



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:33 PM GMT

PDB ID : 4P6X
Title : Crystal Structure of cortisol-bound glucocorticoid receptor ligand binding domain
Authors : He, Y.; Zhou, X.E.; Tolbert, W.D.; Powell, K.; Melcher, K.; Xu, H.E.
Deposited on : 2014-03-25
Resolution : 2.50 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

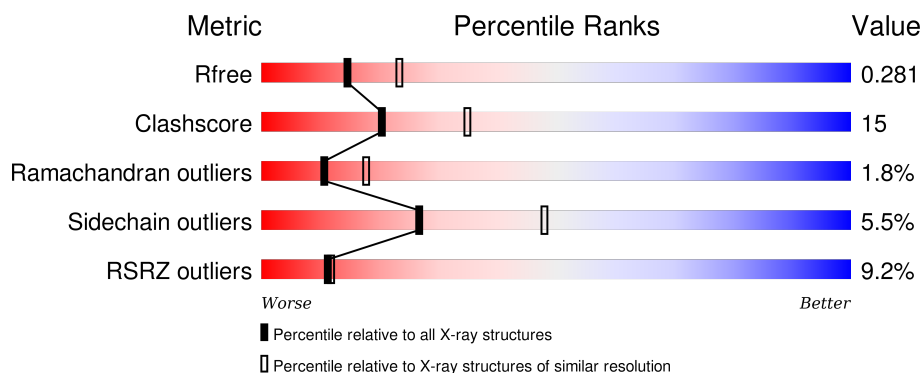
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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 $\leq 5\%$. 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	255	<div> <div>17%</div> <div>52%</div> <div>40%</div> <div>7%</div> </div>
1	C	255	<div> <div>4%</div> <div>76%</div> <div>22%</div> </div>
1	E	255	<div> <div>15%</div> <div>53%</div> <div>44%</div> </div>
1	G	255	<div> <div>6%</div> <div>69%</div> <div>27%</div> </div>
1	I	255	<div> <div>5%</div> <div>79%</div> <div>18%</div> </div>

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Mol	Chain	Length	Quality of chain
1	K	255	
2	B	14	
2	D	14	
2	F	14	
2	H	14	
2	J	14	
2	L	14	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	HCY	G	900	-	-	-	X
3	HCY	I	900	-	-	-	X
3	HCY	K	900	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13848 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 Glucocorticoid receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	252	Total	C	N	O	S	0	0	0
			2052	1327	338	370	17			
1	C	255	Total	C	N	O	S	0	0	0
			2073	1340	341	375	17			
1	E	255	Total	C	N	O	S	0	0	0
			2072	1340	341	374	17			
1	G	254	Total	C	N	O	S	0	0	0
			2063	1334	339	373	17			
1	I	255	Total	C	N	O	S	0	0	0
			2073	1340	341	375	17			
1	K	255	Total	C	N	O	S	0	0	0
			2072	1340	341	374	17			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	602	ALA	PHE	engineered mutation	UNP P04150
A	622	TYR	CYS	engineered mutation	UNP P04150
A	668	VAL	THR	engineered mutation	UNP P04150
A	674	THR	SER	engineered mutation	UNP P04150
A	675	ILE	VAL	engineered mutation	UNP P04150
A	684	ALA	GLU	engineered mutation	UNP P04150
A	688	ALA	GLU	engineered mutation	UNP P04150
C	602	ALA	PHE	engineered mutation	UNP P04150
C	622	TYR	CYS	engineered mutation	UNP P04150
C	668	VAL	THR	engineered mutation	UNP P04150
C	674	THR	SER	engineered mutation	UNP P04150
C	675	ILE	VAL	engineered mutation	UNP P04150
C	684	ALA	GLU	engineered mutation	UNP P04150
C	688	ALA	GLU	engineered mutation	UNP P04150
E	602	ALA	PHE	engineered mutation	UNP P04150
E	622	TYR	CYS	engineered mutation	UNP P04150
E	668	VAL	THR	engineered mutation	UNP P04150

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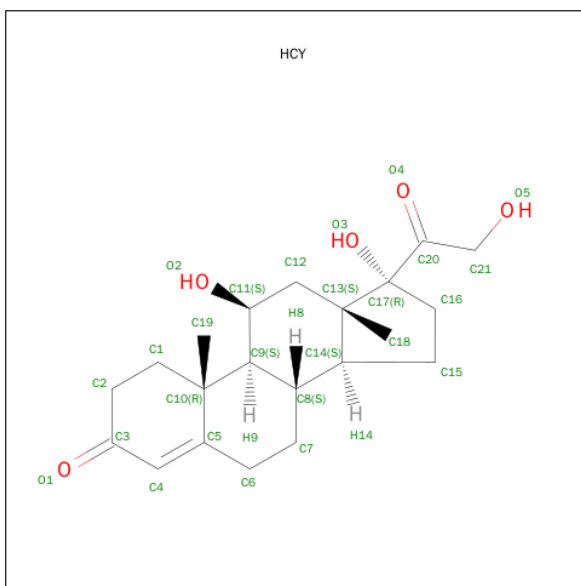
Chain	Residue	Modelled	Actual	Comment	Reference
E	674	THR	SER	engineered mutation	UNP P04150
E	675	ILE	VAL	engineered mutation	UNP P04150
E	684	ALA	GLU	engineered mutation	UNP P04150
E	688	ALA	GLU	engineered mutation	UNP P04150
G	602	ALA	PHE	engineered mutation	UNP P04150
G	622	TYR	CYS	engineered mutation	UNP P04150
G	668	VAL	THR	engineered mutation	UNP P04150
G	674	THR	SER	engineered mutation	UNP P04150
G	675	ILE	VAL	engineered mutation	UNP P04150
G	684	ALA	GLU	engineered mutation	UNP P04150
G	688	ALA	GLU	engineered mutation	UNP P04150
I	602	ALA	PHE	engineered mutation	UNP P04150
I	622	TYR	CYS	engineered mutation	UNP P04150
I	668	VAL	THR	engineered mutation	UNP P04150
I	674	THR	SER	engineered mutation	UNP P04150
I	675	ILE	VAL	engineered mutation	UNP P04150
I	684	ALA	GLU	engineered mutation	UNP P04150
I	688	ALA	GLU	engineered mutation	UNP P04150
K	602	ALA	PHE	engineered mutation	UNP P04150
K	622	TYR	CYS	engineered mutation	UNP P04150
K	668	VAL	THR	engineered mutation	UNP P04150
K	674	THR	SER	engineered mutation	UNP P04150
K	675	ILE	VAL	engineered mutation	UNP P04150
K	684	ALA	GLU	engineered mutation	UNP P04150
K	688	ALA	GLU	engineered mutation	UNP P04150

- Molecule 2 is a protein called Nuclear receptor coactivator 2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	12	Total	C	N	O	0	0	0
			101	64	17	20			
2	D	14	Total	C	N	O	0	0	0
			119	75	20	24			
2	F	14	Total	C	N	O	0	0	0
			119	75	20	24			
2	H	13	Total	C	N	O	0	0	0
			110	69	18	23			
2	J	12	Total	C	N	O	0	0	0
			101	64	17	20			
2	L	14	Total	C	N	O	0	0	0
			119	75	20	24			

- Molecule 3 is (11alpha,14beta)-11,17,21-trihydroxypregn-4-ene-3,20-dione (three-letter code:

HCY) (formula: C₂₁H₃₀O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			26	21	5		
3	C	1	Total	C	O	0	0
			26	21	5		
3	E	1	Total	C	O	0	0
			26	21	5		
3	G	1	Total	C	O	0	0
			26	21	5		
3	I	1	Total	C	O	0	0
			26	21	5		
3	K	1	Total	C	O	0	0
			26	21	5		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	64	Total	O	0	0
			64	64		
4	B	3	Total	O	0	0
			3	3		
4	C	109	Total	O	0	0
			109	109		
4	D	2	Total	O	0	0
			2	2		
4	E	68	Total	O	0	0
			68	68		

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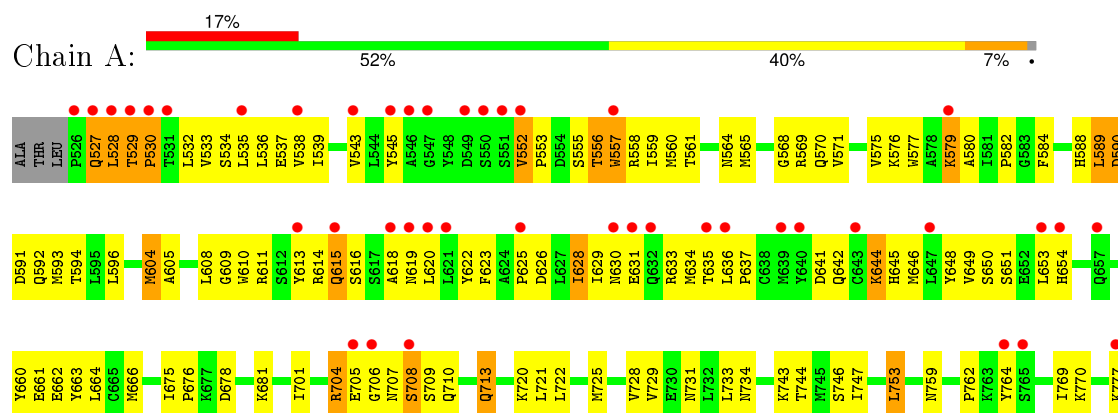
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	F	5	Total 5	O 5	0	0
4	G	102	Total 102	O 102	0	0
4	H	9	Total 9	O 9	0	0
4	I	119	Total 119	O 119	0	0
4	J	7	Total 7	O 7	0	0
4	K	127	Total 127	O 127	0	0
4	L	3	Total 3	O 3	0	0

