	B	140	GLU	3.3
1	A	6	PRO	3.2
1	C	173	PHE	3.2
1	A	170	TRP	3.2
1	B	116	ALA	3.1
1	C	411	THR	3.1
1	D	173	PHE	3.1
1	C	128	PRO	3.0
1	C	124	PRO	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	135	TYR	2.9
1	A	174	PHE	2.9
1	D	215	ILE	2.8
1	B	170	TRP	2.8
1	B	6	PRO	2.8
1	B	161	LEU	2.8
1	D	122	THR	2.8
1	B	169	TYR	2.6
1	B	138	SER	2.5
1	D	121	PRO	2.5
1	A	186	LYS	2.5
1	A	220	THR	2.4
1	A	168	TYR	2.4
1	B	168	TYR	2.4
1	A	161	LEU	2.4
1	C	168	TYR	2.4
1	D	220	THR	2.4
1	C	172	ARG	2.4
1	C	169	TYR	2.3
1	C	215	ILE	2.3
1	A	264	GLY	2.3
1	B	119	ARG	2.3
1	C	122	THR	2.3
1	D	136	VAL	2.3
1	C	397	ASP	2.3
1	C	175	ALA	2.2
1	D	69	ALA	2.2
1	B	159	TRP	2.2
1	B	215	ILE	2.2
1	D	170	TRP	2.2
1	D	168	TYR	2.2
1	D	318	HIS	2.2
1	C	158	ASN	2.2
1	B	114	PHE	2.2
1	B	117	ALA	2.1
1	C	121	PRO	2.1
1	D	182	TYR	2.1
1	D	219	GLY	2.1
1	D	397	ASP	2.1
1	A	221	SER	2.1
1	D	131	TYR	2.1
1	D	134	TYR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	132	HIS	2.1
1	C	137	TRP	2.1
1	D	478	GLY	2.1
1	D	237	ALA	2.1
1	C	6	PRO	2.1
1	C	220	THR	2.0
1	A	219	GLY	2.0
1	B	478	GLY	2.0
1	C	131	TYR	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	CA	A	600	1/1	0.91	0.08	87,87,87,87	0
2	CA	B	600	1/1	0.91	0.06	81,81,81,81	0
2	CA	D	600	1/1	0.91	0.07	68,68,68,68	0
3	MG	C	601	1/1	0.93	0.07	38,38,38,38	0
2	CA	C	600	1/1	0.97	0.05	60,60,60,60	0
3	MG	B	601	1/1	0.99	0.03	19,19,19,19	0
3	MG	A	601	1/1	0.99	0.02	20,20,20,20	0
3	MG	D	601	1/1	0.99	0.03	32,32,32,32	0

6.5 Other polymers (i)

There are no such residues in this entry.