Full wwPDB X-ray Structure Validation Report (i)

Aug 23, 2023 – 05:53 AM EDT

PDB ID	:	3BTJ
Title	:	crystal structure of QacR(E58Q) bound to dequalinium
Authors	:	Schumacher, M.A.; Schuman, J.T.; Brennan, R.G.
Deposited on	:	2007-12-28
Resolution	:	2.98 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

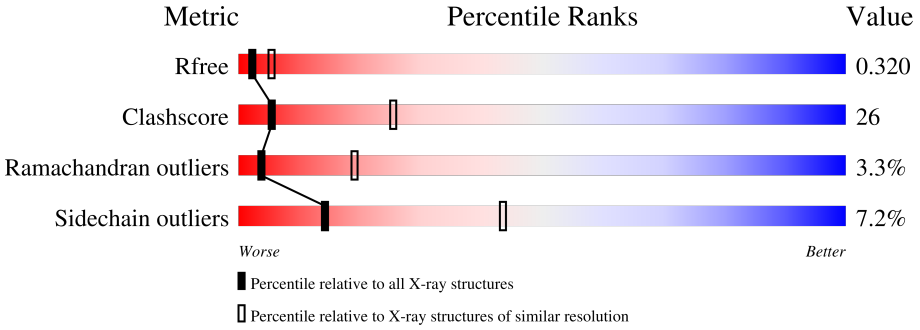
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.98 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	2754 (3.00-2.96)
Clashscore	141614	3103 (3.00-2.96)
Ramachandran outliers	138981	2993 (3.00-2.96)
Sidechain outliers	138945	2996 (3.00-2.96)

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%

Mol	Chain	Length	Quality of chain
1	A	188	61% 35%
1	B	188	43% 45% 9%
1	D	188	48% 45% 5%
1	E	188	55% 39% 5%

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
3	DEQ	A	201	-	X	-	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6313 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.

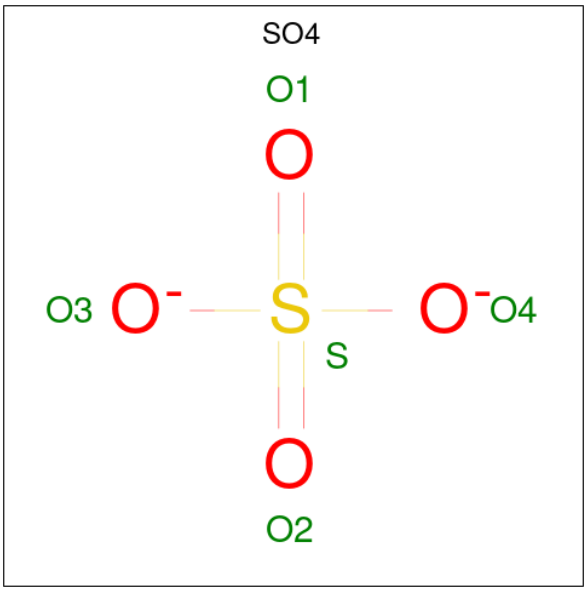
- Molecule 1 is a protein called HTH-type transcriptional regulator qacR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	186	1547	998	253	294	2	0	0	0
1	D	186	1547	998	253	294	2	0	0	0
1	A	186	1547	998	253	294	2	0	0	0
1	E	186	1547	998	253	294	2	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	58	GLN	GLU	engineered mutation	UNP P0A0N3
B	72	ALA	CYS	engineered mutation	UNP P0A0N3
B	141	SER	CYS	engineered mutation	UNP P0A0N3
D	58	GLN	GLU	engineered mutation	UNP P0A0N3
D	72	ALA	CYS	engineered mutation	UNP P0A0N3
D	141	SER	CYS	engineered mutation	UNP P0A0N3
A	58	GLN	GLU	engineered mutation	UNP P0A0N3
A	72	ALA	CYS	engineered mutation	UNP P0A0N3
A	141	SER	CYS	engineered mutation	UNP P0A0N3
E	58	GLN	GLU	engineered mutation	UNP P0A0N3
E	72	ALA	CYS	engineered mutation	UNP P0A0N3
E	141	SER	CYS	engineered mutation	UNP P0A0N3

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	B	1	5	4	1	0	0
2	D	1	5	4	1	0	0
2	D	1	5	4	1	0	0
2	D	1	5	4	1	0	0
2	D	1	5	4	1	0	0
2	D	1	5	4	1	0	0
2	A	1	5	4	1	0	0
2	A	1	5	4	1	0	0
2	A	1	5	4	1	0	0
2	A	1	5	4	1	0	0
2	A	1	5	4	1	0	0
2	A	1	5	4	1	0	0
2	E	1	5	4	1	0	0
2	E	1	5	4	1	0	0

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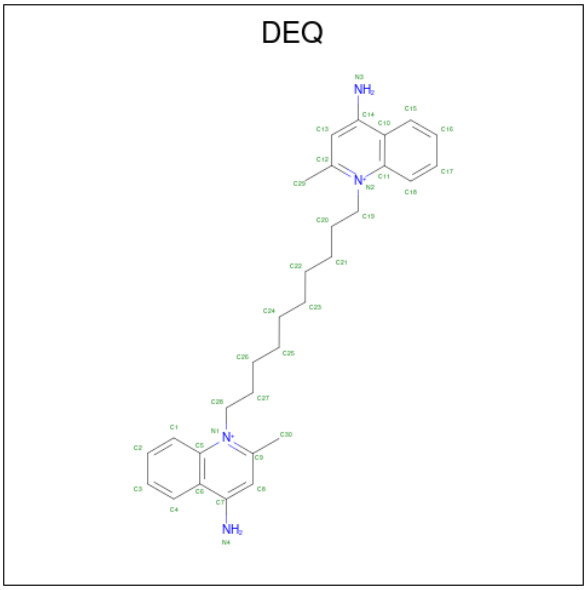
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0

- Molecule 3 is DEQUALINIUM (three-letter code: DEQ) (formula: $C_{30}H_{40}N_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N 34 30 4	0	0

- Molecule 4 is water.

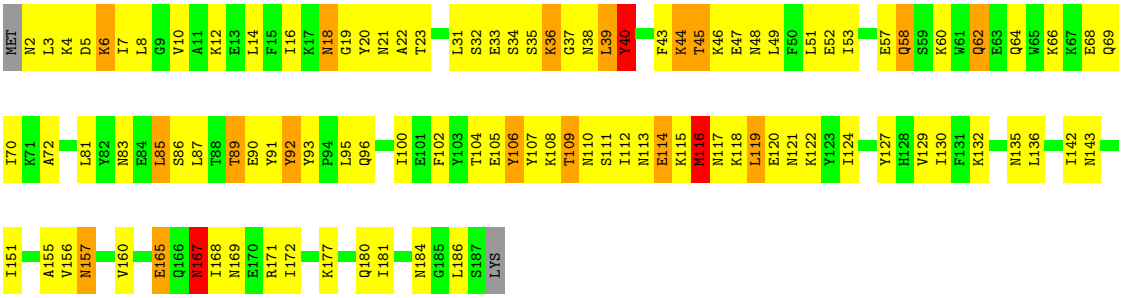
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total O 1 1	0	0
4	A	4	Total O 4 4	0	0
4	E	1	Total O 1 1	0	0

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. 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. 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.

