



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 22, 2026 – 08:30 PM EDT

PDB ID : 3TAF / pdb_00003taf
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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

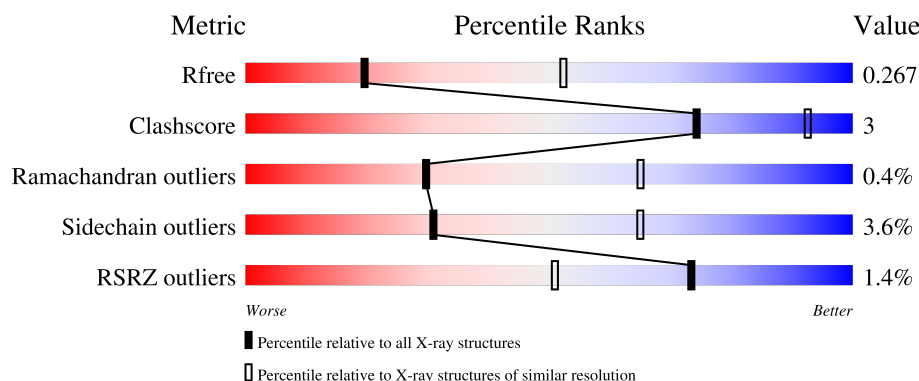
1 Overall quality at a glance

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.



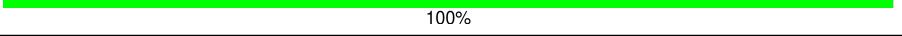
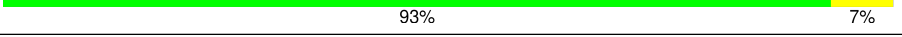
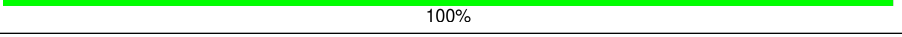
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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 $\leq 5\%$. 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	
1	B	906	
1	C	906	
1	D	906	
2	E	18	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	G	18	 67% 28% 6%
2	I	18	 83% 17%
2	K	18	 89% 6% 6%
3	F	15	 87% 13%
3	H	15	 100%
3	J	15	 93% 7%
3	L	15	 100%

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-directed 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

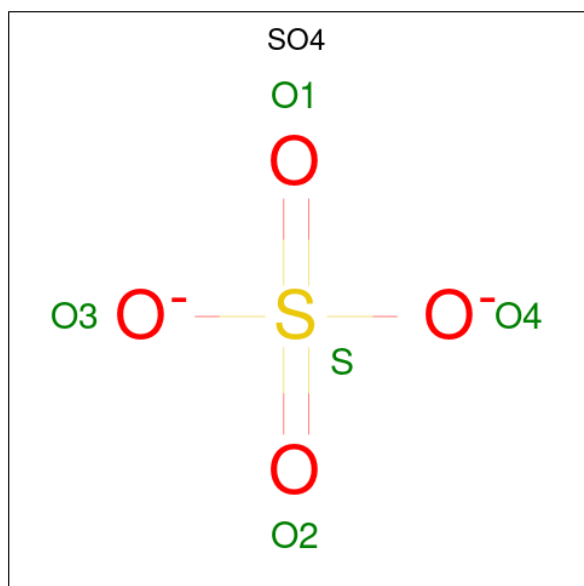
- Molecule 2 is a DNA chain called DNA (5'-D(*CP*CP*(C37)P*GP*GP*TP*AP*TP*GP*AP*CP*AP*GP*CP*CP*GP*CP*G)-3').

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 (CCD ID: SO4) (formula: O₄S).



