Full wwPDB X-ray Structure Validation Report (i)

Feb 18, 2024 – 08:49 AM EST

PDB ID	:	3TAF
Title	:	5-fluorocytosine paired with ddGMP in RB69 gp43
Authors	:	Zahn, K.E.
Deposited on	:	2011-08-04
Resolution	:	3.00 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:

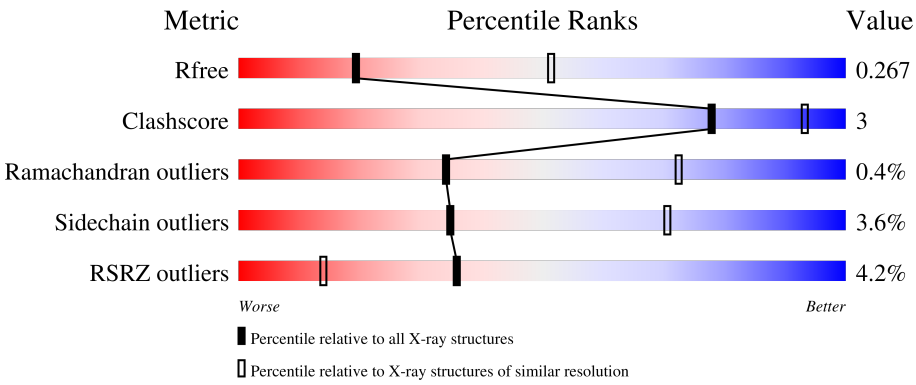
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	906	5% 88% 11% •
1	B	906	3% 88% 11% •
1	C	906	2% 89% 10% •
1	D	906	7% 90% 9% •
2	E	18	11% 89% 11%

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Mol	Chain	Length	Quality of chain
2	G	18	61% 33% 6%
2	I	18	78% 22%
2	K	18	17% 89% 6% 6%
3	F	15	87% 13%
3	H	15	100%
3	J	15	7% 100%
3	L	15	40% 100%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 32340 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 DNA-directed DNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	904	7384	4743	1229	1379	33	0	0	0
1	B	904	7384	4743	1229	1379	33	0	0	0
1	C	903	7374	4737	1226	1378	33	0	0	0
1	D	903	7374	4737	1226	1378	33	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	222	ALA	ASP	engineered mutation	UNP Q38087
A	327	ALA	ASP	engineered mutation	UNP Q38087
A	904	HIS	-	expression tag	UNP Q38087
A	905	HIS	-	expression tag	UNP Q38087
A	906	HIS	-	expression tag	UNP Q38087
B	222	ALA	ASP	engineered mutation	UNP Q38087
B	327	ALA	ASP	engineered mutation	UNP Q38087
B	904	HIS	-	expression tag	UNP Q38087
B	905	HIS	-	expression tag	UNP Q38087
B	906	HIS	-	expression tag	UNP Q38087
C	222	ALA	ASP	engineered mutation	UNP Q38087
C	327	ALA	ASP	engineered mutation	UNP Q38087
C	904	HIS	-	expression tag	UNP Q38087
C	905	HIS	-	expression tag	UNP Q38087
C	906	HIS	-	expression tag	UNP Q38087
D	222	ALA	ASP	engineered mutation	UNP Q38087
D	327	ALA	ASP	engineered mutation	UNP Q38087
D	904	HIS	-	expression tag	UNP Q38087
D	905	HIS	-	expression tag	UNP Q38087
D	906	HIS	-	expression tag	UNP Q38087

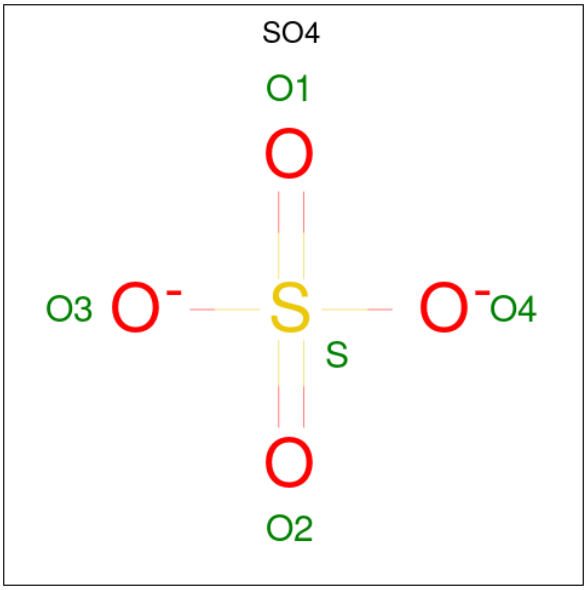
- Molecule 2 is a DNA chain called DNA (5'-D(*CP*CP*(C37)P*GP*GP*TP*AP*TP*GP*AP*CP*AP*GP*CP*CP*GP*CP*G)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	F	N	O	P			
2	E	18	366	173	1	70	105	17	0	0	0
2	G	18	370	173	1	70	108	18	0	0	0
2	I	18	370	173	1	70	108	18	0	0	0
2	K	18	366	173	1	70	105	17	0	0	0

- Molecule 3 is a DNA chain called DNA (5'-D(*GP*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*AP*CP*CP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	F	15	303	145	56	88	14	0	0	0
3	H	15	303	145	56	88	14	0	0	0
3	J	15	303	145	56	88	14	0	0	0
3	L	15	303	145	56	88	14	0	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
4	E	1	5	4	1	0	0
			Total	O	S		
4	G	1	5	4	1	0	0
			Total	O	S		
4	I	1	5	4	1	0	0
			Total	O	S		
4	K	1	5	4	1	0	0

- Molecule 5 is water.

