



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:00 AM GMT

PDB ID : 3GR9
Title : Crystal structure of ColD H188K S187N
Authors : Holden, H.M.; Cook, P.D.; Kubiak, R.L.; Toomey, D.P.
Deposited on : 2009-03-25
Resolution : 2.20 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

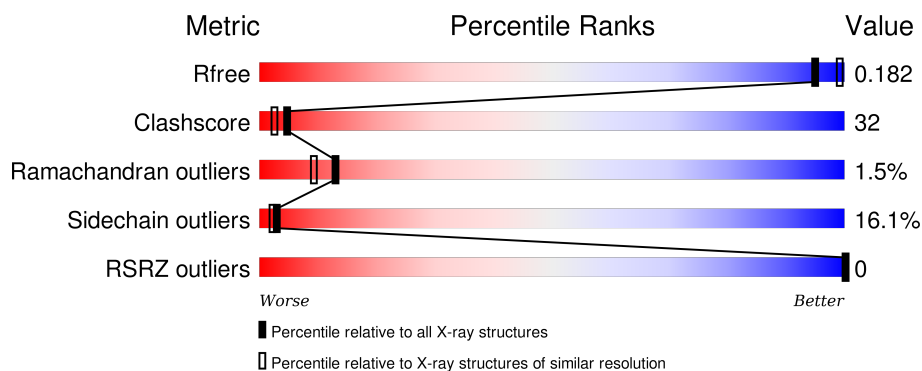
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	390	
1	B	390	
1	C	390	
1	D	390	
1	E	390	

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Mol	Chain	Length	Quality of chain
1	F	390	
1	G	390	
1	H	390	

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
1	IT1	F	188	-	-	X	-
2	AKG	A	401	-	-	-	X
2	AKG	B	402	-	-	X	-
2	AKG	F	405	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 25205 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 ColD.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	384	Total	C	N	O	P	S	0	1	0
			3092	1983	505	589	1	14			
1	B	385	Total	C	N	O	P	S	0	1	0
			3104	1992	506	591	1	14			
1	C	388	Total	C	N	O	P	S	0	1	0
			3128	2007	510	595	1	15			
1	D	381	Total	C	N	O	P	S	0	1	0
			3072	1969	502	586	1	14			
1	E	383	Total	C	N	O	P	S	0	1	0
			3082	1977	503	587	1	14			
1	F	386	Total	C	N	O	P	S	0	1	0
			3112	1996	508	593	1	14			
1	G	387	Total	C	N	O	P	S	0	1	0
			3120	2002	509	594	1	14			
1	H	381	Total	C	N	O	P	S	0	1	0
			3072	1969	502	586	1	14			

There are 32 discrepancies between the modelled and reference sequences:

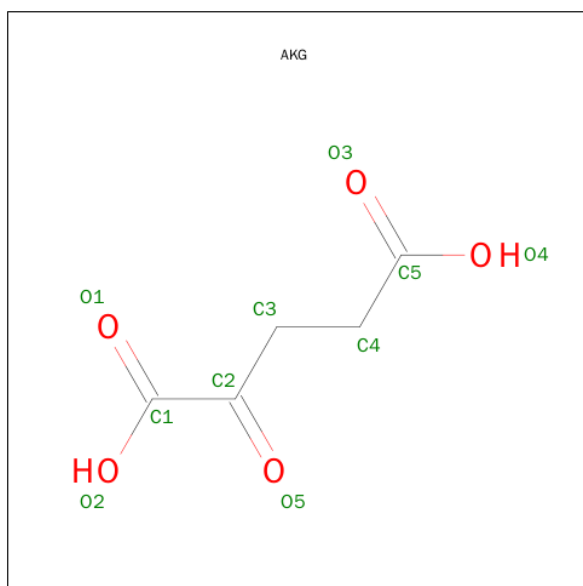
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP Q9F118
A	0	HIS	-	EXPRESSION TAG	UNP Q9F118
A	187	ASN	SER	ENGINEERED	UNP Q9F118
A	188	IT1	HIS	ENGINEERED	UNP Q9F118
B	-1	GLY	-	EXPRESSION TAG	UNP Q9F118
B	0	HIS	-	EXPRESSION TAG	UNP Q9F118
B	187	ASN	SER	ENGINEERED	UNP Q9F118
B	188	IT1	HIS	ENGINEERED	UNP Q9F118
C	-1	GLY	-	EXPRESSION TAG	UNP Q9F118
C	0	HIS	-	EXPRESSION TAG	UNP Q9F118
C	187	ASN	SER	ENGINEERED	UNP Q9F118
C	188	IT1	HIS	ENGINEERED	UNP Q9F118
D	-1	GLY	-	EXPRESSION TAG	UNP Q9F118

