



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 01:53 AM UTC

PDB ID : 3GR9 / pdb_00003gr9
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

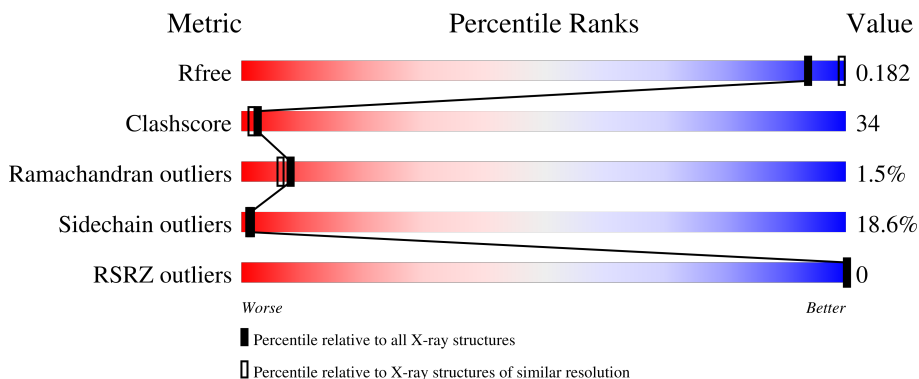
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


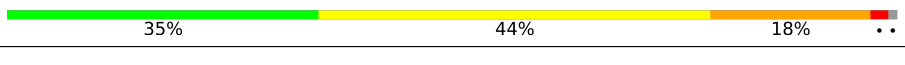
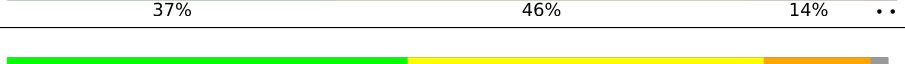
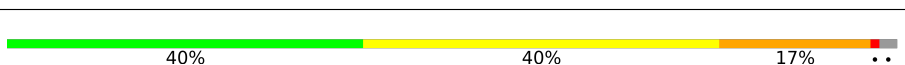

The reported resolution of this entry is 2.20 Å.

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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	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	34%	48%	15% ..
1	G	390	31%	47%	20% ..
1	H	390	36%	45%	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
2	AKG	B	402	-	-	X	-

2 Entry composition [i](#)

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

There are 32 discrepancies between the modelled and reference sequences:

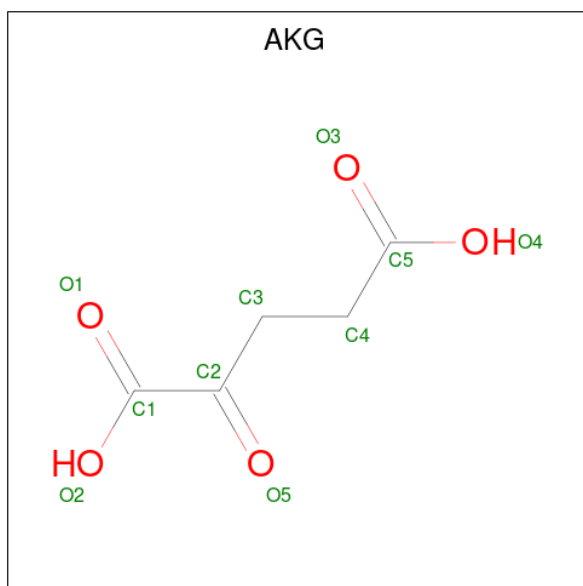
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q9F118
A	0	HIS	-	expression tag	UNP Q9F118
A	187	ASN	SER	engineered mutation	UNP Q9F118
A	188	LLP	HIS	engineered mutation	UNP Q9F118
B	-1	GLY	-	expression tag	UNP Q9F118
B	0	HIS	-	expression tag	UNP Q9F118
B	187	ASN	SER	engineered mutation	UNP Q9F118
B	188	LLP	HIS	engineered mutation	UNP Q9F118
C	-1	GLY	-	expression tag	UNP Q9F118
C	0	HIS	-	expression tag	UNP Q9F118
C	187	ASN	SER	engineered mutation	UNP Q9F118
C	188	LLP	HIS	engineered mutation	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 mutation	UNP Q9F118
D	188	LLP	HIS	engineered mutation	UNP Q9F118
E	-1	GLY	-	expression tag	UNP Q9F118
E	0	HIS	-	expression tag	UNP Q9F118
E	187	ASN	SER	engineered mutation	UNP Q9F118
E	188	LLP	HIS	engineered mutation	UNP Q9F118
F	-1	GLY	-	expression tag	UNP Q9F118
F	0	HIS	-	expression tag	UNP Q9F118
F	187	ASN	SER	engineered mutation	UNP Q9F118
F	188	LLP	HIS	engineered mutation	UNP Q9F118
G	-1	GLY	-	expression tag	UNP Q9F118
G	0	HIS	-	expression tag	UNP Q9F118
G	187	ASN	SER	engineered mutation	UNP Q9F118
G	188	LLP	HIS	engineered mutation	UNP Q9F118
H	-1	GLY	-	expression tag	UNP Q9F118
H	0	HIS	-	expression tag	UNP Q9F118
H	187	ASN	SER	engineered mutation	UNP Q9F118
H	188	LLP	HIS	engineered mutation	UNP Q9F118

