Full wwPDB X-ray Structure Validation Report (i)

Nov 5, 2023 – 08:26 AM EST

PDB ID	:	6OIV
Title	:	XFEL structure of Escherichia coli dGTPase
Authors	:	Barnes, C.O.; Wu, Y.; Calero, G.
Deposited on	:	2019-04-09
Resolution	:	3.06 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:

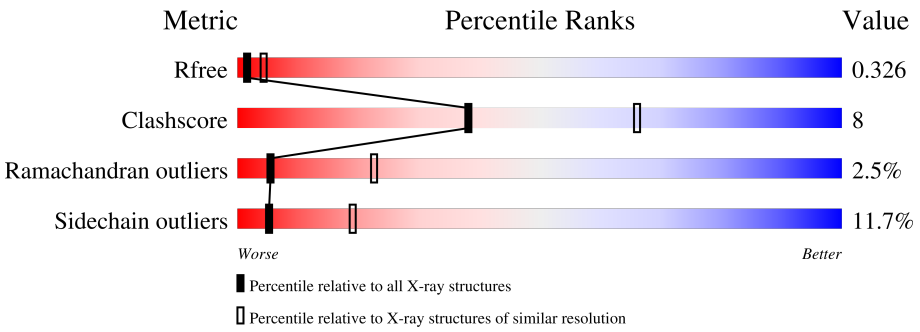
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.06 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	1754 (3.10-3.02)
Clashscore	141614	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)

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	505	70% 25% • •
1	B	505	70% 23% • •
1	C	505	70% 24% • •
1	D	505	70% 24% • •
1	E	505	73% 22% • •
1	F	505	74% 21% • •

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	SO4	C	602	-	-	X	-
3	SO4	D	602	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 24778 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 Deoxyguanosinetriphosphate triphosphohydrolase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	498	4135	2639	737	743	6	10	0	0	0
1	B	488	4042	2586	720	720	6	10	0	0	0
1	C	497	4125	2633	736	740	6	10	0	0	0
1	D	495	4118	2630	734	738	6	10	0	0	0
1	E	497	4130	2636	736	742	6	10	0	0	0
1	F	502	4169	2658	745	750	6	10	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	initiating methionine	UNP P15723
B	1	MSE	-	initiating methionine	UNP P15723
C	1	MSE	-	initiating methionine	UNP P15723
D	1	MSE	-	initiating methionine	UNP P15723
E	1	MSE	-	initiating methionine	UNP P15723
F	1	MSE	-	initiating methionine	UNP P15723

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

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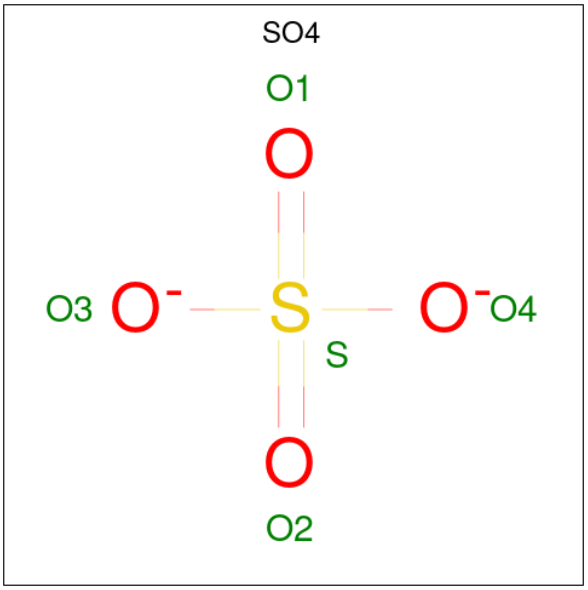
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total Mn 1 1	0	0
2	E	1	Total Mn 1 1	0	0
2	F	1	Total Mn 1 1	0	0

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



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

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

- Molecule 4 is water.

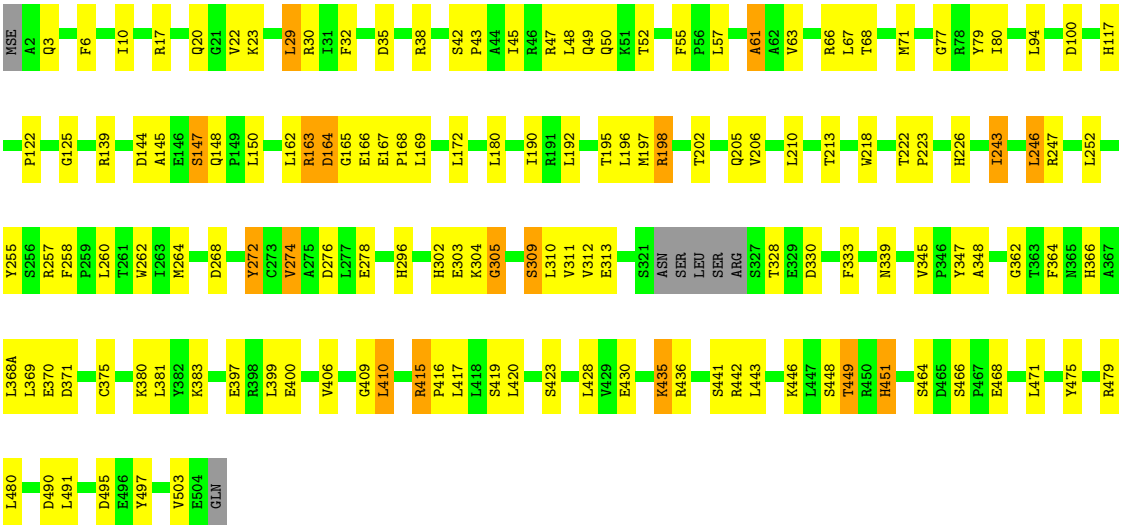
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	C	3	3	3	0	0
			Total	O		
4	E	3	3	3	0	0
			Total	O		
4	F	2	2	2	0	0

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.

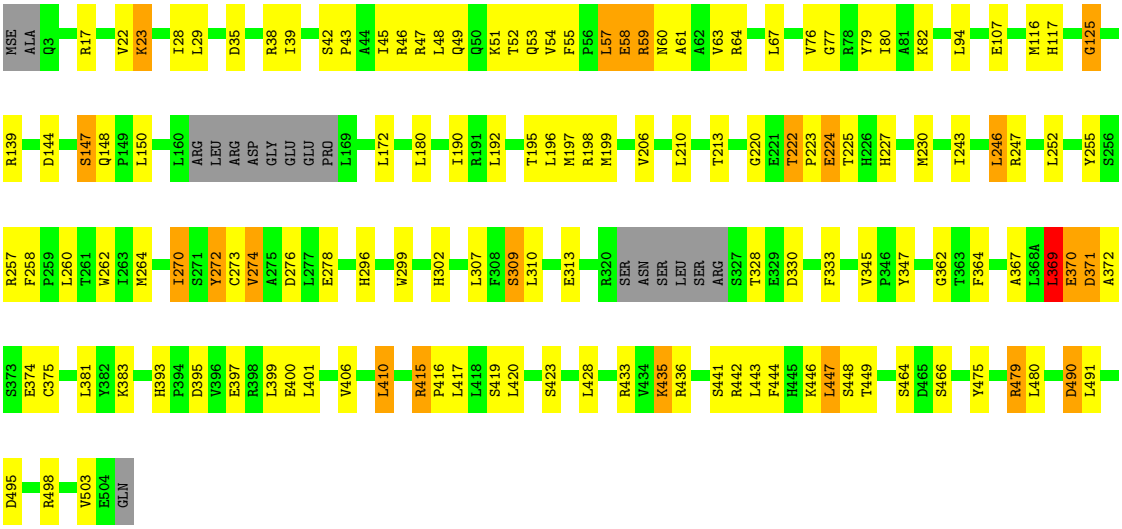
- Molecule 1: Deoxyguanosinetriphosphate triphosphohydrolase