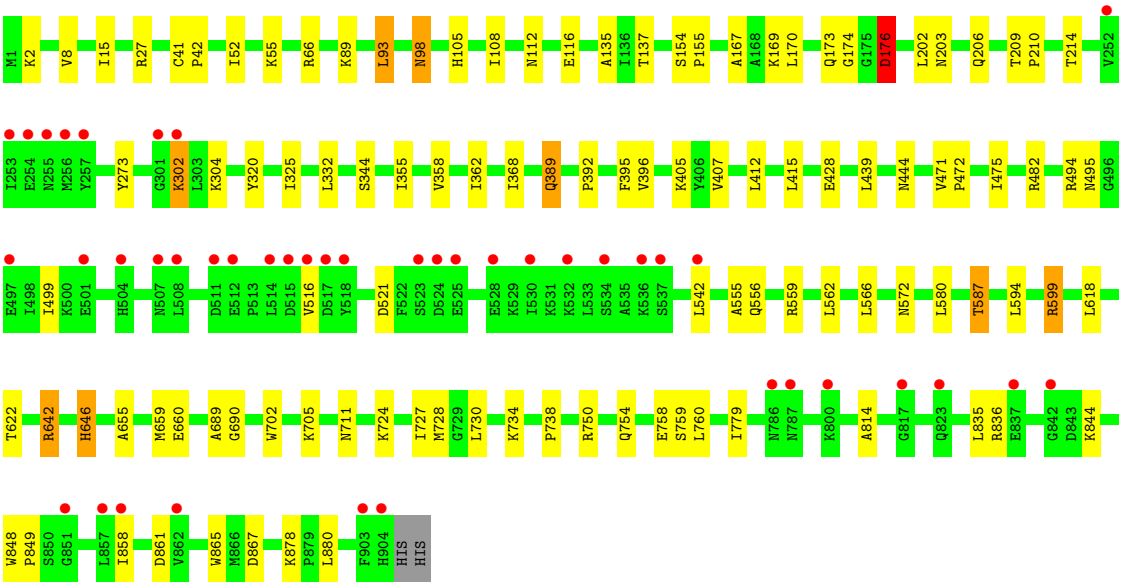
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	9	9	9	0	0
			Total	O		
5	E	1	1	1	0	0
			Total	O		
5	F	1	1	1	0	0
			Total	O		
5	B	47	47	47	0	0
			Total	O		
5	G	13	13	13	0	0
			Total	O		
5	H	18	18	18	0	0
			Total	O		
5	C	12	12	12	0	0
			Total	O		
5	I	3	3	3	0	0
			Total	O		
5	J	4	4	4	0	0
			Total	O		
5	D	8	8	8	0	0
			Total	O		
5	K	1	1	1	0	0
			Total	O		
5	L	3	3	3	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.

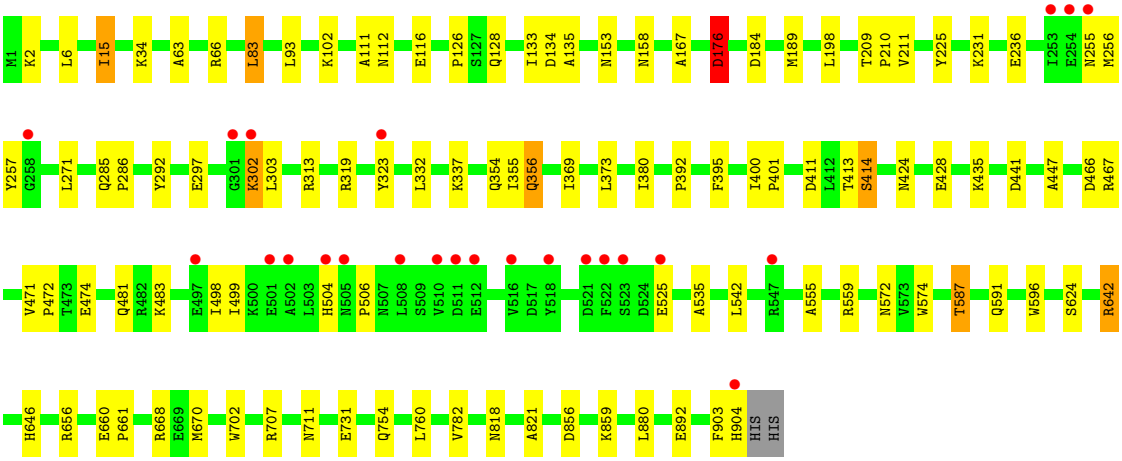
• Molecule 1: DNA-directed DNA polymerase

Chain A:



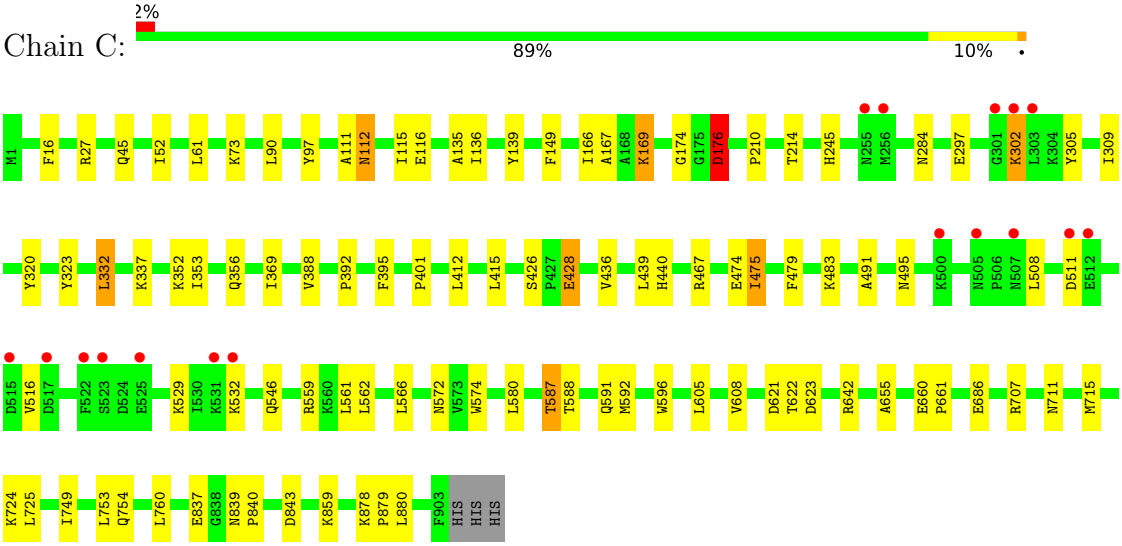
• Molecule 1: DNA-directed DNA polymerase

Chain B:



