Full wwPDB X-ray Structure Validation Report (i)

Oct 17, 2021 – 02:55 AM EDT

PDB ID	:	1JT0
Title	:	Crystal structure of a cooperative QacR-DNA complex
Authors	:	Schumacher, M.A.; Miller, M.C.; Grkovic, S.; Brown, M.H.; Skurray, R.A.; Brennan, R.G.
Deposited on	:	2001-08-20
Resolution	:	2.90 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 following versions of software and data (see references (i)) were used in the production of this report:

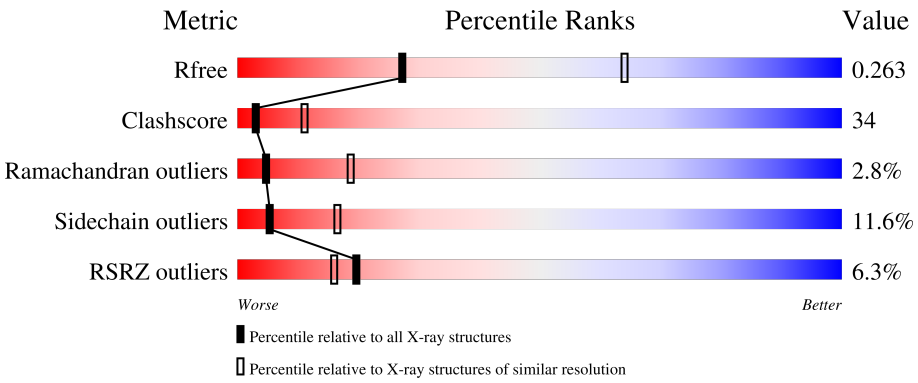
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.90 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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	E	28	18% 71% 11%
1	F	28	46% 46% 7%
2	A	194	10% 34% 57% 6% • •
2	B	194	4% 52% 37% 8% •
2	C	194	8% 37% 53% 6% • •

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Mol	Chain	Length	Quality of chain
2	D	194	5% 42% 41% 12% 5%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7451 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 DNA chain called QACA operator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	E	28	571	274	104	166	27	0	0	0
1	F	28	571	274	104	166	27	0	0	0

- Molecule 2 is a protein called HYPOTHETICAL TRANSCRIPTIONAL REGULATOR IN QACA 5'REGION.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	188	1566	1010	257	297	2	0	0	0
2	B	188	1566	1010	257	297	2	0	0	0
2	C	188	1566	1010	257	297	2	0	0	0
2	D	185	1541	995	251	293	2	0	0	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	72	ALA	CYS	engineered mutation	UNP P0A0N4
A	141	SER	CYS	engineered mutation	UNP P0A0N4
A	189	HIS	-	expression tag	UNP P0A0N4
A	190	HIS	-	expression tag	UNP P0A0N4
A	191	HIS	-	expression tag	UNP P0A0N4
A	192	HIS	-	expression tag	UNP P0A0N4
A	193	HIS	-	expression tag	UNP P0A0N4
A	194	HIS	-	expression tag	UNP P0A0N4
B	72	ALA	CYS	engineered mutation	UNP P0A0N4
B	141	SER	CYS	engineered mutation	UNP P0A0N4
B	189	HIS	-	expression tag	UNP P0A0N4

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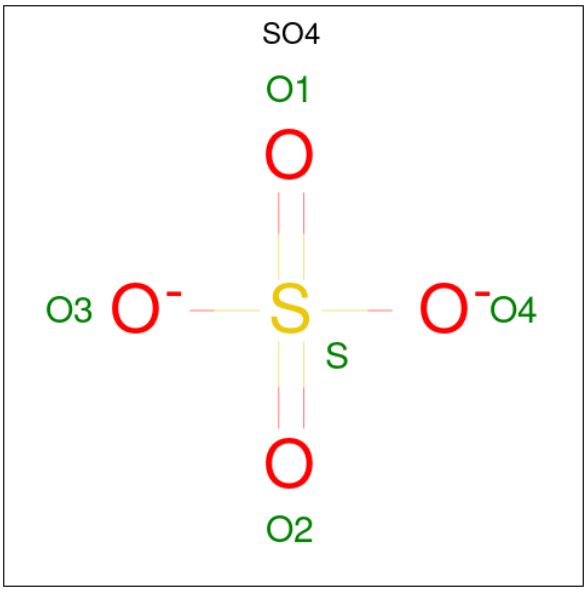
Chain	Residue	Modelled	Actual	Comment	Reference
B	190	HIS	-	expression tag	UNP P0A0N4
B	191	HIS	-	expression tag	UNP P0A0N4
B	192	HIS	-	expression tag	UNP P0A0N4
B	193	HIS	-	expression tag	UNP P0A0N4
B	194	HIS	-	expression tag	UNP P0A0N4
C	72	ALA	CYS	engineered mutation	UNP P0A0N4
C	141	SER	CYS	engineered mutation	UNP P0A0N4
C	189	HIS	-	expression tag	UNP P0A0N4
C	190	HIS	-	expression tag	UNP P0A0N4
C	191	HIS	-	expression tag	UNP P0A0N4
C	192	HIS	-	expression tag	UNP P0A0N4
C	193	HIS	-	expression tag	UNP P0A0N4
C	194	HIS	-	expression tag	UNP P0A0N4
D	72	ALA	CYS	engineered mutation	UNP P0A0N4
D	141	SER	CYS	engineered mutation	UNP P0A0N4
D	189	HIS	-	expression tag	UNP P0A0N4
D	190	HIS	-	expression tag	UNP P0A0N4
D	191	HIS	-	expression tag	UNP P0A0N4
D	192	HIS	-	expression tag	UNP P0A0N4
D	193	HIS	-	expression tag	UNP P0A0N4
D	194	HIS	-	expression tag	UNP P0A0N4

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
3	A	1	5	4	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
3	B	1	5	4	1	0	0
			Total	O	S		
3	B	1	5	4	1	0	0
			Total	O	S		
3	C	1	5	4	1	0	0
			Total	O	S		
3	D	1	5	4	1	0	0

- Molecule 4 is water.

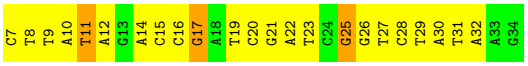
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	E	2	2	2	0	0
			Total	O		
4	F	1	1	1	0	0
			Total	O		
4	A	6	6	6	0	0
			Total	O		
4	B	13	13	13	0	0
			Total	O		
4	C	9	9	9	0	0
			Total	O		
4	D	14	14	14	0	0

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.

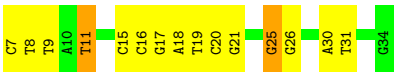
• Molecule 1: QACA operator

Chain E: 18% 71% 11%



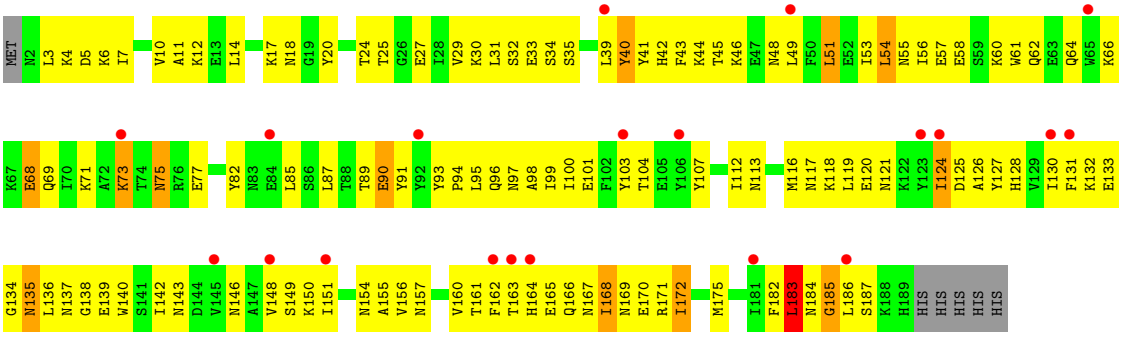
• Molecule 1: QACA operator

Chain F: 46% 46% 7%



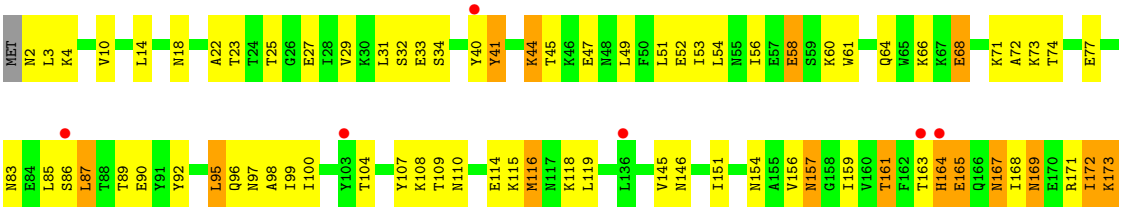
• Molecule 2: HYPOTHETICAL TRANSCRIPTIONAL REGULATOR IN QACA 5'REGION