Chain A:



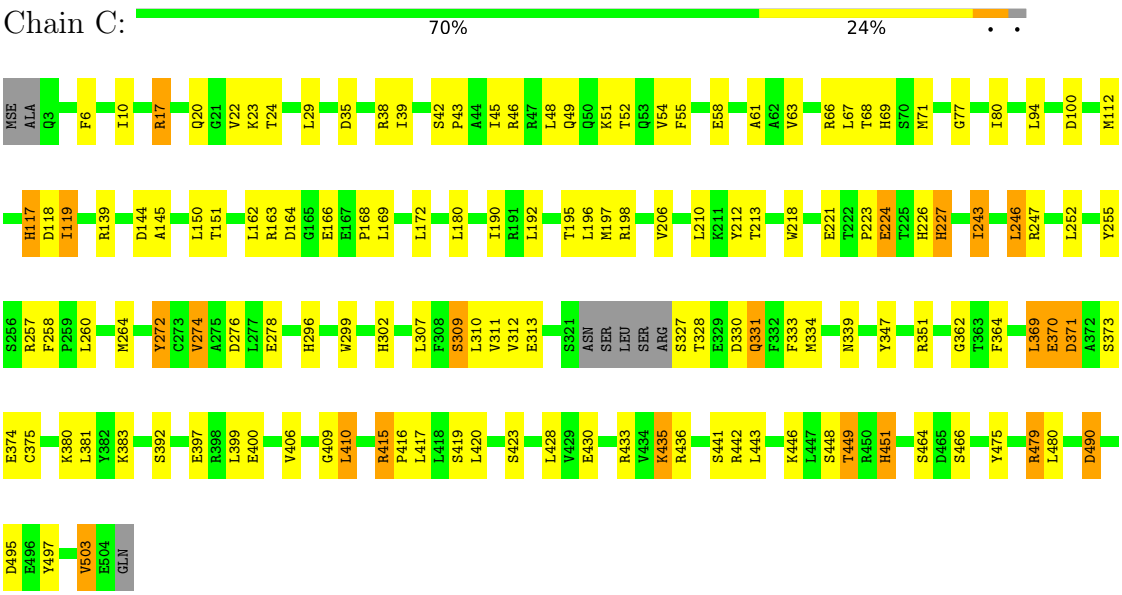
- Molecule 1: Deoxyguanosinetriphosphate triphosphohydrolase

Chain B:



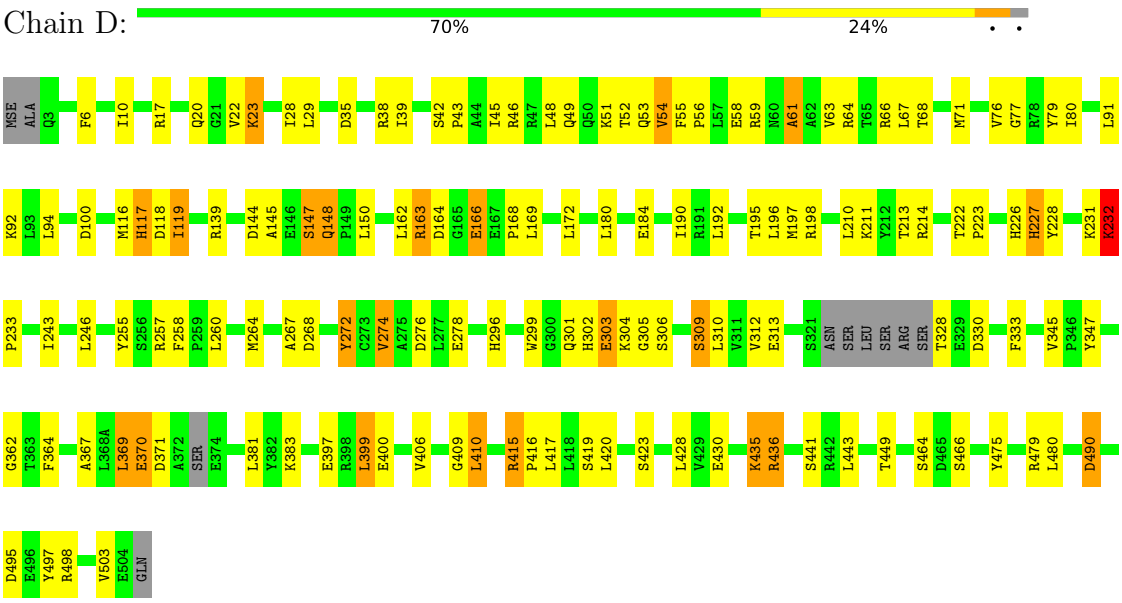
• Molecule 1: Deoxyguanosinetriphosphate triphosphohydrolase

Chain C:



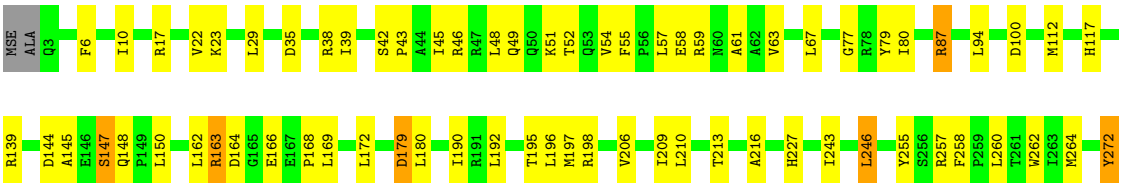
• Molecule 1: Deoxyguanosinetriphosphate triphosphohydrolase

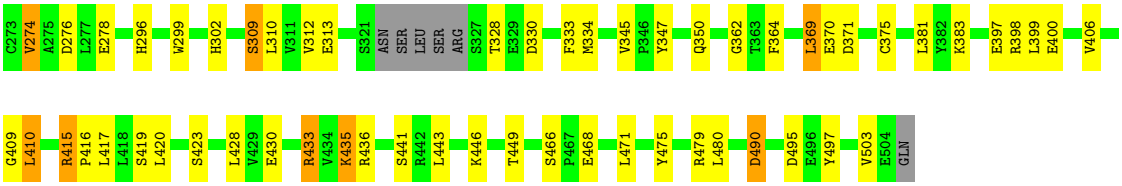
Chain D:



• Molecule 1: Deoxyguanosinetriphosphate triphosphohydrolase

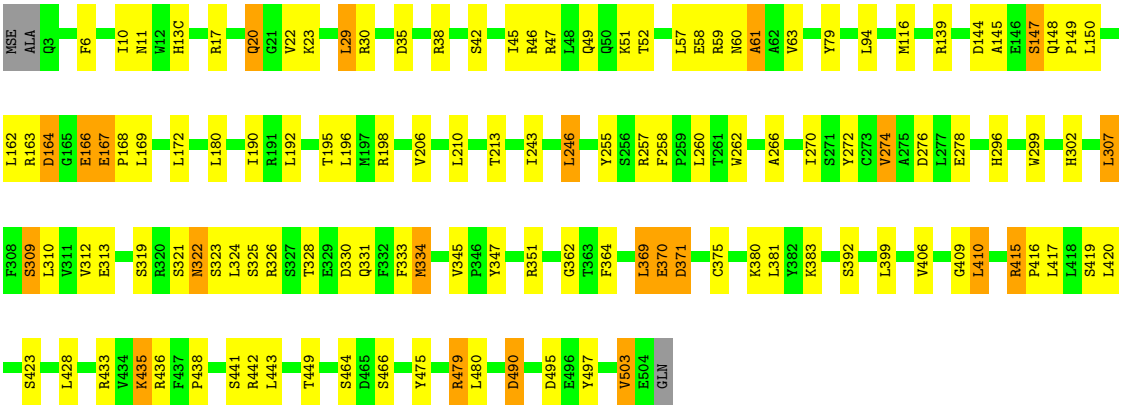
Chain E:





• Molecule 1: Deoxyguanosinetriphosphate triphosphohydrolase

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	192.59Å 192.59Å 291.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	61.20 – 3.06 96.29 – 3.06	Depositor EDS
% Data completeness (in resolution range)	92.3 (61.20-3.06) 92.4 (96.29-3.06)	Depositor EDS
R_{merge}	0.66	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.39 (at 3.07Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.225 , 0.248 0.302 , 0.326	Depositor DCC
R_{free} test set	2922 reflections (3.06%)	wwPDB-VP
Wilson B-factor (Å^2)	29.1	Xtriage
Anisotropy	0.268	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 78.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.31$, $< L^2 > = 0.15$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.72	EDS
Total number of atoms	24778	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.84% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MN, 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	0.55	0/4227	0.76	2/5699 (0.0%)
1	B	0.49	0/4132	0.73	2/5572 (0.0%)
1	C	0.55	0/4217	0.76	1/5685 (0.0%)
1	D	0.49	2/4209 (0.0%)	0.73	1/5673 (0.0%)
1	E	0.54	0/4222	0.72	1/5692 (0.0%)
1	F	0.55	0/4262	0.75	2/5747 (0.0%)
All	All	0.53	2/25269 (0.0%)	0.74	9/34068 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	231	LYS	C-N	-5.86	1.20	1.34
1	D	232	LYS	C-N	5.24	1.44	1.34

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	307	LEU	CA-CB-CG	6.99	131.37	115.30
1	A	163	ARG	C-N-CA	6.75	138.58	121.70
1	B	369	LEU	C-N-CA	-6.57	105.29	121.70
1	D	231	LYS	O-C-N	-6.14	112.87	122.70
1	A	305	GLY	N-CA-C	-6.00	98.10	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	125	GLY	C-N-CA	5.96	136.59	121.70
1	F	163	ARG	C-N-CA	5.51	135.48	121.70
1	C	151	THR	N-CA-CB	5.30	120.38	110.30
1	E	370	GLU	C-N-CA	5.05	134.34	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	47	ARG	Sidechain
1	A	66	ARG	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	A	4135	0	4091	71	0
1	B	4042	0	3996	73	0
1	C	4125	0	4080	69	0
1	D	4118	0	4074	75	0
1	E	4130	0	4086	48	0
1	F	4169	0	4127	62	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	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	20	0	0	3	0
3	D	5	0	0	2	0
3	E	5	0	0	0	0
3	F	5	0	0	0	0
4	C	3	0	0	0	0
4	E	3	0	0	1	0
4	F	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	24778	0	24454	375	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 8.