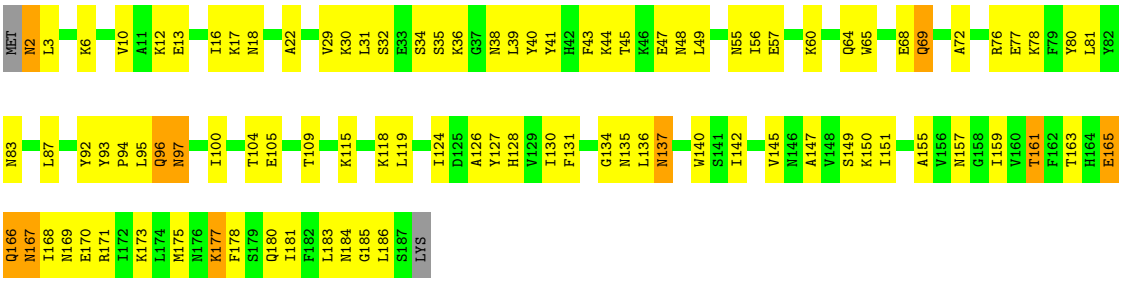
• Molecule 1: HTH-type transcriptional regulator qacR

Chain B:



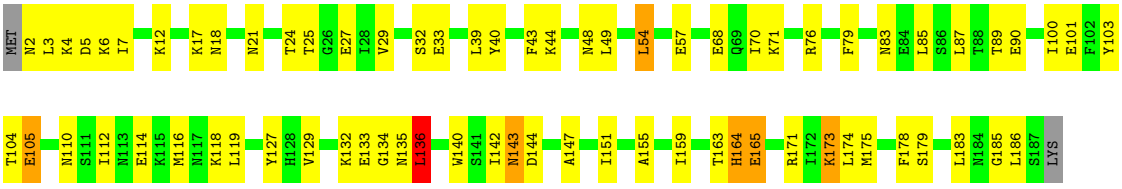
• Molecule 1: HTH-type transcriptional regulator qacR

Chain D:



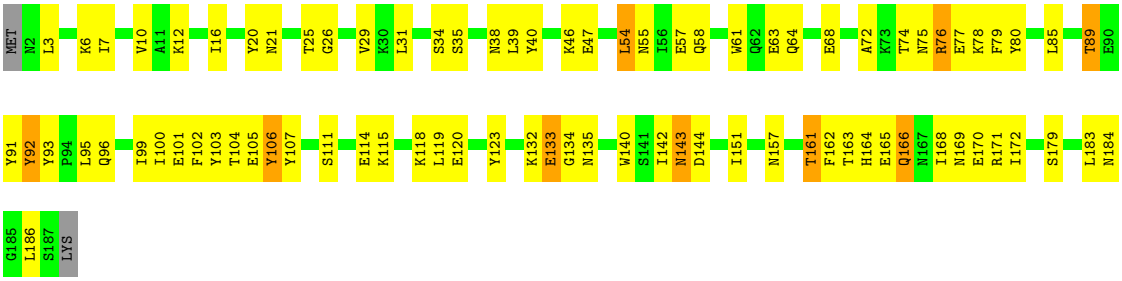
• Molecule 1: HTH-type transcriptional regulator qacR

Chain A:



• Molecule 1: HTH-type transcriptional regulator qacR

Chain E:


MET
N2
L3
K6
I7
V10
A11
K12
I16
Y20
N21
T25
G26
V29
K30
L31
S34
S35
N38
L39
Y40
K46
E47
L54
N55
I56
E57
Q58
W61
Q62
E63
Q64
E68
A72
K73
T74
N75
R76
E77
K78
F79
Y80
L85
T89
E90
Y91
Y92
Y93
P94
L95
Q96
I99
I100
E101
F102
Y103
T104
E105
Y106
Y107
S111
E114
K115
K118
L119
E120
Y123
K132
E133
G134
N135
W140
S141
I142
N143
D144
I151
N157
T161
F162
T163
H164
E165
Q166
N167
I168
N169
E170
R171
I172
S179
L183
N184
G185
L186
S187
LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α, β, γ	171.90Å 171.90Å 94.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	76.88 – 2.98 76.88 – 2.98	Depositor EDS
% Data completeness (in resolution range)	99.3 (76.88-2.98) 99.4 (76.88-2.98)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	1.98 (at 2.96Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.216 , 0.264 0.297 , 0.320	Depositor DCC
R_{free} test set	1439 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å^2)	77.6	Xtriage
Anisotropy	0.170	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 85.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	6313	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% 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: DEQ, 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	A	0.44	0/1578	0.61	0/2126
1	B	0.38	0/1578	0.56	0/2126
1	D	0.40	0/1578	0.60	0/2126
1	E	0.42	0/1578	0.60	0/2126
All	All	0.41	0/6312	0.59	0/8504

There are no bond length outliers.

There are no bond angle outliers.

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	1547	0	1538	72	0
1	B	1547	0	1538	116	0
1	D	1547	0	1538	77	2
1	E	1547	0	1538	78	0
2	A	30	0	0	2	0
2	B	5	0	0	0	0
2	D	25	0	0	0	1
2	E	25	0	0	2	0
3	A	34	0	40	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	4	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
All	All	6313	0	6192	326	2

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 26.