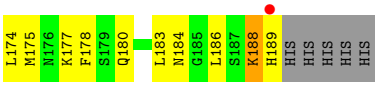
Chain A: 10% 34% 57% 6%



• Molecule 2: HYPOTHETICAL TRANSCRIPTIONAL REGULATOR IN QACA 5'REGION

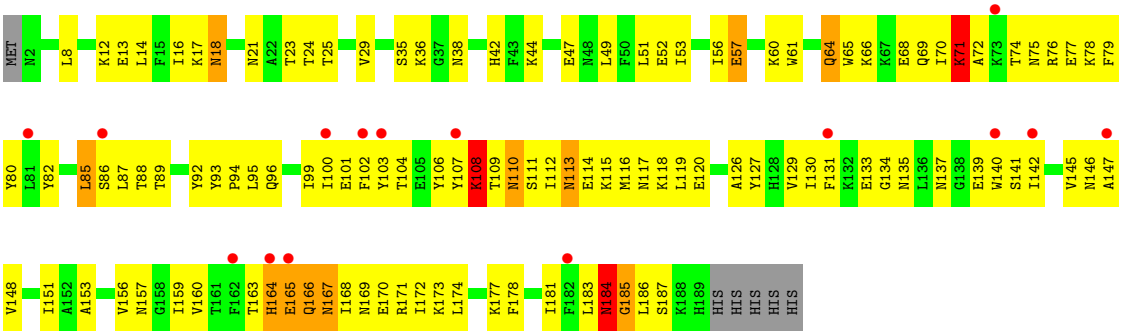
Chain B: 4% 52% 37% 8%





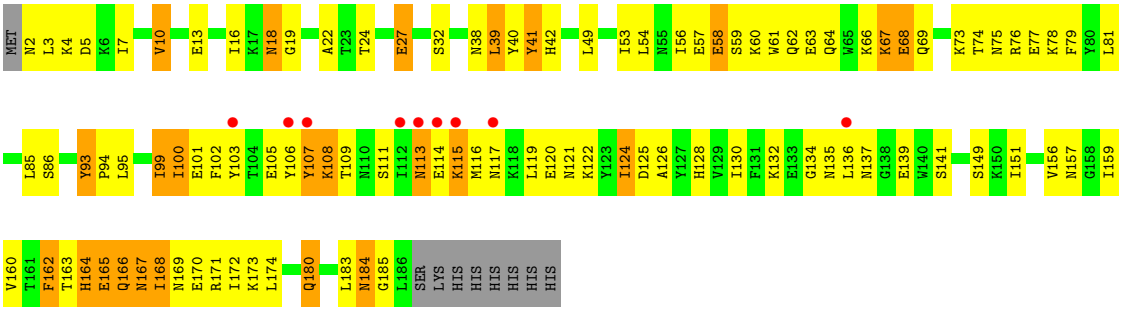
• Molecule 2: HYPOTHETICAL TRANSCRIPTIONAL REGULATOR IN QACA 5'REGION

Chain C:



• Molecule 2: HYPOTHETICAL TRANSCRIPTIONAL REGULATOR IN QACA 5'REGION

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	174.70Å 174.70Å 151.95Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	75.73 – 2.90 75.73 – 2.87	Depositor EDS
% Data completeness (in resolution range)	98.7 (75.73-2.90) 98.7 (75.73-2.87)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	1.89 (at 2.86Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.222 , 0.258 0.228 , 0.263	Depositor DCC
R_{free} test set	5846 reflections (9.85%)	wwPDB-VP
Wilson B-factor (Å^2)	76.7	Xtriage
Anisotropy	0.267	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 83.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.017 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7451	wwPDB-VP
Average B, all atoms (Å^2)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	E	0.80	0/640	1.06	2/986 (0.2%)
1	F	0.74	0/640	0.95	1/986 (0.1%)
2	A	0.44	0/1598	0.61	0/2152
2	B	0.53	0/1598	0.64	0/2152
2	C	0.46	0/1598	0.67	0/2152
2	D	0.50	0/1572	0.66	0/2118
All	All	0.54	0/7646	0.73	3/10546 (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	E	0	3
1	F	0	1
2	A	0	2
2	B	0	1
2	D	0	1
All	All	0	8

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	19	DT	C1'-O4'-C4'	-6.00	104.09	110.10
1	E	25	DG	C5'-C4'-C3'	-5.92	103.45	114.10
1	F	25	DG	C5'-C4'-C3'	-5.08	104.96	114.10

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	40	TYR	Sidechain
2	A	41	TYR	Sidechain
2	B	41	TYR	Sidechain
2	D	41	TYR	Sidechain
1	E	11	DT	Sidechain
1	E	14	DA	Sidechain
1	E	17	DG	Sidechain
1	F	11	DT	Sidechain

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	E	571	0	318	28	0
1	F	571	0	318	23	0
2	A	1566	0	1556	141	0
2	B	1566	0	1556	76	0
2	C	1566	0	1556	130	0
2	D	1541	0	1531	116	0
3	A	5	0	0	0	0
3	B	10	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
4	A	6	0	0	0	0
4	B	13	0	0	1	0
4	C	9	0	0	0	0
4	D	14	0	0	0	0
4	E	2	0	0	0	0
4	F	1	0	0	0	0
All	All	7451	0	6835	484	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 34.

