Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:14 PM GMT

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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

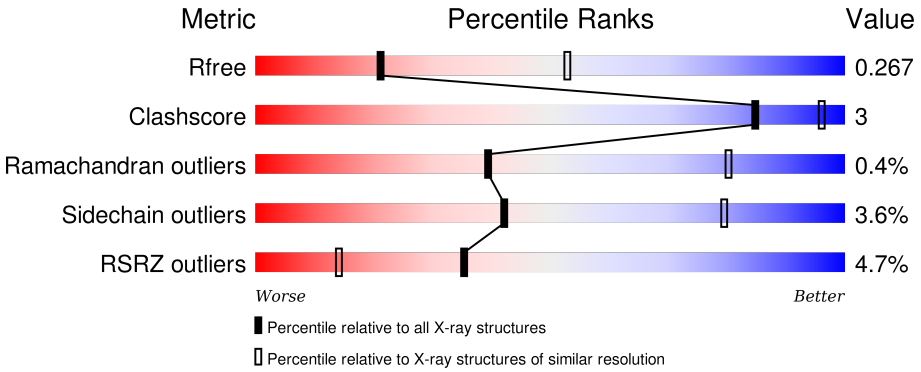
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	4% 88% 11%
1	C	906	2% 89% 10%
1	D	906	7% 90% 9%
2	E	18	11% 94% 6%

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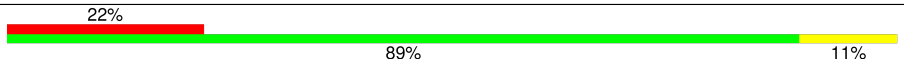
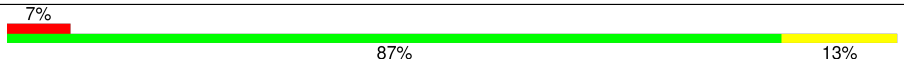
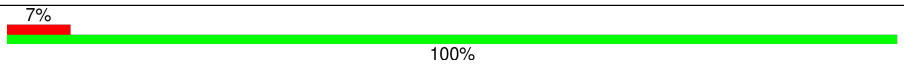
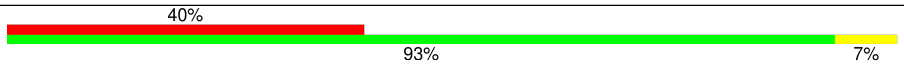
Mol	Chain	Length	Quality of chain
2	G	18	
2	I	18	
2	K	18	
3	F	15	
3	H	15	
3	J	15	
3	L	15	

2 Entry composition

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 polymerase.

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

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

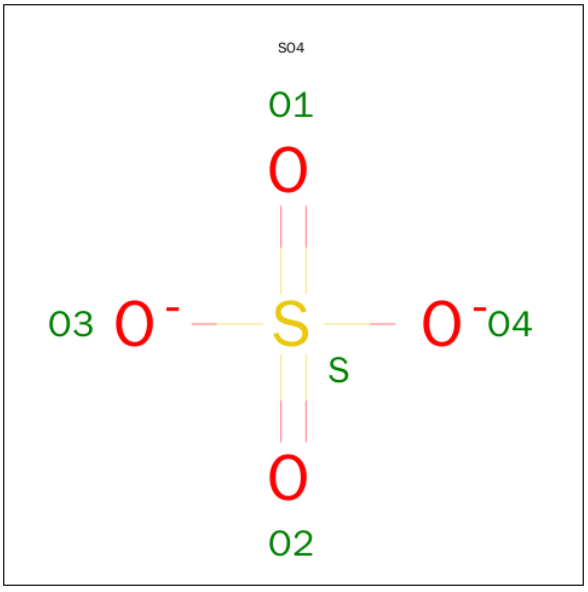
- Molecule 2 is a DNA chain called DNA (5'-D(*CP*CP*(C37)P*GP*GP*TP*AP*TP*GP*AP*CP*AP*GP*CP*CP*GP*CP*G)-3').

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

- 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
3	F	15	Total	C	N	O	P	0	0	0
			303	145	56	88	14			
3	H	15	Total	C	N	O	P	0	0	0
			303	145	56	88	14			
3	J	15	Total	C	N	O	P	0	0	0
			303	145	56	88	14			
3	L	15	Total	C	N	O	P	0	0	0
			303	145	56	88	14			

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



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

- Molecule 5 is water.