- Molecule 2 is 2-OXOGLUTARIC ACID (CCD ID: 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.

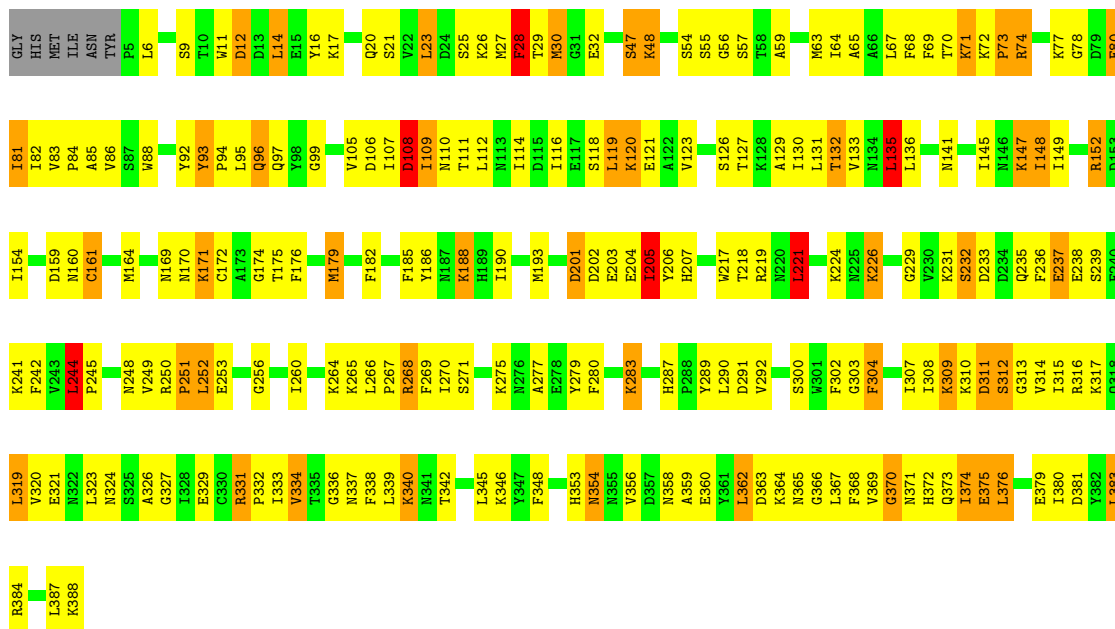
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	42	Total	O	0	0
			42	42		
3	B	52	Total	O	0	0
			52	52		
3	C	50	Total	O	0	0
			50	50		
3	D	55	Total	O	0	0
			55	55		
3	E	37	Total	O	0	0
			37	37		
3	F	43	Total	O	0	0
			43	43		
3	G	41	Total	O	0	0
			41	41		
3	H	43	Total	O	0	0
			43	43		

3 Residue-property plots

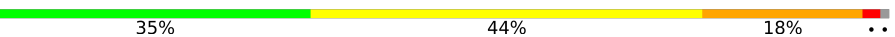
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