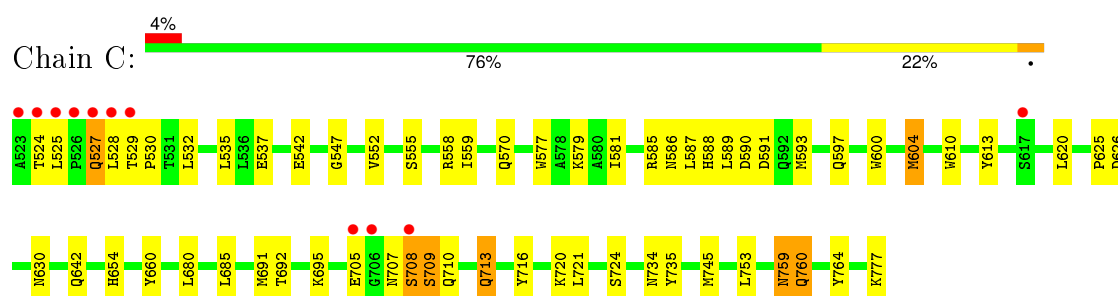
3 Residue-property plots

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.

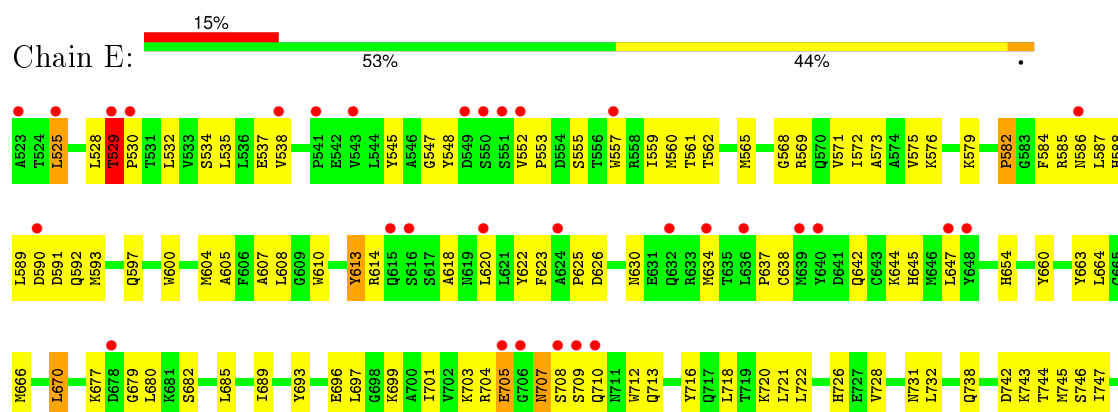
• Molecule 1: Glucocorticoid receptor

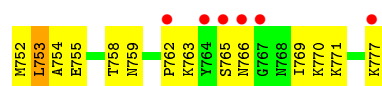


• Molecule 1: Glucocorticoid receptor

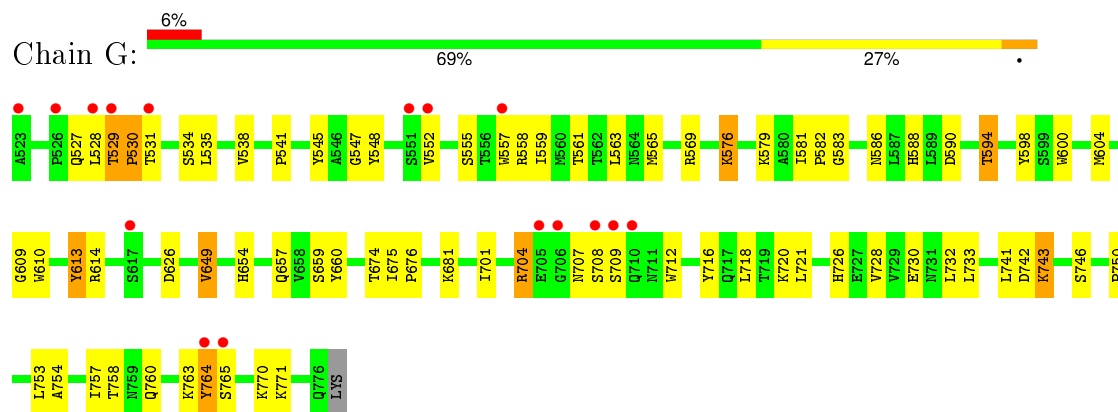


• Molecule 1: Glucocorticoid receptor

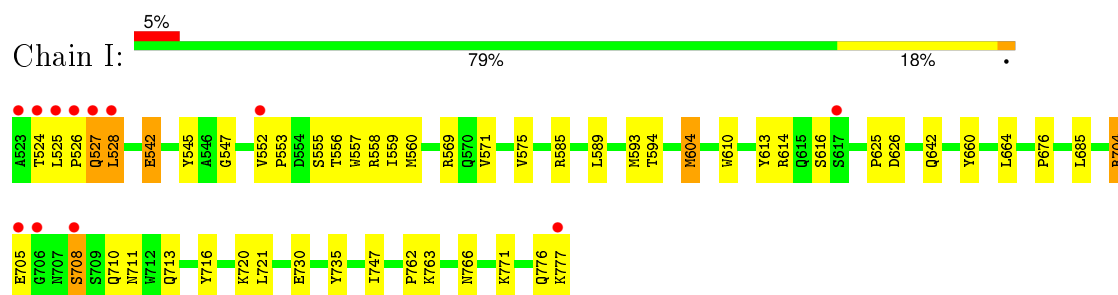




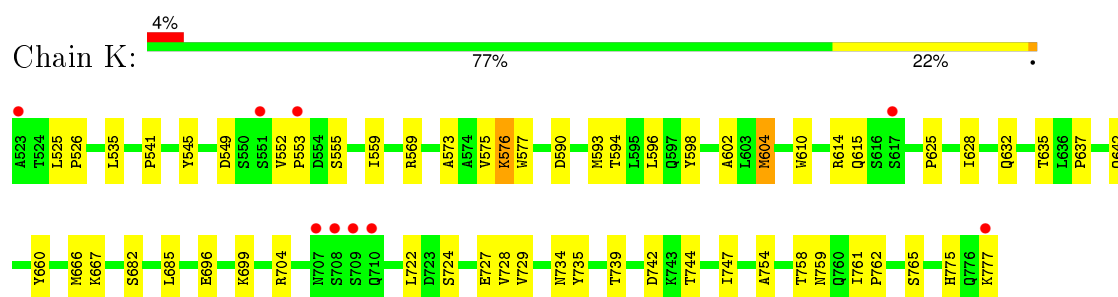
- Molecule 1: Glucocorticoid receptor



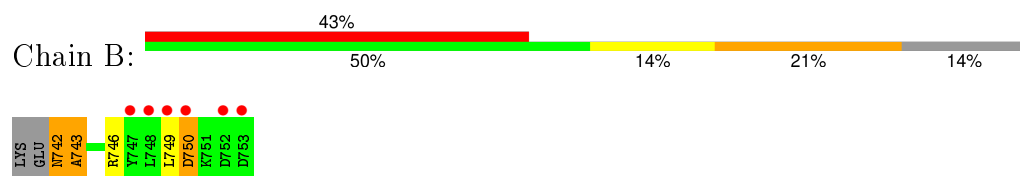
- Molecule 1: Glucocorticoid receptor



- Molecule 1: Glucocorticoid receptor

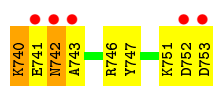


- Molecule 2: Nuclear receptor coactivator 2

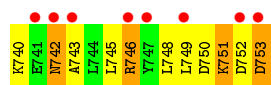
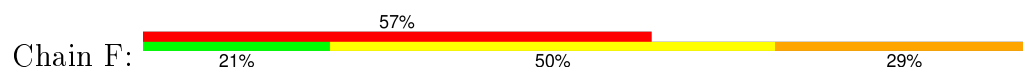


- Molecule 2: Nuclear receptor coactivator 2

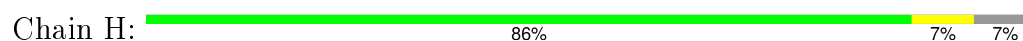




- Molecule 2: Nuclear receptor coactivator 2



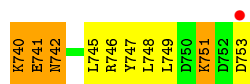
- Molecule 2: Nuclear receptor coactivator 2