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Chain	Residue	Modelled	Actual	Comment	Reference
D	0	HIS	-	EXPRESSION TAG	UNP Q9F118
D	187	ASN	SER	ENGINEERED	UNP Q9F118
D	188	IT1	HIS	ENGINEERED	UNP Q9F118
E	-1	GLY	-	EXPRESSION TAG	UNP Q9F118
E	0	HIS	-	EXPRESSION TAG	UNP Q9F118
E	187	ASN	SER	ENGINEERED	UNP Q9F118
E	188	IT1	HIS	ENGINEERED	UNP Q9F118
F	-1	GLY	-	EXPRESSION TAG	UNP Q9F118
F	0	HIS	-	EXPRESSION TAG	UNP Q9F118
F	187	ASN	SER	ENGINEERED	UNP Q9F118
F	188	IT1	HIS	ENGINEERED	UNP Q9F118
G	-1	GLY	-	EXPRESSION TAG	UNP Q9F118
G	0	HIS	-	EXPRESSION TAG	UNP Q9F118
G	187	ASN	SER	ENGINEERED	UNP Q9F118
G	188	IT1	HIS	ENGINEERED	UNP Q9F118
H	-1	GLY	-	EXPRESSION TAG	UNP Q9F118
H	0	HIS	-	EXPRESSION TAG	UNP Q9F118
H	187	ASN	SER	ENGINEERED	UNP Q9F118
H	188	IT1	HIS	ENGINEERED	UNP Q9F118

- Molecule 2 is 2-OXOGLUTARIC ACID (three-letter code: AKG) (formula: C₅H₆O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	5	5		
2	B	1	Total	C	O	0	0
			10	5	5		

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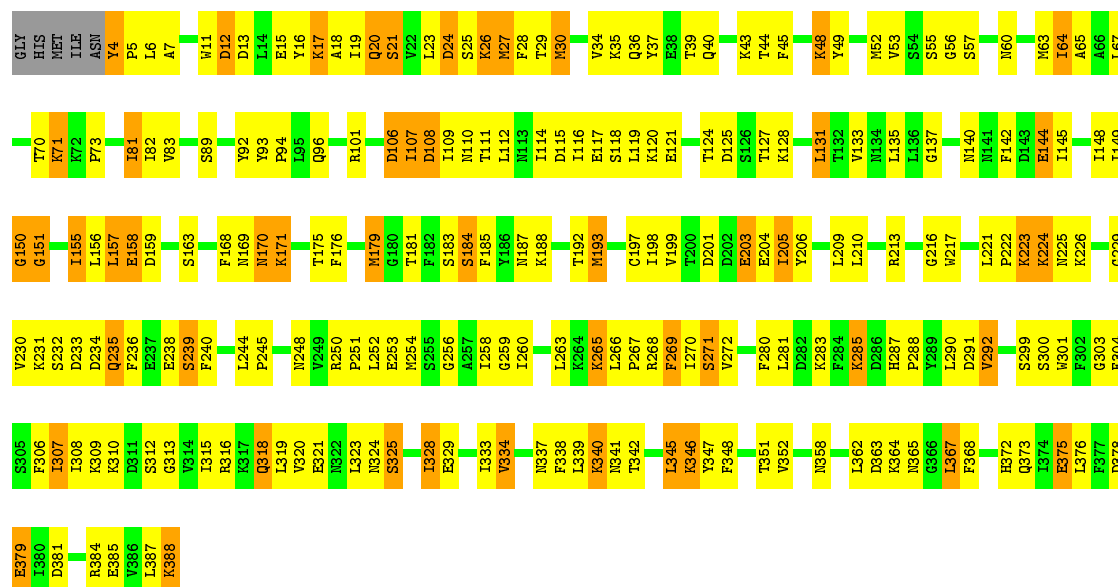
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			10	5	5		
2	D	1	Total	C	O	0	0
			10	5	5		
2	F	1	Total	C	O	0	0
			10	5	5		
2	H	1	Total	C	O	0	0
			10	5	5		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	42	Total	O	0	0
			42	42		
3	B	52	Total	O	0	0
			52	52		
3	C	50	Total	O	0	0
			50	50		
3	D	55	Total	O	0	0
			55	55		
3	E	37	Total	O	0	0
			37	37		
3	F	43	Total	O	0	0
			43	43		
3	G	41	Total	O	0	0
			41	41		
3	H	43	Total	O	0	0
			43	43		

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 ($\text{RSRZ} > 2$). 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.