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

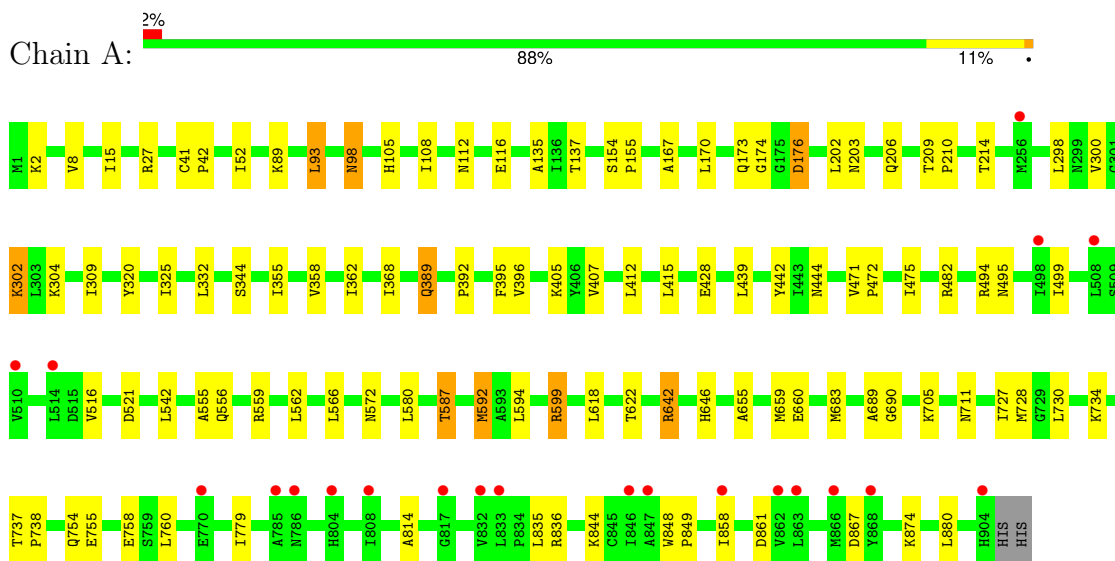
- Molecule 5 is water.

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

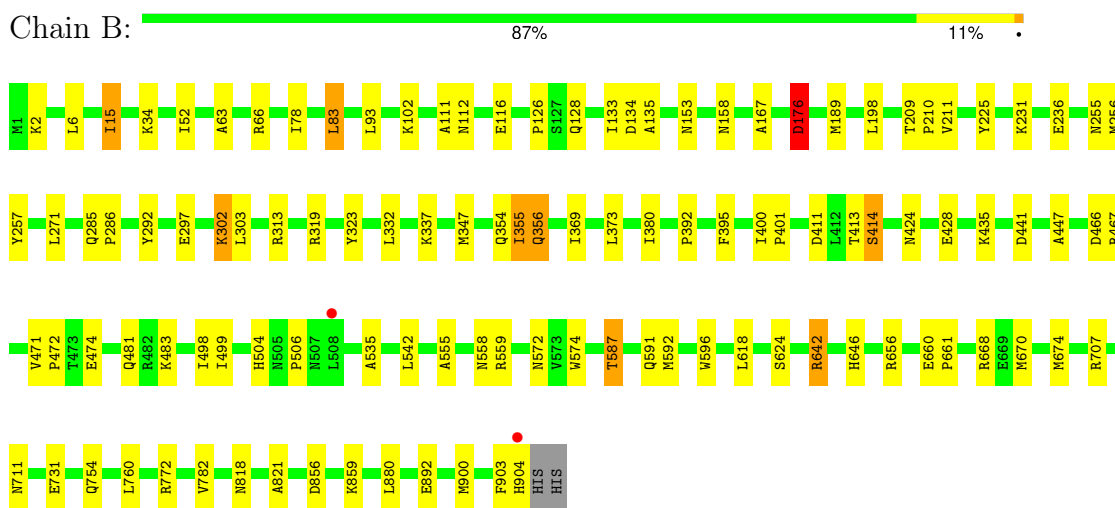
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

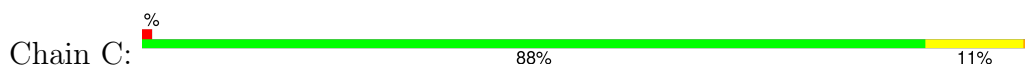
• Molecule 1: DNA-directed DNA polymerase