All (326) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:THR:HG22	1:B:91:TYR:H	1.16	1.09
1:D:142:ILE:HD11	1:D:186:LEU:HD13	1.35	1.05
1:A:135:ASN:HD21	1:A:142:ILE:H	0.95	0.92
1:D:157:ASN:O	1:D:161:THR:HG23	1.78	0.83
1:E:3:LEU:O	1:E:7:ILE:HG12	1.77	0.83
1:B:3:LEU:HD11	1:B:38:ASN:HD22	1.44	0.82
1:E:142:ILE:HD11	1:E:186:LEU:HD13	1.62	0.81
1:E:143:ASN:ND2	1:E:144:ASP:H	1.79	0.79
1:A:135:ASN:ND2	1:A:142:ILE:H	1.78	0.79
1:B:66:LYS:HA	1:B:69:GLN:HE21	1.47	0.79
1:B:96:GLN:HG3	1:B:157:ASN:HD21	1.49	0.78
1:B:87:LEU:HD23	1:B:160:VAL:HG13	1.66	0.78
1:D:76:ARG:HG3	1:D:183:LEU:HD13	1.68	0.76
1:B:167:ASN:HD22	1:B:168:ILE:N	1.85	0.74
1:B:89:THR:HG22	1:B:91:TYR:N	1.99	0.74
1:E:68:GLU:HG2	1:E:85:LEU:HD21	1.69	0.74
1:A:135:ASN:HD21	1:A:142:ILE:N	1.79	0.74
1:E:157:ASN:O	1:E:161:THR:HG23	1.88	0.73
1:D:167:ASN:ND2	1:D:169:ASN:H	1.84	0.73
1:B:10:VAL:HG13	1:B:31:LEU:HD23	1.69	0.73
1:B:36:LYS:H	1:B:36:LYS:HD3	1.54	0.73
1:E:3:LEU:HD13	1:E:38:ASN:ND2	2.04	0.73
1:B:81:LEU:HG	1:B:85:LEU:CD2	2.20	0.72
1:B:177:LYS:O	1:B:181:ILE:HG13	1.89	0.72
1:A:173:LYS:HD3	1:A:173:LYS:C	2.10	0.71
1:B:118:LYS:HA	1:B:121:ASN:ND2	2.05	0.71
1:D:64:GLN:O	1:D:68:GLU:HG3	1.91	0.70
1:B:38:ASN:HB2	1:B:39:LEU:HD22	1.74	0.70
1:D:17:LYS:HE3	1:D:18:ASN:OD1	1.92	0.70
1:E:58:GLN:HB3	1:E:123:TYR:OH	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:LYS:HD2	2:A:595:SO4:O3	1.91	0.69
1:B:89:THR:HG22	1:B:90:GLU:N	2.09	0.68
1:B:177:LYS:HE3	1:B:181:ILE:HD11	1.75	0.68
1:E:25:THR:HG21	1:E:40:TYR:OH	1.94	0.68
1:B:39:LEU:HD22	1:B:39:LEU:N	2.09	0.67
1:A:142:ILE:HD11	1:A:186:LEU:HD13	1.77	0.67
1:B:100:ILE:O	1:B:104:THR:HG23	1.95	0.66
1:A:134:GLY:HA3	1:A:140:TRP:CE2	2.30	0.66
1:B:89:THR:HG22	1:B:90:GLU:H	1.59	0.66
1:B:109:THR:HG23	1:B:112:ILE:HG12	1.77	0.66
1:A:143:ASN:HD22	1:A:144:ASP:N	1.94	0.65
1:B:45:THR:HG23	1:B:48:ASN:HB2	1.79	0.64
1:D:177:LYS:O	1:D:181:ILE:HG13	1.96	0.64
1:E:3:LEU:HD13	1:E:38:ASN:HD21	1.62	0.64
1:B:6:LYS:HE3	1:B:6:LYS:HA	1.79	0.64
1:A:76:ARG:HG3	1:A:183:LEU:HD23	1.78	0.64
1:E:163:THR:HA	1:E:165:GLU:OE1	1.98	0.64
1:A:89:THR:HB	3:A:201:DEQ:HN31	1.63	0.64
1:B:2:ASN:O	1:B:6:LYS:HB2	1.98	0.63
1:A:17:LYS:HG2	1:A:18:ASN:OD1	1.98	0.63
1:D:185:GLY:HA2	1:E:184:ASN:OD1	1.97	0.63
1:B:181:ILE:HD13	1:A:186:LEU:HD21	1.80	0.63
1:B:156:VAL:O	1:B:160:VAL:HG23	1.98	0.62
1:B:177:LYS:HE2	1:A:144:ASP:OD2	2.00	0.62
1:D:43:PHE:O	1:D:44:LYS:HB2	2.00	0.62
1:D:56:ILE:HG22	1:D:60:LYS:HD2	1.80	0.61
1:A:134:GLY:HA3	1:A:140:TRP:CZ2	2.35	0.61
1:B:83:ASN:O	1:B:86:SER:HB2	2.00	0.61
1:B:106:TYR:O	1:B:112:ILE:HG13	2.01	0.61
1:D:167:ASN:HD22	1:D:168:ILE:N	1.99	0.61
1:B:12:LYS:O	1:B:16:ILE:HG13	2.01	0.60
1:A:129:VAL:O	1:A:133:GLU:HG2	2.01	0.60
1:A:57:GLU:HB3	3:A:201:DEQ:H192	1.83	0.60
1:D:2:ASN:CG	1:D:3:LEU:H	2.03	0.60
1:D:39:LEU:HD21	1:D:49:LEU:HD22	1.83	0.60
1:A:164:HIS:HA	1:A:171:ARG:NH2	2.17	0.60
1:B:10:VAL:HG21	1:B:32:SER:HB2	1.84	0.60
1:B:167:ASN:HD22	1:B:167:ASN:C	2.03	0.59
1:B:62:GLN:HE21	1:B:122:LYS:HB3	1.67	0.59
1:E:72:ALA:HB3	1:E:78:LYS:HG2	1.85	0.59
1:B:115:LYS:C	1:B:117:ASN:H	2.06	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:100:ILE:O	1:E:104:THR:HG23	2.03	0.59
1:D:165:GLU:HB3	1:E:103:TYR:CE1	2.37	0.59
1:E:64:GLN:HE22	1:E:89:THR:HB	1.68	0.59
1:D:2:ASN:ND2	1:D:3:LEU:N	2.51	0.58
1:D:3:LEU:O	1:D:3:LEU:HD13	2.03	0.58
1:B:39:LEU:HD22	1:B:39:LEU:H	1.68	0.58
1:E:20:TYR:CZ	1:E:46:LYS:HE2	2.38	0.58
1:D:65:TRP:HZ3	1:D:81:LEU:HD23	1.68	0.58
1:B:47:GLU:HB2	1:B:102:PHE:HE2	1.68	0.58
1:B:60:LYS:HD3	1:B:91:TYR:CZ	2.38	0.58
1:B:118:LYS:HA	1:B:121:ASN:HD22	1.68	0.58
1:D:55:ASN:OD1	1:D:119:LEU:HD21	2.02	0.58
1:B:167:ASN:ND2	1:B:169:ASN:H	2.02	0.58
1:B:100:ILE:CG2	1:A:100:ILE:HD12	2.34	0.57
1:D:45:THR:HG23	1:D:47:GLU:HG3	1.86	0.57
1:A:25:THR:O	1:A:29:VAL:HG23	2.05	0.57
1:B:21:ASN:HD21	1:B:105:GLU:CD	2.08	0.57
1:B:106:TYR:C	1:B:108:LYS:H	2.06	0.57
1:A:163:THR:O	1:A:165:GLU:N	2.38	0.57
1:B:36:LYS:HD3	1:B:36:LYS:N	2.20	0.57
1:D:165:GLU:HG2	1:D:166:GLN:H	1.70	0.57
1:D:134:GLY:HA3	1:D:140:TRP:CZ2	2.40	0.56
1:E:165:GLU:HB2	1:E:166:GLN:OE1	2.05	0.56
1:B:112:ILE:C	1:B:114:GLU:H	2.08	0.55
1:D:2:ASN:ND2	1:D:3:LEU:H	2.05	0.55
1:A:112:ILE:HD12	1:A:112:ILE:N	2.22	0.55
1:B:89:THR:CG2	1:B:91:TYR:H	2.06	0.55
1:D:167:ASN:HD22	1:D:167:ASN:C	2.10	0.55
1:D:76:ARG:O	1:D:80:TYR:HD2	1.90	0.55
1:B:3:LEU:HD21	1:B:34:SER:OG	2.06	0.55
1:D:45:THR:HG23	1:D:48:ASN:HB2	1.87	0.55
1:D:165:GLU:HG2	1:D:166:GLN:OE1	2.07	0.55
1:E:61:TRP:HH2	1:E:85:LEU:HB3	1.72	0.55
1:A:54:LEU:HB3	1:A:119:LEU:HD21	1.89	0.55
1:B:19:GLY:O	1:B:23:THR:HG22	2.06	0.54
1:B:8:LEU:HG	1:B:43:PHE:HZ	1.72	0.54
1:B:181:ILE:HD13	1:A:186:LEU:CD2	2.36	0.54
1:B:6:LYS:HE3	1:B:6:LYS:CA	2.37	0.54