Chain A: 48% 42% 8% ..



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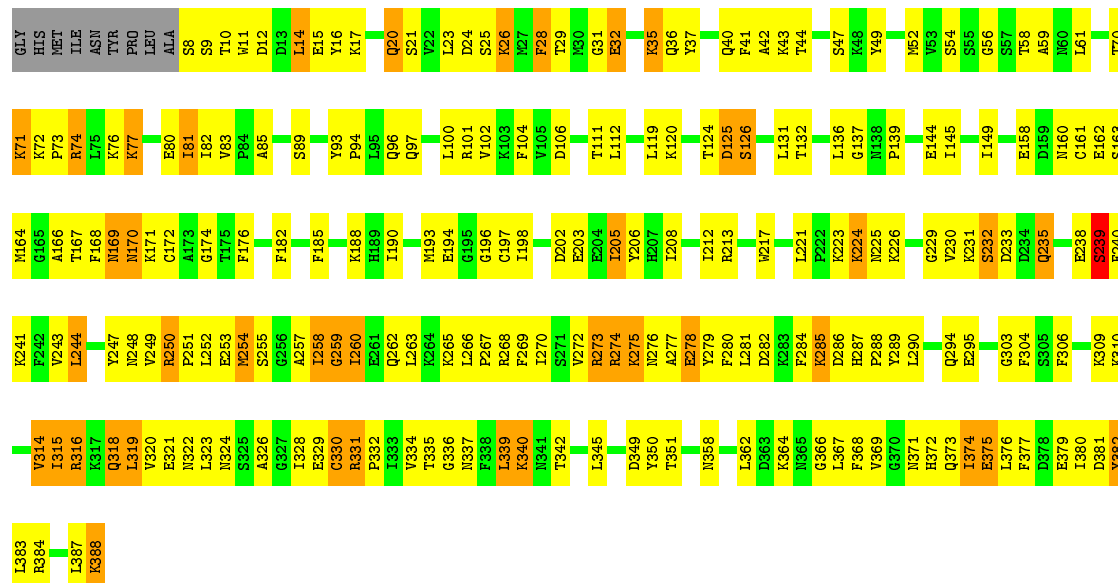
Chain D:

Amino Acid	Category
GLY	Grey
HIS	Green
MET	Green
ILE	Green
ASN	Green
THR	Green
PRO	Green
LEU	Green
ALA	Green
S8	Green
S9	Green
T10	Green
D13	Green
L14	Green
E15	Green
A18	Green
V22	Green
L23	Green
D24	Green
S25	Green
K26	Green
M27	Green
F28	Green
T29	Green
Y33	Green
V34	Green
K35	Green
Q36	Green
Y37	Green
E38	Green
T39	Green
Q40	Green
F41	Green
A42	Green
K43	Green
T44	Green
F45	Green
K48	Green
S54	Green
S55	Green
G56	Green
S57	Green
T58	Green
L62	Green
F69	Green
T70	Green
K71	Green
K72	Green
P73	Green
R74	Green
L75	Green
V76	Green
D79	Green
S80	Green
T81	Green
T82	Green
V83	Green
H86	Green
S87	Green
H88	Green
Y92	Green
Y93	Green
P94	Green
L95	Green
L100	Green
D106	Green
I107	Green
D108	Green
I109	Green
L119	Green
K120	Green
V123	Green
T124	Green
D125	Green
S126	Green
T127	Green
K128	Green
A129	Green
L131	Green
L135	Green
L136	Green
G137	Green
L145	Green
H146	Green
K147	Green
L148	Green
I149	Green
I154	Green
I155	Green
L156	Green
L157	Green
G161	Green
F162	Green
S163	Green
T167	Green
F168	Green
N169	Green
H170	Green
V171	Green
C172	Green
F176	Green
G177	Green
L178	Green
S183	Green
S184	Green
F186	Green
Y186	Green
H187	Green
K188	Green
H189	Green
I190	Green
M193	Green
E194	Green
I198	Green
D202	Green
E203	Green
D204	Green
I205	Green
I206	Green
H207	Green
L208	Green
L209	Green
L210	Green
G211	Green
R212	Green
R213	Green
H217	Green
L218	Green
R219	Green
N220	Green
L221	Green
K224	Green
N225	Green
K226	Green
V227	Green
T228	Green
G229	Green
V230	Green
K231	Green
S232	Green
D233	Green
D234	Green
Q235	Green
F236	Green
E237	Green
E238	Green
F242	Green
P245	Green
V248	Green
V249	Green
L252	Green
E253	Green
K257	Green
L258	Green
G259	Green
I260	Green
E261	Green
Q262	Green
L263	Green
K264	Green
K265	Green
L266	Green
P267	Green
R268	Green
F269	Green
I270	Green
S271	Green
V272	Green
R273	Green
K274	Green
K275	Green
M276	Green
A277	Green
E278	Green
F279	Green
F280	Green
L281	Green
D282	Green
K283	Green
F284	Green
K285	Green
D286	Green
F287	Green
P288	Green
V289	Green
L290	Green
D291	Green
V292	Green
S300	Green
N301	Green
S305	Green
F306	Green
K310	Green
V314	Green
L315	Green
R316	Green
K317	Green
Q318	Green
E321	Green
N322	Green
R324	Green