- Molecule 2: Nuclear receptor coactivator 2



- Molecule 2: Nuclear receptor coactivator 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	220.82Å 220.82Å 74.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.50 38.25 – 2.12	Depositor EDS
% Data completeness (in resolution range)	99.7 (30.00-2.50) 99.8 (38.25-2.12)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 2.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.246 , 0.276 0.252 , 0.281	Depositor DCC
R_{free} test set	5606 reflections (8.48%)	DCC
Wilson B-factor (Å ²)	23.7	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 53.7	EDS
Estimated twinning fraction	0.037 for h,-h-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	9 of 117572 reflections (0.008%)	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13848	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 74.64 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.4708e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: HCY

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	0.33	0/2098	0.49	0/2839
1	C	0.27	0/2119	0.44	0/2868
1	E	0.33	0/2118	0.49	0/2868
1	G	0.28	0/2109	0.43	0/2857
1	I	0.27	0/2119	0.46	1/2868 (0.0%)
1	K	0.28	0/2118	0.42	0/2868
2	B	0.38	0/101	0.73	0/135
2	D	0.47	0/119	0.52	0/158
2	F	0.44	0/119	0.86	0/158
2	H	0.23	0/110	0.34	0/147
2	J	0.25	0/101	0.40	0/135
2	L	0.36	0/119	0.68	0/158
All	All	0.30	0/13350	0.47	1/18059 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	528	LEU	CA-CB-CG	5.30	127.49	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2052	0	2083	101	0
1	C	2073	0	2105	55	0
1	E	2072	0	2105	97	0
1	G	2063	0	2092	66	0
1	I	2073	0	2105	31	0
1	K	2072	0	2105	35	0
2	B	101	0	101	8	0
2	D	119	0	120	14	0
2	F	119	0	120	22	0
2	H	110	0	107	1	0
2	J	101	0	101	3	0
2	L	119	0	120	10	0
3	A	26	0	30	2	0
3	C	26	0	30	1	0
3	E	26	0	30	0	0
3	G	26	0	30	0	0
3	I	26	0	30	1	0
3	K	26	0	30	1	0
4	A	64	0	0	3	0
4	B	3	0	0	0	0
4	C	109	0	0	4	0
4	D	2	0	0	0	0
4	E	68	0	0	5	0
4	F	5	0	0	1	0
4	G	102	0	0	1	0
4	H	9	0	0	0	0
4	I	119	0	0	2	0
4	J	7	0	0	0	0
4	K	127	0	0	3	0
4	L	3	0	0	0	0
All	All	13848	0	13444	390	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 15.