All (375) 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:F:116:MSE:SE	1:F:116:MSE:CE	2.18	1.40
1:C:334:MSE:SE	1:C:334:MSE:CE	2.21	1.38
1:C:66:ARG:NH1	1:C:118:ASP:OD1	1.58	1.33
1:A:17:ARG:NH2	1:F:326:ARG:HH22	1.54	1.05
1:A:17:ARG:HH21	1:F:326:ARG:NH2	1.62	0.98
1:D:117:HIS:O	1:D:118:ASP:HB2	1.59	0.97
1:C:218:TRP:HE1	1:C:221:GLU:H	1.15	0.94
1:D:116:MSE:O	1:D:119:ILE:HG22	1.67	0.93
1:A:35:ASP:OD2	1:A:202:THR:HG22	1.69	0.91
1:C:448:SER:HB2	1:C:451:HIS:CE1	2.06	0.90
1:B:367:ALA:HB3	1:B:370:GLU:HB3	1.51	0.89
1:B:444:PHE:O	1:B:447:LEU:HD12	1.73	0.89
1:C:448:SER:HB2	1:C:451:HIS:HE1	1.39	0.86
1:A:448:SER:HB2	1:A:451:HIS:CE1	2.10	0.86
1:A:448:SER:HB2	1:A:451:HIS:HE1	1.43	0.83
1:A:50:GLN:HG2	1:A:491:LEU:HD13	1.60	0.82
1:D:223:PRO:HB2	1:D:226:HIS:HB2	1.60	0.82
1:F:13(C):HIS:CE1	1:F:20:GLN:HG2	2.15	0.82
1:A:49:GLN:HB2	1:A:67:LEU:HD22	1.62	0.81
1:B:479:ARG:HH11	1:B:479:ARG:HG3	1.47	0.80
1:F:13(C):HIS:HE1	1:F:20:GLN:HG2	1.45	0.80
1:F:479:ARG:HG3	1:F:479:ARG:HH11	1.47	0.79
1:A:366:HIS:HB3	1:A:370:GLU:HG3	1.65	0.79
1:C:479:ARG:HG3	1:C:479:ARG:HH11	1.47	0.78
1:A:17:ARG:HH21	1:F:326:ARG:HH22	0.82	0.78
1:B:23:LYS:HB2	1:B:28:ILE:HD11	1.67	0.76
1:D:117:HIS:CD2	1:D:268:ASP:OD2	2.38	0.75
1:D:119:ILE:HD13	1:D:192:LEU:HD23	1.67	0.75
1:B:223:PRO:HD2	1:B:227:HIS:HA	1.66	0.75
1:D:23:LYS:HB2	1:D:28:ILE:HD11	1.68	0.74
1:C:66:ARG:NH1	1:C:118:ASP:CG	2.40	0.74
1:E:87:ARG:HH21	1:E:350:GLN:HB2	1.51	0.73
1:E:417:LEU:HD11	1:E:443:LEU:HB3	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:LEU:HD11	1:A:443:LEU:HB3	1.70	0.72
1:C:218:TRP:HE1	1:C:221:GLU:N	1.85	0.72
1:B:444:PHE:HA	1:B:447:LEU:CD1	2.18	0.71
1:C:417:LEU:HD11	1:C:443:LEU:HB3	1.72	0.70
1:A:17:ARG:HH12	1:A:38:ARG:HH22	1.40	0.70
1:B:498:ARG:HE	1:C:503:VAL:HG12	1.57	0.70
1:A:42:SER:O	1:A:45:ILE:HG22	1.92	0.70
1:F:417:LEU:HD11	1:F:443:LEU:HB3	1.74	0.70
1:A:48:LEU:N	1:A:48:LEU:HD23	2.06	0.70
1:B:82:LYS:HE2	1:B:107:GLU:OE2	1.92	0.69
1:D:116:MSE:O	1:D:119:ILE:CG2	2.40	0.69
1:B:417:LEU:HD11	1:B:443:LEU:HB3	1.75	0.68
1:D:17:ARG:HH12	1:D:38:ARG:HH22	1.40	0.68
1:A:50:GLN:HB2	1:F:61:ALA:HB2	1.74	0.68
1:D:417:LEU:HD11	1:D:443:LEU:HB3	1.76	0.68
1:C:55:PHE:HB2	1:C:63:VAL:HG21	1.75	0.67
1:D:119:ILE:CD1	1:D:192:LEU:HD23	2.24	0.67
1:C:213:THR:HB	1:C:255:TYR:HA	1.77	0.66
1:E:55:PHE:HB2	1:E:63:VAL:HG21	1.77	0.66
1:E:17:ARG:HH12	1:E:38:ARG:HH22	1.44	0.66
1:A:17:ARG:HG2	1:F:324:LEU:HD21	1.76	0.66
1:F:213:THR:HB	1:F:255:TYR:HA	1.77	0.66
1:F:17:ARG:HH21	1:F:38:ARG:HH22	1.42	0.65
1:A:213:THR:HB	1:A:255:TYR:HA	1.79	0.65
1:B:401:LEU:HD11	1:C:442:ARG:HB3	1.78	0.65
1:F:145:ALA:HA	1:F:162:LEU:HD11	1.79	0.65
1:C:258:PHE:CE2	1:C:260:LEU:HB2	2.31	0.65
1:D:55:PHE:HB2	1:D:63:VAL:HG21	1.78	0.65
1:F:299:TRP:HB3	1:F:302:HIS:CE1	2.33	0.64
1:F:258:PHE:CE2	1:F:260:LEU:HB2	2.32	0.64
1:D:258:PHE:CE2	1:D:260:LEU:HB2	2.33	0.64
1:B:55:PHE:HB2	1:B:63:VAL:HG21	1.79	0.64
1:E:258:PHE:CE2	1:E:260:LEU:HB2	2.33	0.64
1:C:299:TRP:HB3	1:C:302:HIS:CE1	2.33	0.64
1:E:145:ALA:HA	1:E:162:LEU:HD11	1.79	0.64
1:B:258:PHE:CE2	1:B:260:LEU:HB2	2.33	0.63
1:B:17:ARG:HH12	1:B:38:ARG:HH22	1.44	0.63
1:B:444:PHE:HA	1:B:447:LEU:HD11	1.80	0.63
1:E:213:THR:HB	1:E:255:TYR:HA	1.80	0.63
1:E:299:TRP:HB3	1:E:302:HIS:CE1	2.33	0.62
1:D:299:TRP:HB3	1:D:302:HIS:CE1	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:TRP:HZ2	1:A:222:THR:HB	1.65	0.62
1:B:213:THR:HB	1:B:255:TYR:HA	1.81	0.62
1:C:145:ALA:HA	1:C:162:LEU:HD11	1.80	0.62
1:B:299:TRP:HB3	1:B:302:HIS:CE1	2.35	0.62
1:D:228:TYR:OH	1:D:367:ALA:HB2	1.99	0.61
1:B:444:PHE:HA	1:B:447:LEU:HD12	1.83	0.61
1:D:213:THR:HB	1:D:255:TYR:HA	1.80	0.61
1:A:258:PHE:CE2	1:A:260:LEU:HB2	2.35	0.61
1:D:66:ARG:NH1	1:D:118:ASP:OD2	2.33	0.60
1:D:145:ALA:HA	1:D:162:LEU:HD11	1.83	0.60
1:D:117:HIS:O	1:D:118:ASP:CB	2.39	0.60
1:A:145:ALA:HA	1:A:162:LEU:HD11	1.83	0.59
1:D:232:LYS:HB3	1:D:233:PRO:CD	2.32	0.59
1:E:87:ARG:NH2	1:E:350:GLN:HB2	2.17	0.58
1:B:76:VAL:HG11	1:B:270:ILE:CG2	2.33	0.58
1:C:24:THR:HG22	3:C:602:SO4:O3	2.04	0.58
1:B:23:LYS:HB2	1:B:28:ILE:CD1	2.34	0.58
1:A:32:PHE:CE1	1:A:202:THR:HG21	2.39	0.57
1:D:222:THR:CG2	1:D:227:HIS:HA	2.34	0.57
1:F:309:SER:HA	1:F:313:GLU:HB2	1.87	0.57
1:E:42:SER:O	1:E:45:ILE:HG22	2.05	0.57
1:B:491:LEU:HD23	1:D:59:ARG:HD3	1.88	0.56
1:F:351:ARG:NH2	1:F:370:GLU:HG3	2.20	0.56
1:B:309:SER:HA	1:B:313:GLU:HB2	1.85	0.56
1:B:479:ARG:HG3	1:B:479:ARG:NH1	2.19	0.56
1:D:309:SER:HA	1:D:313:GLU:HB2	1.87	0.56
1:A:168:PRO:HD2	1:A:169:LEU:HD12	1.88	0.56
1:A:309:SER:HA	1:A:313:GLU:HB2	1.87	0.56
1:C:309:SER:HA	1:C:313:GLU:HB2	1.87	0.56
1:C:479:ARG:HG3	1:C:479:ARG:NH1	2.19	0.55
1:E:179:ASP:OD1	1:E:216:ALA:HB3	2.06	0.55
1:A:55:PHE:HB2	1:A:63:VAL:HG21	1.88	0.55
1:A:415:ARG:N	1:A:416:PRO:HD2	2.21	0.55
1:C:168:PRO:HD2	1:C:169:LEU:HD12	1.88	0.55
1:E:168:PRO:HD2	1:E:169:LEU:HD12	1.89	0.55
1:D:428:LEU:HD11	1:D:441:SER:HA	1.88	0.55
1:E:415:ARG:N	1:E:416:PRO:HD2	2.22	0.55
1:F:168:PRO:HD2	1:F:169:LEU:HD12	1.88	0.55
1:F:17:ARG:NH2	1:F:38:ARG:HH12	2.05	0.54
1:E:309:SER:HA	1:E:313:GLU:HB2	1.88	0.54
1:D:168:PRO:HD2	1:D:169:LEU:HD12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:23:LYS:HB2	1:D:28:ILE:CD1	2.35	0.54
1:D:415:ARG:N	1:D:416:PRO:HD2	2.23	0.54
1:A:442:ARG:HG2	1:C:397:GLU:HB3	1.90	0.54
1:B:223:PRO:HG2	1:B:230:MSE:HB2	1.90	0.53
1:B:415:ARG:N	1:B:416:PRO:HD2	2.24	0.53
1:C:351:ARG:NH2	1:C:370:GLU:HG3	2.22	0.53
1:C:180:LEU:HD11	1:C:475:TYR:HA	1.91	0.53
1:C:258:PHE:HE2	1:C:260:LEU:HB2	1.74	0.53
1:D:117:HIS:NE2	1:D:118:ASP:OD1	2.41	0.53
1:C:415:ARG:N	1:C:416:PRO:HD2	2.24	0.53
1:D:258:PHE:HE2	1:D:260:LEU:HB2	1.74	0.53
1:A:122:PRO:HG2	1:A:125:GLY:O	2.09	0.53
1:E:428:LEU:HD11	1:E:441:SER:HA	1.91	0.53
1:F:428:LEU:HD11	1:F:441:SER:HA	1.91	0.52
1:A:218:TRP:CZ2	1:A:222:THR:HB	2.45	0.52
1:D:303:GLU:HG3	1:D:305:GLY:H	1.74	0.52
1:F:166:GLU:HG2	1:F:167:GLU:HG2	1.91	0.52
1:F:180:LEU:HD11	1:F:475:TYR:HA	1.91	0.52
1:B:428:LEU:HD11	1:B:441:SER:HA	1.91	0.52
1:E:180:LEU:HD11	1:E:475:TYR:HA	1.92	0.52
1:D:180:LEU:HD11	1:D:475:TYR:HA	1.92	0.52
1:D:211:LYS:NZ	3:D:602:SO4:O3	2.38	0.52
1:F:479:ARG:HG3	1:F:479:ARG:NH1	2.18	0.52
1:A:68:THR:HA	1:A:71:MSE:HE2	1.92	0.51
1:B:278:GLU:HA	1:B:333:PHE:CZ	2.46	0.51
1:B:59:ARG:HH21	1:E:398:ARG:HH12	1.58	0.51
1:C:69:HIS:CE1	1:C:117:HIS:CE1	2.99	0.51
1:D:222:THR:HG21	1:D:227:HIS:HA	1.92	0.51
1:F:192:LEU:HA	1:F:196:LEU:HB2	1.93	0.51
1:F:415:ARG:N	1:F:416:PRO:HD2	2.26	0.51
1:A:180:LEU:HD11	1:A:475:TYR:HA	1.93	0.51
1:E:17:ARG:NH1	1:E:38:ARG:HH22	2.07	0.51
1:E:258:PHE:HE2	1:E:260:LEU:HB2	1.76	0.50
1:E:192:LEU:HA	1:E:196:LEU:HB2	1.94	0.50
1:F:258:PHE:HE2	1:F:260:LEU:HB2	1.75	0.50
1:C:428:LEU:HD11	1:C:441:SER:HA	1.92	0.50
1:A:428:LEU:HD11	1:A:441:SER:HA	1.92	0.50
1:B:46:ARG:HD3	1:D:64:ARG:HG3	1.94	0.50
1:B:76:VAL:HG11	1:B:270:ILE:HG21	1.93	0.50
1:A:397:GLU:HB3	1:B:442:ARG:HG2	1.93	0.50
1:B:444:PHE:C	1:B:447:LEU:HD12	2.32	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:ASP:O	1:A:272:TYR:HB2	2.12	0.50
1:B:444:PHE:CA	1:B:447:LEU:HD12	2.42	0.50
1:C:278:GLU:HA	1:C:333:PHE:CZ	2.47	0.50
1:A:61:ALA:HB3	1:F:47:ARG:HA	1.94	0.49
1:A:278:GLU:HA	1:A:333:PHE:CZ	2.47	0.49
1:D:42:SER:O	1:D:45:ILE:HG22	2.11	0.49
1:D:211:LYS:CE	3:D:602:SO4:O3	2.60	0.49
1:D:278:GLU:HA	1:D:333:PHE:CZ	2.47	0.49
1:F:319:SER:O	1:F:322:ASN:HB3	2.13	0.49
1:A:258:PHE:HE2	1:A:260:LEU:HB2	1.77	0.49
1:B:47:ARG:HA	1:D:61:ALA:HB3	1.94	0.49
1:C:192:LEU:HA	1:C:196:LEU:HB2	1.93	0.49
1:E:415:ARG:NH2	4:E:701:HOH:O	2.46	0.49
1:F:149:PRO:HG2	1:F:164:ASP:O	2.12	0.49
1:C:42:SER:O	1:C:45:ILE:HG22	2.13	0.49
1:A:166:GLU:HG2	1:A:167:GLU:HG3	1.95	0.49
1:B:180:LEU:HD11	1:B:475:TYR:HA	1.93	0.49
1:D:192:LEU:HA	1:D:196:LEU:HB2	1.95	0.48
1:E:278:GLU:HA	1:E:333:PHE:CZ	2.47	0.48
1:F:278:GLU:HA	1:F:333:PHE:CZ	2.48	0.48
1:A:17:ARG:NH2	1:F:326:ARG:NH2	2.38	0.48
1:B:307:LEU:HD12	1:B:374:GLU:HB3	1.95	0.48
1:B:367:ALA:HB3	1:B:370:GLU:CB	2.35	0.48
1:F:13(C):HIS:HE1	1:F:20:GLN:CG	2.22	0.48
1:B:258:PHE:HE2	1:B:260:LEU:HB2	1.74	0.48
1:B:309:SER:HA	1:B:313:GLU:CB	2.44	0.48
1:B:370:GLU:HG3	1:B:371:ASP:N	2.28	0.48
1:E:43:PRO:HD2	1:E:197:MSE:CE	2.44	0.48
1:D:17:ARG:NH1	1:D:38:ARG:HH22	2.10	0.48
1:D:214:ARG:NH2	1:D:232:LYS:HA	2.28	0.48
1:B:64:ARG:HG3	1:D:46:ARG:HD3	1.95	0.47
1:C:68:THR:HA	1:C:71:MSE:HE2	1.96	0.47
1:D:91:LEU:O	1:D:92:LYS:HG2	2.14	0.47
1:F:51:LYS:HA	1:F:490:ASP:OD1	2.14	0.47
1:B:42:SER:O	1:B:45:ILE:HG22	2.14	0.47