All (484) 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)
2:D:103:TYR:CE1	2:D:107:TYR:CB	2.07	1.35
2:D:103:TYR:CD1	2:D:107:TYR:HB3	1.61	1.35
2:D:103:TYR:CE1	2:D:107:TYR:HB3	1.65	1.28
2:D:103:TYR:CE1	2:D:107:TYR:HB2	1.73	1.20
2:C:164:HIS:HA	2:C:171:ARG:NH2	1.57	1.18
2:D:164:HIS:HA	2:D:171:ARG:HH21	0.99	1.14
2:D:103:TYR:HD2	2:D:116:MET:SD	1.76	1.06
2:C:52:GLU:HG2	2:C:56:ILE:HD11	1.37	1.06
1:E:9:DT:H2"	1:E:10:DA:H5"	1.33	1.05
1:F:18:DA:H2"	1:F:19:DT:H5"	1.35	1.04
2:A:124:ILE:HD11	2:A:150:LYS:HA	1.37	1.03
2:A:89:THR:HG22	2:A:91:TYR:H	1.20	1.03
2:B:154:ASN:ND2	2:D:163:THR:HG22	1.77	0.99
1:E:11:DT:H2"	1:E:12:DA:H5"	1.40	0.98
2:D:164:HIS:CA	2:D:171:ARG:HH21	1.77	0.98
2:A:154:ASN:ND2	2:C:163:THR:HG22	1.79	0.98
2:D:106:TYR:HA	2:D:108:LYS:HE3	1.44	0.97
2:C:164:HIS:HA	2:C:171:ARG:HH21	1.11	0.97
2:C:173:LYS:HE2	2:C:173:LYS:HA	1.48	0.95
2:D:2:ASN:ND2	2:D:3:LEU:H	1.64	0.95
2:A:66:LYS:HA	2:A:69:GLN:HE21	1.29	0.94
1:E:30:DA:H2"	1:E:31:DT:O5'	1.65	0.94
2:D:164:HIS:HA	2:D:171:ARG:NH2	1.84	0.92
1:F:18:DA:C2'	1:F:19:DT:H5"	1.99	0.91
2:D:156:VAL:O	2:D:160:VAL:HG23	1.72	0.89
1:E:11:DT:H2"	1:E:12:DA:C5'	2.03	0.88
2:C:141:SER:H	2:C:187:SER:HB3	1.39	0.86
1:E:9:DT:C2'	1:E:10:DA:H5"	2.06	0.86
2:D:103:TYR:HE1	2:D:107:TYR:HB2	1.41	0.85
2:C:164:HIS:CA	2:C:171:ARG:NH2	2.38	0.85
2:C:76:ARG:HG2	2:C:183:LEU:HD13	1.57	0.85
2:C:147:ALA:O	2:C:151:ILE:HG12	1.78	0.83
2:C:56:ILE:HG22	2:C:60:LYS:NZ	1.94	0.83
2:C:86:SER:HB2	2:C:93:TYR:CE2	2.14	0.83
2:B:95:LEU:O	2:B:99:ILE:HG13	1.77	0.83
2:D:103:TYR:CD2	2:D:116:MET:SD	2.69	0.82
2:A:126:ALA:O	2:A:130:ILE:HG12	1.80	0.82
1:E:9:DT:H2"	1:E:10:DA:C5'	2.09	0.81
2:D:95:LEU:O	2:D:99:ILE:HG12	1.80	0.81
2:B:156:VAL:HG13	2:B:175:MET:CE	2.11	0.80
2:B:110:ASN:O	2:B:114:GLU:HG2	1.82	0.80
2:D:103:TYR:CD1	2:D:107:TYR:CB	2.48	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:96:GLN:O	2:C:100:ILE:HG12	1.81	0.79
1:F:7:DC:H2"	1:F:8:DT:H5'	1.65	0.79
2:D:56:ILE:O	2:D:59:SER:HB3	1.83	0.78
2:C:102:PHE:HE1	2:C:112:ILE:HG21	1.51	0.76
1:E:11:DT:C2'	1:E:12:DA:H5"	2.15	0.75
2:A:10:VAL:HG11	2:A:31:LEU:HB2	1.67	0.75
2:C:135:ASN:HD21	2:C:142:ILE:H	1.34	0.75
2:A:154:ASN:HD21	2:C:163:THR:HG22	1.51	0.74
2:B:156:VAL:HG13	2:B:175:MET:HE3	1.69	0.74
1:F:18:DA:H2"	1:F:19:DT:C5'	2.16	0.73
1:E:15:DC:OP1	2:A:3:LEU:HD23	1.87	0.72
2:A:167:ASN:OD1	2:A:168:ILE:HG13	1.89	0.72
2:D:114:GLU:HA	2:D:117:ASN:HB3	1.70	0.72
2:B:72:ALA:HB1	2:B:77:GLU:HB3	1.72	0.72
1:F:30:DA:H2"	1:F:31:DT:C5'	2.18	0.72
2:A:95:LEU:O	2:A:99:ILE:HG13	1.90	0.72
2:A:154:ASN:ND2	2:C:163:THR:CG2	2.52	0.72
2:B:157:ASN:O	2:B:161:THR:HG23	1.91	0.71
2:A:64:GLN:O	2:A:68:GLU:HB2	1.90	0.71
2:A:167:ASN:OD1	2:A:168:ILE:N	2.24	0.71
2:C:117:ASN:HA	2:C:120:GLU:HG2	1.73	0.71
2:D:19:GLY:H	2:D:22:ALA:HB3	1.56	0.70
2:A:165:GLU:N	2:A:165:GLU:OE2	2.23	0.70
2:B:96:GLN:O	2:B:100:ILE:HG12	1.91	0.70
2:A:64:GLN:HE22	2:A:89:THR:HG23	1.55	0.70
2:A:75:ASN:OD1	2:A:133:GLU:HG3	1.91	0.70
2:A:75:ASN:HB2	2:A:139:GLU:OE1	1.91	0.69
2:D:4:LYS:HB2	2:D:42:HIS:ND1	2.07	0.69
2:C:108:LYS:HE2	2:C:109:THR:HG23	1.73	0.69
2:D:103:TYR:HE1	2:D:107:TYR:CB	1.95	0.69
2:D:136:LEU:HD12	2:D:136:LEU:O	1.92	0.69
2:C:167:ASN:HD21	2:C:169:ASN:ND2	1.91	0.69
2:A:131:PHE:CE2	2:A:148:VAL:HG12	2.28	0.69
2:D:169:ASN:O	2:D:173:LYS:HG2	1.92	0.69
2:C:177:LYS:O	2:C:181:ILE:HG13	1.93	0.68
2:B:14:LEU:HD21	2:B:27:GLU:HG2	1.75	0.68
2:C:184:ASN:O	2:C:186:LEU:N	2.25	0.68
2:A:71:LYS:HD2	2:A:71:LYS:H	1.58	0.68
2:C:168:ILE:O	2:C:172:ILE:HG12	1.93	0.68
2:D:121:ASN:HA	2:D:124:ILE:HG12	1.76	0.67
2:A:124:ILE:HD11	2:A:150:LYS:CA	2.19	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:180:GLN:O	2:D:184:ASN:HB2	1.95	0.67
1:F:30:DA:H2"	1:F:31:DT:H5'	1.74	0.67
2:A:25:THR:O	2:A:29:VAL:HG23	1.93	0.67
2:A:89:THR:HG22	2:A:90:GLU:N	2.10	0.67
1:F:7:DC:H2"	1:F:8:DT:C5'	2.24	0.67
2:A:103:TYR:CE1	2:A:107:TYR:CE2	2.83	0.67
2:A:116:MET:O	2:A:120:GLU:HG2	1.95	0.67
2:A:103:TYR:CE1	2:A:107:TYR:CD2	2.83	0.66
2:D:74:THR:HB	2:D:139:GLU:OE2	1.94	0.66
2:A:132:LYS:O	2:A:135:ASN:HB2	1.94	0.66
2:A:184:ASN:O	2:A:186:LEU:N	2.29	0.66
2:D:58:GLU:OE2	2:D:62:GLN:HG2	1.95	0.66
2:C:164:HIS:CA	2:C:171:ARG:HH21	1.97	0.66
2:C:75:ASN:HD22	2:C:139:GLU:HG3	1.60	0.66
2:A:166:GLN:OE1	2:A:170:GLU:HG2	1.95	0.66
2:D:2:ASN:CG	2:D:3:LEU:H	1.97	0.66
2:A:184:ASN:C	2:A:186:LEU:H	1.98	0.66
2:A:6:LYS:O	2:A:10:VAL:HG23	1.96	0.66
2:C:112:ILE:H	2:C:112:ILE:HD12	1.61	0.65
2:A:124:ILE:CD1	2:A:150:LYS:HA	2.21	0.65
2:C:141:SER:N	2:C:187:SER:HB3	2.10	0.65
1:E:22:DA:H2"	1:E:23:DT:H5'	1.77	0.64
2:A:184:ASN:C	2:A:186:LEU:N	2.49	0.64
2:D:24:THR:OG1	2:D:27:GLU:HB2	1.97	0.64
2:A:156:VAL:HG13	2:A:175:MET:CE	2.27	0.64
2:B:107:TYR:HD1	2:B:108:LYS:HD3	1.62	0.64
2:C:17:LYS:HG2	2:C:18:ASN:OD1	1.97	0.64
2:B:188:LYS:HD2	2:B:188:LYS:O	1.98	0.63
2:B:96:GLN:HG2	2:B:161:THR:HG21	1.79	0.63
2:C:156:VAL:O	2:C:160:VAL:HG23	1.99	0.63
2:B:156:VAL:HG13	2:B:175:MET:HE1	1.78	0.63
2:C:163:THR:O	2:C:165:GLU:N	2.31	0.63
2:A:61:TRP:CZ3	2:A:85:LEU:HD23	2.35	0.62
2:A:49:LEU:O	2:A:53:ILE:HG13	1.98	0.62
2:B:154:ASN:HD22	2:D:163:THR:HG22	1.61	0.62
2:D:126:ALA:O	2:D:130:ILE:HG13	1.99	0.62
2:C:61:TRP:HZ2	2:C:82:TYR:CE1	2.18	0.62
1:E:16:DC:H2"	1:E:17:DG:N7	2.14	0.62
