



wwPDB X-ray Structure Validation Summary 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 wwPDB X-ray Structure Validation Summary 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

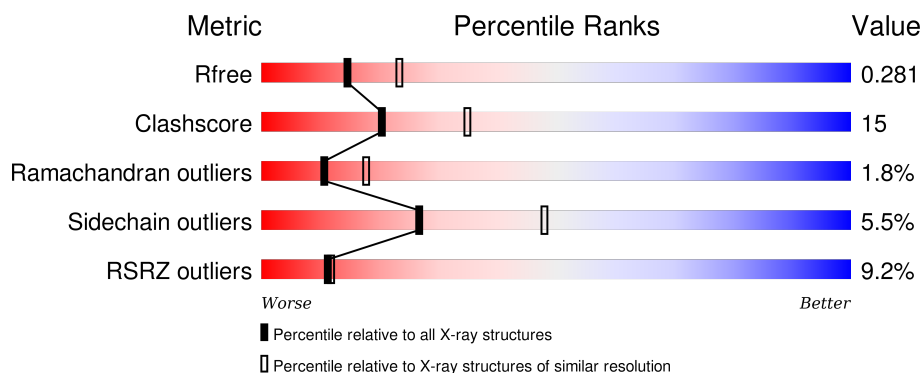
1 Overall quality at a glance ⓘ

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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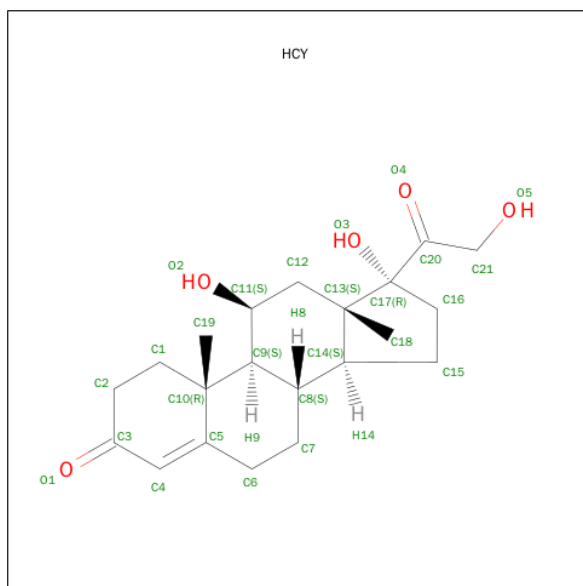
Chain	Residue	Modelled	Actual	Comment	Reference
E	674	THR	SER	engineered mutation	UNP P04150
E	675	ILE	VAL	engineered mutation	UNP P04150
E	684	ALA	GLU	engineered mutation	UNP P04150
E	688	ALA	GLU	engineered mutation	UNP P04150
G	602	ALA	PHE	engineered mutation	UNP P04150
G	622	TYR	CYS	engineered mutation	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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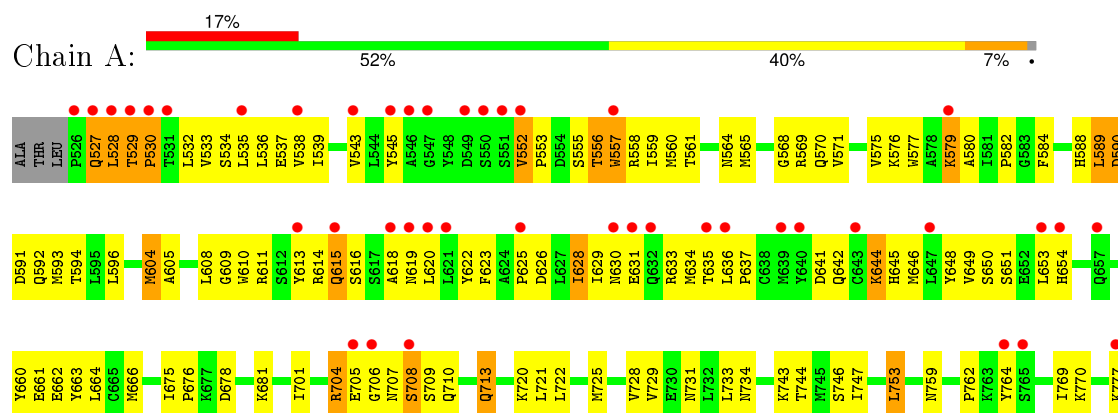
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	F	5	Total 5	O 5	0	0
4	G	102	Total 102	O 102	0	0
4	H	9	Total 9	O 9	0	0
4	I	119	Total 119	O 119	0	0
4	J	7	Total 7	O 7	0	0
4	K	127	Total 127	O 127	0	0
4	L	3	Total 3	O 3	0	0