1:D:232:LYS:HB3	1:D:233:PRO:HD2	1.95	0.47
1:C:24:THR:HA	3:C:602:SO4:O1	2.14	0.47
1:B:59:ARG:NH2	1:E:398:ARG:HH12	2.12	0.47
1:C:66:ARG:HD3	1:C:66:ARG:HA	1.70	0.47
1:C:307:LEU:HD12	1:C:374:GLU:HB3	1.97	0.47
1:C:309:SER:HA	1:C:313:GLU:CB	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:43:PRO:HD2	1:D:197:MSE:CE	2.45	0.47
1:E:163:ARG:HA	1:E:163:ARG:HD3	1.52	0.47
1:B:43:PRO:HD2	1:B:197:MSE:CE	2.45	0.47
1:E:272:TYR:HE2	1:E:383:LYS:HG2	1.80	0.47
1:B:222:THR:HA	1:B:223:PRO:HD3	1.68	0.47
1:C:43:PRO:HD2	1:C:197:MSE:CE	2.45	0.47
1:B:116:MSE:HE1	1:B:199:MSE:SE	2.65	0.47
1:B:262:TRP:CD1	1:B:262:TRP:N	2.81	0.47
1:E:51:LYS:HA	1:E:490:ASP:OD1	2.14	0.47
1:B:46:ARG:O	1:B:49:GLN:HG2	2.16	0.46
1:C:272:TYR:HE2	1:C:383:LYS:HG2	1.80	0.46
1:A:192:LEU:HA	1:A:196:LEU:HB2	1.96	0.46
1:A:202:THR:HG23	1:A:205:GLN:H	1.79	0.46
1:D:309:SER:HA	1:D:313:GLU:CB	2.45	0.46
1:B:192:LEU:HA	1:B:196:LEU:HB2	1.96	0.46
1:D:272:TYR:HE2	1:D:383:LYS:HG2	1.81	0.46
1:F:147:SER:HB3	1:F:148:GLN:H	1.55	0.46
1:B:147:SER:HB3	1:B:148:GLN:H	1.59	0.46
1:B:17:ARG:NH1	1:B:38:ARG:HH22	2.12	0.46
1:D:68:THR:HA	1:D:71:MSE:HE2	1.98	0.46
1:D:222:THR:HG22	1:D:227:HIS:HA	1.97	0.46
1:F:42:SER:O	1:F:45:ILE:HG22	2.16	0.46
1:F:262:TRP:CD1	1:F:262:TRP:N	2.82	0.46
1:A:190:ILE:HD11	1:A:210:LEU:HA	1.98	0.46
1:D:39:ILE:HG12	1:D:116:MSE:HE3	1.98	0.46
1:D:370:GLU:HB3	1:D:371:ASP:H	1.38	0.46
1:E:46:ARG:O	1:E:49:GLN:HG2	2.15	0.46
1:F:266:ALA:O	1:F:270:ILE:HG13	2.16	0.45
1:F:17:ARG:HH21	1:F:38:ARG:HH12	1.62	0.45
1:A:309:SER:HA	1:A:313:GLU:CB	2.46	0.45
1:E:79:TYR:CD2	1:E:345:VAL:HG21	2.51	0.45
1:A:272:TYR:HE2	1:A:383:LYS:HG2	1.81	0.45
1:C:448:SER:CB	1:C:451:HIS:CE1	2.90	0.45
1:E:309:SER:HA	1:E:313:GLU:CB	2.46	0.45
1:B:370:GLU:HG3	1:B:371:ASP:H	1.82	0.45
1:C:17:ARG:HB2	1:C:17:ARG:HH11	1.81	0.45
1:C:212:TYR:HE2	3:C:605:SO4:O3	1.99	0.45
1:F:272:TYR:HE2	1:F:383:LYS:HG2	1.82	0.45
1:C:347:TYR:HD2	1:C:369:LEU:HD13	1.82	0.45
1:D:147:SER:HB3	1:D:148:GLN:H	1.58	0.45
1:A:147:SER:HB3	1:A:148:GLN:H	1.58	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:397:GLU:HA	1:B:400:GLU:OE1	2.16	0.45
1:B:406:VAL:O	1:B:410:LEU:HB2	2.17	0.44
1:A:43:PRO:HD2	1:A:197:MSE:CE	2.47	0.44
1:F:322:ASN:HB2	1:F:331:GLN:HG2	1.99	0.44
1:C:51:LYS:HA	1:C:490:ASP:OD1	2.17	0.44
1:D:53:GLN:HE21	1:D:54:VAL:HG23	1.83	0.44
1:D:347:TYR:HD2	1:D:369:LEU:HD13	1.83	0.44
1:A:247:ARG:HG2	1:A:252:LEU:HB2	1.99	0.44
1:B:347:TYR:HD2	1:B:369:LEU:HD13	1.82	0.44
1:E:433:ARG:HH12	1:F:392:SER:HB3	1.83	0.44
1:F:6:PHE:HB3	1:F:10:ILE:HD12	1.99	0.44
1:F:11:ASN:OD1	1:F:13(C):HIS:HB2	2.18	0.44
1:F:406:VAL:O	1:F:410:LEU:HB2	2.18	0.44
1:B:39:ILE:HG12	1:B:116:MSE:HE3	1.98	0.44
1:E:6:PHE:HB3	1:E:10:ILE:HD12	1.98	0.44
1:F:17:ARG:HH21	1:F:38:ARG:NH2	2.10	0.44
1:A:17:ARG:NH1	1:A:38:ARG:HH22	2.11	0.44
1:B:272:TYR:HE2	1:B:383:LYS:HG2	1.82	0.44
1:C:243:ILE:HD13	1:C:243:ILE:HA	1.93	0.44
1:D:51:LYS:HA	1:D:490:ASP:OD1	2.17	0.44
1:D:303:GLU:HG2	1:D:306:SER:HB3	2.00	0.44
1:A:198:ARG:CD	1:F:325:SER:HB2	2.49	0.43
1:B:39:ILE:HG12	1:B:116:MSE:CE	2.48	0.43
1:C:46:ARG:O	1:C:49:GLN:HG2	2.18	0.43
1:B:77:GLY:HA2	1:B:80:ILE:HD12	2.01	0.43
1:D:79:TYR:CD2	1:D:345:VAL:HG21	2.53	0.43
1:A:262:TRP:CD1	1:A:262:TRP:N	2.81	0.43
1:D:76:VAL:HB	1:D:267:ALA:HB1	1.99	0.43
1:C:48:LEU:HB2	1:C:67:LEU:HB2	2.01	0.43
1:E:347:TYR:HD2	1:E:369:LEU:HD13	1.83	0.43
1:A:304:LYS:HG2	1:A:305:GLY:H	1.83	0.43
1:C:223:PRO:HB2	1:C:226:HIS:HB2	2.00	0.43
1:C:406:VAL:O	1:C:410:LEU:HB2	2.18	0.43
1:E:257:ARG:O	1:E:362:GLY:HA3	2.19	0.43
1:F:309:SER:HA	1:F:313:GLU:CB	2.47	0.43
1:A:79:TYR:CD2	1:A:345:VAL:HG21	2.54	0.43
1:B:51:LYS:HA	1:B:490:ASP:OD1	2.18	0.43
1:D:119:ILE:CD1	1:D:192:LEU:CD2	2.95	0.43
1:A:347:TYR:HD2	1:A:369:LEU:HD13	1.83	0.43
1:C:69:HIS:HE1	1:C:117:HIS:CE1	2.36	0.43
1:C:190:ILE:HD11	1:C:210:LEU:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:PRO:HB2	1:A:226:HIS:HB2	2.01	0.43
1:C:247:ARG:HG2	1:C:252:LEU:HB2	2.00	0.43
1:A:448:SER:CB	1:A:451:HIS:CE1	2.94	0.43
1:B:370:GLU:O	1:B:371:ASP:O	2.37	0.43
1:C:43:PRO:HD2	1:C:197:MSE:HE2	2.01	0.43
1:C:206:VAL:HB	1:C:246:LEU:HD11	2.01	0.43
1:E:206:VAL:HB	1:E:246:LEU:HD11	2.01	0.43
1:F:369:LEU:HD12	1:F:375:CYS:HB3	2.00	0.43
1:B:53:GLN:HE21	1:B:54:VAL:HG23	1.84	0.42
1:C:119:ILE:HD13	1:C:192:LEU:CD2	2.49	0.42
1:C:224:GLU:HA	1:C:227:HIS:ND1	2.34	0.42
1:C:39:ILE:HD13	1:C:112:MSE:HB3	2.01	0.42
1:E:262:TRP:CD1	1:E:262:TRP:N	2.81	0.42
1:F:46:ARG:O	1:F:49:GLN:HG2	2.18	0.42
1:D:190:ILE:HD11	1:D:210:LEU:HA	2.01	0.42
1:E:35:ASP:HA	1:E:38:ARG:HD2	2.01	0.42
1:B:222:THR:HB	1:B:227:HIS:HD2	1.85	0.42
1:E:77:GLY:HA2	1:E:80:ILE:HD12	2.01	0.42
1:A:348:ALA:HB1	1:A:368(A):LEU:HD23	2.01	0.42
1:B:257:ARG:O	1:B:362:GLY:HA3	2.19	0.42
1:A:68:THR:HG21	1:F:46:ARG:HG2	2.01	0.42
1:C:69:HIS:CE1	1:C:117:HIS:HE1	2.37	0.42
1:F:79:TYR:CD2	1:F:345:VAL:HG21	2.55	0.42
1:B:43:PRO:HD2	1:B:197:MSE:HE2	2.02	0.42
1:E:369:LEU:HD12	1:E:375:CYS:HB3	2.02	0.42
1:C:380:LYS:HA	1:C:383:LYS:HD2	2.02	0.42
1:D:184:GLU:OE1	1:D:232:LYS:HD2	2.20	0.42
1:D:409:GLY:HA3	1:D:497:TYR:HE1	1.84	0.42
1:E:147:SER:HB3	1:E:148:GLN:H	1.54	0.42
1:F:35:ASP:HA	1:F:38:ARG:HD2	2.01	0.42
1:F:190:ILE:HD11	1:F:210:LEU:HA	2.01	0.42
1:C:272:TYR:CE2	1:C:383:LYS:HG2	2.55	0.42
1:D:406:VAL:O	1:D:410:LEU:HB2	2.19	0.42
1:E:397:GLU:HA	1:E:400:GLU:OE1	2.20	0.42
1:A:29:LEU:HD23	1:A:30:ARG:HG2	2.02	0.42
1:C:397:GLU:HA	1:C:400:GLU:OE1	2.18	0.42
1:D:6:PHE:HB3	1:D:10:ILE:HD12	2.01	0.42
1:E:43:PRO:HD2	1:E:197:MSE:HE2	2.01	0.42
1:E:406:VAL:O	1:E:410:LEU:HB2	2.20	0.42
1:A:77:GLY:HA2	1:A:80:ILE:HD12	2.02	0.41
1:A:369:LEU:HD12	1:A:375:CYS:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:TYR:CD2	1:B:345:VAL:HG21	2.55	0.41
1:D:39:ILE:HG12	1:D:116:MSE:CE	2.50	0.41
1:F:257:ARG:O	1:F:362:GLY:HA3	2.19	0.41
1:F:347:TYR:HD2	1:F:369:LEU:HD13	1.84	0.41
1:B:48:LEU:HB2	1:B:67:LEU:HB2	2.02	0.41
1:C:257:ARG:O	1:C:362:GLY:HA3	2.20	0.41
1:D:397:GLU:HA	1:D:400:GLU:OE1	2.21	0.41
1:F:380:LYS:HA	1:F:383:LYS:HD2	2.02	0.41
1:C:6:PHE:HB3	1:C:10:ILE:HD12	2.01	0.41
1:C:35:ASP:HA	1:C:38:ARG:HD2	2.03	0.41
1:C:77:GLY:HA2	1:C:80:ILE:HD12	2.01	0.41
1:C:311:VAL:HG13	1:C:339:ASN:HB3	2.03	0.41
1:C:409:GLY:HA3	1:C:497:TYR:HE1	1.85	0.41
1:D:77:GLY:HA2	1:D:80:ILE:HD12	2.02	0.41
1:D:163:ARG:HA	1:D:163:ARG:HD3	1.61	0.41
1:E:39:ILE:HD13	1:E:112:MSE:HB3	2.02	0.41
1:E:468:GLU:HA	1:E:471:LEU:HD13	2.02	0.41
1:A:257:ARG:O	1:A:362:GLY:HA3	2.20	0.41
1:F:206:VAL:HB	1:F:246:LEU:HD11	2.03	0.41
1:B:190:ILE:HD11	1:B:210:LEU:HA	2.02	0.41
1:B:206:VAL:HB	1:B:246:LEU:HD11	2.03	0.41
1:B:369:LEU:HD12	1:B:375:CYS:HB3	2.02	0.41
1:B:498:ARG:NE	1:C:503:VAL:HG12	2.30	0.41
1:D:436:ARG:H	1:D:436:ARG:HG2	1.64	0.41
1:D:498:ARG:HE	1:F:503:VAL:HG12	1.84	0.41
1:A:35:ASP:HA	1:A:38:ARG:HD2	2.03	0.41
1:A:38:ARG:HG2	1:F:334:MSE:HE2	2.02	0.41
1:A:206:VAL:HB	1:A:246:LEU:HD11	2.02	0.41
1:A:406:VAL:O	1:A:410:LEU:HB2	2.20	0.41
1:B:35:ASP:HA	1:B:38:ARG:HD2	2.03	0.41
1:E:48:LEU:HB2	1:E:67:LEU:HB2	2.03	0.41
1:E:190:ILE:HD11	1:E:210:LEU:HA	2.03	0.41
1:A:6:PHE:HB3	1:A:10:ILE:HD12	2.03	0.41
1:A:380:LYS:HA	1:A:383:LYS:HD2	2.02	0.41
1:A:243:ILE:HD13	1:A:243:ILE:HA	1.98	0.41
1:A:397:GLU:HA	1:A:400:GLU:OE1	2.20	0.41
1:A:409:GLY:HA3	1:A:497:TYR:HE1	1.85	0.41
1:B:247:ARG:HG2	1:B:252:LEU:HB2	2.02	0.41
1:D:35:ASP:HA	1:D:38:ARG:HD2	2.02	0.41
1:D:43:PRO:HD2	1:D:197:MSE:HE2	2.03	0.41
1:D:48:LEU:HB2	1:D:67:LEU:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:56:PRO:HG3	1:D:399:LEU:HD22	2.03	0.41
1:D:257:ARG:O	1:D:362:GLY:HA3	2.20	0.41
1:E:409:GLY:HA3	1:E:497:TYR:HE1	1.85	0.41
1:F:29:LEU:HD23	1:F:30:ARG:HG2	2.03	0.41
1:C:331:GLN:HA	1:C:331:GLN:HE21	1.85	0.40
1:D:46:ARG:O	1:D:49:GLN:HG2	2.20	0.40
1:A:311:VAL:HG13	1:A:339:ASN:HB3	2.03	0.40
1:A:468:GLU:HA	1:A:471:LEU:HD13	2.04	0.40
1:B:393:HIS:CE1	1:B:395:ASP:H	2.40	0.40
1:F:409:GLY:HA3	1:F:497:TYR:HE1	1.85	0.40
1:A:43:PRO:HD2	1:A:197:MSE:HE2	2.02	0.40
1:C:369:LEU:HD12	1:C:375:CYS:HB3	2.03	0.40
1:C:370:GLU:OE2	1:C:373:SER:HB3	2.21	0.40
1:F:438:PRO:O	1:F:442:ARG:HD2	2.22	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	494/505 (98%)	434 (88%)	47 (10%)	13 (3%)	5	22
1	B	482/505 (95%)	421 (87%)	46 (10%)	15 (3%)	4	19
1	C	493/505 (98%)	439 (89%)	41 (8%)	13 (3%)	5	22
1	D	489/505 (97%)	432 (88%)	45 (9%)	12 (2%)	5	22
1	E	493/505 (98%)	441 (90%)	40 (8%)	12 (2%)	6	23
1	F	500/505 (99%)	443 (89%)	47 (9%)	10 (2%)	7	27
All	All	2951/3030 (97%)	2610 (88%)	266 (9%)	75 (2%)	5	22