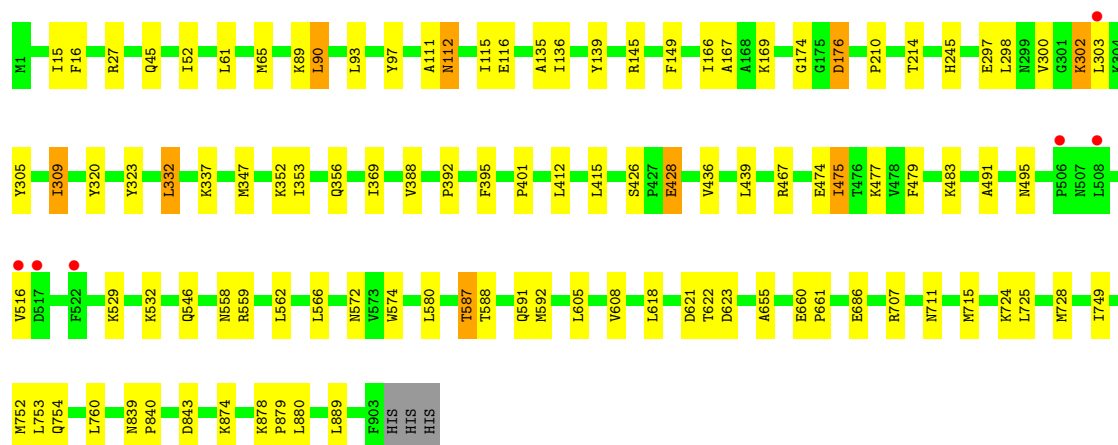


• Molecule 1: DNA-directed DNA polymerase

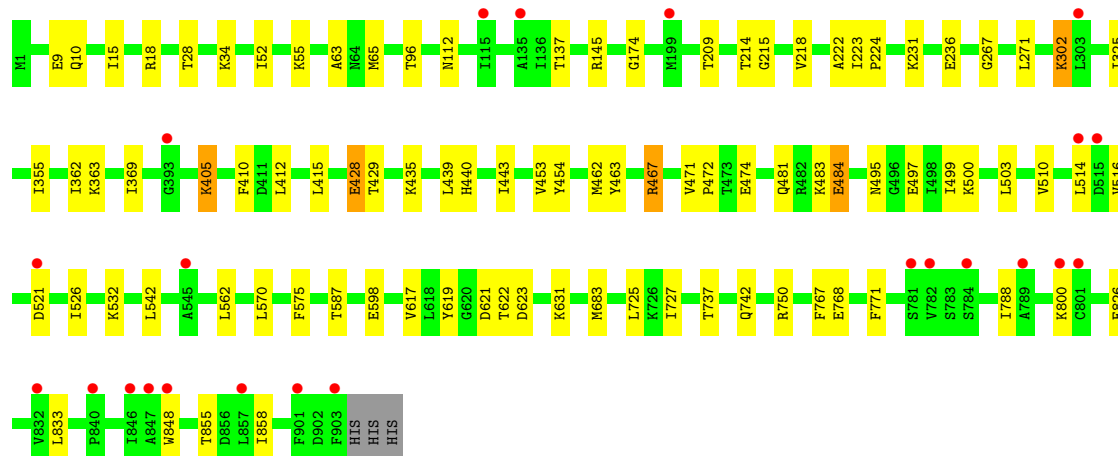
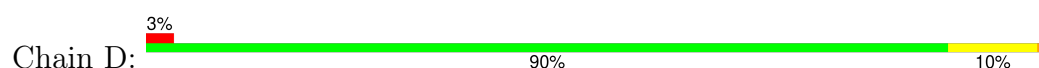


• Molecule 1: DNA-directed DNA polymerase

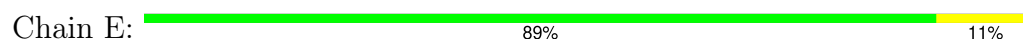




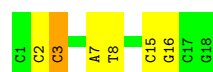
• Molecule 1: DNA-directed DNA polymerase



• 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')

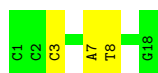


• Molecule 2: DNA (5'-D(*CP*CP*(C37)P*GP*GP*TP*AP*TP*GP*AP*CP*AP*GP*CP*CP*GP*CP*G)-3')



• 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:  83% 17%



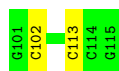
- Molecule 2: DNA (5'-D(*CP*CP*(C37)P*GP*GP*TP*AP*TP*GP*AP*CP*AP*GP*CP*CP*GP*CP*G)-3')