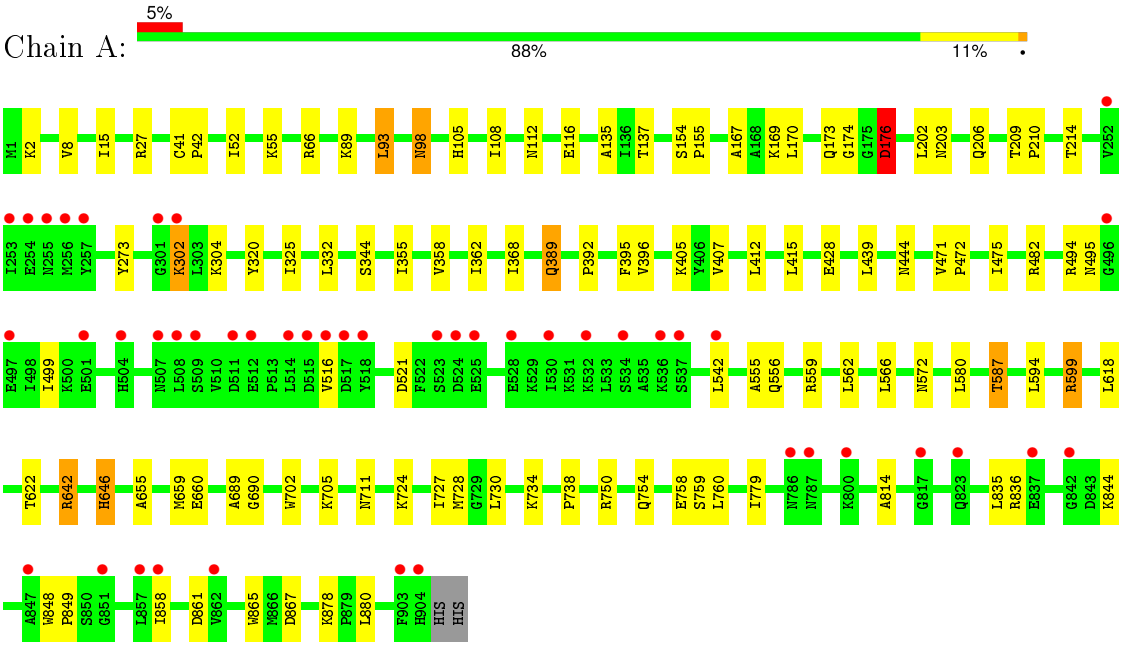
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	9	Total O 9 9	0	0
5	E	1	Total O 1 1	0	0
5	F	1	Total O 1 1	0	0
5	B	47	Total O 47 47	0	0
5	G	13	Total O 13 13	0	0
5	H	18	Total O 18 18	0	0
5	C	12	Total O 12 12	0	0
5	I	3	Total O 3 3	0	0
5	J	4	Total O 4 4	0	0
5	D	8	Total O 8 8	0	0
5	K	1	Total O 1 1	0	0
5	L	3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