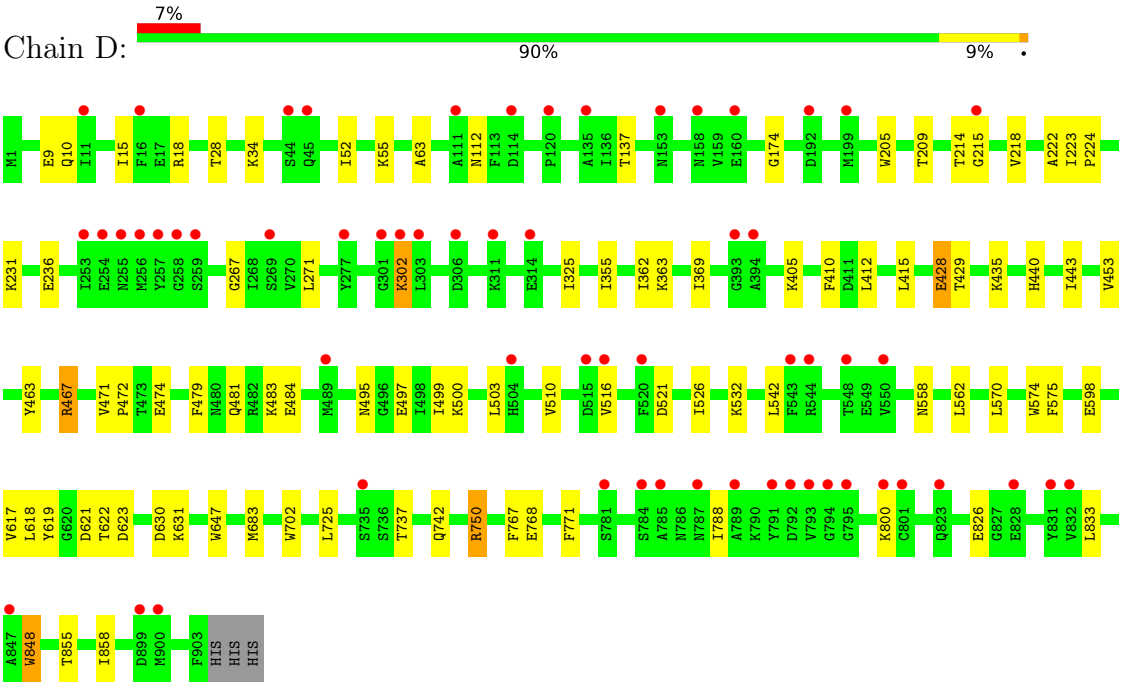
• Molecule 1: DNA-directed DNA polymerase

Chain C:



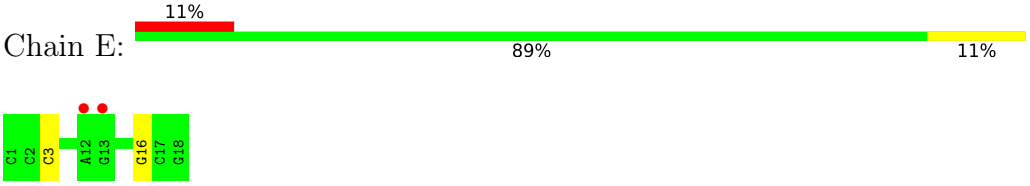
• Molecule 1: DNA-directed DNA polymerase

Chain D:



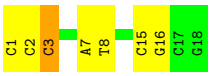
• Molecule 2: DNA (5'-D(*CP*CP*(C37)P*GP*GP*TP*AP*TP*GP*AP*CP*AP*GP*CP*CP*GP*CP*G)-3')

Chain E:



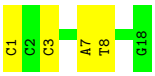
• Molecule 2: DNA (5'-D(*CP*CP*(C37)P*GP*GP*TP*AP*TP*GP*AP*CP*AP*GP*CP*CP*GP*CP*G)-3')

Chain G:



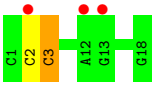
• Molecule 2: DNA (5'-D(*CP*CP*(C37)P*GP*GP*TP*AP*TP*GP*AP*CP*AP*GP*CP*CP*GP*CP*G)-3')

Chain I:



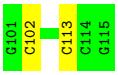
• Molecule 2: DNA (5'-D(*CP*CP*(C37)P*GP*GP*TP*AP*TP*GP*AP*CP*AP*GP*CP*CP*GP*CP*G)-3')

Chain K:

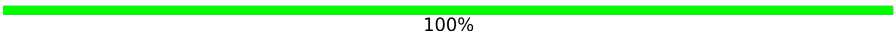


• Molecule 3: DNA (5'-D(*GP*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*AP*CP*CP*G)-3')

Chain F:

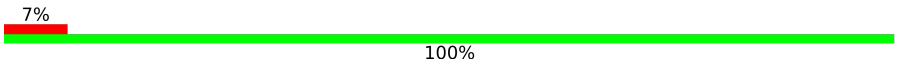


• Molecule 3: DNA (5'-D(*GP*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*AP*CP*CP*G)-3')

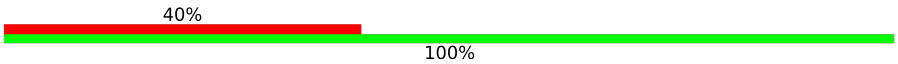
Chain H: 

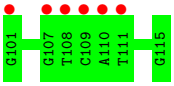
There are no outlier residues recorded for this chain.

• Molecule 3: DNA (5'-D(*GP*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*AP*CP*CP*G)-3')

Chain J: 

• Molecule 3: DNA (5'-D(*GP*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*AP*CP*CP*G)-3')

Chain L: 


G101
G107
T108
C109
A110
T111
G115

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	132.98Å 123.24Å 169.35Å 90.00° 96.96° 90.00°	Depositor
Resolution (Å)	29.99 – 3.00 29.99 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.8 (29.99-3.00) 98.9 (29.99-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.00 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.6.0116, CNS	Depositor
R, R_{free}	0.232 , 0.280 0.219 , 0.267	Depositor DCC
R_{free} test set	10394 reflections (9.67%)	wwPDB-VP
Wilson B-factor (Å^2)	77.2	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 41.5	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	0.93	EDS
Total number of atoms	32340	wwPDB-VP
Average B, all atoms (Å^2)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% 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: C37, 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	0.41	2/7566 (0.0%)	0.47	0/10224
1	B	0.41	1/7566 (0.0%)	0.48	0/10224
1	C	0.41	1/7555 (0.0%)	0.48	0/10209
1	D	0.41	5/7555 (0.1%)	0.45	0/10209
2	E	0.21	0/387	0.77	0/593
2	G	0.55	1/391 (0.3%)	0.77	0/597
2	I	0.55	1/391 (0.3%)	0.76	0/597
2	K	0.21	0/387	0.77	0/593
3	F	0.21	0/339	0.77	0/521
3	H	0.23	0/339	0.82	0/521
3	J	0.23	0/339	0.81	0/521
3	L	0.18	0/339	0.78	0/521
All	All	0.40	11/33154 (0.0%)	0.51	0/45330