1:E:57:GLU:HG3	1:E:95:LEU:HD12	1.88	0.54
1:B:60:LYS:HB3	1:B:91:TYR:CD1	2.42	0.54
1:D:100:ILE:O	1:D:104:THR:HG23	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:THR:OG1	3:A:201:DEQ:H151	2.07	0.54
1:B:81:LEU:HG	1:B:85:LEU:HD23	1.88	0.54
1:B:168:ILE:O	1:B:172:ILE:HG12	2.08	0.54
1:D:115:LYS:O	1:D:118:LYS:HB3	2.08	0.54
1:D:38:ASN:O	1:D:41:TYR:HB3	2.09	0.53
1:D:12:LYS:O	1:D:16:ILE:HG13	2.09	0.53
1:D:65:TRP:CZ3	1:D:81:LEU:HD23	2.44	0.53
1:B:7:ILE:HB	1:B:43:PHE:HE1	1.73	0.53
1:A:54:LEU:HG	3:A:201:DEQ:H232	1.91	0.53
1:A:147:ALA:O	1:A:151:ILE:HG13	2.09	0.53
1:E:92:TYR:CD2	1:E:123:TYR:CZ	2.97	0.53
1:A:100:ILE:HD13	3:A:201:DEQ:H21	1.91	0.53
1:E:74:THR:OG1	1:E:77:GLU:HG3	2.08	0.52
1:D:45:THR:CG2	1:D:47:GLU:HG3	2.39	0.52
1:B:106:TYR:HB3	1:B:112:ILE:HD11	1.90	0.52
1:B:45:THR:OG1	1:B:46:LYS:N	2.43	0.52
1:A:165:GLU:CD	1:A:165:GLU:H	2.13	0.52
1:D:175:MET:O	1:D:178:PHE:HB3	2.10	0.52
1:D:177:LYS:HB3	1:E:151:ILE:HD11	1.92	0.52
1:A:68:GLU:CD	1:A:71:LYS:HE2	2.30	0.52
1:B:114:GLU:OE2	1:B:115:LYS:HG2	2.10	0.52
1:B:132:LYS:HA	1:B:135:ASN:HD22	1.73	0.52
1:E:105:GLU:OE1	1:E:106:TYR:HE2	1.93	0.52
1:D:6:LYS:HG3	1:D:32:SER:HB2	1.91	0.51
1:D:128:HIS:ND1	1:D:145:VAL:HG12	2.25	0.51
1:D:124:ILE:HD12	1:D:150:LYS:HA	1.91	0.51
1:B:4:LYS:O	1:B:4:LYS:HD3	2.10	0.51
1:A:3:LEU:O	1:A:7:ILE:HG13	2.10	0.51
1:A:39:LEU:O	1:A:39:LEU:HD23	2.10	0.51
1:A:76:ARG:HG3	1:A:183:LEU:CD2	2.39	0.51
1:B:19:GLY:H	1:B:22:ALA:HB3	1.75	0.51
1:E:55:ASN:HD22	1:E:119:LEU:HD21	1.75	0.51
1:B:51:LEU:HD23	1:B:115:LYS:HG3	1.91	0.51
1:B:167:ASN:C	1:B:167:ASN:ND2	2.64	0.51
1:A:112:ILE:O	1:A:116:MET:HG3	2.11	0.51
1:E:168:ILE:HG23	1:E:169:ASN:N	2.25	0.51
1:D:34:SER:OG	1:D:35:SER:N	2.44	0.51
1:E:132:LYS:O	1:E:135:ASN:HB2	2.11	0.51
1:D:167:ASN:ND2	1:D:167:ASN:C	2.64	0.50
1:D:22:ALA:HB2	1:E:21:ASN:HB2	1.93	0.50
1:D:165:GLU:CB	1:E:103:TYR:CE1	2.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:HIS:HA	1:A:171:ARG:CZ	2.40	0.50
1:A:110:ASN:O	1:A:114:GLU:HB2	2.11	0.50
1:B:114:GLU:CD	1:B:115:LYS:HG2	2.32	0.50
1:E:12:LYS:O	1:E:16:ILE:HG13	2.12	0.50
1:E:68:GLU:HG2	1:E:85:LEU:HD11	1.94	0.49
1:B:8:LEU:HD21	1:B:52:GLU:HG2	1.92	0.49
1:D:180:GLN:HG2	1:D:184:ASN:ND2	2.28	0.49
1:A:103:TYR:O	1:A:105:GLU:N	2.43	0.49
1:A:179:SER:O	1:A:183:LEU:HB2	2.13	0.49
1:B:2:ASN:N	1:B:6:LYS:HZ2	2.10	0.49
1:B:36:LYS:HG2	1:B:37:GLY:N	2.27	0.49
1:B:112:ILE:O	1:B:116:MET:HB2	2.13	0.49
1:A:163:THR:HB	1:A:171:ARG:HD3	1.95	0.49
1:B:34:SER:HB3	1:B:38:ASN:CG	2.33	0.48
1:B:64:GLN:O	1:B:68:GLU:HG3	2.13	0.48
1:B:115:LYS:C	1:B:117:ASN:N	2.66	0.48
1:E:39:LEU:HD23	1:E:39:LEU:C	2.33	0.48
1:D:171:ARG:HG2	1:D:171:ARG:HH11	1.78	0.48
1:E:75:ASN:HD21	1:E:133:GLU:HB3	1.77	0.48
1:E:134:GLY:HA3	1:E:140:TRP:CE2	2.47	0.48
1:D:165:GLU:HG2	1:D:166:GLN:N	2.28	0.48
1:B:7:ILE:HD13	1:B:32:SER:OG	2.13	0.48
1:A:24:THR:OG1	1:A:27:GLU:HG3	2.14	0.48
1:E:68:GLU:CG	1:E:85:LEU:HD21	2.42	0.48
1:D:134:GLY:HA3	1:D:140:TRP:CE2	2.49	0.48
1:A:103:TYR:C	1:A:105:GLU:H	2.15	0.48
1:E:10:VAL:HG11	1:E:31:LEU:HB2	1.96	0.48
1:E:111:SER:O	1:E:115:LYS:HG3	2.12	0.48
1:D:65:TRP:O	1:D:69:GLN:HG2	2.14	0.48
1:B:39:LEU:N	1:B:39:LEU:CD2	2.77	0.47
1:B:132:LYS:O	1:B:135:ASN:HB2	2.14	0.47
1:D:87:LEU:HD13	1:D:171:ARG:HB3	1.96	0.47
1:E:165:GLU:O	1:E:166:GLN:O	2.32	0.47
1:E:179:SER:O	1:E:183:LEU:HB2	2.14	0.47
1:B:39:LEU:H	1:B:39:LEU:CD2	2.28	0.47
1:B:83:ASN:ND2	1:B:127:TYR:OH	2.47	0.47
1:A:83:ASN:ND2	1:A:127:TYR:OH	2.47	0.47
1:A:89:THR:CB	3:A:201:DEQ:H151	2.45	0.47
1:A:143:ASN:ND2	1:A:144:ASP:OD1	2.47	0.47
1:B:10:VAL:O	1:B:14:LEU:HD13	2.14	0.47
1:B:90:GLU:HG2	1:B:91:TYR:CD2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:LEU:HD23	1:A:39:LEU:C	2.35	0.47
1:B:18:ASN:HB3	1:B:22:ALA:CB	2.44	0.47
1:D:45:THR:CG2	1:D:48:ASN:HB2	2.45	0.47
1:A:68:GLU:OE2	1:A:71:LYS:HE2	2.14	0.47
1:A:163:THR:CG2	1:A:171:ARG:HD3	2.44	0.47
1:B:142:ILE:HD12	1:B:186:LEU:HD22	1.97	0.47
1:D:97:ASN:OD1	1:E:101:GLU:HG3	2.15	0.47
1:A:43:PHE:O	1:A:44:LYS:HB2	2.15	0.47
1:E:47:GLU:HB2	1:E:102:PHE:HE2	1.79	0.46
1:D:155:ALA:O	1:D:159:ILE:HG12	2.15	0.46
1:A:79:PHE:CD2	1:A:183:LEU:HD13	2.50	0.46
1:E:76:ARG:HG2	1:E:76:ARG:HH11	1.80	0.46
1:E:163:THR:O	1:E:171:ARG:HD3	2.15	0.46
1:A:173:LYS:HD3	1:A:173:LYS:O	2.15	0.46
1:E:55:ASN:ND2	1:E:119:LEU:HD21	2.29	0.46
1:B:37:GLY:O	1:B:38:ASN:C	2.54	0.46
1:B:120:GLU:O	1:B:124:ILE:HG23	2.15	0.46
1:E:143:ASN:HD22	1:E:144:ASP:H	1.60	0.46
1:B:100:ILE:HG21	1:A:100:ILE:HD12	1.97	0.46
3:A:201:DEQ:H202	3:A:201:DEQ:H181	1.98	0.45
1:D:72:ALA:HB1	1:D:77:GLU:HB3	1.98	0.45
1:D:39:LEU:HD23	1:D:43:PHE:HD1	1.81	0.45
1:D:57:GLU:HG3	1:D:95:LEU:HD12	1.97	0.45
1:A:136:LEU:N	1:A:136:LEU:CD1	2.80	0.45
1:D:100:ILE:HD11	1:E:162:PHE:CE2	2.51	0.45