[illegible]

● Molecule 1: Cold

Chain H: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	69.73Å 114.66Å 114.57Å 78.98° 76.23° 76.33°	Depositor
Resolution (Å)	50.00 – 2.20 49.10 – 2.20	Depositor EDS
% Data completeness (in resolution range)	90.8 (50.00-2.20) 86.9 (49.10-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.62 (at 2.20Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.177 , 0.272 0.182 , 0.182	Depositor DCC
R_{free} test set	15293 reflections (11.13%)	DCC
Wilson B-factor (Å ²)	19.3	Xtriage
Anisotropy	0.172	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 68.8	EDS
Estimated twinning fraction	0.289 for -h,-l,-k	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 152769 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	25205	wwPDB-VP
Average B, all atoms (Å ²)	43.0	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 35.91 % 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 5.4201e-04. 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: AKG, IT1

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	0.73	0/3134	1.10	7/4230 (0.2%)
1	B	0.74	0/3147	1.09	6/4249 (0.1%)
1	C	0.72	0/3171	1.08	7/4281 (0.2%)
1	D	0.74	0/3113	1.09	6/4201 (0.1%)
1	E	0.70	0/3124	1.06	7/4219 (0.2%)
1	F	0.70	0/3155	1.07	6/4260 (0.1%)
1	G	0.70	1/3163 (0.0%)	1.07	6/4271 (0.1%)
1	H	0.68	0/3113	1.07	6/4201 (0.1%)
All	All	0.71	1/25120 (0.0%)	1.08	51/33912 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	231	LYS	CB-CG	6.07	1.69	1.52

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	213	ARG	NE-CZ-NH1	10.96	125.78	120.30
1	G	339	LEU	CA-CB-CG	-7.37	98.35	115.30
1	C	323	LEU	CA-CB-CG	-7.13	98.90	115.30
1	A	213	ARG	NE-CZ-NH2	-7.09	116.75	120.30
1	E	381	ASP	CB-CG-OD1	-7.00	112.00	118.30

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	3092	0	3062	171	0
1	B	3104	0	3070	201	0
1	C	3128	0	3099	196	0
1	D	3072	0	3038	141	0
1	E	3082	0	3050	185	0
1	F	3112	0	3076	252	0
1	G	3120	0	3088	256	0
1	H	3072	0	3039	205	0
2	A	10	0	4	1	0
2	B	10	0	4	5	0
2	C	10	0	4	1	0
2	D	10	0	4	2	0
2	F	10	0	4	3	0
2	H	10	0	4	0	0
3	A	42	0	0	4	0
3	B	52	0	0	4	0
3	C	50	0	0	4	0
3	D	55	0	0	7	0
3	E	37	0	0	4	0
3	F	43	0	0	4	0
3	G	41	0	0	6	0
3	H	43	0	0	6	0
All	All	25205	0	24546	1569	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 32.