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	1	DC	OP3-P	-10.04	1.49	1.61
2	G	1	DC	OP3-P	-9.99	1.49	1.61
1	A	702	TRP	CD2-CE2	5.14	1.47	1.41
1	A	865	TRP	CD2-CE2	5.14	1.47	1.41
1	D	702	TRP	CD2-CE2	5.09	1.47	1.41
1	C	596	TRP	CD2-CE2	5.09	1.47	1.41
1	D	647	TRP	CD2-CE2	5.07	1.47	1.41
1	B	702	TRP	CD2-CE2	5.07	1.47	1.41
1	D	848	TRP	CD2-CE2	5.02	1.47	1.41
1	D	205	TRP	CD2-CE2	5.02	1.47	1.41
1	D	574	TRP	CD2-CE2	5.00	1.47	1.41

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	7384	0	7274	48	0
1	B	7384	0	7274	48	0
1	C	7374	0	7267	41	0
1	D	7374	0	7267	39	0
2	E	366	0	201	1	0
2	G	370	0	200	3	0
2	I	370	0	200	2	0
2	K	366	0	201	1	0
3	F	303	0	168	2	0
3	H	303	0	168	0	0
3	J	303	0	168	0	0
3	L	303	0	168	0	0
4	E	5	0	0	0	0
4	G	5	0	0	0	0
4	I	5	0	0	0	0
4	K	5	0	0	0	0
5	A	9	0	0	0	0
5	B	47	0	0	1	0
5	C	12	0	0	1	0
5	D	8	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	13	0	0	0	0
5	H	18	0	0	0	0
5	I	3	0	0	0	0
5	J	4	0	0	0	0
5	K	1	0	0	0	0
5	L	3	0	0	0	0
All	All	32340	0	30556	181	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 3.