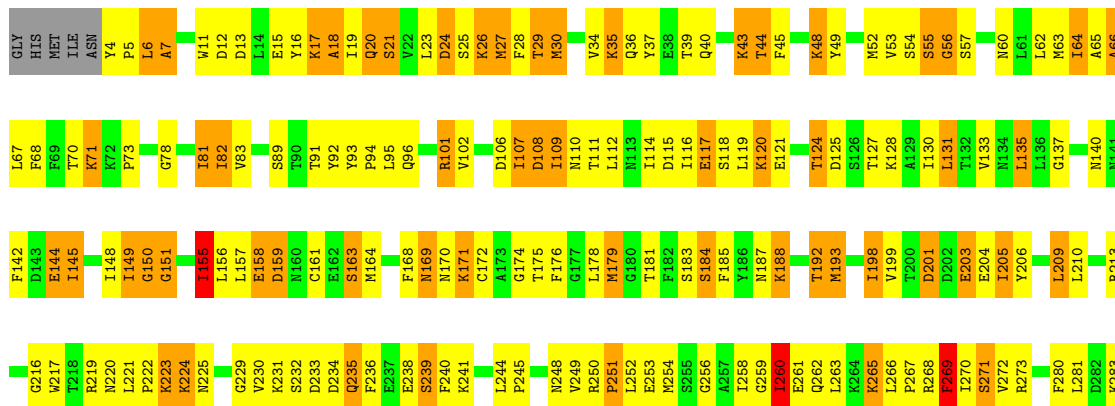
- Molecule 1: Cold

Chain A: 