1:A:2:ASN:O	1:A:5:ASP:N	2.50	0.45
1:B:91:TYR:O	1:B:93:TYR:N	2.47	0.45
1:E:96:GLN:O	1:E:100:ILE:HG22	2.17	0.45
1:E:143:ASN:CG	1:E:144:ASP:H	2.18	0.45
1:D:147:ALA:O	1:D:151:ILE:HG13	2.17	0.45
1:E:54:LEU:HD11	1:E:99:ILE:HG12	1.99	0.45
1:E:166:GLN:OE1	1:E:166:GLN:N	2.49	0.45
1:D:36:LYS:HG2	1:D:40:TYR:CE1	2.52	0.45
1:D:105:GLU:HG3	1:D:105:GLU:O	2.16	0.45
1:A:132:LYS:O	1:A:136:LEU:HD13	2.17	0.45
1:E:75:ASN:ND2	1:E:133:GLU:HB3	2.32	0.45
1:B:109:THR:O	1:B:112:ILE:HG12	2.17	0.44
1:D:135:ASN:C	1:D:137:ASN:H	2.20	0.44
1:A:21:ASN:ND2	1:A:101:GLU:OE1	2.50	0.44
1:A:143:ASN:HD22	1:A:144:ASP:H	1.62	0.44
1:B:151:ILE:CG2	1:A:178:PHE:HB2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:TYR:CZ	1:E:6:LYS:HD3	2.52	0.44
1:A:163:THR:O	1:A:164:HIS:C	2.56	0.44
1:D:170:GLU:OE2	1:D:173:LYS:HD3	2.16	0.44
1:B:89:THR:CG2	1:B:90:GLU:N	2.78	0.44
1:A:4:LYS:N	2:A:279:SO4:O3	2.50	0.44
1:A:143:ASN:ND2	1:A:143:ASN:H	2.15	0.44
1:E:96:GLN:CA	1:E:96:GLN:HE21	2.30	0.44
1:A:6:LYS:HE3	1:A:32:SER:HA	2.00	0.44
1:E:12:LYS:HD2	2:E:399:SO4:O3	2.18	0.44
1:D:96:GLN:HG2	1:D:161:THR:HG21	1.99	0.44
1:E:114:GLU:O	1:E:118:LYS:HG3	2.18	0.44
1:E:29:VAL:HG13	1:E:34:SER:O	2.18	0.43
1:B:40:TYR:O	1:B:44:LYS:HD2	2.17	0.43
1:B:49:LEU:O	1:B:53:ILE:HG12	2.19	0.43
1:E:103:TYR:O	1:E:107:TYR:HB3	2.17	0.43
1:B:6:LYS:HA	1:B:6:LYS:CE	2.46	0.43
1:D:127:TYR:O	1:D:131:PHE:CD2	2.72	0.43
1:B:44:LYS:HB2	1:B:48:ASN:ND2	2.34	0.43
1:B:70:ILE:C	1:B:72:ALA:H	2.21	0.43
1:D:161:THR:O	1:E:100:ILE:HD12	2.18	0.43
1:E:58:GLN:HB3	1:E:123:TYR:CZ	2.53	0.43
1:A:68:GLU:OE1	1:A:71:LYS:HE2	2.19	0.43
1:B:106:TYR:C	1:B:108:LYS:N	2.71	0.43
1:B:168:ILE:HA	1:B:171:ARG:HG3	2.00	0.43
1:A:165:GLU:O	1:A:165:GLU:HG2	2.18	0.43
1:E:76:ARG:HH11	1:E:76:ARG:CG	2.31	0.43
1:B:18:ASN:HB3	1:B:22:ALA:HB1	2.00	0.43
1:B:53:ILE:O	1:B:57:GLU:HG2	2.18	0.43
1:D:29:VAL:HG21	1:D:36:LYS:HA	2.00	0.43
1:D:93:TYR:N	1:D:94:PRO:CD	2.82	0.43
1:D:128:HIS:HA	1:D:149:SER:OG	2.18	0.43
1:B:20:TYR:CE1	1:B:102:PHE:HD2	2.37	0.43
1:B:58:GLN:HG2	1:B:92:TYR:CE2	2.54	0.43
1:E:26:GLY:HA3	2:E:900:SO4:O2	2.19	0.43
1:D:2:ASN:CG	1:D:3:LEU:N	2.71	0.43
1:D:10:VAL:HG21	1:D:32:SER:HB3	2.01	0.43
1:B:58:GLN:HG3	1:B:119:LEU:HD21	2.01	0.42
1:D:163:THR:HA	1:D:165:GLU:OE2	2.19	0.42
1:D:186:LEU:HD23	1:D:186:LEU:HA	1.80	0.42
1:E:61:TRP:CH2	1:E:85:LEU:HB3	2.52	0.42
1:B:106:TYR:O	1:B:108:LYS:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:ILE:HG21	1:A:178:PHE:HB2	2.02	0.42
1:E:105:GLU:HG2	1:E:106:TYR:CE2	2.54	0.42
1:B:62:GLN:NE2	1:B:122:LYS:HB3	2.35	0.42
1:D:36:LYS:CG	1:D:40:TYR:HE1	2.32	0.42
1:E:95:LEU:O	1:E:99:ILE:HG13	2.19	0.42
1:E:96:GLN:HE21	1:E:96:GLN:HA	1.83	0.42
1:D:36:LYS:O	1:D:40:TYR:HD1	2.03	0.42
1:A:2:ASN:O	1:A:6:LYS:N	2.46	0.42
1:E:35:SER:OG	1:E:38:ASN:HB2	2.20	0.42
1:B:16:ILE:HG12	1:B:95:LEU:HD23	2.01	0.42
1:B:184:ASN:ND2	1:A:185:GLY:HA2	2.35	0.42
1:B:49:LEU:O	1:B:49:LEU:HD12	2.20	0.42
1:B:112:ILE:C	1:B:114:GLU:N	2.73	0.42
1:E:16:ILE:O	1:E:16:ILE:HG22	2.19	0.42
1:B:47:GLU:HB2	1:B:102:PHE:CE2	2.52	0.42
1:B:58:GLN:CA	1:B:58:GLN:HE21	2.33	0.42
1:B:142:ILE:HD11	1:B:186:LEU:HD13	2.02	0.42
1:A:87:LEU:C	1:A:87:LEU:HD23	2.39	0.42
1:E:29:VAL:HG23	1:E:39:LEU:HD12	2.02	0.42
1:E:163:THR:OG1	1:E:171:ARG:HD2	2.20	0.41
1:D:31:LEU:HD12	1:D:31:LEU:HA	1.90	0.41
1:D:126:ALA:O	1:D:130:ILE:HG13	2.19	0.41
1:E:96:GLN:HA	1:E:96:GLN:NE2	2.35	0.41
1:A:136:LEU:CD1	1:A:136:LEU:H	2.33	0.41
1:E:12:LYS:HE3	1:E:57:GLU:CD	2.41	0.41
1:E:134:GLY:HA3	1:E:140:TRP:CZ2	2.56	0.41
1:E:63:GLU:HA	1:E:63:GLU:OE1	2.21	0.41
1:E:80:TYR:CE1	1:E:179:SER:HB2	2.55	0.41
1:E:91:TYR:O	1:E:93:TYR:N	2.54	0.41
1:E:183:LEU:HD12	1:E:183:LEU:HA	1.84	0.41
1:B:129:VAL:O	1:B:130:ILE:C	2.59	0.41
1:A:163:THR:HG22	1:A:171:ARG:HD3	2.02	0.41
1:B:89:THR:CG2	1:B:90:GLU:H	2.30	0.41
1:A:159:ILE:HB	1:A:175:MET:HE1	2.03	0.41
1:B:3:LEU:HD11	1:B:38:ASN:ND2	2.24	0.40
1:E:79:PHE:CD2	1:E:183:LEU:HD13	2.54	0.40
1:E:168:ILE:O	1:E:172:ILE:HG13	2.21	0.40
1:B:70:ILE:C	1:B:72:ALA:N	2.75	0.40
1:D:83:ASN:HB3	1:D:175:MET:SD	2.61	0.40
1:B:109:THR:HG23	1:B:112:ILE:CG1	2.47	0.40
1:B:109:THR:O	1:B:111:SER:N	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:72:ALA:HB3	1:D:78:LYS:HG2	2.04	0.40
1:D:177:LYS:O	1:D:177:LYS:HD3	2.22	0.40
1:E:106:TYR:N	1:E:106:TYR:CD2	2.89	0.40
1:D:142:ILE:HD11	1:D:186:LEU:CD1	2.26	0.40
1:B:115:LYS:O	1:B:117:ASN:N	2.54	0.40
1:B:132:LYS:HA	1:B:135:ASN:ND2	2.35	0.40
1:B:132:LYS:O	1:B:136:LEU:HD13	2.22	0.40
1:B:155:ALA:HB1	1:A:155:ALA:HB1	2.04	0.40
1:A:174:LEU:HD23	1:A:174:LEU:HA	1.90	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:30:LYS:CB	2:D:779:SO4:O4[7_556]	1.84	0.36
1:D:13:GLU:CG	1:D:31:LEU:O[7_556]	1.87	0.33