All (181) 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:A:112:ASN:HB3	1:A:214:THR:HG23	1.36	1.05
1:B:302:LYS:HD2	1:B:302:LYS:H	1.48	0.77
1:D:112:ASN:HB3	1:D:214:THR:HG23	1.67	0.77
1:C:711:ASN:HD21	1:C:754:GLN:HE21	1.36	0.74
1:A:8:VAL:HG11	1:A:93:LEU:HD21	1.74	0.69
1:A:302:LYS:H	1:A:302:LYS:HD2	1.60	0.67
1:D:497:GLU:HA	1:D:500:LYS:HE2	1.78	0.66
1:C:116:GLU:HB2	1:C:135:ALA:HB3	1.80	0.64
1:C:475:ILE:HG13	1:C:566:LEU:HD22	1.81	0.63
1:A:170:LEU:H	1:A:173:GLN:HE21	1.46	0.63
1:A:412:LEU:HD13	1:A:415:LEU:HD13	1.81	0.61
1:B:116:GLU:HB2	1:B:135:ALA:HB3	1.82	0.61
1:D:18:ARG:HG2	1:D:28:THR:HG22	1.83	0.61
1:C:529:LYS:HD3	1:C:532:LYS:HD2	1.83	0.60
1:B:642:ARG:HE	1:B:646:HIS:CE1	2.20	0.60
1:D:218:VAL:HA	1:D:222:ALA:HB3	1.83	0.59
1:C:707:ARG:HD2	2:I:7:DA:H4'	1.84	0.59
1:D:137:THR:HG21	1:D:325:ILE:HA	1.86	0.58
1:C:605:LEU:HA	1:C:608:VAL:HG22	1.84	0.57
1:C:52:ILE:HD12	1:C:428:GLU:HG3	1.85	0.57
1:B:441:ASP:HB3	1:B:447:ALA:HB2	1.86	0.57
1:D:440:HIS:HA	1:D:443:ILE:HD12	1.87	0.56
1:B:711:ASN:HD21	1:B:754:GLN:HE21	1.54	0.56
1:A:471:VAL:HB	1:A:472:PRO:HD3	1.88	0.56
1:A:98:ASN:HD22	1:A:98:ASN:H	1.54	0.56
1:B:392:PRO:O	1:B:587:THR:HG21	2.06	0.56
1:A:495:ASN:HD21	1:A:521:ASP:HA	1.71	0.55
1:B:656:ARG:HA	1:B:660:GLU:HG3	1.88	0.55
2:G:7:DA:H2'	2:G:8:DT:C6	2.41	0.55
1:B:354:GLN:HB3	1:B:356:GLN:OE1	2.06	0.55
1:C:167:ALA:HA	1:C:176:ASP:HB2	1.89	0.55
1:D:34:LYS:HE3	1:D:63:ALA:HA	1.88	0.55
1:A:738:PRO:HB3	1:A:779:ILE:HA	1.88	0.54
1:A:112:ASN:HB3	1:A:214:THR:CG2	2.23	0.54
1:A:444:ASN:HA	1:A:599:ARG:HE	1.72	0.54
1:C:90:LEU:HD11	1:C:353:ILE:HG22	1.89	0.54
1:C:878:LYS:HB3	1:C:879:PRO:HD3	1.90	0.53
1:C:115:ILE:HG22	1:C:136:ILE:HG12	1.91	0.52
2:G:15:DC:H2'	2:G:16:DG:C8	2.45	0.52
1:B:231:LYS:HE3	1:B:236:GLU:HG3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:ARG:HH21	1:B:189:MET:HB3	1.76	0.51
1:A:154:SER:HB2	1:A:155:PRO:HD2	1.93	0.51
1:A:392:PRO:O	1:A:587:THR:HG21	2.10	0.51
1:B:167:ALA:HA	1:B:176:ASP:HB2	1.93	0.51
1:D:855:THR:HG23	1:D:858:ILE:HG22	1.93	0.51
1:A:711:ASN:HD21	1:A:754:GLN:HE21	1.58	0.51
1:D:471:VAL:HB	1:D:472:PRO:HD3	1.93	0.51
1:B:856:ASP:HA	1:B:859:LYS:HB3	1.93	0.51
1:C:136:ILE:HB	1:C:149:PHE:HB2	1.93	0.51
1:C:395:PHE:HA	5:C:914:HOH:O	2.11	0.51
1:A:98:ASN:H	1:A:98:ASN:ND2	2.09	0.51
1:A:727:ILE:HG23	1:A:730:LEU:HD12	1.93	0.50
1:B:707:ARG:HH22	1:B:731:GLU:CD	2.15	0.50
1:D:619:TYR:CE2	1:D:621:ASP:HB2	2.46	0.50
1:C:297:GLU:O	1:C:337:LYS:HE2	2.12	0.49
1:A:655:ALA:HA	1:A:659:MET:HB2	1.93	0.49
1:B:66:ARG:HB2	5:B:921:HOH:O	2.12	0.49
1:C:839:ASN:HB2	1:C:840:PRO:HD2	1.94	0.49
1:C:395:PHE:HB2	1:C:591:GLN:HG2	1.93	0.49
1:B:395:PHE:HB2	1:B:591:GLN:HE21	1.77	0.49
1:A:116:GLU:HB2	1:A:135:ALA:HB3	1.94	0.49
1:A:836:ARG:HB3	1:A:867:ASP:HB2	1.94	0.49
1:B:369:ILE:HG12	1:B:474:GLU:HG3	1.95	0.49
1:A:642:ARG:HE	1:A:646:HIS:CE1	2.31	0.49
1:B:555:ALA:O	1:B:559:ARG:HG2	2.13	0.48
1:B:818:ASN:HD22	1:B:821:ALA:H	1.59	0.48
1:D:495:ASN:O	1:D:499:ILE:HG12	2.12	0.48
1:B:303:LEU:HG	1:B:323:TYR:CE2	2.49	0.48
2:G:2:DC:H2"	2:G:3:C37:O1P	2.13	0.48
2:K:2:DC:H2'	2:K:3:C37:C6	2.44	0.48
1:A:848:TRP:HB2	1:A:849:PRO:HD2	1.94	0.48
1:B:373:LEU:HD12	1:B:380:ILE:HG22	1.95	0.48
1:D:369:ILE:HG12	1:D:474:GLU:HG3	1.95	0.48
1:A:202:LEU:O	1:A:206:GLN:HG2	2.13	0.47
1:D:500:LYS:HA	1:D:503:LEU:HB2	1.96	0.47
1:D:598:GLU:HG3	1:D:617:VAL:HG11	1.94	0.47
1:A:814:ALA:HB1	1:A:858:ILE:HG21	1.96	0.47
1:D:833:LEU:HD12	1:D:848:TRP:HH2	1.80	0.47
1:C:725:LEU:HD22	1:C:753:LEU:HD12	1.96	0.47
2:I:7:DA:H2'	2:I:8:DT:H71	1.97	0.47
1:D:800:LYS:O	1:D:800:LYS:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:16:DG:H1	3:F:102:DC:H42	1.62	0.46
1:B:297:GLU:O	1:B:337:LYS:HE2	2.15	0.46
1:A:302:LYS:HG3	1:A:304:LYS:HE3	1.97	0.46
1:D:218:VAL:HG22	1:D:223:ILE:HG13	1.97	0.46
1:D:499:ILE:HG21	1:D:542:LEU:HB2	1.97	0.46
1:B:660:GLU:HB2	1:B:661:PRO:HD3	1.98	0.46
1:C:711:ASN:HD22	1:C:725:LEU:HD23	1.81	0.46
1:C:439:LEU:HD11	1:C:592:MET:HB2	1.97	0.46
1:A:52:ILE:HB	1:A:428:GLU:HG2	1.98	0.45
1:A:396:VAL:O	1:A:705:LYS:NZ	2.49	0.45
1:A:655:ALA:O	1:A:660:GLU:HG2	2.16	0.45
1:C:660:GLU:HB2	1:C:661:PRO:HD3	1.98	0.45
1:D:231:LYS:HG3	1:D:236:GLU:HA	1.98	0.45