2:D:166:GLN:OE1	2:D:166:GLN:HA	1.98	0.62
2:A:185:GLY:HA2	2:C:184:ASN:HB3	1.82	0.62
2:A:58:GLU:HB2	2:A:119:LEU:HD12	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:108:LYS:CD	2:D:109:THR:HG23	2.30	0.62
2:C:61:TRP:CZ3	2:C:85:LEU:HD12	2.35	0.61
2:A:25:THR:HG21	2:A:40:TYR:HE1	1.65	0.61
2:A:166:GLN:CD	2:A:170:GLU:HG2	2.21	0.61
2:A:100:ILE:O	2:A:104:THR:HG23	2.01	0.61
2:A:118:LYS:HZ3	2:A:118:LYS:HB3	1.64	0.61
2:C:21:ASN:ND2	2:C:101:GLU:OE1	2.29	0.61
2:D:19:GLY:N	2:D:22:ALA:HB3	2.16	0.61
2:B:49:LEU:O	2:B:53:ILE:HG13	2.00	0.60
2:D:167:ASN:C	2:D:167:ASN:OD1	2.39	0.60
2:A:3:LEU:HD12	2:A:34:SER:HB2	1.84	0.60
2:C:18:ASN:OD1	2:C:18:ASN:N	2.35	0.60
2:D:100:ILE:HG22	2:D:101:GLU:N	2.17	0.60
2:A:82:TYR:HE2	2:A:127:TYR:CE2	2.19	0.59
2:B:73:LYS:O	2:B:73:LYS:HD3	2.02	0.59
2:C:167:ASN:O	2:C:170:GLU:HB3	2.02	0.59
2:D:49:LEU:O	2:D:53:ILE:HG13	2.02	0.59
2:A:60:LYS:HB3	2:A:91:TYR:CD2	2.37	0.59
2:C:164:HIS:HA	2:C:171:ARG:HH22	1.61	0.59
2:D:75:ASN:HD22	2:D:134:GLY:HA2	1.67	0.59
2:C:25:THR:O	2:C:29:VAL:HG13	2.02	0.59
2:A:97:ASN:ND2	2:A:98:ALA:H	2.01	0.59
2:B:118:LYS:HD3	4:B:408:HOH:O	2.02	0.59
2:C:134:GLY:CA	2:C:139:GLU:HB2	2.33	0.59
2:A:163:THR:HG22	2:A:163:THR:O	2.01	0.58
2:B:107:TYR:HB3	2:B:108:LYS:NZ	2.18	0.58
2:A:135:ASN:ND2	2:A:140:TRP:O	2.36	0.58
2:A:136:LEU:HD12	2:A:137:ASN:N	2.18	0.58
2:A:12:LYS:HE3	2:A:57:GLU:OE2	2.03	0.58
2:A:118:LYS:HZ3	2:A:119:LEU:HD22	1.69	0.57
2:A:135:ASN:HD21	2:A:142:ILE:H	1.52	0.57
2:C:74:THR:HB	2:C:139:GLU:OE2	2.04	0.57
2:C:142:ILE:HG12	2:C:148:VAL:HG21	1.86	0.57
2:C:115:LYS:O	2:C:118:LYS:HG2	2.03	0.57
2:A:156:VAL:O	2:A:160:VAL:HG23	2.03	0.57
2:C:76:ARG:HG3	2:C:140:TRP:HZ3	1.67	0.57
2:C:102:PHE:CE1	2:C:112:ILE:HG21	2.36	0.57
2:A:119:LEU:HD22	2:A:119:LEU:H	1.69	0.57
2:C:93:TYR:HE1	2:C:157:ASN:ND2	2.02	0.57
2:D:164:HIS:N	2:D:171:ARG:HH21	2.03	0.57
2:C:14:LEU:HB3	2:C:23:THR:HG23	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:15:DC:OP1	2:B:3:LEU:HB2	2.05	0.57
2:A:163:THR:C	2:A:171:ARG:HH12	2.07	0.57
1:E:20:DC:H2"	1:E:21:DG:C8	2.40	0.57
2:A:17:LYS:HG2	2:A:18:ASN:OD1	2.05	0.57
2:A:185:GLY:HA2	2:C:184:ASN:CB	2.34	0.57
2:B:68:GLU:O	2:B:71:LYS:HG3	2.05	0.57
2:A:45:THR:HG23	2:A:48:ASN:H	1.69	0.56
2:D:103:TYR:CZ	2:D:107:TYR:HB2	2.35	0.56
2:D:162:PHE:N	2:D:162:PHE:CD1	2.72	0.56
2:D:76:ARG:HG3	2:D:183:LEU:HD13	1.87	0.56
2:A:163:THR:C	2:A:171:ARG:NH1	2.59	0.56
2:D:61:TRP:CH2	2:D:85:LEU:HD23	2.41	0.56
2:A:136:LEU:C	2:A:138:GLY:H	2.08	0.55
2:C:164:HIS:N	2:C:171:ARG:NH2	2.54	0.55
2:B:3:LEU:HG	2:B:34:SER:HB2	1.87	0.55
2:B:40:TYR:HE2	2:B:45:THR:HA	1.71	0.55
2:A:125:ASP:O	2:A:128:HIS:N	2.39	0.55
2:D:124:ILE:HD13	2:D:124:ILE:N	2.21	0.55
2:A:117:ASN:O	2:A:120:GLU:HB2	2.07	0.55
2:B:14:LEU:HD23	2:B:23:THR:HG23	1.89	0.55
1:E:25:DG:H2"	1:E:26:DG:C5'	2.36	0.54
2:B:74:THR:O	2:B:77:GLU:HB2	2.07	0.54
2:C:80:TYR:CE1	2:C:183:LEU:HD12	2.42	0.54
2:A:156:VAL:HG13	2:A:175:MET:HE1	1.88	0.54
2:D:111:SER:O	2:D:115:LYS:HB2	2.07	0.54
1:E:29:DT:H2"	1:E:30:DA:H5'	1.89	0.54
1:F:30:DA:H2"	1:F:31:DT:H5"	1.87	0.54
2:B:116:MET:HA	2:B:116:MET:HE3	1.90	0.54
1:E:29:DT:H2"	1:E:30:DA:C5'	2.38	0.54
2:C:80:TYR:HE1	2:C:183:LEU:HD12	1.73	0.54
2:B:44:LYS:HE2	2:B:44:LYS:H	1.73	0.54
2:C:103:TYR:O	2:C:107:TYR:HB3	2.08	0.54
2:D:81:LEU:O	2:D:85:LEU:HB2	2.07	0.54
2:C:8:LEU:HD22	2:C:53:ILE:HG12	1.90	0.54
2:D:66:LYS:HA	2:D:69:GLN:HE21	1.72	0.54
2:D:168:ILE:O	2:D:172:ILE:HG13	2.08	0.54
2:B:10:VAL:HG11	2:B:31:LEU:HB2	1.89	0.53
2:C:47:GLU:HG3	2:C:102:PHE:HZ	1.72	0.53
2:D:63:GLU:HG2	2:D:67:LYS:NZ	2.23	0.53
2:C:109:THR:C	2:C:111:SER:H	2.12	0.53
2:B:64:GLN:HE22	2:B:89:THR:CB	2.21	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:100:ILE:O	2:C:104:THR:HG23	2.09	0.53
2:B:167:ASN:C	2:B:167:ASN:OD1	2.46	0.53
2:C:164:HIS:N	2:C:171:ARG:HH22	2.06	0.53
2:C:118:LYS:HG3	2:C:119:LEU:N	2.22	0.53
2:C:135:ASN:ND2	2:C:142:ILE:H	2.02	0.53
2:C:14:LEU:CB	2:C:23:THR:HG23	2.39	0.53
2:B:58:GLU:O	2:B:61:TRP:HB3	2.09	0.53
2:D:162:PHE:N	2:D:162:PHE:HD1	2.07	0.53
2:D:10:VAL:HG11	2:D:32:SER:HB3	1.90	0.53
2:A:125:ASP:O	2:A:126:ALA:C	2.48	0.52
2:A:89:THR:HG22	2:A:90:GLU:H	1.74	0.52
2:B:189:HIS:HD2	2:D:184:ASN:ND2	2.06	0.52
1:E:30:DA:C2'	1:E:31:DT:O5'	2.46	0.52
2:A:10:VAL:O	2:A:14:LEU:HD13	2.10	0.52
2:A:96:GLN:HG2	2:A:161:THR:HG21	1.92	0.52
2:D:102:PHE:O	2:D:106:TYR:HD2	1.93	0.52
2:A:135:ASN:HD21	2:A:142:ILE:N	2.07	0.52
2:D:166:GLN:NE2	2:D:170:GLU:HG2	2.25	0.52
2:A:73:LYS:HG3	2:A:77:GLU:OE1	2.10	0.51
2:D:164:HIS:N	2:D:171:ARG:NH2	2.58	0.51
2:C:127:TYR:CE2	2:C:153:ALA:HA	2.45	0.51
2:D:99:ILE:HG22	2:D:116:MET:CE	2.40	0.51
2:D:159:ILE:O	2:D:163:THR:HG23	2.10	0.51
1:F:25:DG:H2"	1:F:26:DG:C5'	2.41	0.51
2:B:44:LYS:H	2:B:44:LYS:CD	2.24	0.51
2:C:163:THR:OG1	2:C:171:ARG:NH1	2.44	0.51
2:A:97:ASN:ND2	2:A:98:ALA:N	2.57	0.51
2:C:177:LYS:HD2	2:C:181:ILE:HD11	1.92	0.51
2:A:125:ASP:O	2:A:127:TYR:N	2.44	0.51
2:A:156:VAL:HG13	2:A:175:MET:HE3	1.93	0.51
1:E:31:DT:H2"	1:E:32:DA:H5'	1.93	0.51
2:D:99:ILE:HG22	2:D:116:MET:HE2	1.93	0.51
2:C:56:ILE:HG22	2:C:60:LYS:HZ2	1.74	0.50
2:C:165:GLU:N	2:C:165:GLU:OE1	2.43	0.50
1:E:21:DG:H2"	1:E:22:DA:O5'	2.10	0.50
2:B:61:TRP:CZ3	2:B:85:LEU:HG	2.46	0.50
2:A:87:LEU:HD13	2:A:171:ARG:HB3	1.94	0.50