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	184/188 (98%)	166 (90%)	15 (8%)	3 (2%)	9 38
1	B	184/188 (98%)	144 (78%)	27 (15%)	13 (7%)	1 5
1	D	184/188 (98%)	161 (88%)	19 (10%)	4 (2%)	6 29
1	E	184/188 (98%)	161 (88%)	19 (10%)	4 (2%)	6 29
All	All	736/752 (98%)	632 (86%)	80 (11%)	24 (3%)	4 19

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	44	LYS
1	B	89	THR
1	A	164	HIS
1	E	166	GLN
1	B	33	GLU
1	B	35	SER
1	B	40	TYR
1	B	92	TYR
1	B	110	ASN
1	B	165	GLU
1	D	166	GLN
1	E	92	TYR
1	E	143	ASN
1	B	106	TYR
1	B	107	TYR
1	D	92	TYR
1	A	104	THR
1	B	113	ASN
1	D	137	ASN
1	A	136	LEU
1	E	89	THR
1	B	116	MET
1	D	136	LEU
1	B	167	ASN

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	169/171 (99%)	156 (92%)	13 (8%)	13 40
1	B	169/171 (99%)	150 (89%)	19 (11%)	6 23
1	D	169/171 (99%)	160 (95%)	9 (5%)	22 56
1	E	169/171 (99%)	161 (95%)	8 (5%)	26 61
All	All	676/684 (99%)	627 (93%)	49 (7%)	14 43