All (390) 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)
2:F:748:LEU:HA	2:F:751:LYS:HD3	1.45	0.97
1:C:530:PRO:HB2	1:G:530:PRO:HB2	1.54	0.89
2:F:740:LYS:HG3	2:F:742:ASN:H	1.39	0.87
1:C:759:ASN:HD22	2:D:740:LYS:HE3	1.39	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:529:THR:HB	1:A:530:PRO:HD3	1.55	0.87
1:E:585:ARG:NH2	2:F:751:LYS:O	2.10	0.84
1:A:704:ARG:HG3	1:A:705:GLU:H	1.45	0.80
1:A:537:GLU:HG3	1:A:660:TYR:HE2	1.46	0.79
1:I:763:LYS:HA	1:I:766:ASN:HB2	1.64	0.79
1:C:692:THR:HG21	1:G:528:LEU:HD11	1.61	0.79
1:A:744:THR:HG21	1:E:743:LYS:HB2	1.65	0.79
1:E:579:LYS:HD3	2:F:749:LEU:HA	1.65	0.77
1:A:576:LYS:HG3	1:A:577:TRP:H	1.48	0.76
1:A:537:GLU:HG3	1:A:660:TYR:CE2	2.21	0.75
1:C:589:LEU:HD11	2:D:746:ARG:HG3	1.69	0.74
1:G:541:PRO:HB3	1:G:576:LYS:HZ2	1.51	0.74
1:A:593:MET:SD	2:B:746:ARG:HA	2.28	0.73
1:E:573:ALA:O	1:E:576:LYS:HG2	1.89	0.73
1:A:557:TRP:HB2	1:A:746:SER:HB2	1.69	0.72
2:D:742:ASN:O	2:D:746:ARG:HB3	1.90	0.71
1:E:699:LYS:O	1:E:703:LYS:HG2	1.90	0.70
1:A:616:SER:HB3	1:A:620:LEU:HD11	1.72	0.70
1:A:615:GLN:HG2	1:A:622:TYR:CZ	2.26	0.69
1:A:588:HIS:CD2	1:A:681:LYS:HD2	2.30	0.67
1:G:531:THR:HG23	1:G:534:SER:H	1.59	0.67
1:E:545:TYR:O	1:E:569:ARG:NH2	2.27	0.67
1:K:742:ASP:OD2	1:K:744:THR:HG22	1.95	0.67
1:E:535:LEU:HD12	1:E:582:PRO:HD3	1.78	0.66
1:G:743:LYS:H	1:G:743:LYS:CE	2.08	0.66
1:I:545:TYR:O	1:I:569:ARG:NH2	2.29	0.66
1:C:692:THR:HG21	1:G:528:LEU:CD1	2.27	0.65
1:I:604:MET:HG2	3:I:900:HCY:H192	1.76	0.65
1:A:720:LYS:NZ	1:A:777:LYS:HD3	2.12	0.64
2:F:740:LYS:HG3	2:F:742:ASN:N	2.12	0.64
1:A:543:VAL:HG11	1:A:625:PRO:HD3	1.78	0.64
1:A:593:MET:HG2	2:B:749:LEU:HD12	1.79	0.64
1:G:760:GLN:HB3	1:G:764:TYR:HE1	1.61	0.64
1:E:630:ASN:O	1:E:634:MET:HG2	1.97	0.63
2:L:740:LYS:NZ	2:L:741:GLU:HB3	2.13	0.63
1:E:529:THR:OG1	1:E:530:PRO:HA	1.98	0.63
1:C:586:ASN:OD1	1:G:527:GLN:HG3	1.99	0.63
1:G:741:LEU:O	1:G:743:LYS:NZ	2.31	0.62
1:A:633:ARG:HA	1:A:636:LEU:HD23	1.79	0.62
1:A:701:ILE:O	1:A:704:ARG:HG2	1.99	0.62
1:E:568:GLY:O	1:E:572:ILE:HG13	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:589:LEU:HD23	1:E:590:ASP:H	1.66	0.61
1:I:560:MET:CE	1:I:747:ILE:HD11	2.30	0.61
1:I:716:TYR:OH	1:I:777:LYS:HE3	2.00	0.61
2:F:746:ARG:NH1	4:F:804:HOH:O	2.34	0.61
1:K:604:MET:HG2	3:K:900:HCY:H192	1.81	0.61
1:K:724:SER:O	1:K:727:GLU:HG2	2.01	0.61
1:E:593:MET:HG2	1:E:597:GLN:NE2	2.15	0.61
1:E:644:LYS:HD2	1:E:645:HIS:CE1	2.36	0.61
1:K:590:ASP:OD1	2:L:746:ARG:NH2	2.33	0.60
1:E:555:SER:O	1:E:559:ILE:HG12	2.01	0.60
1:G:659:SER:HB3	1:G:704:ARG:HD3	1.82	0.60
1:A:528:LEU:H	1:A:528:LEU:HD22	1.66	0.60
1:A:620:LEU:HD22	1:A:628:ILE:HD11	1.83	0.60
1:A:759:ASN:ND2	4:A:1038:HOH:O	2.35	0.60
1:G:557:TRP:CD1	1:G:746:SER:HB2	2.36	0.60
2:L:742:ASN:HB3	2:L:745:LEU:HB3	1.84	0.60
1:E:707:ASN:O	1:E:707:ASN:ND2	2.31	0.59
1:A:675:ILE:HD11	1:A:770:LYS:HD2	1.84	0.59
1:E:532:LEU:HB3	1:E:696:GLU:OE1	2.02	0.59
1:E:537:GLU:HG3	1:E:664:LEU:HD11	1.84	0.59
1:E:591:ASP:OD1	1:E:680:LEU:HB2	2.03	0.59
1:A:533:VAL:HG21	1:A:661:GLU:HG2	1.83	0.59
1:C:759:ASN:HD22	2:D:740:LYS:CE	2.15	0.59
1:E:525:LEU:HB2	1:E:528:LEU:HD12	1.85	0.59
1:K:739:THR:HB	1:K:747:ILE:HD12	1.85	0.58
1:C:720:LYS:NZ	1:C:777:LYS:HE3	2.19	0.58
1:A:704:ARG:HG3	1:A:705:GLU:N	2.15	0.58
1:A:615:GLN:HG2	1:A:622:TYR:CE1	2.39	0.57
1:G:743:LYS:H	1:G:743:LYS:HE2	1.68	0.57
2:L:747:TYR:O	2:L:751:LYS:HG3	2.04	0.57
1:A:527:GLN:HG3	1:A:528:LEU:N	2.19	0.57
1:A:618:ALA:HB3	1:A:620:LEU:HG	1.87	0.57
1:I:762:PRO:HB2	4:I:1100:HOH:O	2.03	0.57
1:E:759:ASN:HD22	2:F:740:LYS:HB3	1.70	0.57
1:G:541:PRO:HB3	1:G:576:LYS:NZ	2.18	0.57
1:I:585:ARG:HG3	4:I:1079:HOH:O	2.04	0.57
1:A:545:TYR:O	1:A:569:ARG:NH2	2.38	0.57
1:G:760:GLN:HB3	1:G:764:TYR:CE1	2.39	0.57
2:J:751:LYS:HG2	2:J:752:ASP:H	1.69	0.57
1:C:691:MET:HG3	1:C:695:LYS:NZ	2.19	0.57
1:I:555:SER:OG	1:I:558:ARG:HB2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:545:TYR:CE1	1:K:625:PRO:HB2	2.40	0.56
2:L:740:LYS:HG3	2:L:741:GLU:N	2.20	0.56
2:D:740:LYS:HB3	2:D:740:LYS:NZ	2.20	0.56
1:A:528:LEU:N	1:A:528:LEU:HD22	2.19	0.56
1:C:537:GLU:HG3	1:C:660:TYR:HE2	1.70	0.56
1:K:614:ARG:NH1	4:K:1091:HOH:O	2.38	0.56
1:G:529:THR:HG23	1:G:531:THR:N	2.20	0.56
1:C:710:GLN:HA	4:C:1076:HOH:O	2.05	0.56
1:A:611:ARG:O	1:A:615:GLN:HB2	2.05	0.56
1:A:660:TYR:O	1:A:664:LEU:HG	2.06	0.56
1:A:618:ALA:C	1:A:620:LEU:H	2.08	0.56
1:C:579:LYS:HB2	1:C:585:ARG:HD2	1.88	0.56
1:E:568:GLY:HA2	1:E:753:LEU:HD13	1.88	0.56
1:G:707:ASN:O	1:G:709:SER:N	2.39	0.56
1:A:744:THR:CG2	1:E:743:LYS:HB2	2.35	0.55
1:E:645:HIS:CD2	1:E:731:ASN:HD22	2.24	0.55
1:E:759:ASN:HB2	2:F:740:LYS:CE	2.35	0.55
1:A:576:LYS:O	1:A:579:LYS:HG3	2.05	0.55
1:K:759:ASN:HD22	2:L:740:LYS:N	2.05	0.55
2:L:751:LYS:NZ	2:L:753:ASP:HB3	2.22	0.55
1:E:623:PHE:N	4:E:1022:HOH:O	2.39	0.55
1:A:530:PRO:HB3	4:A:1002:HOH:O	2.06	0.55
1:A:649:VAL:O	1:A:653:LEU:HG	2.07	0.54
1:E:742:ASP:HB3	1:E:745:MET:HE3	1.88	0.54
1:E:589:LEU:HD12	2:F:746:ARG:NH2	2.22	0.54
1:A:620:LEU:HB2	1:A:628:ILE:HD11	1.89	0.54
1:A:743:LYS:HB2	1:E:744:THR:HG21	1.89	0.54
1:E:720:LYS:NZ	1:E:777:LYS:HD3	2.22	0.54
1:C:593:MET:SD	2:D:746:ARG:HB2	2.48	0.54
1:G:742:ASP:HA	1:G:743:LYS:NZ	2.22	0.54
1:G:569:ARG:HG2	1:K:632:GLN:OE1	2.08	0.54
1:G:588:HIS:HD2	1:G:590:ASP:HB2	1.72	0.54
1:C:708:SER:OG	1:E:777:LYS:HD2	2.07	0.54
1:A:610:TRP:HB2	1:A:663:TYR:CE1	2.43	0.54
1:I:642:GLN:HG2	1:I:735:TYR:CG	2.43	0.54
1:A:588:HIS:HD2	1:A:590:ASP:HB2	1.73	0.53
1:E:607:ALA:HA	1:E:663:TYR:OH	2.08	0.53
2:D:742:ASN:HA	2:D:746:ARG:H	1.72	0.53
1:A:576:LYS:HG3	1:A:577:TRP:N	2.22	0.53
1:C:525:LEU:HD21	1:G:586:ASN:HB2	1.90	0.53
1:E:677:LYS:HB2	1:E:769:ILE:N	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:570:GLN:NE2	1:C:604:MET:HG3	2.23	0.53
1:I:560:MET:HE1	1:I:747:ILE:HD11	1.89	0.53
1:C:535:LEU:HD22	1:G:538:VAL:HG21	1.89	0.53
1:A:645:HIS:CD2	1:A:731:ASN:HD22	2.26	0.53
1:A:536:LEU:O	1:A:539:ILE:HG12	2.09	0.52
1:A:611:ARG:HH21	1:A:623:PHE:HA	1.74	0.52
1:G:760:GLN:O	1:G:764:TYR:HD1	1.92	0.52
1:E:618:ALA:HB3	1:E:620:LEU:HD13	1.90	0.52
1:C:528:LEU:HD13	1:G:582:PRO:O	2.09	0.52
1:A:613:TYR:CD1	1:A:654:HIS:HB2	2.44	0.52
2:D:747:TYR:O	2:D:751:LYS:HG2	2.09	0.52
1:I:525:LEU:C	1:I:527:GLN:H	2.12	0.52
1:G:716:TYR:O	1:G:720:LYS:HB2	2.09	0.52
1:K:541:PRO:HB3	1:K:576:LYS:NZ	2.24	0.52
2:F:746:ARG:HB2	2:F:746:ARG:NH1	2.23	0.52
1:C:707:ASN:O	1:C:709:SER:N	2.42	0.52
1:C:579:LYS:NZ	2:D:753:ASP:OD1	2.42	0.52
1:C:527:GLN:OE1	1:G:586:ASN:ND2	2.39	0.52
1:E:582:PRO:HG2	1:E:693:TYR:OH	2.10	0.51
1:A:720:LYS:HZ3	1:A:777:LYS:HD3	1.74	0.51
1:A:545:TYR:HE1	1:A:625:PRO:HB2	1.74	0.51
1:A:604:MET:HG2	3:A:900:HCY:H192	1.91	0.51
1:A:729:VAL:O	1:A:733:LEU:HB2	2.10	0.51
1:E:613:TYR:CD2	1:E:614:ARG:HG2	2.45	0.51
1:E:754:ALA:O	1:E:758:THR:HG23	2.10	0.51
1:A:532:LEU:O	1:A:536:LEU:HG	2.10	0.51
2:L:740:LYS:CE	2:L:741:GLU:HB3	2.40	0.51
1:K:575:VAL:HG22	1:K:596:LEU:HD13	1.93	0.51
1:A:609:GLY:HA2	1:A:650:SER:HB2	1.93	0.51
1:C:642:GLN:HG2	1:C:735:TYR:CG	2.46	0.51
1:K:545:TYR:O	1:K:569:ARG:NH2	2.44	0.51
1:G:743:LYS:H	1:G:743:LYS:NZ	2.08	0.50
1:C:713:GLN:NE2	1:E:712:TRP:CD1	2.79	0.50
1:C:530:PRO:O	1:G:530:PRO:HG2	2.11	0.50
1:A:713:GLN:NE2	1:G:712:TRP:CE2	2.80	0.50
1:A:725:MET:HA	1:A:728:VAL:HG13	1.93	0.50
1:C:705:GLU:OE1	1:C:707:ASN:ND2	2.44	0.50
1:E:726:HIS:CE1	1:E:771:LYS:HB3	2.47	0.50
1:I:524:THR:C	1:I:526:PRO:HD3	2.32	0.50
1:C:591:ASP:CG	1:C:680:LEU:HB3	2.32	0.50
1:E:759:ASN:HB2	2:F:740:LYS:HD2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:535:LEU:HD21	1:G:535:LEU:HA	1.93	0.50
1:A:710:GLN:O	1:A:713:GLN:HB3	2.11	0.50
1:K:775:HIS:HE1	4:K:1018:HOH:O	1.94	0.50
1:A:556:THR:HG23	1:A:557:TRP:H	1.76	0.49
1:C:720:LYS:HZ1	1:C:777:LYS:HE3	1.76	0.49
1:A:535:LEU:HD12	1:A:582:PRO:HG3	1.94	0.49
1:I:730:GLU:OE2	1:I:771:LYS:NZ	2.43	0.49
1:G:701:ILE:HD11	1:G:718:LEU:HD12	1.93	0.49
1:A:534:SER:O	1:A:538:VAL:HG12	2.12	0.49
1:E:579:LYS:NZ	2:F:749:LEU:O	2.40	0.49
1:G:654:HIS:O	1:G:657:GLN:NE2	2.45	0.49
1:C:593:MET:HE1	2:D:742:ASN:HB3	1.95	0.49
1:A:552:VAL:HG23	1:A:553:PRO:HD2	1.94	0.49
1:A:631:GLU:O	1:A:635:THR:HG23	2.12	0.49
1:A:543:VAL:CG1	1:A:625:PRO:HD3	2.42	0.49
1:E:589:LEU:HD12	2:F:746:ARG:CZ	2.42	0.49
1:E:670:LEU:HD13	1:E:722:LEU:HD22	1.94	0.49
1:C:585:ARG:NE	4:C:1086:HOH:O	2.46	0.49
1:E:638:CYS:HB3	4:E:1013:HOH:O	2.13	0.49
1:E:584:PHE:CE2	1:E:592:GLN:HB3	2.48	0.49
1:I:555:SER:O	1:I:559:ILE:HG12	2.13	0.49
1:A:743:LYS:HB2	1:E:744:THR:CG2	2.43	0.49
1:E:605:ALA:O	1:E:608:LEU:HB3	2.13	0.48
1:A:613:TYR:CD2	1:A:614:ARG:HG2	2.48	0.48
1:K:775:HIS:HB3	1:K:777:LYS:NZ	2.29	0.48
1:G:728:VAL:O	1:G:732:LEU:HG	2.13	0.48
1:E:588:HIS:HD2	1:E:590:ASP:HB2	1.78	0.48
1:E:759:ASN:O	1:E:762:PRO:HD2	2.14	0.48
1:G:594:THR:HG23	1:G:598:TYR:CE1	2.48	0.48
1:E:587:LEU:O	1:E:592:GLN:NE2	2.46	0.48
1:C:610:TRP:CZ2	1:C:660:TYR:HD1	2.30	0.48
1:G:588:HIS:CD2	1:G:590:ASP:H	2.31	0.48
1:E:685:LEU:O	1:E:689:ILE:HG13	2.13	0.48
1:G:579:LYS:HE3	2:H:753:ASP:OD2	2.14	0.48