The worst 5 of 1569 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:C:52:MET:SD	1:C:52:MET:CE	2.03	1.46
1:F:188:IT1:H4A	2:F:405:AKG:O5	1.36	1.25
1:B:124:THR:HG22	1:B:125:ASP:H	1.11	1.15
1:C:152:ARG:HH21	1:C:152:ARG:CG	1.59	1.12
1:F:222:PRO:HG2	1:F:225:ASN:HB3	1.26	1.09

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	382/390 (98%)	352 (92%)	25 (6%)	5 (1%)	15	11
1	B	383/390 (98%)	342 (89%)	35 (9%)	6 (2%)	12	8
1	C	386/390 (99%)	336 (87%)	43 (11%)	7 (2%)	11	7
1	D	379/390 (97%)	354 (93%)	22 (6%)	3 (1%)	24	22
1	E	381/390 (98%)	337 (88%)	37 (10%)	7 (2%)	11	7
1	F	384/390 (98%)	338 (88%)	41 (11%)	5 (1%)	15	11
1	G	385/390 (99%)	339 (88%)	40 (10%)	6 (2%)	12	8
1	H	379/390 (97%)	327 (86%)	46 (12%)	6 (2%)	12	8
All	All	3059/3120 (98%)	2725 (89%)	289 (9%)	45 (2%)	13	9

5 of 45 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	312	SER
1	C	152	ARG
1	G	354	ASN
1	A	311	ASP
1	B	150	GLY

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	340/344 (99%)	287 (84%)	53 (16%)	3	2
1	B	341/344 (99%)	284 (83%)	57 (17%)	3	2
1	C	344/344 (100%)	291 (85%)	53 (15%)	3	2
1	D	338/344 (98%)	293 (87%)	45 (13%)	5	4
1	E	339/344 (98%)	292 (86%)	47 (14%)	4	3
1	F	342/344 (99%)	285 (83%)	57 (17%)	3	2
1	G	343/344 (100%)	282 (82%)	61 (18%)	2	1
1	H	338/344 (98%)	269 (80%)	69 (20%)	1	1
All	All	2725/2752 (99%)	2283 (84%)	442 (16%)	3	2

5 of 442 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	355	ASN
1	E	360	GLU
1	H	235	GLN
1	D	378	ASP
1	E	170	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	97	GLN
1	F	170	ASN
1	H	322	ASN
1	F	3	ASN
1	F	207	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 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
1	IT1	A	188	1	23,24,25	1.52	4 (17%)	28,32,34	1.43	5 (17%)
1	IT1	B	188	1	23,24,25	1.09	2 (8%)	28,32,34	1.22	4 (14%)
1	IT1	C	188	1	23,24,25	1.11	1 (4%)	28,32,34	1.04	1 (3%)
1	IT1	D	188	1	23,24,25	1.20	2 (8%)	28,32,34	1.08	2 (7%)
1	IT1	E	188	1	23,24,25	1.31	3 (13%)	28,32,34	1.13	0
1	IT1	F	188	1	23,24,25	1.11	1 (4%)	28,32,34	1.14	1 (3%)
1	IT1	G	188	1	23,24,25	1.18	2 (8%)	28,32,34	1.02	1 (3%)
1	IT1	H	188	1	23,24,25	1.41	4 (17%)	28,32,34	1.00	1 (3%)

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
1	IT1	A	188	1	-	0/15/17/19	0/1/1/1
1	IT1	B	188	1	-	0/15/17/19	0/1/1/1
1	IT1	C	188	1	-	0/15/17/19	0/1/1/1
1	IT1	D	188	1	-	0/15/17/19	0/1/1/1
1	IT1	E	188	1	-	0/15/17/19	0/1/1/1
1	IT1	F	188	1	-	0/15/17/19	0/1/1/1
1	IT1	G	188	1	-	0/15/17/19	0/1/1/1
1	IT1	H	188	1	-	0/15/17/19	0/1/1/1

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	188	IT1	C3-C2	-3.50	1.38	1.40
1	F	188	IT1	C3-C2	-2.98	1.38	1.40
1	H	188	IT1	C3-C2	-2.28	1.39	1.40
1	A	188	IT1	P-OP3	2.10	1.62	1.54
1	E	188	IT1	P-OP2	2.31	1.63	1.54