All (75) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	164	ASP
1	A	371	ASP
1	B	58	GLU
1	B	125	GLY
1	B	222	THR
1	B	371	ASP
1	C	58	GLU
1	C	371	ASP
1	D	370	GLU
1	E	371	ASP
1	F	164	ASP
1	F	371	ASP
1	A	22	VAL
1	A	57	LEU
1	A	435	LYS
1	B	22	VAL
1	B	224	GLU
1	B	435	LYS
1	C	22	VAL
1	C	166	GLU
1	C	435	LYS
1	D	22	VAL
1	D	272	TYR
1	D	435	LYS
1	E	22	VAL
1	E	166	GLU
1	E	435	LYS
1	F	22	VAL
1	F	435	LYS
1	A	61	ALA
1	B	61	ALA
1	B	372	ALA
1	C	61	ALA
1	C	100	ASP
1	D	61	ALA
1	D	166	GLU
1	D	232	LYS
1	E	61	ALA
1	E	272	TYR
1	F	61	ALA
1	A	23	LYS
1	A	100	ASP
1	A	272	TYR

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Mol	Chain	Res	Type
1	A	449	THR
1	B	23	LYS
1	B	57	LEU
1	B	220	GLY
1	B	272	TYR
1	B	364	PHE
1	C	23	LYS
1	C	272	TYR
1	D	23	LYS
1	E	57	LEU
1	E	100	ASP
1	F	23	LYS
1	A	364	PHE
1	C	274	VAL
1	C	449	THR
1	D	100	ASP
1	D	364	PHE
1	E	23	LYS
1	F	57	LEU
1	F	167	GLU
1	F	364	PHE
1	A	165	GLY
1	A	274	VAL
1	B	274	VAL
1	C	364	PHE
1	D	274	VAL
1	E	364	PHE
1	E	274	VAL
1	F	274	VAL
1	C	54	VAL
1	E	54	VAL
1	D	54	VAL