2:C:25:THR:O	2:C:29:VAL:CG1	2.59	0.50
1:F:7:DC:H2'	1:F:8:DT:C6	2.46	0.50
2:A:24:THR:HG23	2:A:27:GLU:H	1.76	0.50
2:D:2:ASN:CG	2:D:3:LEU:N	2.64	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:58:GLU:OE1	2:D:122:LYS:HD2	2.11	0.50
2:D:106:TYR:HA	2:D:108:LYS:CE	2.29	0.50
2:A:60:LYS:HG2	2:A:91:TYR:CE2	2.46	0.50
1:F:16:DC:H2"	1:F:17:DG:N7	2.27	0.50
2:A:164:HIS:N	2:A:171:ARG:HH12	2.09	0.50
2:C:53:ILE:O	2:C:57:GLU:HB2	2.12	0.50
2:A:39:LEU:O	2:A:39:LEU:HD12	2.12	0.49
2:A:151:ILE:HD12	2:C:178:PHE:HB2	1.93	0.49
2:D:116:MET:HA	2:D:119:LEU:HD12	1.94	0.49
2:C:173:LYS:HA	2:C:173:LYS:CE	2.30	0.49
2:D:86:SER:HB2	2:D:93:TYR:CD2	2.47	0.49
2:D:125:ASP:O	2:D:128:HIS:N	2.46	0.49
2:B:18:ASN:O	2:B:22:ALA:HB3	2.12	0.49
2:C:131:PHE:CE2	2:C:148:VAL:HG12	2.48	0.49
2:A:75:ASN:OD1	2:A:134:GLY:HA2	2.13	0.48
2:B:172:ILE:HD13	2:B:173:LYS:HD2	1.95	0.48
1:E:22:DA:H2"	1:E:23:DT:C5'	2.42	0.48
2:B:72:ALA:HA	2:B:77:GLU:OE2	2.13	0.48
2:A:103:TYR:HE1	2:A:107:TYR:CE2	2.29	0.48
2:B:2:ASN:C	2:B:4:LYS:N	2.66	0.48
2:C:112:ILE:O	2:C:116:MET:HG2	2.13	0.48
2:C:164:HIS:CA	2:C:171:ARG:HH22	2.23	0.48
2:A:164:HIS:HA	2:A:171:ARG:NH1	2.29	0.48
2:C:85:LEU:C	2:C:87:LEU:H	2.17	0.48
2:D:86:SER:HB2	2:D:93:TYR:CE2	2.49	0.48
2:D:93:TYR:HE1	2:D:157:ASN:OD1	1.96	0.48
2:D:100:ILE:HD13	2:D:100:ILE:HA	1.66	0.48
1:F:8:DT:H2'	1:F:9:DT:H72	1.95	0.48
2:A:89:THR:HG22	2:A:91:TYR:N	2.06	0.48
2:B:151:ILE:HG13	2:D:174:LEU:HD12	1.96	0.48
2:B:167:ASN:OD1	2:B:167:ASN:O	2.31	0.48
2:C:86:SER:HB2	2:C:93:TYR:CZ	2.48	0.48
2:A:39:LEU:HD11	2:A:49:LEU:HD22	1.95	0.48
2:A:135:ASN:HD22	2:A:135:ASN:HA	1.53	0.48
2:C:44:LYS:NZ	2:C:44:LYS:HB3	2.28	0.48
1:E:7:DC:H2"	1:E:8:DT:H5'	1.95	0.47
2:A:151:ILE:CD1	2:C:174:LEU:HD22	2.44	0.47
2:C:95:LEU:O	2:C:99:ILE:HG13	2.14	0.47
2:D:56:ILE:HG22	2:D:60:LYS:HD2	1.97	0.47
2:A:64:GLN:NE2	2:A:89:THR:HG23	2.26	0.47
2:A:117:ASN:HA	2:A:120:GLU:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:108:LYS:HD3	2:D:109:THR:HG23	1.94	0.47
2:A:45:THR:OG1	2:A:46:LYS:N	2.46	0.47
2:A:154:ASN:HD22	2:C:163:THR:CG2	2.27	0.47
2:A:182:PHE:C	2:A:184:ASN:H	2.18	0.47
2:D:135:ASN:C	2:D:137:ASN:H	2.18	0.47
1:F:19:DT:H2"	1:F:20:DC:C6	2.49	0.47
2:A:89:THR:CG2	2:A:90:GLU:N	2.77	0.47
2:B:51:LEU:HD13	2:B:115:LYS:HD3	1.96	0.47
2:C:85:LEU:HD22	2:C:85:LEU:HA	1.76	0.47
2:B:184:ASN:OD1	2:D:185:GLY:HA2	2.14	0.47
2:C:25:THR:OG1	2:C:36:LYS:HE2	2.15	0.47
2:D:19:GLY:H	2:D:22:ALA:CB	2.27	0.47
2:C:16:ILE:HG12	2:C:94:PRO:O	2.15	0.47
2:D:108:LYS:HD2	2:D:109:THR:N	2.30	0.47
2:A:53:ILE:O	2:A:57:GLU:HG2	2.15	0.46
2:A:151:ILE:HD11	2:C:174:LEU:O	2.14	0.46
2:A:184:ASN:HB2	2:C:185:GLY:HA3	1.97	0.46
2:C:12:LYS:HE2	2:C:16:ILE:HD11	1.97	0.46
2:C:137:ASN:C	2:C:139:GLU:H	2.19	0.46
2:A:103:TYR:CE1	2:A:107:TYR:HE2	2.33	0.46
2:C:93:TYR:HE1	2:C:157:ASN:HD22	1.63	0.46
1:F:30:DA:C2'	1:F:31:DT:H5"	2.46	0.46
2:A:68:GLU:OE2	2:A:68:GLU:O	2.34	0.46
2:A:103:TYR:CE1	2:A:107:TYR:HD2	2.32	0.46
2:C:75:ASN:O	2:C:78:LYS:HB2	2.15	0.46
1:F:19:DT:H2"	1:F:20:DC:H6	1.80	0.46
2:A:11:ALA:HB3	2:A:53:ILE:HD11	1.97	0.46
2:A:101:GLU:O	2:A:104:THR:OG1	2.33	0.46
2:A:75:ASN:OD1	2:A:134:GLY:CA	2.64	0.46
2:C:117:ASN:HA	2:C:120:GLU:CG	2.42	0.46
1:E:7:DC:H2"	1:E:8:DT:C5'	2.45	0.46
2:B:25:THR:O	2:B:29:VAL:HG22	2.16	0.46
2:D:2:ASN:HD22	2:D:3:LEU:H	1.57	0.46
2:B:40:TYR:CE2	2:B:45:THR:HA	2.50	0.46
2:C:53:ILE:HA	2:C:56:ILE:HD12	1.97	0.46
2:A:167:ASN:OD1	2:A:169:ASN:N	2.49	0.46
2:D:168:ILE:CG2	2:D:169:ASN:N	2.78	0.46
2:B:168:ILE:HG23	2:B:169:ASN:N	2.31	0.46
2:C:52:GLU:O	2:C:56:ILE:HG13	2.16	0.46
2:C:64:GLN:O	2:C:68:GLU:HG2	2.16	0.46
2:C:106:TYR:O	2:C:112:ILE:HD13	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:110:ASN:O	2:C:114:GLU:HG2	2.16	0.46
1:E:27:DT:H2"	1:E:28:DC:C6	2.50	0.45
2:D:117:ASN:O	2:D:120:GLU:HG3	2.16	0.45
2:A:125:ASP:C	2:A:127:TYR:N	2.69	0.45
2:C:38:ASN:ND2	2:C:42:HIS:CE1	2.85	0.45
2:A:43:PHE:O	2:A:44:LYS:C	2.54	0.45
2:A:136:LEU:HD12	2:A:136:LEU:C	2.37	0.45
2:B:116:MET:HA	2:B:116:MET:CE	2.46	0.45
2:B:175:MET:O	2:B:178:PHE:HB3	2.16	0.45
2:B:64:GLN:HE22	2:B:89:THR:HB	1.81	0.45
2:D:56:ILE:O	2:D:60:LYS:HG3	2.16	0.45
1:F:20:DC:H2"	1:F:21:DG:C8	2.52	0.45
2:D:62:GLN:OE1	2:D:62:GLN:HA	2.16	0.45
2:A:154:ASN:HD22	2:C:163:THR:HG22	1.76	0.45
2:B:97:ASN:CG	2:B:98:ALA:H	2.20	0.45
2:D:64:GLN:HG2	2:D:68:GLU:HG3	1.98	0.45
2:A:54:LEU:CD1	2:A:95:LEU:HD11	2.46	0.45
2:B:174:LEU:HD12	2:D:151:ILE:CG1	2.46	0.45
1:E:11:DT:OP2	2:D:2:ASN:ND2	2.50	0.45
2:A:121:ASN:O	2:A:124:ILE:HG22	2.16	0.45
2:A:162:PHE:CE2	2:C:157:ASN:OD1	2.69	0.45
2:B:154:ASN:HD22	2:D:163:THR:CG2	2.29	0.45
2:D:75:ASN:O	2:D:78:LYS:HB2	2.16	0.45
2:D:99:ILE:HG12	2:D:99:ILE:H	1.64	0.45
2:C:183:LEU:O	2:C:184:ASN:C	2.55	0.45
2:C:126:ALA:O	2:C:130:ILE:HG12	2.17	0.44
2:C:166:GLN:HB3	2:C:170:GLU:OE1	2.16	0.44
2:A:121:ASN:HA	2:A:124:ILE:HB	1.99	0.44
2:D:64:GLN:HE21	2:D:85:LEU:HD21	1.82	0.44
2:C:71:LYS:HZ2	2:C:71:LYS:HA	1.82	0.44
2:B:44:LYS:H	2:B:44:LYS:CE	2.30	0.44
2:A:163:THR:O	2:A:163:THR:CG2	2.65	0.44
2:A:169:ASN:HA	2:A:172:ILE:HG22	1.99	0.44
2:B:52:GLU:O	2:B:56:ILE:HG12	2.17	0.44
2:D:105:GLU:O	2:D:105:GLU:HG2	2.18	0.44
2:A:163:THR:C	2:A:165:GLU:OE2	2.56	0.44
2:B:174:LEU:HD12	2:D:151:ILE:HG12	2.00	0.44
2:C:93:TYR:N	2:C:94:PRO:CD	2.80	0.44