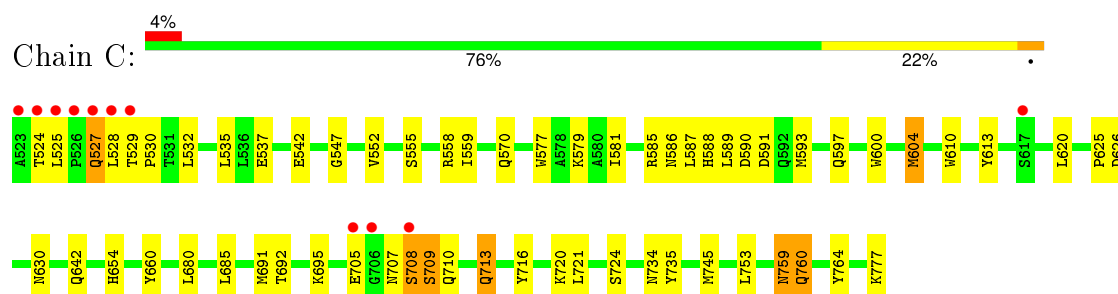
3 Residue-property plots [i](#)

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.

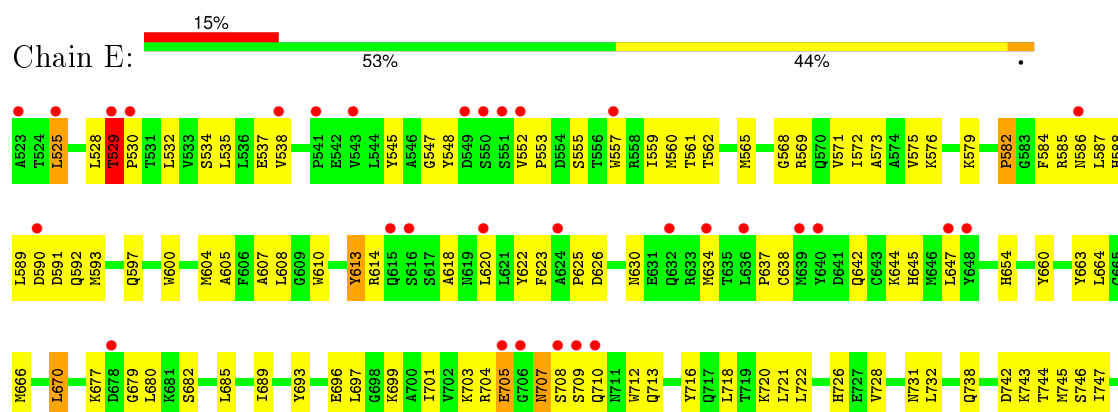
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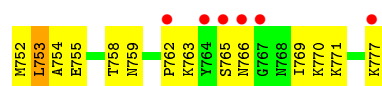