Chain K:  89% 6% 6%



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

Chain F:  87% 13%



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

Chain H:  100%

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:  93% 7%



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

Chain L:  100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

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) 98.8 (29.99-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 (9.56%)	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 , 38.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.51	0/7566	0.76	2/10224 (0.0%)
1	B	0.51	0/7566	0.76	0/10224
1	C	0.50	0/7555	0.75	0/10209
1	D	0.51	0/7555	0.75	0/10209
2	E	0.28	0/387	0.58	0/593
2	G	0.28	0/391	0.62	0/597
2	I	0.28	0/391	0.59	0/597
2	K	0.28	0/387	0.57	0/593
3	F	0.27	0/339	0.59	0/521
3	H	0.28	0/339	0.67	0/521
3	J	0.28	0/339	0.67	0/521
3	L	0.28	0/339	0.60	0/521
All	All	0.50	0/33154	0.74	2/45330 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	737	THR	CA-C-N	5.71	125.72	119.89
1	A	737	THR	C-N-CA	5.71	125.72	119.89

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	51	0
1	B	7384	0	7274	49	0
1	C	7374	0	7267	47	0
1	D	7374	0	7267	41	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	1	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	193	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 (193) 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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:711:ASN:HD21	1:C:754:GLN:HE21	1.36	0.74
1:B:347:MET:HE2	1:B:558:ASN:HD22	1.56	0.71
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:442:TYR:HB3	1:A:592:MET:HE2	1.81	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:C:347:MET:HE2	1:C:558:ASN:ND2	2.21	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:B:707:ARG:HH22	1:B:731:GLU:CD	2.15	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:728:MET:HE2	3:J:115:DG:OP2	2.09	0.53
1:A:412:LEU:HG	1:A:683:MET:HE3	1.90	0.53
1:C:115:ILE:HG22	1:C:136:ILE:HG12	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:D:15:ILE:HG23	1:D:65:MET:HE1	1.93	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: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:OP1	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:B:413:THR:O	1:B:414:SER:C	2.57	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:752:MET:HE3	1:C:889:LEU:HD11	1.97	0.46
1:D:800:LYS:O	1:D:800:LYS:HG3	2.15	0.46
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:B:15:ILE:C	1:B:15:ILE:HD12	2.40	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:B:592:MET:SD	1:B:674:MET:HE3	2.58	0.43
1:C:298:LEU:C	1:C:300:VAL:H	2.26	0.43
1:C:655:ALA:O	1:C:660:GLU:HG2	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:454:TYR:CD2	1:D:462:MET:HE2	2.53	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: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:C:15:ILE:HG23	1:C:65:MET:HE1	2.01	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: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:A:298:LEU:C	1:A:300:VAL:H	2.28	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:428:GLU:CD	1:C:428:GLU:H	2.29	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: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%)	36	70
1	B	902/906 (100%)	860 (95%)	38 (4%)	4 (0%)	30	65
1	C	901/906 (99%)	867 (96%)	30 (3%)	4 (0%)	30	65
1	D	901/906 (99%)	859 (95%)	39 (4%)	3 (0%)	36	70
All	All	3606/3624 (100%)	3440 (95%)	152 (4%)	14 (0%)	30	65

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 ⓘ

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%)	774 (97%)	27 (3%)	32	66
1	B	801/803 (100%)	771 (96%)	30 (4%)	30	64
1	C	800/803 (100%)	766 (96%)	34 (4%)	26	60
1	D	800/803 (100%)	777 (97%)	23 (3%)	37	70
All	All	3202/3212 (100%)	3088 (96%)	114 (4%)	31	65