1:C:491:ALA:O	1:C:495:ASN:HB2	2.16	0.45
1:B:596:TRP:CE2	1:B:670:MET:HB2	2.52	0.45
1:C:112:ASN:CB	1:C:214:THR:HG23	2.47	0.45
1:D:9:GLU:HG3	1:D:267:GLY:H	1.81	0.45
1:D:412:LEU:HD13	1:D:415:LEU:HD13	1.99	0.45
1:C:621:ASP:O	1:C:623:ASP:N	2.49	0.45
1:A:41:CYS:HB2	1:A:42:PRO:HD2	1.98	0.45
1:A:362:ILE:HG13	1:A:572:ASN:HD22	1.82	0.45
1:A:344:SER:HB2	1:A:358:VAL:HG21	1.99	0.44
1:B:471:VAL:HB	1:B:472:PRO:HD3	1.98	0.44
1:C:16:PHE:HB3	1:C:245:HIS:CE1	2.52	0.44
1:D:725:LEU:HD11	1:D:750:ARG:HG3	1.98	0.44
1:A:368:ILE:HD13	1:A:562:LEU:HD21	1.99	0.44
1:B:286:PRO:HB3	1:B:782:VAL:HG21	1.98	0.44
1:A:209:THR:HA	1:A:210:PRO:HD3	1.85	0.44
1:D:223:ILE:N	1:D:224:PRO:HD2	2.32	0.44
1:A:734:LYS:HG2	3:F:113:DC:H5'	1.98	0.44
1:B:411:ASP:OD1	1:B:624:SER:HB3	2.18	0.44
1:C:309:ILE:H	1:C:309:ILE:HG13	1.66	0.44
1:A:355:ILE:H	1:A:355:ILE:HD12	1.83	0.43
1:C:655:ALA:O	1:C:660:GLU:HG2	2.18	0.43
1:D:471:VAL:HG11	1:D:570:LEU:HD11	1.99	0.43
1:B:134:ASP:HB2	1:B:313:ARG:NH1	2.33	0.43
1:D:788:ILE:HD12	1:D:826:GLU:HG2	1.99	0.43
1:B:506:PRO:HB3	1:B:535:ALA:HB2	2.00	0.43
1:C:97:TYR:O	1:C:352:LYS:HE2	2.19	0.43
1:B:34:LYS:HE3	1:B:63:ALA:HA	2.00	0.43
1:C:587:THR:HG22	1:C:588:THR:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:749:ILE:O	1:C:753:LEU:HG	2.18	0.43
1:D:214:THR:OG1	1:D:215:GLY:N	2.51	0.43
1:B:285:GLN:HE21	1:B:292:TYR:HE2	1.65	0.43
1:A:89:LYS:O	1:A:93:LEU:HD22	2.18	0.43
1:A:555:ALA:O	1:A:559:ARG:HG2	2.19	0.43
1:C:412:LEU:HD13	1:C:415:LEU:HD13	2.00	0.43
1:D:737:THR:HB	1:D:742:GLN:HE21	1.83	0.43
1:B:153:ASN:HD22	1:B:158:ASN:HB3	1.82	0.43
1:D:481:GLN:O	1:D:484:GLU:HB3	2.19	0.43
1:A:105:HIS:HA	1:A:108:ILE:HD12	2.01	0.43
1:A:405:LYS:O	1:A:690:GLY:HA2	2.19	0.43
1:B:133:ILE:HD12	1:B:198:LEU:HD21	2.01	0.42
1:B:903:PHE:HB3	1:B:904:HIS:H	1.61	0.42
1:A:389:GLN:HE21	1:A:389:GLN:HB3	1.66	0.42
1:B:481:GLN:HE21	1:B:559:ARG:HH11	1.67	0.42
1:D:302:LYS:H	1:D:302:LYS:HD2	1.84	0.42
1:B:413:THR:O	1:B:414:SER:C	2.57	0.42
1:C:166:ILE:HA	1:C:169:LYS:HD3	2.00	0.42
1:B:111:ALA:HB3	1:B:210:PRO:HB3	2.01	0.42
1:C:302:LYS:H	1:C:302:LYS:HD2	1.83	0.42
1:D:429:THR:O	1:D:463:TYR:HA	2.20	0.42
1:D:467:ARG:H	1:D:467:ARG:HD2	1.85	0.42
1:B:83:LEU:H	1:B:83:LEU:HD23	1.85	0.42
1:D:362:ILE:HG23	1:D:575:PHE:HD1	1.85	0.42
1:B:126:PRO:HA	1:B:225:TYR:HD2	1.85	0.42
1:B:499:ILE:HG21	1:B:542:LEU:HB2	2.02	0.42
1:C:572:ASN:ND2	1:C:574:TRP:H	2.18	0.42
1:A:116:GLU:HB3	1:A:320:TYR:OH	2.20	0.41
1:A:475:ILE:HD13	1:A:566:LEU:HD22	2.02	0.41
1:A:482:ARG:HH11	1:A:556:GLN:HG2	1.84	0.41
1:B:572:ASN:ND2	1:B:574:TRP:HB2	2.35	0.41
1:A:167:ALA:HA	1:A:176:ASP:HB2	2.02	0.41
1:A:499:ILE:HG21	1:A:542:LEU:HB2	2.02	0.41
1:C:369:ILE:HG12	1:C:474:GLU:HG3	2.02	0.41
1:C:116:GLU:HB3	1:C:320:TYR:OH	2.21	0.41
1:C:392:PRO:O	1:C:587:THR:HG21	2.21	0.41
1:C:475:ILE:CG1	1:C:566:LEU:HD22	2.48	0.41
1:D:10:GLN:HA	1:D:15:ILE:HG22	2.01	0.41
1:B:400:ILE:HA	1:B:401:PRO:HD3	1.95	0.41
1:C:305:TYR:HD2	1:C:323:TYR:HE2	1.67	0.41
1:B:15:ILE:C	1:B:15:ILE:HD12	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:LEU:HD11	1:B:355:ILE:CG2	2.51	0.41
1:B:6:LEU:HD22	1:B:211:VAL:HG11	2.03	0.41
1:C:111:ALA:HB3	1:C:210:PRO:HB3	2.03	0.41
1:D:767:PHE:O	1:D:771:PHE:HB2	2.21	0.41
1:B:319:ARG:HD2	1:B:323:TYR:CE1	2.56	0.41
1:B:209:THR:HA	1:B:210:PRO:HD3	1.91	0.41
1:B:255:ASN:HB3	1:B:256:MET:H	1.67	0.41
1:C:686:GLU:HG3	1:C:715:MET:SD	2.61	0.41
1:D:621:ASP:O	1:D:623:ASP:N	2.53	0.41
1:A:137:THR:HG21	1:A:325:ILE:HA	2.03	0.40
1:A:395:PHE:HD2	1:A:594:LEU:HD23	1.86	0.40
1:D:52:ILE:HD12	1:D:428:GLU:HG3	2.03	0.40
1:D:271:LEU:HD11	1:D:355:ILE:HG22	2.03	0.40
1:D:516:VAL:HG21	1:D:526:ILE:HG21	2.02	0.40
1:A:407:VAL:HB	1:A:689:ALA:HB3	2.04	0.40
1:C:139:TYR:CD2	1:C:332:LEU:HD21	2.56	0.40
1:B:176:ASP:N	1:B:176:ASP:OD1	2.55	0.40
1:D:410:PHE:HB3	1:D:683:MET:HG2	2.04	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	902/906 (100%)	854 (95%)	45 (5%)	3 (0%)	41	76
1	B	902/906 (100%)	860 (95%)	38 (4%)	4 (0%)	34	72
1	C	901/906 (99%)	867 (96%)	30 (3%)	4 (0%)	34	72
1	D	901/906 (99%)	859 (95%)	39 (4%)	3 (0%)	41	76
All	All	3606/3624 (100%)	3440 (95%)	152 (4%)	14 (0%)	34	72