2:D:128:HIS:HA	2:D:149:SER:OG	2.18	0.44
2:D:165:GLU:CD	2:D:165:GLU:H	2.20	0.44
2:B:108:LYS:HD3	2:B:108:LYS:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:41:TYR:CD1	2:D:41:TYR:C	2.91	0.44
2:A:61:TRP:HZ2	2:A:82:TYR:CE1	2.36	0.43
2:B:183:LEU:O	2:B:186:LEU:HB2	2.18	0.43
2:D:79:PHE:CD2	2:D:183:LEU:HD21	2.53	0.43
1:F:25:DG:H2"	1:F:26:DG:O4'	2.18	0.43
2:A:75:ASN:OD1	2:A:134:GLY:N	2.51	0.43
2:A:4:LYS:HG3	2:A:42:HIS:CG	2.53	0.43
2:A:183:LEU:HD12	2:A:183:LEU:HA	1.77	0.43
2:C:74:THR:OG1	2:C:77:GLU:HB2	2.18	0.43
1:F:7:DC:H2'	1:F:8:DT:H71	2.01	0.43
2:A:75:ASN:HD22	2:A:75:ASN:HA	1.52	0.43
2:A:97:ASN:HB2	2:C:104:THR:HG21	2.01	0.43
2:B:83:ASN:OD1	2:B:156:VAL:HG21	2.17	0.43
2:B:100:ILE:HD11	2:D:162:PHE:CZ	2.54	0.43
2:D:16:ILE:HG13	2:D:95:LEU:HD23	2.00	0.43
2:D:54:LEU:HD11	2:D:99:ILE:CD1	2.48	0.43
2:B:172:ILE:O	2:B:172:ILE:HG12	2.17	0.43
2:C:131:PHE:CB	2:C:145:VAL:HG13	2.47	0.43
1:E:16:DC:H2"	1:E:17:DG:C8	2.53	0.43
2:A:29:VAL:HG12	2:A:34:SER:O	2.19	0.43
2:A:55:ASN:O	2:A:56:ILE:C	2.57	0.43
2:D:114:GLU:C	2:D:116:MET:H	2.22	0.43
2:A:29:VAL:HG11	2:A:35:SER:HA	1.99	0.43
2:B:14:LEU:HB3	2:B:23:THR:CG2	2.49	0.43
2:C:56:ILE:HG22	2:C:60:LYS:HZ1	1.77	0.43
2:C:65:TRP:HA	2:C:65:TRP:CE3	2.53	0.43
2:C:74:THR:O	2:C:78:LYS:HG2	2.19	0.43
2:C:112:ILE:HD12	2:C:112:ILE:N	2.30	0.43
2:A:14:LEU:HD21	2:A:27:GLU:HG2	2.00	0.43
2:C:93:TYR:CE1	2:C:157:ASN:ND2	2.85	0.43
1:F:26:DG:H2'	2:D:40:TYR:CE2	2.54	0.43
2:B:171:ARG:C	2:B:173:LYS:N	2.71	0.43
2:C:57:GLU:HG3	2:C:92:TYR:H	1.84	0.43
2:A:155:ALA:HB2	2:C:159:ILE:HD11	1.99	0.43
2:A:54:LEU:HD12	2:A:54:LEU:HA	1.72	0.42
2:B:177:LYS:O	2:B:180:GLN:HB3	2.18	0.42
2:D:103:TYR:O	2:D:107:TYR:N	2.48	0.42
2:A:117:ASN:HA	2:A:120:GLU:CG	2.50	0.42
2:A:136:LEU:C	2:A:138:GLY:N	2.73	0.42
2:A:146:ASN:HA	2:A:149:SER:OG	2.19	0.42
2:B:173:LYS:NZ	2:B:173:LYS:HA	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:38:ASN:HD21	2:C:42:HIS:HE1	1.67	0.42
2:C:118:LYS:CG	2:C:119:LEU:N	2.82	0.42
2:D:3:LEU:HA	2:D:3:LEU:HD12	1.63	0.42
2:B:87:LEU:O	2:B:168:ILE:HD11	2.20	0.42
2:B:163:THR:C	2:B:165:GLU:OE2	2.58	0.42
2:D:7:ILE:HG21	2:D:39:LEU:HD23	2.00	0.42
2:C:70:ILE:C	2:C:72:ALA:H	2.22	0.42
2:D:109:THR:O	2:D:113:ASN:HB2	2.20	0.42
2:A:96:GLN:O	2:A:99:ILE:HB	2.19	0.42
2:C:38:ASN:ND2	2:C:42:HIS:HE1	2.18	0.42
2:C:64:GLN:HE22	2:C:89:THR:CB	2.33	0.42
2:C:65:TRP:O	2:C:69:GLN:HG2	2.20	0.42
2:D:103:TYR:HD2	2:D:116:MET:CG	2.32	0.42
2:A:118:LYS:HB3	2:A:118:LYS:NZ	2.32	0.42
2:B:171:ARG:C	2:B:173:LYS:H	2.23	0.42
2:D:106:TYR:C	2:D:108:LYS:H	2.23	0.42
2:D:132:LYS:O	2:D:135:ASN:HB2	2.20	0.42
2:D:135:ASN:OD1	2:D:141:SER:HA	2.20	0.42
1:E:27:DT:H2"	1:E:28:DC:H6	1.85	0.42
2:B:159:ILE:O	2:B:163:THR:HG23	2.20	0.42
2:C:168:ILE:HG23	2:C:169:ASN:N	2.35	0.42
2:D:41:TYR:HD1	2:D:42:HIS:CD2	2.37	0.42
2:D:120:GLU:C	2:D:122:LYS:N	2.72	0.42
1:F:25:DG:H2"	1:F:26:DG:H5'	2.02	0.41
2:C:74:THR:O	2:C:77:GLU:HB3	2.20	0.41
2:A:184:ASN:O	2:A:185:GLY:C	2.59	0.41
2:C:51:LEU:HA	2:C:51:LEU:HD23	1.82	0.41
1:F:18:DA:C1'	1:F:19:DT:H5"	2.50	0.41
2:A:99:ILE:HG23	2:A:116:MET:CE	2.50	0.41
2:B:44:LYS:CD	2:B:44:LYS:N	2.82	0.41
2:C:79:PHE:O	2:C:80:TYR:C	2.58	0.41
2:D:60:LYS:HG3	2:D:60:LYS:H	1.56	0.41
1:E:11:DT:H6	2:D:38:ASN:HD22	1.68	0.41
2:A:29:VAL:HG11	2:A:35:SER:CA	2.51	0.41
2:C:166:GLN:OE1	2:C:170:GLU:CD	2.58	0.41
2:A:6:LYS:HD2	2:A:32:SER:HA	2.03	0.41
2:A:7:ILE:HG21	2:A:39:LEU:HD13	2.02	0.41
2:A:112:ILE:O	2:A:116:MET:HG3	2.20	0.41
2:D:18:ASN:OD1	2:D:18:ASN:N	2.52	0.41
2:D:108:LYS:HD2	2:D:109:THR:HG23	2.01	0.41
2:B:107:TYR:HB3	2:B:108:LYS:HZ2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:169:ASN:HD22	2:B:169:ASN:HA	1.57	0.41
2:C:75:ASN:ND2	2:C:134:GLY:HA2	2.35	0.41
1:E:25:DG:OP1	2:C:24:THR:HA	2.21	0.41
2:A:51:LEU:HD13	2:A:51:LEU:HA	1.86	0.41
2:B:52:GLU:OE1	2:B:52:GLU:HA	2.20	0.41
2:B:73:LYS:H	2:B:77:GLU:CD	2.21	0.41
2:D:93:TYR:N	2:D:94:PRO:CD	2.84	0.41
2:D:100:ILE:CG2	2:D:101:GLU:N	2.83	0.41
2:A:66:LYS:HA	2:A:69:GLN:NE2	2.13	0.41
2:A:93:TYR:N	2:A:94:PRO:CD	2.84	0.41
2:B:107:TYR:HB3	2:B:108:LYS:HZ1	1.83	0.41
2:A:103:TYR:O	2:A:107:TYR:HB2	2.21	0.41
2:C:102:PHE:HE1	2:C:112:ILE:CG2	2.26	0.41
2:C:137:ASN:C	2:C:139:GLU:N	2.74	0.41
1:E:8:DT:C6	1:E:9:DT:H72	2.55	0.41
2:C:110:ASN:HA	2:C:113:ASN:CB	2.50	0.41
2:D:85:LEU:HA	2:D:85:LEU:HD12	1.84	0.41
1:F:11:DT:OP2	2:C:42:HIS:CE1	2.74	0.40
2:B:32:SER:O	2:B:33:GLU:HB2	2.21	0.40
2:B:97:ASN:CG	2:B:98:ALA:N	2.74	0.40
2:C:111:SER:OG	2:C:112:ILE:HD12	2.20	0.40
2:A:30:LYS:HB3	2:A:30:LYS:HE2	1.80	0.40
2:A:44:LYS:HE3	2:A:44:LYS:HB2	1.95	0.40
2:B:114:GLU:HG2	2:B:114:GLU:H	1.72	0.40
2:D:74:THR:HG23	2:D:77:GLU:OE1	2.21	0.40
1:E:8:DT:H2'	1:E:9:DT:H72	2.04	0.40
2:A:32:SER:O	2:A:33:GLU:HB2	2.21	0.40
2:B:184:ASN:C	2:B:186:LEU:H	2.25	0.40
2:C:36:LYS:HD3	2:C:36:LYS:HA	1.85	0.40
2:C:131:PHE:HB3	2:C:145:VAL:HG13	2.04	0.40
2:C:129:VAL:HG12	2:C:130:ILE:N	2.36	0.40
2:D:106:TYR:C	2:D:108:LYS:N	2.74	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
2	A	186/194 (96%)	150 (81%)	30 (16%)	6 (3%)	4 16
2	B	186/194 (96%)	166 (89%)	18 (10%)	2 (1%)	14 42
2	C	186/194 (96%)	152 (82%)	26 (14%)	8 (4%)	2 10
2	D	183/194 (94%)	153 (84%)	25 (14%)	5 (3%)	5 19
All	All	741/776 (96%)	621 (84%)	99 (13%)	21 (3%)	5 19