• Molecule 1: Glucocorticoid receptor



• Molecule 1: Glucocorticoid receptor

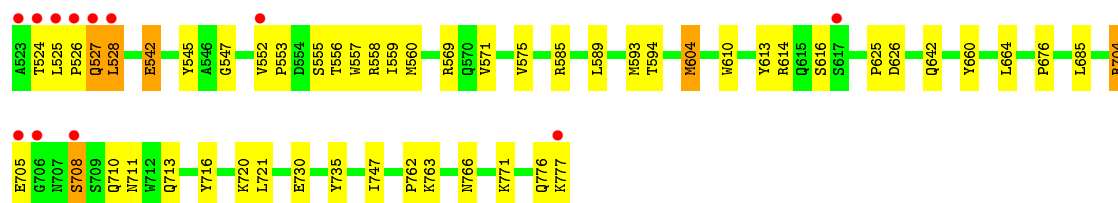
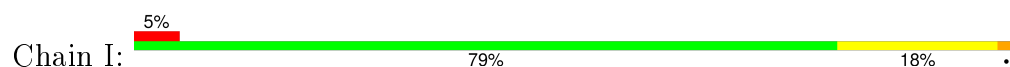




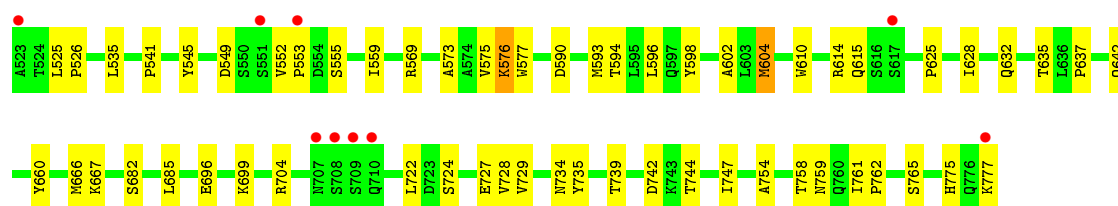
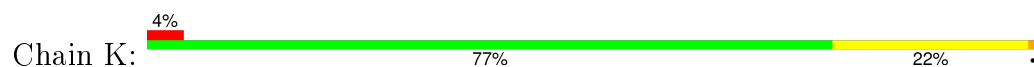
• Molecule 1: Glucocorticoid receptor



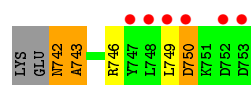
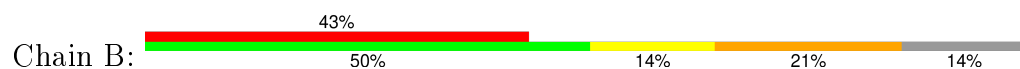
• Molecule 1: Glucocorticoid receptor



• Molecule 1: Glucocorticoid receptor

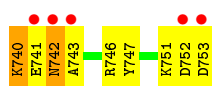


• Molecule 2: Nuclear receptor coactivator 2

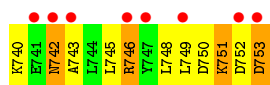
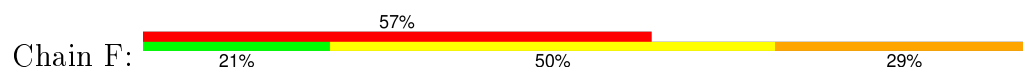


• Molecule 2: Nuclear receptor coactivator 2

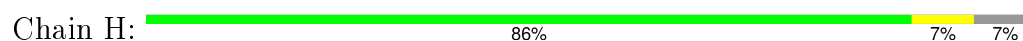




- Molecule 2: Nuclear receptor coactivator 2



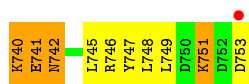
- Molecule 2: Nuclear receptor coactivator 2



- 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.

The worst 5 of 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

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	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
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

5 of 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

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Mol	Chain	Res	Type
2	F	743	ALA

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

5 of 80 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	529	THR
2	F	746	ARG
1	K	734	ASN
1	E	613	TYR
1	E	705	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	713	GLN
1	C	759	ASN
1	E	760	GLN
1	C	570	GLN
1	G	586	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

The worst 5 of 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

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 ⓘ

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	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

The worst 5 of 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

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(\AA^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.