1:K:642:GLN:HG2	1:K:735:TYR:CG	2.49	0.48
1:E:572:ILE:HG12	1:E:752:MET:CE	2.44	0.48
1:E:591:ASP:CG	1:E:680:LEU:HD13	2.34	0.48
1:G:742:ASP:HA	1:G:743:LYS:HZ1	1.77	0.48
1:E:634:MET:HB2	4:E:1002:HOH:O	2.13	0.48
1:A:594:THR:HG21	1:A:676:PRO:HG3	1.96	0.48
1:K:593:MET:HG2	2:L:749:LEU:HD12	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:593:MET:HG2	2:B:749:LEU:CD1	2.44	0.47
1:C:527:GLN:CD	1:G:583:GLY:H	2.18	0.47
1:K:754:ALA:O	1:K:758:THR:HG23	2.14	0.47
1:C:620:LEU:HG	1:C:630:ASN:HA	1.96	0.47
1:K:727:GLU:HG3	1:K:728:VAL:N	2.29	0.47
1:A:529:THR:HB	1:A:530:PRO:CD	2.36	0.47
1:E:660:TYR:O	1:E:664:LEU:HG	2.14	0.47
1:C:760:GLN:HG3	1:C:764:TYR:HE1	1.79	0.47
1:A:620:LEU:HA	1:A:634:MET:HE1	1.97	0.47
2:B:742:ASN:N	2:B:742:ASN:HD22	2.13	0.47
1:E:716:TYR:O	1:E:720:LYS:HB2	2.14	0.47
1:C:625:PRO:HG3	4:C:1027:HOH:O	2.13	0.47
1:A:579:LYS:HD2	1:A:579:LYS:C	2.35	0.47
1:C:579:LYS:HZ2	2:D:753:ASP:CG	2.17	0.47
1:G:588:HIS:CD2	1:G:681:LYS:HD2	2.50	0.47
1:K:576:LYS:HD2	1:K:577:TRP:N	2.28	0.47
1:C:555:SER:OG	1:C:558:ARG:HG2	2.14	0.47
1:C:525:LEU:HD21	1:G:586:ASN:CB	2.44	0.47
1:C:600:TRP:CZ3	1:C:753:LEU:HD11	2.49	0.47
1:E:552:VAL:HG23	1:E:553:PRO:HD2	1.96	0.47
1:A:561:THR:O	1:A:565:MET:HG2	2.15	0.47
1:E:666:MET:HB3	1:E:722:LEU:HD21	1.97	0.46
2:F:751:LYS:HZ2	2:F:751:LYS:HB2	1.80	0.46
1:E:535:LEU:HD13	1:E:535:LEU:O	2.15	0.46
1:E:610:TRP:HB2	1:E:663:TYR:CE1	2.50	0.46
1:A:764:TYR:CE2	1:A:769:ILE:HD12	2.51	0.46
1:A:608:LEU:HD23	1:A:646:MET:HB3	1.97	0.46
1:E:677:LYS:HB2	1:E:769:ILE:H	1.79	0.46
1:C:691:MET:HG3	1:C:695:LYS:HZ1	1.80	0.46
1:A:645:HIS:HD2	1:A:731:ASN:HD22	1.62	0.46
1:G:548:TYR:OH	1:G:558:ARG:NH2	2.48	0.46
1:I:610:TRP:CE2	1:I:614:ARG:HG3	2.50	0.46
1:K:667:LYS:HD2	4:K:1092:HOH:O	2.16	0.46
1:I:594:THR:HG21	1:I:676:PRO:HG3	1.98	0.46
1:E:634:MET:HE2	1:E:647:LEU:HD11	1.96	0.46
1:G:545:TYR:O	1:G:569:ARG:NH2	2.34	0.46
1:I:552:VAL:HG23	1:I:553:PRO:HD2	1.98	0.46
1:E:591:ASP:OD2	1:E:680:LEU:HD13	2.16	0.46
1:A:605:ALA:O	1:A:608:LEU:HB3	2.16	0.46
1:I:542:GLU:HG3	1:I:542:GLU:H	1.60	0.46
1:I:593:MET:HG3	2:J:745:LEU:HD23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:587:LEU:HD23	1:C:685:LEU:HD12	1.98	0.46
1:A:557:TRP:CG	1:A:558:ARG:N	2.84	0.46
1:I:545:TYR:CE1	1:I:625:PRO:HB2	2.51	0.46
1:E:597:GLN:HE21	2:F:745:LEU:HD23	1.81	0.46
1:G:609:GLY:HA3	1:G:649:VAL:HG22	1.98	0.46
1:A:620:LEU:HA	1:A:634:MET:CE	2.46	0.45
1:A:645:HIS:O	1:A:648:TYR:HB3	2.16	0.45
1:C:555:SER:O	1:C:559:ILE:HG12	2.16	0.45
1:G:750:PRO:HB2	4:G:1049:HOH:O	2.16	0.45
1:G:594:THR:HG23	1:G:598:TYR:CD1	2.51	0.45
1:E:561:THR:O	1:E:565:MET:HG2	2.16	0.45
1:E:561:THR:OG1	1:E:747:ILE:HA	2.17	0.45
1:A:666:MET:HB3	1:A:722:LEU:HD21	1.98	0.45
1:C:532:LEU:HD11	1:G:528:LEU:HD11	1.99	0.45
1:A:555:SER:O	1:A:559:ILE:HG13	2.16	0.45
1:I:720:LYS:NZ	1:I:777:LYS:HD2	2.31	0.45
1:A:535:LEU:O	1:A:535:LEU:HD13	2.17	0.45
1:G:561:THR:O	1:G:565:MET:HG2	2.17	0.45
1:E:572:ILE:HG12	1:E:752:MET:HE3	1.99	0.45
1:G:763:LYS:C	1:G:765:SER:H	2.20	0.45
1:E:545:TYR:CE1	1:E:625:PRO:HB2	2.52	0.45
1:E:530:PRO:HG2	1:E:534:SER:OG	2.16	0.45
1:I:556:THR:HG22	1:I:560:MET:HE2	1.98	0.45
1:C:528:LEU:HD12	1:C:528:LEU:HA	1.84	0.45
1:G:552:VAL:HG23	1:G:558:ARG:NH2	2.32	0.44
1:C:547:GLY:N	1:C:626:ASP:OD2	2.50	0.44
1:I:660:TYR:O	1:I:664:LEU:HG	2.17	0.44
1:E:579:LYS:HD3	2:F:749:LEU:HD23	1.99	0.44
1:A:596:LEU:HD12	2:B:749:LEU:HD11	1.99	0.44
1:K:594:THR:O	1:K:598:TYR:HD1	2.00	0.44
1:E:759:ASN:C	1:E:762:PRO:HD2	2.38	0.44
1:I:593:MET:HE1	2:J:746:ARG:HB2	1.99	0.44
1:E:571:VAL:O	1:E:575:VAL:HG23	2.17	0.44
1:E:697:LEU:O	1:E:701:ILE:HG13	2.17	0.44
1:A:588:HIS:CD2	1:A:590:ASP:HB2	2.50	0.44
1:A:588:HIS:HB3	1:A:591:ASP:OD2	2.17	0.44
1:C:716:TYR:O	1:C:720:LYS:HB2	2.18	0.44
1:K:525:LEU:HD12	1:K:526:PRO:HD2	2.00	0.44
1:E:634:MET:CE	1:E:647:LEU:HD11	2.48	0.44
1:A:579:LYS:HD2	1:A:580:ALA:N	2.32	0.44
1:K:602:ALA:HB2	1:K:729:VAL:HG21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:549:ASP:OD2	1:K:552:VAL:HG13	2.17	0.44
1:I:556:THR:HG22	1:I:560:MET:CE	2.48	0.43
1:E:600:TRP:O	1:E:604:MET:HG2	2.18	0.43
1:E:707:ASN:O	1:E:709:SER:N	2.51	0.43
1:I:571:VAL:O	1:I:575:VAL:HG23	2.18	0.43
1:G:594:THR:HG21	1:G:676:PRO:HD3	2.00	0.43
1:G:754:ALA:O	1:G:758:THR:HG23	2.18	0.43
1:C:527:GLN:C	1:C:529:THR:H	2.21	0.43
1:E:560:MET:CE	1:E:642:GLN:HE22	2.32	0.43
1:I:716:TYR:O	1:I:720:LYS:HB2	2.18	0.43
1:A:584:PHE:CE2	1:A:592:GLN:HB3	2.53	0.43
1:I:547:GLY:N	1:I:626:ASP:OD2	2.51	0.43
1:E:557:TRP:NE1	1:E:746:SER:O	2.51	0.43
1:G:730:GLU:OE2	1:G:771:LYS:NZ	2.50	0.43
1:E:585:ARG:C	1:E:587:LEU:H	2.22	0.43
2:B:742:ASN:CG	2:B:743:ALA:H	2.22	0.43
1:A:568:GLY:HA2	1:A:753:LEU:HD13	2.00	0.43
1:C:530:PRO:HB3	4:C:1057:HOH:O	2.18	0.43
2:D:740:LYS:N	2:D:742:ASN:OD1	2.52	0.43
1:A:707:ASN:O	1:A:709:SER:N	2.51	0.43
1:E:548:TYR:HD1	1:E:562:THR:HG21	1.83	0.43
1:K:761:ILE:HB	1:K:762:PRO:HD3	2.01	0.43
1:G:555:SER:O	1:G:559:ILE:HG12	2.19	0.43
1:A:642:GLN:C	1:A:644:LYS:H	2.22	0.43
1:C:588:HIS:HE1	1:C:590:ASP:OD2	2.02	0.43
1:A:734:ASN:HB3	1:E:765:SER:HB3	2.00	0.43
1:K:682:SER:HB3	1:K:685:LEU:HB3	2.01	0.43
1:G:753:LEU:O	1:G:757:ILE:HG13	2.19	0.42
1:E:705:GLU:H	1:E:705:GLU:CD	2.22	0.42
1:C:597:GLN:HG2	2:D:741:GLU:OE1	2.19	0.42
2:F:742:ASN:HD22	2:F:746:ARG:CG	2.32	0.42
1:A:537:GLU:HG2	1:A:537:GLU:O	2.19	0.42
1:E:535:LEU:HA	1:E:538:VAL:HG12	2.01	0.42
1:E:613:TYR:CE1	1:E:654:HIS:HA	2.54	0.42
1:A:660:TYR:CE2	1:A:664:LEU:HD11	2.54	0.42
1:A:533:VAL:CG2	1:A:661:GLU:HG2	2.48	0.42
1:G:600:TRP:O	1:G:604:MET:HG2	2.19	0.42
1:I:704:ARG:HG3	1:I:705:GLU:N	2.34	0.42
1:E:535:LEU:CD1	1:E:582:PRO:HD3	2.47	0.42
1:A:613:TYR:HD1	1:A:654:HIS:HB2	1.83	0.42
1:G:528:LEU:HD12	1:G:528:LEU:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:742:ASN:ND2	2:B:743:ALA:H	2.17	0.42
1:G:581:ILE:HA	1:G:582:PRO:HD2	1.91	0.42
1:G:598:TYR:HB3	1:G:674:THR:HB	2.02	0.42
1:G:552:VAL:HG23	1:G:558:ARG:CZ	2.50	0.42
4:A:1038:HOH:O	2:B:742:ASN:N	2.53	0.42
1:E:728:VAL:O	1:E:732:LEU:HG	2.19	0.42
2:D:742:ASN:HB2	2:D:746:ARG:CZ	2.50	0.42
1:E:535:LEU:HD12	1:E:582:PRO:CD	2.47	0.42
1:E:701:ILE:HD11	1:E:718:LEU:HD12	2.02	0.42
1:C:613:TYR:CE1	1:C:654:HIS:HA	2.55	0.42
1:I:710:GLN:O	1:I:713:GLN:HB3	2.20	0.41
1:C:604:MET:HG2	3:C:900:HCY:H192	2.00	0.41
1:K:573:ALA:O	1:K:576:LYS:HE3	2.20	0.41
1:A:589:LEU:HD22	1:A:589:LEU:HA	1.94	0.41
1:A:571:VAL:O	1:A:575:VAL:HG23	2.20	0.41
1:K:628:ILE:N	1:K:628:ILE:HD12	2.35	0.41
2:F:742:ASN:HB2	2:F:746:ARG:HB3	2.01	0.41
1:E:608:LEU:HD11	4:E:1022:HOH:O	2.19	0.41
1:K:552:VAL:HB	1:K:553:PRO:HD2	2.02	0.41
1:C:721:LEU:HD12	1:C:724:SER:OG	2.21	0.41
1:E:710:GLN:O	1:E:713:GLN:HB3	2.19	0.41
1:A:545:TYR:HD1	1:A:626:ASP:OD1	2.03	0.41
1:E:530:PRO:HB3	4:E:1001:HOH:O	2.19	0.41
1:E:738:GLN:HG2	1:E:745:MET:HE1	2.01	0.41
1:A:713:GLN:NE2	1:G:712:TRP:CD2	2.89	0.41
1:A:662:GLU:O	1:A:666:MET:HG3	2.21	0.41
1:G:733:LEU:HD23	1:G:733:LEU:HA	1.94	0.41
2:F:740:LYS:HB2	2:F:740:LYS:HE2	1.76	0.41
1:A:616:SER:OG	1:A:620:LEU:HD21	2.21	0.41
1:A:561:THR:OG1	1:A:747:ILE:HA	2.20	0.41
1:G:610:TRP:CZ2	1:G:660:TYR:HD1	2.39	0.41
1:E:755:GLU:O	2:F:740:LYS:HE3	2.21	0.41
1:A:629:ILE:HG22	1:A:634:MET:HE2	2.02	0.41
1:E:680:LEU:HD12	1:E:682:SER:H	1.85	0.41
1:A:564:ASN:OD1	3:A:900:HCY:H121	2.21	0.41
1:A:570:GLN:NE2	1:A:604:MET:HG3	2.35	0.41
1:I:708:SER:HA	1:I:711:ASN:CG	2.42	0.41
1:G:547:GLY:N	1:G:626:ASP:OD2	2.47	0.41
1:G:675:ILE:HD11	1:G:770:LYS:CE	2.51	0.41
1:K:576:LYS:C	1:K:576:LYS:HD2	2.41	0.41
1:E:685:LEU:HD22	1:E:689:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:610:TRP:CZ2	1:K:660:TYR:HD1	2.39	0.41
1:K:759:ASN:HB2	2:L:740:LYS:N	2.36	0.40
1:G:726:HIS:CE1	1:G:771:LYS:HB3	2.56	0.40
1:E:547:GLY:N	1:E:626:ASP:OD2	2.45	0.40
1:A:706:GLY:O	1:A:708:SER:N	2.54	0.40
1:C:707:ASN:O	1:C:708:SER:C	2.59	0.40
1:G:559:ILE:O	1:G:563:LEU:HG	2.21	0.40
1:A:642:GLN:C	1:A:644:LYS:N	2.74	0.40
2:F:753:ASP:N	2:F:753:ASP:OD2	2.54	0.40
1:G:613:TYR:CE1	1:G:654:HIS:HA	2.56	0.40
1:C:577:TRP:CZ2	1:C:581:ILE:HD11	2.56	0.40
2:F:751:LYS:NZ	2:F:751:LYS:HB2	2.36	0.40
1:E:763:LYS:HA	1:E:766:ASN:HB3	2.04	0.40
1:K:696:GLU:HA	1:K:699:LYS:HD2	2.03	0.40
1:E:770:LYS:O	1:E:770:LYS:HG3	2.21	0.40
1:K:555:SER:O	1:K:559:ILE:HG13	2.22	0.40
1:K:666:MET:HB3	1:K:722:LEU:HD21	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	250/255 (98%)	214 (86%)	29 (12%)	7 (3%)	6	9
1	C	253/255 (99%)	241 (95%)	10 (4%)	2 (1%)	24	41
1	E	253/255 (99%)	216 (85%)	30 (12%)	7 (3%)	6	9
1	G	252/255 (99%)	239 (95%)	9 (4%)	4 (2%)	12	21
1	I	253/255 (99%)	240 (95%)	12 (5%)	1 (0%)	39	61
1	K	253/255 (99%)	241 (95%)	10 (4%)	2 (1%)	24	41
2	B	10/14 (71%)	6 (60%)	2 (20%)	2 (20%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	12/14 (86%)	9 (75%)	2 (17%)	1 (8%)	1	1
2	F	12/14 (86%)	7 (58%)	2 (17%)	3 (25%)	0	0
2	H	11/14 (79%)	11 (100%)	0	0	100	100
2	J	10/14 (71%)	8 (80%)	2 (20%)	0	100	100
2	L	12/14 (86%)	11 (92%)	1 (8%)	0	100	100
All	All	1581/1614 (98%)	1443 (91%)	109 (7%)	29 (2%)	11	18