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	443/439 (101%)	395 (89%)	48 (11%)	6	22
1	B	431/439 (98%)	379 (88%)	52 (12%)	5	17
1	C	442/439 (101%)	387 (88%)	55 (12%)	4	17
1	D	441/439 (100%)	389 (88%)	52 (12%)	5	18
1	E	443/439 (101%)	392 (88%)	51 (12%)	5	20
1	F	448/439 (102%)	396 (88%)	52 (12%)	5	19
All	All	2648/2634 (100%)	2338 (88%)	310 (12%)	5	19

All (310) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	20	GLN
1	A	29	LEU
1	A	52	THR
1	A	94	LEU
1	A	117	HIS
1	A	139	ARG
1	A	144	ASP
1	A	147	SER
1	A	150	LEU
1	A	163	ARG
1	A	164	ASP
1	A	172	LEU
1	A	195	THR
1	A	198	ARG
1	A	243	ILE
1	A	246	LEU
1	A	264	MSE
1	A	274	VAL
1	A	276	ASP
1	A	296	HIS
1	A	302	HIS
1	A	303	GLU
1	A	309	SER
1	A	310	LEU
1	A	312	VAL
1	A	328	THR
1	A	330	ASP
1	A	381	LEU
1	A	399	LEU

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Mol	Chain	Res	Type
1	A	410	LEU
1	A	415	ARG
1	A	419	SER
1	A	420	LEU
1	A	423	SER
1	A	430	GLU
1	A	435	LYS
1	A	436	ARG
1	A	446	LYS
1	A	449	THR
1	A	451	HIS
1	A	464	SER
1	A	466	SER
1	A	479	ARG
1	A	480	LEU
1	A	490	ASP
1	A	495	ASP
1	A	503	VAL
1	B	29	LEU
1	B	52	THR
1	B	57	LEU
1	B	58	GLU
1	B	59	ARG
1	B	60	ASN
1	B	94	LEU
1	B	117	HIS
1	B	139	ARG
1	B	144	ASP
1	B	147	SER
1	B	150	LEU
1	B	172	LEU
1	B	195	THR
1	B	198	ARG
1	B	224	GLU
1	B	225	THR
1	B	243	ILE
1	B	246	LEU
1	B	264	MSE
1	B	270	ILE
1	B	273	CYS
1	B	274	VAL
1	B	276	ASP