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	15	ILE
1	A	93	LEU
1	A	98	ASN
1	A	203	ASN
1	A	302	LYS
1	A	309	ILE
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	592	MET
1	A	599	ARG
1	A	618	LEU
1	A	642	ARG
1	A	728	MET
1	A	755	GLU
1	A	758	GLU
1	A	760	LEU
1	A	835	LEU
1	A	844	LYS
1	A	861	ASP
1	A	874	LYS
1	A	880	LEU
1	B	2	LYS
1	B	15	ILE
1	B	52	ILE
1	B	78	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	257	TYR
1	B	302	LYS
1	B	332	LEU
1	B	355	ILE
1	B	356	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	428	GLU
1	B	435	LYS
1	B	466	ASP
1	B	467	ARG
1	B	483	LYS
1	B	498	ILE
1	B	504	HIS
1	B	587	THR
1	B	618	LEU
1	B	642	ARG
1	B	668	ARG
1	B	760	LEU
1	B	772	ARG
1	B	880	LEU
1	B	900	MET
1	C	27	ARG
1	C	45	GLN
1	C	61	LEU
1	C	89	LYS
1	C	90	LEU
1	C	93	LEU
1	C	112	ASN
1	C	145	ARG
1	C	302	LYS
1	C	303	LEU
1	C	309	ILE
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	467	ARG
1	C	475	ILE
1	C	477	LYS
1	C	479	PHE
1	C	483	LYS
1	C	516	VAL
1	C	546	GLN
1	C	559	ARG
1	C	562	LEU
1	C	580	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	587	THR
1	C	618	LEU
1	C	724	LYS
1	C	760	LEU
1	C	843	ASP
1	C	874	LYS
1	C	880	LEU
1	D	55	LYS
1	D	96	THR
1	D	145	ARG
1	D	209	THR
1	D	302	LYS
1	D	363	LYS
1	D	405	LYS
1	D	428	GLU
1	D	435	LYS
1	D	439	LEU
1	D	453	VAL
1	D	467	ARG
1	D	483	LYS
1	D	484	GLU
1	D	510	VAL
1	D	514	LEU
1	D	521	ASP
1	D	532	LYS
1	D	562	LEU
1	D	587	THR
1	D	631	LYS
1	D	727	ILE
1	D	768	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (83) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	98	ASN
1	A	112	ASN
1	A	131	HIS
1	A	158	ASN
1	A	173	GLN
1	A	245	HIS
1	A	284	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	285	GLN
1	A	376	GLN
1	A	389	GLN
1	A	480	ASN
1	A	481	GLN
1	A	493	GLN
1	A	495	ASN
1	A	556	GLN
1	A	572	ASN
1	A	646	HIS
1	A	675	ASN
1	A	678	GLN
1	A	679	HIS
1	A	711	ASN
1	A	733	GLN
1	A	786	ASN
1	A	787	ASN
1	B	45	GLN
1	B	153	ASN
1	B	158	ASN
1	B	203	ASN
1	B	217	ASN
1	B	245	HIS
1	B	284	ASN
1	B	285	GLN
1	B	377	ASN
1	B	386	HIS
1	B	481	GLN
1	B	539	ASN
1	B	558	ASN
1	B	591	GLN
1	B	595	GLN
1	B	646	HIS
1	B	678	GLN
1	B	711	ASN
1	B	761	GLN
1	B	818	ASN
1	C	23	ASN
1	C	40	HIS
1	C	153	ASN
1	C	158	ASN
1	C	173	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	193	ASN
1	C	203	ASN
1	C	206	GLN
1	C	217	ASN
1	C	245	HIS
1	C	284	ASN
1	C	317	HIS
1	C	539	ASN
1	C	556	GLN
1	C	558	ASN
1	C	572	ASN
1	C	595	GLN
1	C	646	HIS
1	C	678	GLN
1	C	679	HIS
1	C	711	ASN
1	C	775	ASN
1	C	864	HIS
1	D	112	ASN
1	D	153	ASN
1	D	203	ASN
1	D	207	GLN
1	D	245	HIS
1	D	285	GLN
1	D	339	GLN
1	D	354	GLN
1	D	371	ASN
1	D	386	HIS
1	D	539	ASN
1	D	675	ASN
1	D	742	GLN
1	D	787	ASN
1	D	818	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	K	3	3,2	18,21,22	0.45	0	25,30,33	1.81	3 (12%)
2	C37	E	3	3,2	18,21,22	0.47	0	25,30,33	1.77	3 (12%)
2	C37	I	3	3,2	18,21,22	0.46	0	25,30,33	1.80	3 (12%)
2	C37	G	3	3,2	18,21,22	0.46	0	25,30,33	1.75	3 (12%)

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	K	3	3,2	-	0/7/21/22	0/2/2/2
2	C37	E	3	3,2	-	0/7/21/22	0/2/2/2
2	C37	I	3	3,2	-	0/7/21/22	0/2/2/2
2	C37	G	3	3,2	-	0/7/21/22	0/2/2/2

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	3	C37	F-C5-C4	7.02	122.56	118.09
2	I	3	C37	F-C5-C4	7.00	122.55	118.09
2	E	3	C37	F-C5-C4	6.88	122.47	118.09
2	G	3	C37	F-C5-C4	6.75	122.39	118.09
2	K	3	C37	C6-C5-C4	-3.89	117.44	120.25
2	I	3	C37	C6-C5-C4	-3.85	117.47	120.25
2	E	3	C37	C6-C5-C4	-3.81	117.50	120.25
2	G	3	C37	C6-C5-C4	-3.79	117.51	120.25
2	K	3	C37	C5-C4-N3	3.64	121.96	119.59
2	I	3	C37	C5-C4-N3	3.53	121.89	119.59
2	G	3	C37	C5-C4-N3	3.52	121.88	119.59
2	E	3	C37	C5-C4-N3	3.51	121.88	119.59