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

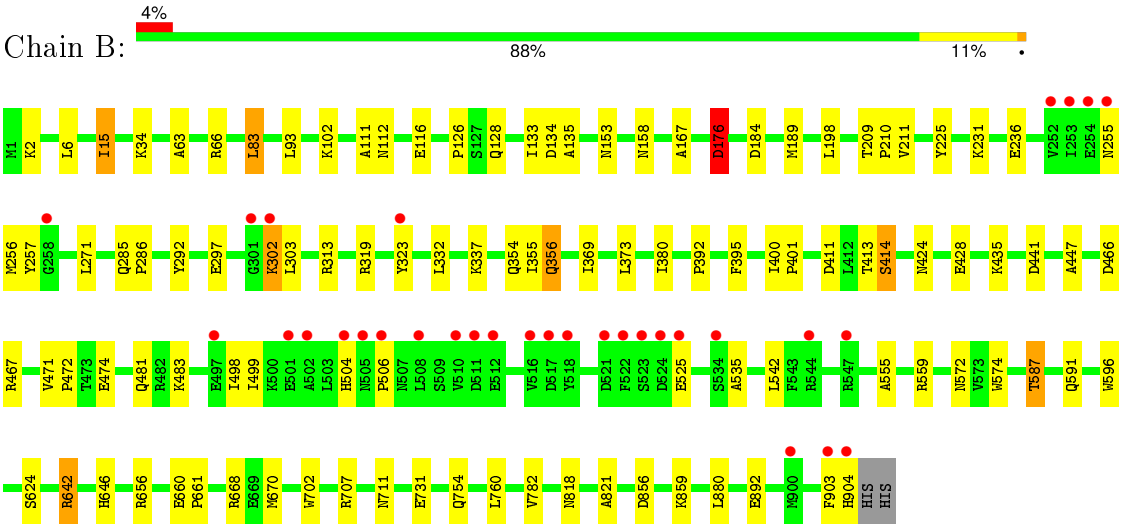
- Molecule 1: DNA polymerase

Chain A:



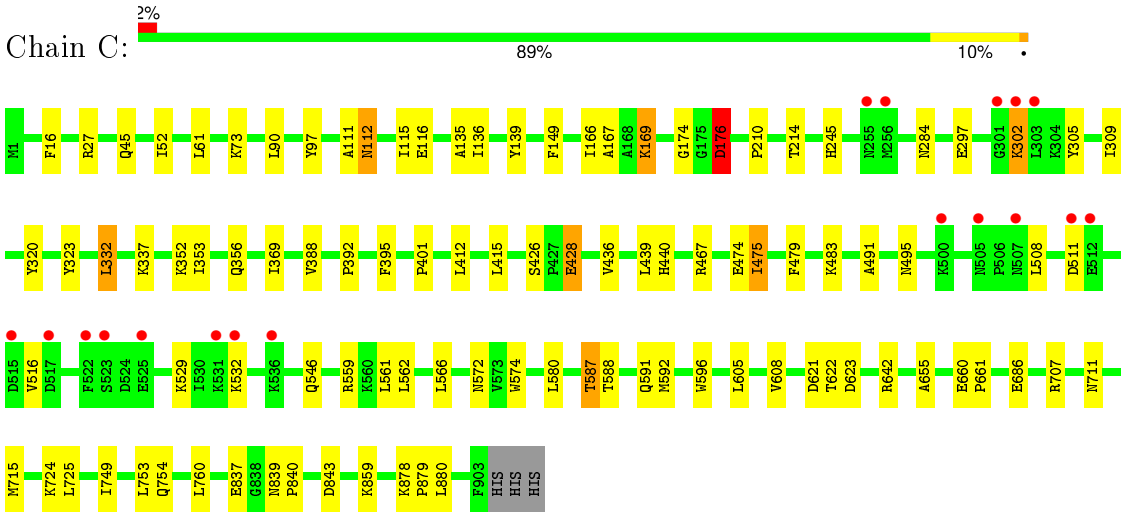
- Molecule 1: DNA polymerase

Chain B:



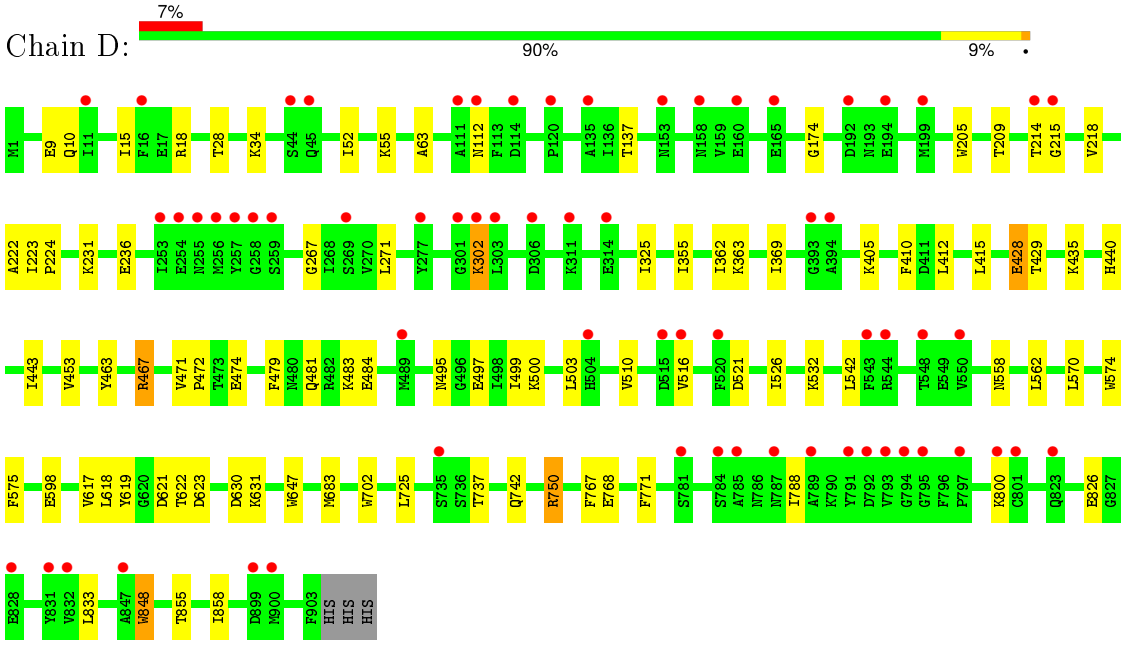
- Molecule 1: DNA polymerase

Chain C:



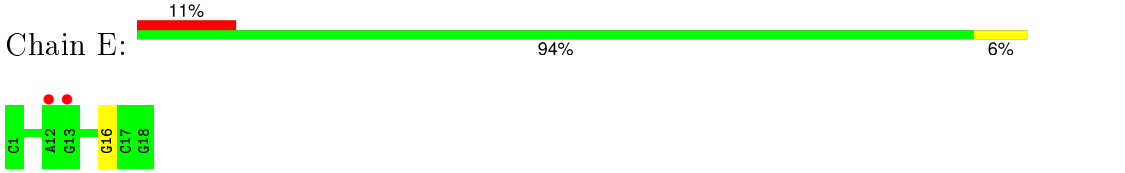
• Molecule 1: DNA polymerase

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:

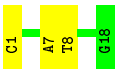


• Molecule 2: DNA (5'-D(*CP*CP*(C37)P*GP*GP*TP*AP*TP*GP*AP*CP*AP*GP*CP*CP*GP*CP*G)-3')

Chain G:

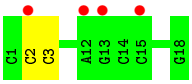
• Molecule 2: DNA (5'-D(*CP*CP*(C37)P*GP*GP*TP*AP*TP*GP*AP*CP*AP*GP*CP*CP*GP*CP*G)-3')

Chain I:



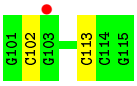
• Molecule 2: DNA (5'-D(*CP*CP*(C37)P*GP*GP*TP*AP*TP*GP*AP*CP*AP*GP*CP*CP*GP*CP*G)-3')

Chain K:



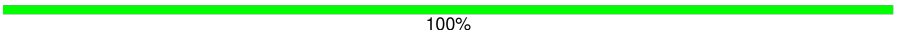
• Molecule 3: DNA (5'-D(*GP*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*AP*CP*CP*G)-3')

Chain F:



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

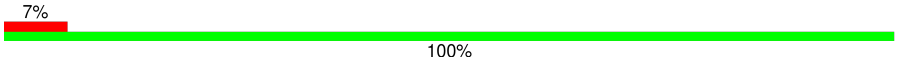
Chain H:



There are no outlier residues recorded for this chain.

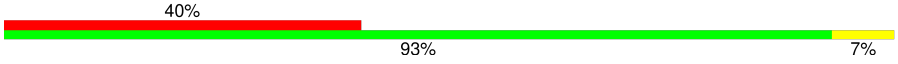
• Molecule 3: DNA (5'-D(*GP*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*AP*CP*CP*G)-3')

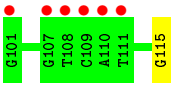
Chain J:



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

Chain L:





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	Depositor
R, R_{free}	0.232 , 0.280 0.219 , 0.267	Depositor DCC
R_{free} test set	10394 reflections (10.71%)	DCC
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
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 107458 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	2	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	1	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	182	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 (182) 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:H	1:B:302:LYS:HD2	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:H	1:A:98:ASN:HD22	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
2:G:7:DA:H2'	2:G:8:DT:C6	2.41	0.55
1:B:656:ARG:HA	1:B:660:GLU:HG3	1.88	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:392:PRO:O	1:A:587:THR:HG21	2.10	0.51
1:A:154:SER:HB2	1:A:155:PRO:HD2	1.93	0.51
1:D:855:THR:HG23	1:D:858:ILE:HG22	1.93	0.51
1:A:27:ARG:HH21	1:B:189:MET:HB3	1.76	0.51
1:B:167:ALA:HA	1:B:176:ASP:HB2	1.93	0.51
1:D:471:VAL:HB	1:D:472:PRO:HD3	1.93	0.51
1:A:711:ASN:HD21	1:A:754:GLN:HE21	1.58	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:ND2	1:A:98:ASN:H	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:818:ASN:HD22	1:B:821:ALA:H	1.59	0.48
1:B:555:ALA:O	1:B:559:ARG:HG2	2.13	0.48
1:D:495:ASN:O	1:D:499:ILE:HG12	2.12	0.48
2:G:2:DC:H2"	2:G:3:C37:O1P	2.13	0.48
1:B:303:LEU:HG	1:B:323:TYR:CE2	2.49	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:HG3	1:D:800:LYS:O	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
2:K:3:C37:O2	3:L:115:DG:N2	2.37	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:D:231:LYS:HG3	1:D:236:GLU:HA	1.98	0.45
1:C:660:GLU:HB2	1:C:661:PRO:HD3	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:D:9:GLU:HG3	1:D:267:GLY:H	1.81	0.45
1:C:112:ASN:CB	1:C:214:THR:HG23	2.47	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: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:B:471:VAL:HB	1:B:472:PRO:HD3	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:HG13	1:C:309:ILE:H	1.66	0.44
1:D:471:VAL:HG11	1:D:570:LEU:HD11	1.99	0.43
1:C:655:ALA:O	1:C:660:GLU:HG2	2.18	0.43
1:A:355:ILE:HD12	1:A:355:ILE:H	1.83	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:C:97:TYR:O	1:C:352:LYS:HE2	2.19	0.43
1:B:506:PRO:HB3	1:B:535:ALA:HB2	2.00	0.43
1:D:214:THR:OG1	1:D:215:GLY:N	2.51	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: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
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:D:737:THR:HB	1:D:742:GLN:HE21	1.83	0.43
1:C:412:LEU:HD13	1:C:415:LEU:HD13	2.00	0.43
1:A:555:ALA:O	1:A:559:ARG:HG2	2.19	0.43
1:D:481:GLN:O	1:D:484:GLU:HB3	2.19	0.43
1:B:153:ASN:HD22	1:B:158:ASN:HB3	1.82	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:903:PHE:HB3	1:B:904:HIS:H	1.61	0.42
1:B:133:ILE:HD12	1:B:198:LEU:HD21	2.01	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:A:389:GLN:HB3	1:A:389:GLN:HE21	1.66	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:C:302:LYS:H	1:C:302:LYS:HD2	1.83	0.42
1:B:111:ALA:HB3	1:B:210:PRO:HB3	2.01	0.42
1:D:467:ARG:HD2	1:D:467:ARG:H	1.85	0.42
1:D:429:THR:O	1:D:463:TYR:HA	2.20	0.42
1:B:83:LEU:HD23	1:B:83:LEU:H	1.85	0.42
1:D:362:ILE:HG23	1:D:575:PHE:HD1	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:B:126:PRO:HA	1:B:225:TYR:HD2	1.85	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:C:369:ILE:HG12	1:C:474:GLU:HG3	2.02	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: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

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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:15:ILE:C	1:B:15:ILE:HD12	2.40	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:D:621:ASP:O	1:D:623:ASP:N	2.53	0.41
1:B:209:THR:HA	1:B:210:PRO:HD3	1.91	0.41
1:C:686:GLU:HG3	1:C:715:MET:SD	2.61	0.41
1:B:255:ASN:HB3	1:B:256:MET:H	1.67	0.41
1:D:516:VAL:HG21	1:D:526:ILE:HG21	2.02	0.40
1:A:395:PHE:HD2	1:A:594:LEU:HD23	1.86	0.40
1:A:137:THR:HG21	1:A:325:ILE:HA	2.03	0.40
1:D:271:LEU:HD11	1:D:355:ILE:HG22	2.03	0.40
1:D:52:ILE:HD12	1:D:428:GLU:HG3	2.03	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:OD1	1:B:176:ASP:N	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%)	46 84
1	B	902/906 (100%)	860 (95%)	38 (4%)	4 (0%)	39 80
1	C	901/906 (99%)	867 (96%)	30 (3%)	4 (0%)	39 80
1	D	901/906 (99%)	859 (95%)	39 (4%)	3 (0%)	46 84
All	All	3606/3624 (100%)	3440 (95%)	152 (4%)	14 (0%)	39 80