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	622	THR
1	A	622	THR
1	D	622	THR
1	B	176	ASP
1	B	424	ASN
1	B	892	GLU
1	C	176	ASP
1	D	174	GLY
1	A	176	ASP
1	B	414	SER
1	D	405	LYS
1	A	174	GLY
1	C	174	GLY
1	C	401	PRO

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	801/803 (100%)	768 (96%)	33 (4%)	30	67
1	B	801/803 (100%)	775 (97%)	26 (3%)	39	74
1	C	800/803 (100%)	764 (96%)	36 (4%)	27	64
1	D	800/803 (100%)	780 (98%)	20 (2%)	47	79
All	All	3202/3212 (100%)	3087 (96%)	115 (4%)	35	70

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	15	ILE
1	A	55	LYS
1	A	66	ARG
1	A	93	LEU
1	A	98	ASN
1	A	169	LYS
1	A	176	ASP

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Mol	Chain	Res	Type
1	A	203	ASN
1	A	273	TYR
1	A	302	LYS
1	A	332	LEU
1	A	389	GLN
1	A	439	LEU
1	A	494	ARG
1	A	516	VAL
1	A	580	LEU
1	A	587	THR
1	A	599	ARG
1	A	618	LEU
1	A	642	ARG
1	A	646	HIS
1	A	724	LYS
1	A	728	MET
1	A	750	ARG
1	A	758	GLU
1	A	759	SER
1	A	760	LEU
1	A	835	LEU
1	A	844	LYS
1	A	861	ASP
1	A	878	LYS
1	A	880	LEU
1	B	2	LYS
1	B	15	ILE
1	B	83	LEU
1	B	93	LEU
1	B	102	LYS
1	B	112	ASN
1	B	128	GLN
1	B	176	ASP
1	B	184	ASP
1	B	257	TYR
1	B	302	LYS
1	B	332	LEU
1	B	356	GLN
1	B	428	GLU
1	B	435	LYS
1	B	466	ASP
1	B	467	ARG

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Mol	Chain	Res	Type
1	B	483	LYS
1	B	498	ILE
1	B	504	HIS
1	B	525	GLU
1	B	587	THR
1	B	642	ARG
1	B	668	ARG
1	B	760	LEU
1	B	880	LEU
1	C	27	ARG
1	C	45	GLN
1	C	61	LEU
1	C	73	LYS
1	C	112	ASN
1	C	169	LYS
1	C	176	ASP
1	C	284	ASN
1	C	302	LYS
1	C	332	LEU
1	C	356	GLN
1	C	388	VAL
1	C	426	SER
1	C	428	GLU
1	C	436	VAL
1	C	440	HIS
1	C	467	ARG
1	C	475	ILE
1	C	479	PHE
1	C	483	LYS
1	C	508	LEU
1	C	511	ASP
1	C	516	VAL
1	C	546	GLN
1	C	559	ARG
1	C	561	LEU
1	C	562	LEU
1	C	580	LEU
1	C	587	THR
1	C	642	ARG
1	C	724	LYS
1	C	760	LEU
1	C	837	GLU

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Mol	Chain	Res	Type
1	C	843	ASP
1	C	859	LYS
1	C	880	LEU
1	D	55	LYS
1	D	209	THR
1	D	302	LYS
1	D	363	LYS
1	D	428	GLU
1	D	435	LYS
1	D	453	VAL
1	D	467	ARG
1	D	479	PHE
1	D	483	LYS
1	D	510	VAL
1	D	521	ASP
1	D	532	LYS
1	D	558	ASN
1	D	562	LEU
1	D	618	LEU
1	D	630	ASP
1	D	631	LYS
1	D	750	ARG
1	D	768	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	ASN
1	A	153	ASN
1	A	158	ASN
1	A	173	GLN
1	A	285	GLN
1	A	389	GLN
1	A	481	GLN
1	A	495	ASN
1	A	572	ASN
1	A	646	HIS
1	A	678	GLN
1	A	711	ASN
1	B	45	GLN
1	B	131	HIS
1	B	153	ASN

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Mol	Chain	Res	Type
1	B	158	ASN
1	B	203	ASN
1	B	245	HIS
1	B	284	ASN
1	B	285	GLN
1	B	481	GLN
1	B	558	ASN
1	B	572	ASN
1	B	591	GLN
1	B	646	HIS
1	B	675	ASN
1	B	678	GLN
1	B	711	ASN
1	B	818	ASN
1	C	40	HIS
1	C	112	ASN
1	C	153	ASN
1	C	158	ASN
1	C	173	GLN
1	C	203	ASN
1	C	245	HIS
1	C	284	ASN
1	C	285	GLN
1	C	481	GLN
1	C	539	ASN
1	C	556	GLN
1	C	558	ASN
1	C	572	ASN
1	C	646	HIS
1	C	678	GLN
1	C	679	HIS
1	C	711	ASN
1	C	864	HIS
1	D	153	ASN
1	D	158	ASN
1	D	203	ASN
1	D	207	GLN
1	D	285	GLN
1	D	481	GLN
1	D	539	ASN
1	D	711	ASN
1	D	742	GLN

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Mol	Chain	Res	Type
1	D	787	ASN
1	D	812	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)

4 non-standard protein/DNA/RNA residues 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	C37	G	3	2,3	18,21,22	0.54	0	25,30,33	1.55	2 (8%)
2	C37	I	3	2,3	18,21,22	0.54	0	25,30,33	1.60	2 (8%)
2	C37	E	3	2,3	18,21,22	0.53	0	25,30,33	1.58	2 (8%)
2	C37	K	3	2,3	18,21,22	0.52	0	25,30,33	1.61	2 (8%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	C37	G	3	2,3	-	0/7/21/22	0/2/2/2
2	C37	I	3	2,3	-	0/7/21/22	0/2/2/2
2	C37	E	3	2,3	-	0/7/21/22	0/2/2/2
2	C37	K	3	2,3	-	0/7/21/22	0/2/2/2

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	K	3	C37	F-C5-C4	6.95	122.56	118.02
2	I	3	C37	F-C5-C4	6.92	122.55	118.02
2	E	3	C37	F-C5-C4	6.81	122.47	118.02
2	G	3	C37	F-C5-C4	6.69	122.39	118.02
2	K	3	C37	C5-C4-N3	3.58	121.96	119.60
2	I	3	C37	C5-C4-N3	3.48	121.89	119.60
2	G	3	C37	C5-C4-N3	3.46	121.88	119.60
2	E	3	C37	C5-C4-N3	3.45	121.88	119.60

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	3	C37	1	0
2	K	3	C37	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

4 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	$\#\|Z\| > 2$
4	SO4	I	19	-	4,4,4	0.34	0	6,6,6	0.12	0
4	SO4	G	19	-	4,4,4	0.33	0	6,6,6	0.05	0
4	SO4	E	19	-	4,4,4	0.33	0	6,6,6	0.07	0
4	SO4	K	19	-	4,4,4	0.32	0	6,6,6	0.05	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	A	904/906 (99%)	-0.00	43 (4%)	30	11	40, 76, 159, 244	0
1	B	904/906 (99%)	-0.21	24 (2%)	54	26	33, 60, 163, 357	0
1	C	903/906 (99%)	-0.24	17 (1%)	66	37	32, 62, 126, 219	0
1	D	903/906 (99%)	0.31	60 (6%)	18	5	62, 117, 170, 199	0
2	E	17/18 (94%)	0.35	2 (11%)	4	1	62, 88, 140, 143	0
2	G	17/18 (94%)	-0.56	0	100	100	34, 49, 70, 80	0
2	I	17/18 (94%)	-0.13	0	100	100	43, 56, 84, 96	0
2	K	17/18 (94%)	1.22	3 (17%)	1	0	83, 113, 138, 147	0
3	F	15/15 (100%)	0.49	0	100	100	69, 103, 168, 170	0
3	H	15/15 (100%)	-0.49	0	100	100	39, 50, 78, 84	0
3	J	15/15 (100%)	-0.01	1 (6%)	17	5	44, 64, 102, 103	0
3	L	15/15 (100%)	1.77	6 (40%)	0	0	102, 133, 169, 170	0
All	All	3742/3756 (99%)	-0.02	156 (4%)	36	14	32, 77, 163, 357	0