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	529	THR
1	A	530	PRO
1	C	708	SER
1	E	704	ARG
2	F	743	ALA
1	G	704	ARG
1	G	708	SER
1	K	704	ARG
1	A	708	SER
1	C	709	SER
2	D	743	ALA
1	E	529	THR
1	E	708	SER
2	F	742	ASN
1	A	762	PRO
2	B	743	ALA
1	E	679	GLY
2	F	752	ASP
1	K	637	PRO
1	A	619	ASN
1	A	637	PRO
1	A	644	LYS
2	B	750	ASP
1	E	582	PRO
1	E	586	ASN
1	G	764	TYR
1	I	708	SER
1	E	637	PRO
1	G	530	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	229/231 (99%)	209 (91%)	20 (9%)	13	24
1	C	231/231 (100%)	221 (96%)	10 (4%)	35	61
1	E	231/231 (100%)	222 (96%)	9 (4%)	39	66
1	G	230/231 (100%)	222 (96%)	8 (4%)	43	70
1	I	231/231 (100%)	219 (95%)	12 (5%)	29	51
1	K	231/231 (100%)	224 (97%)	7 (3%)	48	76
2	B	11/13 (85%)	9 (82%)	2 (18%)	2	3
2	D	13/13 (100%)	10 (77%)	3 (23%)	1	1
2	F	13/13 (100%)	9 (69%)	4 (31%)	0	0
2	H	12/13 (92%)	12 (100%)	0	100	100
2	J	11/13 (85%)	11 (100%)	0	100	100
2	L	13/13 (100%)	8 (62%)	5 (38%)	0	0
All	All	1456/1464 (100%)	1376 (94%)	80 (6%)	27	48