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%)	37	76
1	B	801/803 (100%)	775 (97%)	26 (3%)	46	82
1	C	800/803 (100%)	764 (96%)	36 (4%)	34	74
1	D	800/803 (100%)	780 (98%)	20 (2%)	55	86
All	All	3202/3212 (100%)	3087 (96%)	115 (4%)	42	79

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

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Mol	Chain	Res	Type
1	A	169	LYS
1	A	176	ASP
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

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Mol	Chain	Res	Type
1	B	466	ASP
1	B	467	ARG
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

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Mol	Chain	Res	Type
1	C	760	LEU
1	C	837	GLU
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

Some 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

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Mol	Chain	Res	Type
1	B	131	HIS
1	B	153	ASN
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

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Mol	Chain	Res	Type
1	D	711	ASN
1	D	742	GLN
1	D	787	ASN
1	D	812	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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	E	3	3,2	13,21,22	1.04	2 (15%)	17,30,33	1.83	4 (23%)
2	C37	G	3	3,2	13,21,22	1.03	2 (15%)	17,30,33	1.81	4 (23%)
2	C37	I	3	3,2	13,21,22	1.04	2 (15%)	17,30,33	1.85	4 (23%)
2	C37	K	3	3,2	13,21,22	1.02	2 (15%)	17,30,33	1.87	4 (23%)

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	E	3	3,2	-	0/3/21/22	0/2/2/2
2	C37	G	3	3,2	-	0/3/21/22	0/2/2/2
2	C37	I	3	3,2	-	0/3/21/22	0/2/2/2
2	C37	K	3	3,2	-	0/3/21/22	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	3	C37	C6-C5	-2.17	1.34	1.38
2	E	3	C37	C6-C5	-2.16	1.34	1.38
2	G	3	C37	C6-C5	-2.13	1.34	1.38
2	K	3	C37	C6-C5	-2.11	1.34	1.38
2	G	3	C37	C4-C5	2.10	1.43	1.40
2	K	3	C37	C4-C5	2.12	1.43	1.40
2	E	3	C37	C4-C5	2.16	1.43	1.40
2	I	3	C37	C4-C5	2.17	1.43	1.40

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	K	3	C37	C5-C4-N4	-4.04	120.11	122.63
2	K	3	C37	C6-C5-C4	-4.03	117.44	121.48
2	I	3	C37	C6-C5-C4	-4.00	117.47	121.48
2	I	3	C37	C5-C4-N4	-4.00	120.14	122.63
2	E	3	C37	C6-C5-C4	-3.98	117.50	121.48
2	G	3	C37	C6-C5-C4	-3.96	117.51	121.48
2	E	3	C37	C5-C4-N4	-3.96	120.16	122.63
2	G	3	C37	C5-C4-N4	-3.89	120.21	122.63
2	E	3	C37	C5-C4-N3	3.35	121.88	118.51
2	G	3	C37	C5-C4-N3	3.36	121.88	118.51
2	I	3	C37	C5-C4-N3	3.37	121.89	118.51
2	K	3	C37	C5-C4-N3	3.44	121.96	118.51
2	G	3	C37	F-C5-C4	3.47	122.39	119.70
2	E	3	C37	F-C5-C4	3.57	122.47	119.70
2	I	3	C37	F-C5-C4	3.67	122.55	119.70
2	K	3	C37	F-C5-C4	3.69	122.56	119.70