All (156) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	904	HIS	11.9
1	A	256	MET	9.3
1	D	789	ALA	7.9
1	D	847	ALA	7.8
1	A	904	HIS	7.0
1	D	256	MET	6.2
1	A	514	LEU	6.1
1	A	257	TYR	5.5
1	C	511	ASP	5.4
1	D	800	LYS	5.3
1	A	516	VAL	5.3

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Mol	Chain	Res	Type	RSRZ
1	D	900	MET	5.2
1	B	523	SER	5.2
1	A	523	SER	4.6
1	D	787	ASN	4.4
1	D	515	ASP	4.4
1	D	795	GLY	4.4
1	D	257	TYR	4.2
1	D	120	PRO	4.0
1	C	512	GLU	4.0
1	D	258	GLY	3.9
1	D	111	ALA	3.9
1	A	524	ASP	3.9
1	B	510	VAL	3.8
1	D	302	LYS	3.8
1	A	508	LEU	3.7
1	D	199	MET	3.6
1	A	507	ASN	3.6
1	D	301	GLY	3.6
1	D	794	GLY	3.6
1	D	828	GLU	3.5
1	D	253	ILE	3.5
1	A	302	LYS	3.5
1	D	269	SER	3.4
1	C	515	ASP	3.4
1	A	255	ASN	3.4
1	B	512	GLU	3.4
1	D	255	ASN	3.3
1	D	44	SER	3.3
1	C	302	LYS	3.3
1	D	543	PHE	3.3
1	D	801	CYS	3.3
1	A	528	GLU	3.2
1	C	523	SER	3.2
1	A	512	GLU	3.2
1	D	823	GLN	3.2
1	D	11	ILE	3.2
1	B	302	LYS	3.2
1	D	899	ASP	3.2
3	L	108	DT	3.1
1	A	515	ASP	3.1
1	A	501	GLU	3.1
1	D	785	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	16	PHE	3.0
1	D	394	ALA	3.0
3	L	101	DG	3.0
1	C	525	GLU	3.0
1	D	314	GLU	3.0
1	B	525	GLU	2.9
1	D	158	ASN	2.9
1	B	516	VAL	2.9
1	B	505	ASN	2.8
1	A	858	ILE	2.8
1	A	504	HIS	2.8
1	B	511	ASP	2.8
1	C	531	LYS	2.8
1	A	537	SER	2.8
1	C	256	MET	2.7
1	D	793	VAL	2.7
3	J	101	DG	2.7
1	B	255	ASN	2.7
2	K	13	DG	2.7
2	K	12	DA	2.7
1	D	306	ASP	2.6
1	D	254	GLU	2.6
1	A	786	ASN	2.6
2	E	13	DG	2.6
1	D	544	ARG	2.6
1	D	792	ASP	2.6
1	A	530	ILE	2.6
1	B	508	LEU	2.6
3	L	109	DC	2.6
1	A	301	GLY	2.6
1	D	504	HIS	2.5
1	A	817	GLY	2.5
1	A	842	GLY	2.5
1	D	548	THR	2.5
1	C	522	PHE	2.5
1	A	800	LYS	2.5
1	D	135	ALA	2.5
1	D	215	GLY	2.5
2	E	12	DA	2.5
2	K	2	DC	2.5
3	L	111	DT	2.5
1	A	511	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	393	GLY	2.4
1	C	301	GLY	2.4
1	A	823	GLN	2.4
1	D	114	ASP	2.4
1	A	857	LEU	2.4
1	B	521	ASP	2.4
1	D	781	SER	2.4
1	D	277	TYR	2.4
1	D	550	VAL	2.4
1	D	791	TYR	2.4
1	D	192	ASP	2.4
3	L	110	DA	2.4
1	B	323	TYR	2.4
1	D	831	TYR	2.3
1	B	502	ALA	2.3
1	A	536	LYS	2.3
1	D	303	LEU	2.3
1	A	862	VAL	2.3
1	D	735	SER	2.3
1	A	837	GLU	2.2
1	A	787	ASN	2.2
1	C	507	ASN	2.2
1	D	153	ASN	2.2
1	A	532	LYS	2.2
1	B	518	TYR	2.2
1	D	160	GLU	2.2
1	B	504	HIS	2.2
1	D	520	PHE	2.2
1	A	497	GLU	2.2
1	A	851	GLY	2.2
1	A	254	GLU	2.2
1	D	784	SER	2.2
1	B	253	ILE	2.2
1	C	303	LEU	2.2
1	C	532	LYS	2.2
3	L	107	DG	2.2
1	B	301	GLY	2.2
1	A	252	VAL	2.1
1	D	311	LYS	2.1
1	A	518	TYR	2.1
1	A	517	ASP	2.1
1	A	253	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	534	SER	2.1
1	A	542	LEU	2.1
1	A	903	PHE	2.1
1	B	254	GLU	2.1
1	B	547	ARG	2.1
1	D	259	SER	2.1
1	B	522	PHE	2.1
1	A	525	GLU	2.1
1	B	497	GLU	2.1
1	C	517	ASP	2.1
1	D	489	MET	2.1
1	C	255	ASN	2.1
1	C	505	ASN	2.1
1	D	45	GLN	2.0
1	B	501	GLU	2.0
1	D	832	VAL	2.0
1	C	500	LYS	2.0
1	D	516	VAL	2.0
1	B	258	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
2	C37	K	3	20/21	0.85	0.33	104,111,114,114	0
2	C37	E	3	20/21	0.90	0.25	78,90,93,93	0
2	C37	I	3	20/21	0.94	0.15	55,59,62,64	0
2	C37	G	3	20/21	0.98	0.12	37,38,45,46	0

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
4	SO4	E	19	5/5	0.80	0.21	110,112,112,113	0
4	SO4	K	19	5/5	0.82	0.22	133,133,134,134	0
4	SO4	I	19	5/5	0.89	0.22	86,87,88,88	0
4	SO4	G	19	5/5	0.91	0.16	92,93,94,96	0

6.5 Other polymers (i)

There are no such residues in this entry.