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	527	GLN
1	A	528	LEU
1	A	552	VAL
1	A	556	THR
1	A	557	TRP
1	A	560	MET
1	A	579	LYS
1	A	589	LEU
1	A	590	ASP
1	A	604	MET
1	A	615	GLN
1	A	628	ILE
1	A	630	ASN
1	A	641	ASP

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Mol	Chain	Res	Type
1	A	651	SER
1	A	678	ASP
1	A	704	ARG
1	A	713	GLN
1	A	721	LEU
1	A	753	LEU
2	B	742	ASN
2	B	750	ASP
1	C	524	THR
1	C	527	GLN
1	C	542	GLU
1	C	552	VAL
1	C	604	MET
1	C	713	GLN
1	C	734	ASN
1	C	745	MET
1	C	759	ASN
1	C	760	GLN
2	D	740	LYS
2	D	742	ASN
2	D	752	ASP
1	E	525	LEU
1	E	529	THR
1	E	613	TYR
1	E	622	TYR
1	E	670	LEU
1	E	705	GLU
1	E	707	ASN
1	E	721	LEU
1	E	753	LEU
2	F	746	ARG
2	F	750	ASP
2	F	751	LYS
2	F	753	ASP
1	G	529	THR
1	G	576	LYS
1	G	594	THR
1	G	613	TYR
1	G	614	ARG
1	G	649	VAL
1	G	721	LEU
1	G	743	LYS

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Mol	Chain	Res	Type
1	I	527	GLN
1	I	528	LEU
1	I	542	GLU
1	I	557	TRP
1	I	589	LEU
1	I	604	MET
1	I	613	TYR
1	I	616	SER
1	I	685	LEU
1	I	704	ARG
1	I	721	LEU
1	I	776	GLN
1	K	535	LEU
1	K	576	LYS
1	K	604	MET
1	K	615	GLN
1	K	635	THR
1	K	734	ASN
1	K	765	SER
2	L	740	LYS
2	L	741	GLU
2	L	742	ASN
2	L	748	LEU
2	L	751	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	570	GLN
1	A	588	HIS
1	A	713	GLN
1	A	731	ASN
2	B	742	ASN
1	C	527	GLN
1	C	570	GLN
1	C	713	GLN
1	C	759	ASN
1	C	760	GLN
2	D	742	ASN
1	E	597	GLN
1	E	731	ASN
1	E	760	GLN

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Mol	Chain	Res	Type
1	G	586	ASN
1	G	588	HIS
2	L	742	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

6 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
3	HCY	A	900	-	29,29,29	0.81	0	48,48,48	1.84	10 (20%)
3	HCY	C	900	-	29,29,29	0.81	1 (3%)	48,48,48	1.84	10 (20%)
3	HCY	E	900	-	29,29,29	0.80	0	48,48,48	1.86	10 (20%)
3	HCY	G	900	-	29,29,29	0.80	0	48,48,48	1.85	10 (20%)
3	HCY	I	900	-	29,29,29	0.81	0	48,48,48	1.80	12 (25%)
3	HCY	K	900	-	29,29,29	0.79	0	48,48,48	1.87	11 (22%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical

component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HCY	A	900	-	-	0/8/73/73	0/4/4/4
3	HCY	C	900	-	-	0/8/73/73	0/4/4/4
3	HCY	E	900	-	-	0/8/73/73	0/4/4/4
3	HCY	G	900	-	-	0/8/73/73	0/4/4/4
3	HCY	I	900	-	-	0/8/73/73	0/4/4/4
3	HCY	K	900	-	-	0/8/73/73	0/4/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	900	HCY	C16-C17	-2.01	1.50	1.54