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

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

5.5 Carbohydrates (i)

There are no carbohydrates 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	E	19	-	4,4,4	0.37	0	6,6,6	0.10	0
4	SO4	G	19	-	4,4,4	0.36	0	6,6,6	0.07	0
4	SO4	I	19	-	4,4,4	0.36	0	6,6,6	0.15	0
4	SO4	K	19	-	4,4,4	0.35	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
4	SO4	E	19	-	-	0/0/0/0	0/0/0/0
4	SO4	G	19	-	-	0/0/0/0	0/0/0/0
4	SO4	I	19	-	-	0/0/0/0	0/0/0/0
4	SO4	K	19	-	-	0/0/0/0	0/0/0/0

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

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	904/906 (99%)	0.02	46 (5%) 32 12	40, 76, 159, 244	0
1	B	904/906 (99%)	-0.18	32 (3%) 48 21	33, 60, 163, 357	0
1	C	903/906 (99%)	-0.22	18 (1%) 68 39	32, 62, 126, 219	0
1	D	903/906 (99%)	0.35	65 (7%) 18 7	62, 117, 170, 199	0
2	E	17/18 (94%)	0.42	2 (11%) 6 2	62, 88, 140, 143	0
2	G	17/18 (94%)	-0.53	0 100 100	34, 49, 70, 80	0
2	I	17/18 (94%)	-0.08	0 100 100	43, 56, 84, 96	0
2	K	17/18 (94%)	1.32	4 (23%) 1 1	83, 113, 138, 147	0
3	F	15/15 (100%)	0.57	1 (6%) 21 7	69, 103, 168, 170	0
3	H	15/15 (100%)	-0.47	0 100 100	39, 50, 78, 84	0
3	J	15/15 (100%)	0.04	1 (6%) 21 7	44, 64, 102, 103	0
3	L	15/15 (100%)	1.89	6 (40%) 0 0	102, 133, 169, 170	0
All	All	3742/3756 (99%)	0.01	175 (4%) 35 14	32, 77, 163, 357	0

All (175) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	904	HIS	12.0
1	A	256	MET	9.8
1	D	789	ALA	8.2
1	D	847	ALA	8.1
1	A	904	HIS	6.9
1	D	256	MET	6.5
1	A	514	LEU	6.3
1	A	257	TYR	5.8
1	C	511	ASP	5.5
1	D	800	LYS	5.5
1	D	900	MET	5.5