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	188	IT1	OP4-C5A-C5	-3.12	103.84	108.99
1	G	188	IT1	CD-CE-NZ	-2.90	106.22	110.98
1	B	188	IT1	CD-CE-NZ	-2.82	106.35	110.98
1	A	188	IT1	CD-CE-NZ	-2.76	106.45	110.98
1	C	188	IT1	OP4-C5A-C5	-2.51	104.85	108.99

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	188	IT1	4	0
1	B	188	IT1	6	0
1	C	188	IT1	5	0
1	D	188	IT1	1	0
1	E	188	IT1	1	0
1	F	188	IT1	9	0
1	G	188	IT1	3	0
1	H	188	IT1	3	0

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	$\# Z > 2$
2	AKG	A	401	-	3,9,9	0.35	0	4,11,11	1.08	0
2	AKG	B	402	-	3,9,9	1.08	0	4,11,11	1.98	2 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	AKG	C	403	-	3,9,9	0.44	0	4,11,11	1.17	0
2	AKG	D	404	-	3,9,9	0.32	0	4,11,11	2.13	1 (25%)
2	AKG	F	405	-	3,9,9	0.25	0	4,11,11	1.54	1 (25%)
2	AKG	H	406	-	3,9,9	1.00	0	4,11,11	2.59	3 (75%)

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	AKG	A	401	-	-	0/3/9/9	0/0/0/0
2	AKG	B	402	-	-	0/3/9/9	0/0/0/0
2	AKG	C	403	-	-	0/3/9/9	0/0/0/0
2	AKG	D	404	-	-	0/3/9/9	0/0/0/0
2	AKG	F	405	-	-	0/3/9/9	0/0/0/0
2	AKG	H	406	-	-	0/3/9/9	0/0/0/0

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	404	AKG	C3-C4-C5	-3.57	106.20	112.75
2	H	406	AKG	C4-C3-C2	-3.34	104.53	112.98
2	H	406	AKG	C3-C4-C5	-3.29	106.72	112.75
2	B	402	AKG	C3-C4-C5	-3.00	107.24	112.75
2	F	405	AKG	C4-C3-C2	-2.82	105.86	112.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	AKG	1	0
2	B	402	AKG	5	0
2	C	403	AKG	1	0
2	D	404	AKG	2	0
2	F	405	AKG	3	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 [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	383/390 (98%)	-1.57	0 100 100	11, 37, 67, 96	0
1	B	384/390 (98%)	-1.57	0 100 100	14, 36, 70, 88	0
1	C	387/390 (99%)	-1.56	0 100 100	10, 38, 73, 89	0
1	D	380/390 (97%)	-1.58	0 100 100	11, 37, 66, 94	0
1	E	382/390 (97%)	-1.54	0 100 100	13, 42, 72, 94	0
1	F	385/390 (98%)	-1.55	0 100 100	13, 40, 73, 92	0
1	G	386/390 (98%)	-1.53	0 100 100	15, 45, 74, 98	0
1	H	380/390 (97%)	-1.52	0 100 100	14, 45, 77, 100	0
All	All	3067/3120 (98%)	-1.55	0 100 100	10, 40, 73, 100	0

There are no RSRZ outliers to report.

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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
1	IT1	D	188	24/25	1.00	0.05	-	14,36,61,69	0
1	IT1	E	188	24/25	1.00	0.05	-	5,40,99,99	0
1	IT1	F	188	24/25	0.99	0.06	-	32,59,99,99	0
1	IT1	G	188	24/25	1.00	0.05	-	13,26,57,66	0
1	IT1	A	188	24/25	1.00	0.05	-	7,34,55,78	0
1	IT1	B	188	24/25	1.00	0.05	-	11,28,86,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
1	IT1	C	188	24/25	1.00	0.05	-	10,26,55,83	0
1	IT1	H	188	24/25	1.00	0.05	-	13,39,98,99	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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
2	AKG	A	401	10/10	0.99	0.07	5.98	34,66,99,99	0
2	AKG	F	405	10/10	0.99	0.06	2.95	43,62,99,99	0
2	AKG	B	402	10/10	0.99	0.05	0.61	16,32,70,79	0
2	AKG	D	404	10/10	0.99	0.05	0.40	23,42,99,99	0
2	AKG	C	403	10/10	0.99	0.04	-1.26	16,32,99,99	0
2	AKG	H	406	10/10	0.99	0.04	-1.60	15,37,99,99	0

6.5 Other polymers [i](#)

There are no such residues in this entry.