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Mol	Chain	Res	Type
1	B	296	HIS
1	B	309	SER
1	B	310	LEU
1	B	328	THR
1	B	330	ASP
1	B	369	LEU
1	B	370	GLU
1	B	381	LEU
1	B	399	LEU
1	B	410	LEU
1	B	415	ARG
1	B	419	SER
1	B	420	LEU
1	B	423	SER
1	B	433	ARG
1	B	435	LYS
1	B	436	ARG
1	B	446	LYS
1	B	447	LEU
1	B	448	SER
1	B	449	THR
1	B	464	SER
1	B	466	SER
1	B	479	ARG
1	B	480	LEU
1	B	490	ASP
1	B	495	ASP
1	B	503	VAL
1	C	17	ARG
1	C	20	GLN
1	C	29	LEU
1	C	52	THR
1	C	94	LEU
1	C	117	HIS
1	C	119	ILE
1	C	139	ARG
1	C	144	ASP
1	C	150	LEU
1	C	163	ARG
1	C	164	ASP
1	C	172	LEU
1	C	195	THR

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Mol	Chain	Res	Type
1	C	198	ARG
1	C	224	GLU
1	C	227	HIS
1	C	243	ILE
1	C	246	LEU
1	C	264	MSE
1	C	274	VAL
1	C	276	ASP
1	C	296	HIS
1	C	309	SER
1	C	310	LEU
1	C	312	VAL
1	C	327	SER
1	C	328	THR
1	C	330	ASP
1	C	331	GLN
1	C	369	LEU
1	C	370	GLU
1	C	371	ASP
1	C	381	LEU
1	C	392	SER
1	C	399	LEU
1	C	410	LEU
1	C	415	ARG
1	C	419	SER
1	C	420	LEU
1	C	423	SER
1	C	430	GLU
1	C	433	ARG
1	C	435	LYS
1	C	436	ARG
1	C	446	LYS
1	C	449	THR
1	C	451	HIS
1	C	464	SER
1	C	466	SER
1	C	479	ARG
1	C	480	LEU
1	C	490	ASP
1	C	495	ASP
1	C	503	VAL
1	D	20	GLN

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Mol	Chain	Res	Type
1	D	29	LEU
1	D	52	THR
1	D	58	GLU
1	D	94	LEU
1	D	117	HIS
1	D	119	ILE
1	D	139	ARG
1	D	144	ASP
1	D	147	SER
1	D	148	GLN
1	D	150	LEU
1	D	163	ARG
1	D	164	ASP
1	D	166	GLU
1	D	172	LEU
1	D	195	THR
1	D	198	ARG
1	D	227	HIS
1	D	243	ILE
1	D	246	LEU
1	D	264	MSE
1	D	274	VAL
1	D	276	ASP
1	D	296	HIS
1	D	301	GLN
1	D	303	GLU
1	D	304	LYS
1	D	309	SER
1	D	310	LEU
1	D	312	VAL
1	D	328	THR
1	D	330	ASP
1	D	369	LEU
1	D	381	LEU
1	D	399	LEU
1	D	410	LEU
1	D	415	ARG
1	D	419	SER
1	D	420	LEU
1	D	423	SER
1	D	430	GLU
1	D	435	LYS

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Mol	Chain	Res	Type
1	D	436	ARG
1	D	449	THR
1	D	464	SER
1	D	466	SER
1	D	479	ARG
1	D	480	LEU
1	D	490	ASP
1	D	495	ASP
1	D	503	VAL
1	E	29	LEU
1	E	52	THR
1	E	58	GLU
1	E	59	ARG
1	E	87	ARG
1	E	94	LEU
1	E	117	HIS
1	E	139	ARG
1	E	144	ASP
1	E	147	SER
1	E	150	LEU
1	E	163	ARG
1	E	164	ASP
1	E	172	LEU
1	E	179	ASP
1	E	195	THR
1	E	198	ARG
1	E	209	ILE
1	E	227	HIS
1	E	243	ILE
1	E	246	LEU
1	E	264	MSE
1	E	274	VAL
1	E	276	ASP
1	E	296	HIS
1	E	309	SER
1	E	310	LEU
1	E	312	VAL
1	E	328	THR
1	E	330	ASP
1	E	334	MSE
1	E	369	LEU
1	E	381	LEU

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Mol	Chain	Res	Type
1	E	399	LEU
1	E	410	LEU
1	E	415	ARG
1	E	419	SER
1	E	420	LEU
1	E	423	SER
1	E	430	GLU
1	E	433	ARG
1	E	435	LYS
1	E	436	ARG
1	E	446	LYS
1	E	449	THR
1	E	466	SER
1	E	479	ARG
1	E	480	LEU
1	E	490	ASP
1	E	495	ASP
1	E	503	VAL
1	F	20	GLN
1	F	29	LEU
1	F	52	THR
1	F	58	GLU
1	F	59	ARG
1	F	60	ASN
1	F	63	VAL
1	F	94	LEU
1	F	139	ARG
1	F	144	ASP
1	F	147	SER
1	F	150	LEU
1	F	166	GLU
1	F	172	LEU
1	F	195	THR
1	F	198	ARG
1	F	243	ILE
1	F	246	LEU
1	F	274	VAL
1	F	276	ASP
1	F	296	HIS
1	F	307	LEU
1	F	309	SER
1	F	310	LEU

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Mol	Chain	Res	Type
1	F	312	VAL
1	F	321	SER
1	F	322	ASN
1	F	323	SER
1	F	328	THR
1	F	330	ASP
1	F	334	MSE
1	F	369	LEU
1	F	370	GLU
1	F	371	ASP
1	F	381	LEU
1	F	399	LEU
1	F	410	LEU
1	F	415	ARG
1	F	419	SER
1	F	420	LEU
1	F	423	SER
1	F	433	ARG
1	F	435	LYS
1	F	436	ARG
1	F	449	THR
1	F	464	SER
1	F	466	SER
1	F	479	ARG
1	F	480	LEU
1	F	490	ASP
1	F	495	ASP
1	F	503	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	182	HIS
1	A	339	ASN
1	A	451	HIS
1	B	53	GLN
1	B	60	ASN
1	B	227	HIS
1	B	302	HIS
1	B	339	ASN
1	C	53	GLN
1	C	69	HIS

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Mol	Chain	Res	Type
1	C	117	HIS
1	C	302	HIS
1	C	331	GLN
1	C	355	ASN
1	C	451	HIS
1	D	53	GLN
1	D	69	HIS
1	D	182	HIS
1	D	186	ASN
1	D	302	HIS
1	D	355	ASN
1	E	182	HIS
1	E	302	HIS
1	E	339	ASN
1	F	13(C)	HIS
1	F	60	ASN
1	F	339	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)

Of 15 ligands modelled in this entry, 6 are monoatomic - leaving 9 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	SO4	A	602	-	4,4,4	0.29	0	6,6,6	0.21	0
3	SO4	E	602	-	4,4,4	0.18	0	6,6,6	0.11	0
3	SO4	F	602	-	4,4,4	0.22	0	6,6,6	0.09	0
3	SO4	C	605	-	4,4,4	0.36	0	6,6,6	0.31	0
3	SO4	C	602	-	4,4,4	0.29	0	6,6,6	0.37	0
3	SO4	B	602	-	4,4,4	0.17	0	6,6,6	0.11	0
3	SO4	C	604	-	4,4,4	0.23	0	6,6,6	0.34	0
3	SO4	D	602	-	4,4,4	0.62	0	6,6,6	0.10	0
3	SO4	C	603	-	4,4,4	0.25	0	6,6,6	0.35	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.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	605	SO4	1	0
3	C	602	SO4	2	0
3	D	602	SO4	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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.

6.5 Other polymers (i)

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