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	143	ASN
2	A	187	SER
2	C	108	LYS
2	C	164	HIS
2	C	166	GLN
2	C	184	ASN
2	D	68	GLU
2	C	165	GLU
2	C	185	GLY
2	D	113	ASN
2	D	164	HIS
2	A	20	TYR
2	A	113	ASN
2	B	164	HIS
2	C	110	ASN
2	A	183	LEU
2	B	92	TYR
2	D	67	LYS
2	D	115	LYS
2	A	185	GLY
2	C	71	LYS

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
2	A	171/177 (97%)	157 (92%)	14 (8%)	11 32
2	B	171/177 (97%)	144 (84%)	27 (16%)	2 8
2	C	171/177 (97%)	155 (91%)	16 (9%)	8 26
2	D	168/177 (95%)	146 (87%)	22 (13%)	4 12
All	All	681/708 (96%)	602 (88%)	79 (12%)	5 16

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	5	ASP
2	A	51	LEU
2	A	54	LEU
2	A	62	GLN
2	A	68	GLU
2	A	73	LYS
2	A	75	ASN
2	A	90	GLU
2	A	124	ILE
2	A	135	ASN
2	A	157	ASN
2	A	168	ILE
2	A	172	ILE
2	A	183	LEU
2	B	41	TYR
2	B	44	LYS
2	B	47	GLU
2	B	54	LEU
2	B	58	GLU
2	B	60	LYS
2	B	66	LYS
2	B	68	GLU
2	B	86	SER
2	B	87	LEU
2	B	90	GLU
2	B	95	LEU
2	B	104	THR
2	B	109	THR
2	B	116	MET
2	B	119	LEU
2	B	145	VAL