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	5	ASP
1	B	6	LYS
1	B	18	ASN
1	B	36	LYS
1	B	39	LEU
1	B	40	TYR
1	B	45	THR
1	B	58	GLN
1	B	62	GLN
1	B	85	LEU
1	B	109	THR
1	B	114	GLU
1	B	116	MET
1	B	119	LEU
1	B	143	ASN
1	B	157	ASN
1	B	165	GLU
1	B	167	ASN
1	B	180	GLN
1	D	2	ASN
1	D	69	GLN
1	D	96	GLN
1	D	97	ASN
1	D	109	THR
1	D	161	THR
1	D	165	GLU
1	D	167	ASN
1	D	177	LYS
1	A	33	GLU
1	A	48	ASN
1	A	49	LEU
1	A	54	LEU
1	A	70	ILE
1	A	85	LEU
1	A	90	GLU
1	A	105	GLU
1	A	118	LYS
1	A	136	LEU
1	A	143	ASN
1	A	165	GLU
1	A	173	LYS
1	E	54	LEU
1	E	76	ARG

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Mol	Chain	Res	Type
1	E	106	TYR
1	E	120	GLU
1	E	133	GLU
1	E	161	THR
1	E	164	HIS
1	E	170	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	21	ASN
1	B	38	ASN
1	B	48	ASN
1	B	58	GLN
1	B	62	GLN
1	B	69	GLN
1	B	75	ASN
1	B	83	ASN
1	B	96	GLN
1	B	110	ASN
1	B	121	ASN
1	B	137	ASN
1	B	154	ASN
1	B	157	ASN
1	B	166	GLN
1	B	167	ASN
1	B	184	ASN
1	D	2	ASN
1	D	64	GLN
1	D	75	ASN
1	D	83	ASN
1	D	117	ASN
1	D	143	ASN
1	D	154	ASN
1	D	167	ASN
1	D	176	ASN
1	D	184	ASN
1	A	21	ASN
1	A	62	GLN
1	A	83	ASN
1	A	113	ASN
1	A	121	ASN

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Mol	Chain	Res	Type
1	A	135	ASN
1	A	143	ASN
1	A	166	GLN
1	A	180	GLN
1	E	18	ASN
1	E	55	ASN
1	E	58	GLN
1	E	64	GLN
1	E	75	ASN
1	E	83	ASN
1	E	96	GLN
1	E	117	ASN
1	E	121	ASN
1	E	143	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)

18 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	D	899	-	4,4,4	0.26	0	6,6,6	0.07	0
2	SO4	E	239	-	4,4,4	0.27	0	6,6,6	0.11	0
2	SO4	E	249	-	4,4,4	0.33	0	6,6,6	0.14	0
2	SO4	A	801	-	4,4,4	0.30	0	6,6,6	0.10	0
2	SO4	A	599	-	4,4,4	0.27	0	6,6,6	0.12	0
2	SO4	D	999	-	4,4,4	0.26	0	6,6,6	0.10	0
2	SO4	D	280	-	4,4,4	0.25	0	6,6,6	0.05	0
2	SO4	A	279	-	4,4,4	0.30	0	6,6,6	0.12	0
2	SO4	A	595	-	4,4,4	0.22	0	6,6,6	0.11	0
2	SO4	D	779	-	4,4,4	0.27	0	6,6,6	0.08	0
2	SO4	A	699	-	4,4,4	0.31	0	6,6,6	0.13	0
2	SO4	E	399	-	4,4,4	0.25	0	6,6,6	0.08	0
2	SO4	A	299	-	4,4,4	0.29	0	6,6,6	0.08	0
2	SO4	D	400	-	4,4,4	0.26	0	6,6,6	0.07	0
2	SO4	E	799	-	4,4,4	0.29	0	6,6,6	0.14	0
2	SO4	E	900	-	4,4,4	0.29	0	6,6,6	0.23	0
3	DEQ	A	201	-	35,37,37	5.54	15 (42%)	42,50,50	4.67	24 (57%)
2	SO4	B	1000	-	4,4,4	0.25	0	6,6,6	0.09	0

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
3	DEQ	A	201	-	-	4/13/13/13	0/4/4/4

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	201	DEQ	C12-N2	17.62	1.57	1.36
3	A	201	DEQ	C11-N2	17.30	1.62	1.40
3	A	201	DEQ	C5-N1	14.21	1.58	1.40
3	A	201	DEQ	C9-N1	11.17	1.49	1.36
3	A	201	DEQ	C10-C11	4.39	1.49	1.42
3	A	201	DEQ	C6-C5	3.90	1.48	1.42
3	A	201	DEQ	C2-C1	3.23	1.44	1.36
3	A	201	DEQ	C18-C11	3.18	1.47	1.41
3	A	201	DEQ	C3-C4	3.14	1.43	1.36
3	A	201	DEQ	C17-C18	3.08	1.43	1.36
3	A	201	DEQ	C30-C9	2.99	1.56	1.49
3	A	201	DEQ	C16-C15	2.97	1.43	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	201	DEQ	C8-C7	2.97	1.42	1.39
3	A	201	DEQ	C1-C5	2.91	1.46	1.41
3	A	201	DEQ	C14-N3	2.23	1.45	1.38