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	K	3	C37	1	0
2	G	3	C37	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	K	19	-	4,4,4	0.43	0	6,6,6	0.09	0
4	SO4	E	19	-	4,4,4	0.43	0	6,6,6	0.09	0
4	SO4	I	19	-	4,4,4	0.44	0	6,6,6	0.14	0
4	SO4	G	19	-	4,4,4	0.43	0	6,6,6	0.07	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

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, 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%)	-0.09	21 (2%) 61 38	40, 76, 159, 244	0
1	B	904/906 (99%)	-0.37	2 (0%) 91 83	33, 60, 163, 357	0
1	C	903/906 (99%)	-0.32	6 (0%) 84 66	32, 62, 126, 219	0
1	D	903/906 (99%)	0.27	23 (2%) 58 35	62, 117, 170, 199	0
2	E	17/18 (94%)	0.27	0 100 100	62, 88, 140, 143	0
2	G	17/18 (94%)	-0.52	0 100 100	34, 49, 70, 80	0
2	I	17/18 (94%)	-0.34	0 100 100	43, 56, 84, 96	0
2	K	17/18 (94%)	0.21	0 100 100	83, 113, 138, 147	0
3	F	15/15 (100%)	0.31	0 100 100	69, 103, 168, 170	0
3	H	15/15 (100%)	-0.58	0 100 100	39, 50, 78, 84	0
3	J	15/15 (100%)	-0.40	0 100 100	44, 64, 102, 103	0
3	L	15/15 (100%)	0.22	0 100 100	102, 133, 169, 170	0
All	All	3742/3756 (99%)	-0.13	52 (1%) 73 51	32, 77, 163, 357	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	847	ALA	7.5
1	A	862	VAL	4.2
1	A	858	ILE	4.1
1	D	789	ALA	4.0
1	D	514	LEU	3.7
1	A	847	ALA	3.7
1	D	832	VAL	3.6
1	A	786	ASN	3.5
1	C	303	LEU	3.5
1	B	904	HIS	3.5
1	A	508	LEU	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	115	ILE	3.2
1	C	517	ASP	3.0
1	D	199	MET	3.0
1	D	901	PHE	3.0
1	D	545	ALA	2.9
1	D	303	LEU	2.9
1	D	784	SER	2.8
1	D	800	LYS	2.7
1	C	522	PHE	2.7
1	D	135	ALA	2.7
1	A	510	VAL	2.7
1	A	832	VAL	2.6
1	D	782	VAL	2.6
1	A	846	ILE	2.6
1	D	846	ILE	2.6
1	A	833	LEU	2.5
1	A	804	HIS	2.5
1	A	770	GLU	2.5
1	A	785	ALA	2.4
1	A	868	TYR	2.4
1	A	808	ILE	2.4
1	A	514	LEU	2.4
1	D	840	PRO	2.4
1	B	508	LEU	2.4
1	D	857	LEU	2.4
1	A	817	GLY	2.3
1	D	781	SER	2.3
1	C	508	LEU	2.3
1	D	801	CYS	2.3
1	D	393	GLY	2.2
1	A	904	HIS	2.2
1	A	498	ILE	2.2
1	D	903	PHE	2.1
1	A	256	MET	2.1
1	C	506	PRO	2.1
1	A	866	MET	2.1
1	D	515	ASP	2.0
1	D	848	TRP	2.0
1	D	521	ASP	2.0
1	C	516	VAL	2.0
1	A	863	LEU	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	0.83	0.10	104,111,114,114	0
2	C37	E	3	20/21	0.87	0.12	78,90,93,93	0
2	C37	I	3	20/21	0.94	0.07	55,59,62,64	0
2	C37	G	3	20/21	0.97	0.05	37,38,45,46	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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	0.71	0.10	110,112,112,113	0
4	SO4	K	19	5/5	0.83	0.07	133,133,134,134	0
4	SO4	I	19	5/5	0.87	0.08	86,87,88,88	0
4	SO4	G	19	5/5	0.88	0.09	92,93,94,96	0

6.5 Other polymers [i](#)

There are no such residues in this entry.