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Mol	Chain	Res	Type
2	B	146	ASN
2	B	157	ASN
2	B	161	THR
2	B	164	HIS
2	B	165	GLU
2	B	167	ASN
2	B	169	ASN
2	B	172	ILE
2	B	173	LYS
2	B	188	LYS
2	C	13	GLU
2	C	18	ASN
2	C	35	SER
2	C	49	LEU
2	C	57	GLU
2	C	64	GLN
2	C	66	LYS
2	C	71	LYS
2	C	85	LEU
2	C	88	THR
2	C	108	LYS
2	C	113	ASN
2	C	133	GLU
2	C	146	ASN
2	C	167	ASN
2	C	184	ASN
2	D	5	ASP
2	D	10	VAL
2	D	13	GLU
2	D	18	ASN
2	D	27	GLU
2	D	39	LEU
2	D	57	GLU
2	D	58	GLU
2	D	73	LYS
2	D	93	TYR
2	D	99	ILE
2	D	100	ILE
2	D	107	TYR
2	D	108	LYS
2	D	124	ILE
2	D	162	PHE

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Mol	Chain	Res	Type
2	D	165	GLU
2	D	166	GLN
2	D	167	ASN
2	D	168	ILE
2	D	180	GLN
2	D	184	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	2	ASN
2	A	55	ASN
2	A	62	GLN
2	A	64	GLN
2	A	69	GLN
2	A	96	GLN
2	A	97	ASN
2	A	113	ASN
2	A	117	ASN
2	A	128	HIS
2	A	135	ASN
2	A	154	ASN
2	A	176	ASN
2	B	38	ASN
2	B	55	ASN
2	B	64	GLN
2	B	69	GLN
2	B	117	ASN
2	B	128	HIS
2	B	137	ASN
2	B	154	ASN
2	B	169	ASN
2	B	180	GLN
2	B	189	HIS
2	C	42	HIS
2	C	48	ASN
2	C	64	GLN
2	C	69	GLN
2	C	97	ASN
2	C	113	ASN
2	C	135	ASN
2	C	146	ASN

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Mol	Chain	Res	Type
2	C	154	ASN
2	C	157	ASN
2	C	164	HIS
2	C	169	ASN
2	C	176	ASN
2	C	180	GLN
2	D	2	ASN
2	D	38	ASN
2	D	64	GLN
2	D	75	ASN
2	D	137	ASN
2	D	184	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

5 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	$\#\|Z\| > 2$
3	SO4	D	899	-	4,4,4	0.25	0	6,6,6	0.05	0
3	SO4	C	699	-	4,4,4	0.27	0	6,6,6	0.05	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	SO4	B	399	-	4,4,4	0.27	0	6,6,6	0.05	0
3	SO4	A	999	-	4,4,4	0.27	0	6,6,6	0.05	0
3	SO4	B	299	-	4,4,4	0.26	0	6,6,6	0.07	0

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 (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	E	28/28 (100%)	0.30	0 100 100	44, 59, 68, 69	0
1	F	28/28 (100%)	0.29	0 100 100	47, 60, 72, 77	0
2	A	188/194 (96%)	0.81	20 (10%) 6 4	59, 93, 148, 168	0
2	B	188/194 (96%)	0.59	7 (3%) 41 37	41, 66, 118, 146	0
2	C	188/194 (96%)	0.70	15 (7%) 12 9	45, 87, 134, 153	0
2	D	185/194 (95%)	0.70	9 (4%) 29 26	41, 70, 133, 163	0
All	All	805/832 (96%)	0.67	51 (6%) 20 16	41, 77, 135, 168	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	164	HIS	8.8
2	D	115	LYS	5.9
2	B	164	HIS	5.2
2	D	107	TYR	5.2
2	C	164	HIS	5.0
2	D	103	TYR	4.4
2	C	103	TYR	4.0
2	D	112	ILE	3.9
2	C	107	TYR	3.6
2	C	86	SER	3.4
2	A	131	PHE	3.4
2	A	106	TYR	3.3
2	C	131	PHE	3.2
2	D	106	TYR	3.2
2	C	165	GLU	3.1
2	B	103	TYR	3.0
2	D	113	ASN	2.9
2	A	103	TYR	2.8
2	C	100	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
2	A	163	THR	2.7
2	A	123	TYR	2.6
2	C	140	TRP	2.6
2	A	148	VAL	2.6
2	A	73	LYS	2.5
2	D	114	GLU	2.5
2	A	186	LEU	2.5
2	B	189	HIS	2.5
2	A	92	TYR	2.5
2	A	124	ILE	2.4
2	A	84	GLU	2.4
2	B	86	SER	2.4
2	A	162	PHE	2.3
2	D	117	ASN	2.3
2	C	142	ILE	2.3
2	C	147	ALA	2.3
2	A	151	ILE	2.3
2	C	182	PHE	2.2
2	A	130	ILE	2.2
2	A	65	TRP	2.2
2	A	49	LEU	2.2
2	C	81	LEU	2.2
2	A	181	ILE	2.2
2	A	39	LEU	2.2
2	C	102	PHE	2.2
2	B	40	TYR	2.2
2	C	162	PHE	2.1
2	B	136	LEU	2.1
2	A	145	VAL	2.1
2	D	136	LEU	2.1
2	C	73	LYS	2.0
2	B	163	THR	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 monosaccharides 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
3	SO4	B	399	5/5	0.59	0.33	189,189,190,190	0
3	SO4	A	999	5/5	0.63	0.24	198,198,198,198	0
3	SO4	B	299	5/5	0.65	0.26	175,176,176,176	0
3	SO4	D	899	5/5	0.77	0.26	188,188,189,189	0
3	SO4	C	699	5/5	0.84	0.21	163,164,164,164	0

6.5 Other polymers (i)

There are no such residues in this entry.