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	900	HCY	C7-C8-C14	-3.35	106.46	112.02
3	A	900	HCY	C16-C17-C20	-3.35	110.10	113.81
3	C	900	HCY	C7-C8-C14	-3.30	106.55	112.02
3	A	900	HCY	C7-C8-C14	-3.30	106.56	112.02
3	G	900	HCY	C7-C8-C14	-3.28	106.59	112.02
3	E	900	HCY	C7-C8-C14	-3.27	106.60	112.02
3	K	900	HCY	C16-C17-C20	-3.26	110.20	113.81
3	G	900	HCY	C16-C17-C20	-3.25	110.21	113.81
3	K	900	HCY	C7-C8-C14	-3.23	106.66	112.02
3	E	900	HCY	C16-C17-C20	-3.19	110.28	113.81
3	C	900	HCY	C16-C17-C20	-3.14	110.33	113.81
3	I	900	HCY	C16-C17-C20	-3.12	110.35	113.81
3	A	900	HCY	C6-C5-C4	-3.03	117.05	120.89
3	E	900	HCY	C6-C5-C4	-3.02	117.06	120.89
3	G	900	HCY	C6-C5-C4	-2.93	117.17	120.89
3	K	900	HCY	C6-C5-C4	-2.92	117.19	120.89
3	I	900	HCY	C6-C5-C4	-2.89	117.22	120.89
3	C	900	HCY	C6-C5-C4	-2.87	117.25	120.89
3	I	900	HCY	O3-C17-C16	-2.02	105.97	110.65
3	K	900	HCY	O3-C17-C16	-2.00	106.01	110.65
3	I	900	HCY	O2-C11-C9	2.04	115.29	110.91
3	G	900	HCY	C1-C10-C5	2.13	112.88	108.80
3	I	900	HCY	C1-C10-C5	2.22	113.04	108.80
3	A	900	HCY	C1-C10-C5	2.22	113.05	108.80
3	I	900	HCY	C7-C8-C9	2.25	113.75	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	900	HCY	C1-C10-C5	2.27	113.14	108.80
3	E	900	HCY	C1-C10-C5	2.28	113.17	108.80
3	A	900	HCY	C7-C8-C9	2.28	113.80	109.60
3	C	900	HCY	C7-C8-C9	2.30	113.84	109.60
3	E	900	HCY	C7-C8-C9	2.31	113.85	109.60
3	G	900	HCY	C7-C8-C9	2.32	113.88	109.60
3	C	900	HCY	C1-C10-C5	2.37	113.35	108.80
3	K	900	HCY	C7-C8-C9	2.43	114.07	109.60
3	G	900	HCY	C2-C3-C4	2.66	120.79	116.70
3	A	900	HCY	C2-C3-C4	2.72	120.88	116.70
3	I	900	HCY	C2-C3-C4	2.74	120.91	116.70
3	E	900	HCY	C2-C3-C4	2.78	120.98	116.70
3	K	900	HCY	C2-C3-C4	2.80	121.01	116.70
3	C	900	HCY	C2-C3-C4	2.80	121.01	116.70
3	G	900	HCY	C6-C5-C10	2.83	119.92	116.71
3	I	900	HCY	C6-C5-C10	2.85	119.94	116.71
3	C	900	HCY	C6-C5-C10	2.91	120.02	116.71
3	A	900	HCY	C6-C5-C10	2.97	120.08	116.71
3	E	900	HCY	C6-C5-C10	2.99	120.11	116.71
3	K	900	HCY	C6-C5-C10	3.03	120.15	116.71
3	A	900	HCY	C2-C1-C10	3.17	117.88	113.41
3	E	900	HCY	C2-C1-C10	3.17	117.89	113.41
3	K	900	HCY	C2-C1-C10	3.31	118.07	113.41
3	I	900	HCY	C2-C1-C10	3.31	118.08	113.41
3	G	900	HCY	C2-C1-C10	3.33	118.11	113.41
3	C	900	HCY	C2-C1-C10	3.37	118.17	113.41
3	G	900	HCY	C13-C17-C20	4.33	117.12	112.83
3	K	900	HCY	C13-C17-C20	4.35	117.14	112.83
3	I	900	HCY	C13-C17-C20	4.47	117.25	112.83
3	C	900	HCY	C13-C17-C20	4.47	117.25	112.83
3	E	900	HCY	C13-C17-C20	4.52	117.31	112.83
3	A	900	HCY	C13-C17-C20	4.57	117.35	112.83
3	I	900	HCY	C12-C13-C17	5.76	120.42	116.17
3	C	900	HCY	C12-C13-C17	6.08	120.65	116.17
3	A	900	HCY	C12-C13-C17	6.14	120.69	116.17
3	G	900	HCY	C12-C13-C17	6.35	120.85	116.17
3	E	900	HCY	C12-C13-C17	6.39	120.88	116.17
3	K	900	HCY	C12-C13-C17	6.42	120.90	116.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	900	HCY	2	0
3	C	900	HCY	1	0
3	I	900	HCY	1	0
3	K	900	HCY	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	252/255 (98%)	0.63	43 (17%) 2 2	10, 39, 70, 86	0
1	C	255/255 (100%)	-0.27	11 (4%) 39 44	8, 24, 51, 87	0
1	E	255/255 (100%)	0.81	37 (14%) 3 3	9, 41, 67, 88	0
1	G	254/255 (99%)	-0.20	16 (6%) 23 26	8, 24, 53, 80	0
1	I	255/255 (100%)	-0.27	12 (4%) 35 40	7, 22, 53, 90	0
1	K	255/255 (100%)	-0.18	9 (3%) 48 53	9, 25, 51, 76	0
2	B	12/14 (85%)	1.87	6 (50%) 0 0	45, 58, 78, 81	0
2	D	14/14 (100%)	1.43	5 (35%) 0 0	26, 45, 66, 71	0
2	F	14/14 (100%)	2.59	8 (57%) 0 0	51, 61, 70, 80	0
2	H	13/14 (92%)	-0.52	0 100 100	17, 24, 36, 45	0
2	J	12/14 (85%)	-0.12	0 100 100	21, 25, 42, 52	0
2	L	14/14 (100%)	0.55	1 (7%) 19 21	27, 38, 67, 69	0
All	All	1605/1614 (99%)	0.13	148 (9%) 11 12	7, 27, 64, 90	0

All (148) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	706	GLY	11.3
1	E	765	SER	8.7
1	I	523	ALA	8.5
1	C	526	PRO	7.6
1	A	765	SER	7.2
2	D	742	ASN	6.4
1	A	526	PRO	6.1
1	E	525	LEU	5.8
1	E	777	LYS	5.7
1	A	620	LEU	5.7
1	A	640	TYR	5.6

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Mol	Chain	Res	Type	RSRZ
1	E	706	GLY	5.4
1	E	615	GLN	5.4
1	A	706	GLY	5.4
2	F	753	ASP	5.1
1	E	557	TRP	5.0
2	F	749	LEU	4.9
1	K	707	ASN	4.9
1	E	762	PRO	4.9
1	C	617	SER	4.9
2	B	752	ASP	4.9
1	K	709	SER	4.8
1	G	706	GLY	4.7
1	G	764	TYR	4.6
2	D	743	ALA	4.6
1	K	710	GLN	4.5
1	E	639	MET	4.5
1	A	708	SER	4.4
1	I	617	SER	4.3
1	C	525	LEU	4.2
1	I	524	THR	4.1
1	A	550	SER	4.1
1	C	527	GLN	4.1
1	I	525	LEU	4.0
1	C	524	THR	3.9
1	A	647	LEU	3.9
1	K	617	SER	3.9
1	E	620	LEU	3.8
1	C	528	LEU	3.8
1	A	549	ASP	3.8
1	E	710	GLN	3.7
1	E	764	TYR	3.7
2	D	753	ASP	3.6
1	A	529	THR	3.6
1	E	549	ASP	3.6
1	C	529	THR	3.6
1	I	708	SER	3.6
1	E	550	SER	3.5
1	E	551	SER	3.4
1	G	528	LEU	3.4
1	G	529	THR	3.4
1	G	710	GLN	3.4
1	I	526	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
2	F	742	ASN	3.3
2	F	752	ASP	3.3
1	E	616	SER	3.3
1	C	708	SER	3.2
1	E	538	VAL	3.1
1	A	530	PRO	3.1
1	G	557	TRP	3.1
1	A	631	GLU	3.1
1	A	527	GLN	3.1
1	E	709	SER	3.1
1	G	709	SER	3.0
1	I	705	GLU	3.0
1	A	538	VAL	3.0
1	E	543	VAL	3.0
2	F	746	ARG	3.0
1	A	653	LEU	3.0
1	A	528	LEU	2.9
1	I	552	VAL	2.9
2	L	753	ASP	2.9
2	D	741	GLU	2.9
1	A	654	HIS	2.9
1	G	526	PRO	2.9
1	E	708	SER	2.8
1	C	706	GLY	2.8
1	K	551	SER	2.8
2	B	747	TYR	2.8
1	A	551	SER	2.8
1	K	777	LYS	2.7
1	K	523	ALA	2.7
2	F	743	ALA	2.7
1	E	640	TYR	2.7
1	A	615	GLN	2.7
1	A	625	PRO	2.7
1	E	705	GLU	2.7
1	A	639	MET	2.6
2	B	750	ASP	2.6
1	E	632	GLN	2.6
1	E	523	ALA	2.6
1	A	557	TRP	2.6
1	E	586	ASN	2.6
1	C	523	ALA	2.6
1	E	636	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	705	GLU	2.6
1	G	705	GLU	2.6
1	I	528	LEU	2.5
1	E	678	ASP	2.5
1	A	535	LEU	2.5
2	B	749	LEU	2.5
1	A	777	LYS	2.5
1	I	777	LYS	2.5
2	F	747	TYR	2.5
1	G	617	SER	2.5
1	E	541	PRO	2.4
2	B	753	ASP	2.4
1	A	657	GLN	2.4
1	A	545	TYR	2.4
1	A	636	LEU	2.4
1	G	765	SER	2.3
1	A	619	ASN	2.3
1	K	553	PRO	2.3
1	A	613	TYR	2.3
1	E	647	LEU	2.3
1	A	543	VAL	2.3
1	E	767	GLY	2.3
1	G	523	ALA	2.3
2	D	752	ASP	2.2
1	E	529	THR	2.2
1	E	766	ASN	2.2
1	E	624	ALA	2.2
1	A	547	GLY	2.2
2	B	748	LEU	2.2
1	A	552	VAL	2.1
1	E	552	VAL	2.1
1	G	708	SER	2.1
1	A	618	ALA	2.1
1	G	552	VAL	2.1
1	E	634	MET	2.1
1	A	643	CYS	2.1
1	A	531	THR	2.1
1	G	551	SER	2.1
1	G	531	THR	2.1
1	K	708	SER	2.1
1	E	590	ASP	2.1
1	A	546	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	I	527	GLN	2.1
1	A	635	THR	2.1
1	A	579	LYS	2.0
1	E	530	PRO	2.0
1	A	764	TYR	2.0
1	C	705	GLU	2.0
1	A	632	GLN	2.0
2	F	741	GLU	2.0
1	A	621	LEU	2.0
1	E	648	TYR	2.0
1	A	630	ASN	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

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, 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	LLDF	B-factors(Å ²)	Q<0.9
3	HCY	G	900	26/26	0.87	0.17	3.26	15,21,26,28	0
3	HCY	I	900	26/26	0.91	0.17	3.04	15,20,24,28	0
3	HCY	K	900	26/26	0.90	0.18	3.03	15,21,27,28	0
3	HCY	C	900	26/26	0.87	0.16	1.45	18,22,28,29	0
3	HCY	A	900	26/26	0.90	0.15	0.14	15,23,28,29	0
3	HCY	E	900	26/26	0.89	0.15	-0.09	19,25,29,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.