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	201	DEQ	C19-N2-C11	18.77	135.64	118.90
3	A	201	DEQ	C12-N2-C11	-10.92	111.39	122.15
3	A	201	DEQ	C28-N1-C5	9.88	127.72	118.90
3	A	201	DEQ	C27-C26-C25	6.83	149.12	114.42
3	A	201	DEQ	C14-C10-C11	5.49	121.68	118.35
3	A	201	DEQ	C18-C11-N2	5.37	126.63	121.36
3	A	201	DEQ	C1-C5-N1	5.12	126.39	121.36
3	A	201	DEQ	C13-C14-N3	-4.67	109.26	120.21
3	A	201	DEQ	C8-C7-C6	4.48	121.06	117.96
3	A	201	DEQ	C13-C14-C10	4.18	120.85	117.96
3	A	201	DEQ	C9-N1-C5	-4.11	118.10	122.15
3	A	201	DEQ	C30-C9-N1	4.08	126.26	119.85
3	A	201	DEQ	C10-C14-N3	3.97	129.89	120.40
3	A	201	DEQ	C29-C12-C13	-3.90	113.07	121.54
3	A	201	DEQ	C18-C11-C10	-3.75	114.73	119.41
3	A	201	DEQ	C30-C9-C8	-3.02	115.00	121.54
3	A	201	DEQ	C7-C6-C5	2.83	120.06	118.35
3	A	201	DEQ	C1-C5-C6	-2.64	116.11	119.41
3	A	201	DEQ	C17-C18-C11	2.60	124.43	119.44
3	A	201	DEQ	C15-C10-C14	-2.43	118.95	122.72
3	A	201	DEQ	C8-C7-N4	-2.35	114.71	120.21
3	A	201	DEQ	C29-C12-N2	2.25	123.38	119.85
3	A	201	DEQ	C24-C23-C22	-2.14	103.58	114.42
3	A	201	DEQ	C22-C21-C20	-2.04	104.05	114.42

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	201	DEQ	C27-C28-N1-C5
3	A	201	DEQ	C27-C28-N1-C9
3	A	201	DEQ	C20-C19-N2-C11
3	A	201	DEQ	C20-C19-N2-C12

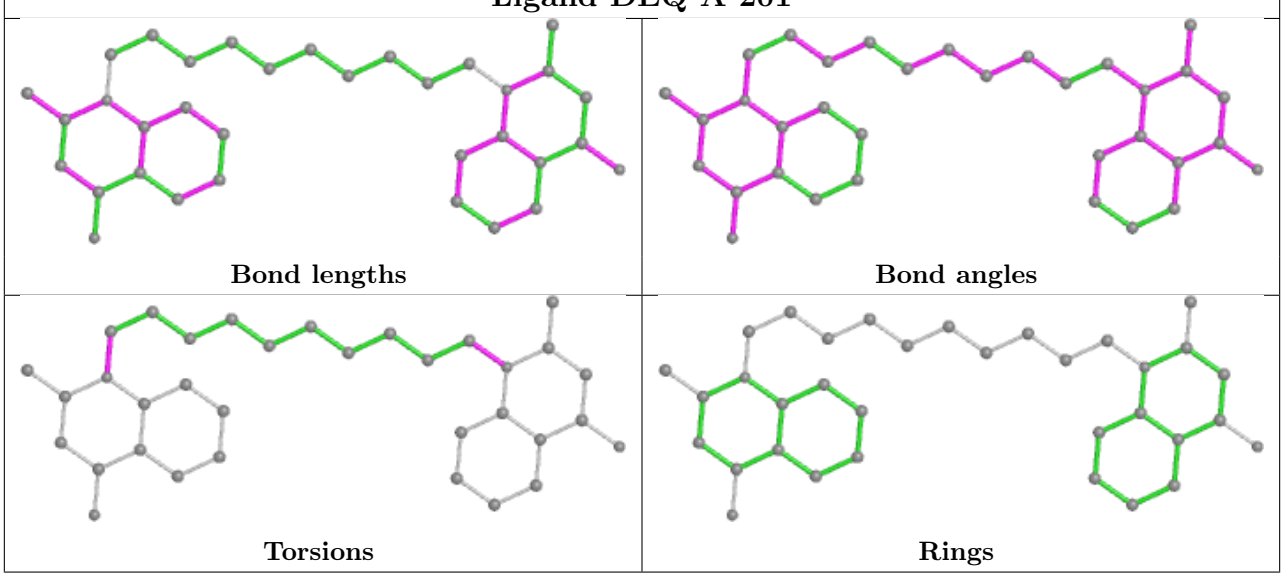
There are no ring outliers.

6 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	279	SO4	1	0
2	A	595	SO4	1	0
2	D	779	SO4	0	1
2	E	399	SO4	1	0
2	E	900	SO4	1	0
3	A	201	DEQ	7	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand DEQ A 201



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)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

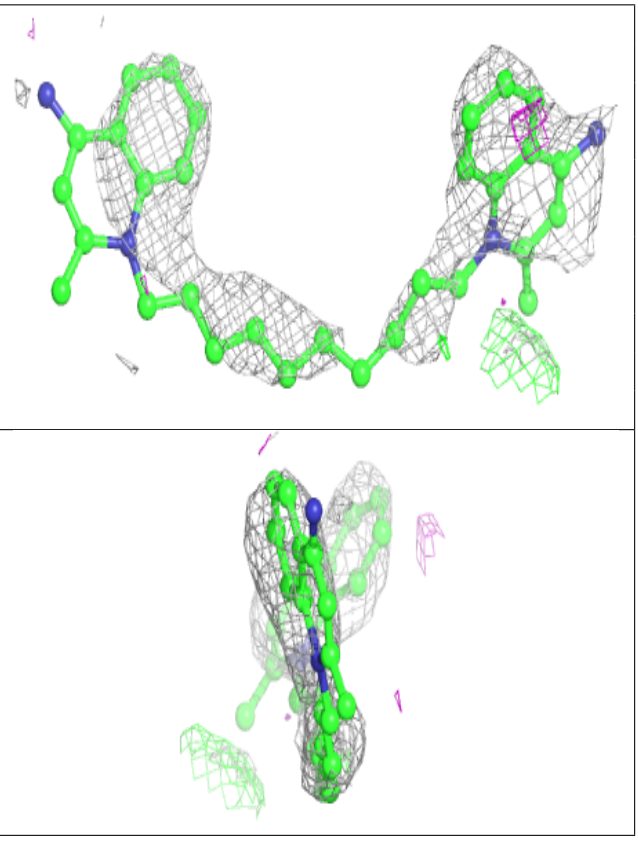
6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around DEQ A 201:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.