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Mol	Chain	Res	Type	RSRZ
1	A	516	VAL	5.5
1	B	523	SER	5.4
1	A	523	SER	4.9
1	D	787	ASN	4.7
1	D	515	ASP	4.5
1	D	795	GLY	4.5
1	D	257	TYR	4.5
1	D	258	GLY	4.2
1	C	512	GLU	4.1
1	B	510	VAL	4.1
1	D	111	ALA	4.1
1	A	524	ASP	4.0
1	D	120	PRO	3.9
1	A	508	LEU	3.9
1	D	302	LYS	3.9
1	D	301	GLY	3.7
1	D	794	GLY	3.7
1	D	199	MET	3.7
1	D	269	SER	3.6
1	A	302	LYS	3.6
1	D	828	GLU	3.6
1	D	255	ASN	3.6
1	D	253	ILE	3.6
1	C	515	ASP	3.6
1	A	255	ASN	3.5
1	D	801	CYS	3.5
1	B	512	GLU	3.5
1	D	543	PHE	3.5
1	A	507	ASN	3.4
1	D	11	ILE	3.4
1	A	528	GLU	3.4
1	C	302	LYS	3.4
3	L	108	DT	3.3
1	B	302	LYS	3.3
1	D	44	SER	3.3
1	D	899	ASP	3.3
1	D	823	GLN	3.3
1	D	785	ALA	3.3
1	A	512	GLU	3.2
1	D	16	PHE	3.2
1	D	314	GLU	3.2
1	C	523	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	501	GLU	3.2
1	A	515	ASP	3.2
3	L	101	DG	3.1
1	D	394	ALA	3.1
1	D	158	ASN	3.1
1	B	525	GLU	3.0
1	B	505	ASN	3.0
1	B	516	VAL	3.0
1	C	525	GLU	2.9
1	A	504	HIS	2.9
1	C	256	MET	2.9
2	E	13	DG	2.9
1	B	511	ASP	2.9
1	C	531	LYS	2.9
1	B	255	ASN	2.9
3	J	101	DG	2.9
1	A	537	SER	2.9
1	A	858	ILE	2.8
2	K	13	DG	2.8
2	K	12	DA	2.8
2	K	2	DC	2.8
3	L	109	DC	2.7
1	B	508	LEU	2.7
1	D	793	VAL	2.7
1	D	254	GLU	2.7
1	A	786	ASN	2.7
1	A	301	GLY	2.7
1	D	792	ASP	2.7
1	D	544	ARG	2.7
1	A	817	GLY	2.6
1	D	215	GLY	2.6
1	D	393	GLY	2.6
2	E	12	DA	2.6
1	D	306	ASP	2.6
1	D	114	ASP	2.6
1	D	277	TYR	2.6
1	B	521	ASP	2.6
1	A	530	ILE	2.6
3	L	111	DT	2.5
1	D	548	THR	2.5
1	A	800	LYS	2.5
1	D	192	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	323	TYR	2.5
1	D	791	TYR	2.5
1	C	301	GLY	2.5
1	A	823	GLN	2.5
1	C	522	PHE	2.5
1	D	135	ALA	2.5
1	A	842	GLY	2.5
1	A	511	ASP	2.5
1	D	504	HIS	2.5
1	A	857	LEU	2.5
1	A	862	VAL	2.5
1	B	504	HIS	2.5
1	D	781	SER	2.5
1	D	550	VAL	2.5
1	D	831	TYR	2.4
1	B	502	ALA	2.4
3	L	110	DA	2.4
1	C	507	ASN	2.4
1	D	153	ASN	2.4
1	A	787	ASN	2.4
1	A	837	GLU	2.4
1	B	518	TYR	2.3
1	B	522	PHE	2.3
1	A	536	LYS	2.3
1	A	497	GLU	2.3
3	L	107	DG	2.3
1	D	160	GLU	2.3
1	D	303	LEU	2.3
1	D	520	PHE	2.3
1	C	532	LYS	2.3
1	D	784	SER	2.3
1	A	851	GLY	2.3
1	A	532	LYS	2.3
1	C	303	LEU	2.3
1	A	518	TYR	2.3
1	A	252	VAL	2.3
1	B	253	ILE	2.3
1	D	311	LYS	2.2
1	B	301	GLY	2.2
1	B	254	GLU	2.2
1	A	542	LEU	2.2
1	B	497	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	903	PHE	2.2
1	A	254	GLU	2.2
1	A	253	ILE	2.2
1	A	534	SER	2.2
1	B	547	ARG	2.2
1	D	735	SER	2.2
1	D	194	GLU	2.1
1	C	255	ASN	2.1
1	B	900	MET	2.1
1	D	259	SER	2.1
1	A	517	ASP	2.1
1	C	517	ASP	2.1
1	D	45	GLN	2.1
1	B	517	ASP	2.1
3	F	103	DG	2.1
1	B	506	PRO	2.1
1	B	501	GLU	2.1
1	A	496	GLY	2.1
1	A	525	GLU	2.1
1	B	524	ASP	2.1
1	B	544	ARG	2.1
1	C	505	ASN	2.1
1	D	112	ASN	2.1
1	D	797	PRO	2.1
1	B	252	VAL	2.1
1	D	516	VAL	2.1
1	C	500	LYS	2.1
1	D	832	VAL	2.1
1	D	214	THR	2.1
1	B	258	GLY	2.0
1	A	847	ALA	2.0
1	B	534	SER	2.0
1	D	165	GLU	2.0
1	C	536	LYS	2.0
1	B	903	PHE	2.0
2	K	15	DC	2.0
1	D	489	MET	2.0
1	A	509	SER	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	C37	E	3	20/21	0.90	0.25	-	78,90,93,93	0
2	C37	G	3	20/21	0.98	0.12	-	37,38,45,46	0
2	C37	I	3	20/21	0.94	0.16	-	55,59,62,64	0
2	C37	K	3	20/21	0.85	0.33	-	104,111,114,114	0

6.3 Carbohydrates (i)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	SO4	E	19	5/5	0.80	0.21	-	110,112,112,113	0
4	SO4	G	19	5/5	0.91	0.16	-	92,93,94,96	0
4	SO4	I	19	5/5	0.89	0.22	-	86,87,88,88	0
4	SO4	K	19	5/5	0.82	0.22	-	133,133,134,134	0

6.5 Other polymers (i)

There are no such residues in this entry.