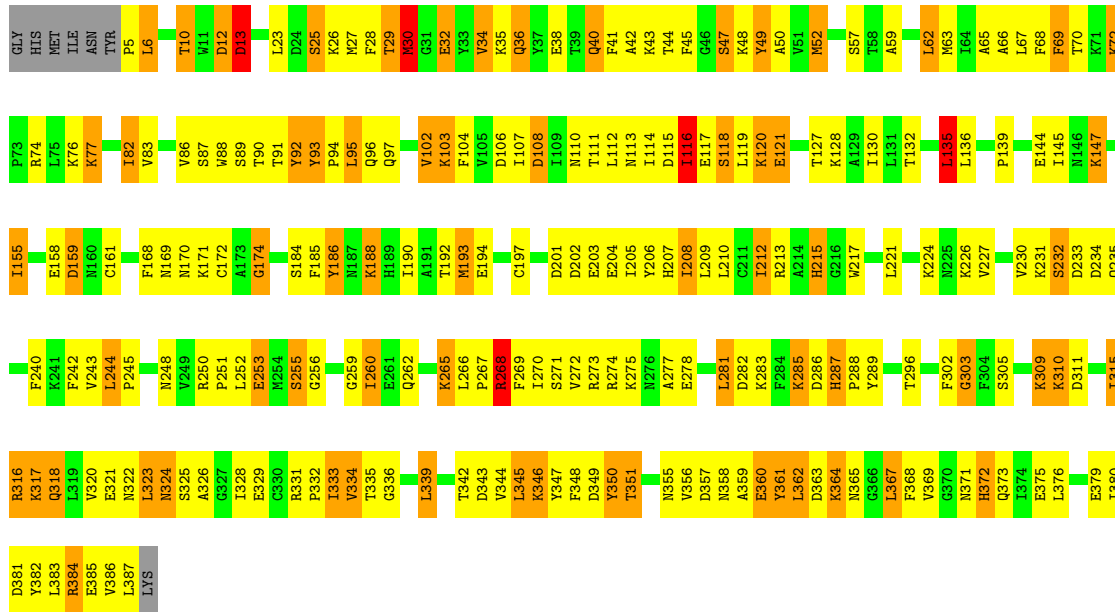


- Molecule 1: Cold

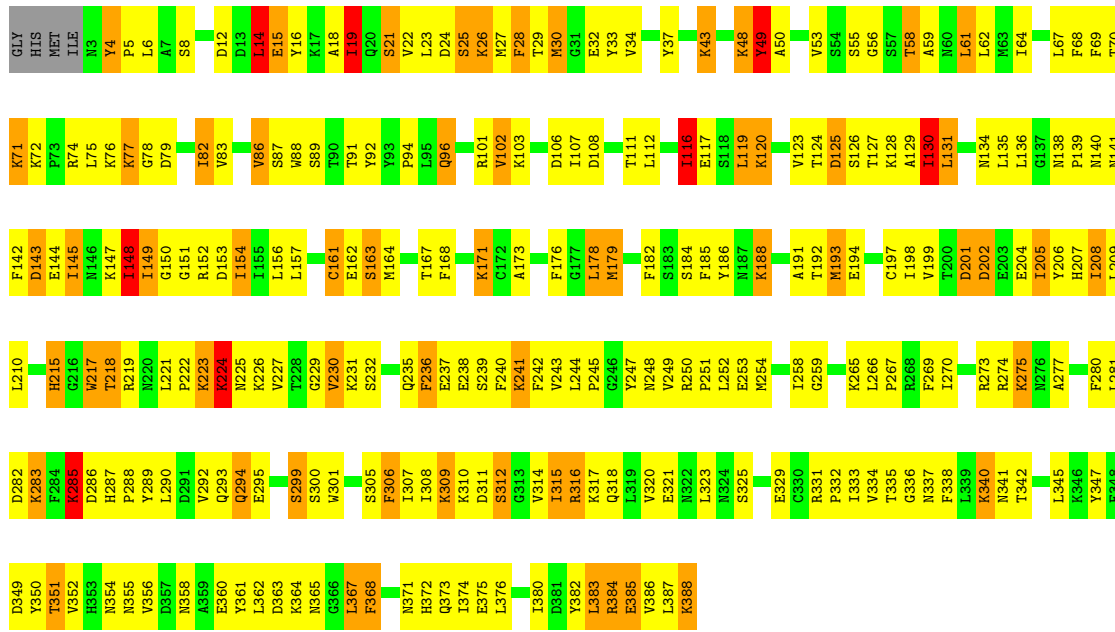
Chain B: 



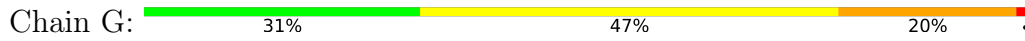
● Molecule 1: Cold



● Molecule 1: Cold



● Molecule 1: Cold



4 Data and refinement statistics i

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 50.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	90.8 (50.00-2.20) 90.7 (50.00-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.62 (at 2.20Å)	Xtrriage
Refinement program	TNT	Depositor
R, R_{free}	0.177 , 0.272 0.182 , 0.182	Depositor DCC
R_{free} test set	15300 reflections (10.02%)	wwPDB-VP
Wilson B-factor (Å ²)	19.3	Xtrriage
Anisotropy	0.172	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 54.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	0.289 for -h,-l,-k	Xtrriage
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

Xtrriage'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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: AKG, LLP

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	0.90	2/3134 (0.1%)	1.48	39/4230 (0.9%)
1	B	0.90	1/3147 (0.0%)	1.49	49/4249 (1.2%)
1	C	0.90	3/3171 (0.1%)	1.49	54/4281 (1.3%)
1	D	0.92	2/3113 (0.1%)	1.50	43/4201 (1.0%)
1	E	0.86	3/3124 (0.1%)	1.46	41/4219 (1.0%)
1	F	0.86	2/3155 (0.1%)	1.46	48/4260 (1.1%)
1	G	0.86	2/3163 (0.1%)	1.46	48/4271 (1.1%)
1	H	0.83	2/3113 (0.1%)	1.50	44/4201 (1.0%)
All	All	0.88	17/25120 (0.1%)	1.48	366/33912 (1.1%)

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	52	MET	SD-CE	9.59	2.03	1.79
1	F	164	MET	SD-CE	7.42	1.98	1.79
1	D	179	MET	SD-CE	6.99	1.97	1.79
1	A	164	MET	SD-CE	6.68	1.96	1.79
1	E	52	MET	SD-CE	6.63	1.96	1.79

The worst 5 of 366 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	25	SER	N-CA-C	-12.39	99.14	114.75
1	E	227	VAL	N-CA-C	11.34	121.99	111.45
1	B	178	LEU	N-CA-C	-11.12	98.98	112.54
1	G	13	ASP	N-CA-C	-10.95	100.66	114.56
1	B	249	VAL	N-CA-C	10.80	121.52	111.91

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	3063	178	0
1	B	3104	0	3070	217	0
1	C	3128	0	3099	203	0
1	D	3072	0	3039	149	0
1	E	3082	0	3050	198	0
1	F	3112	0	3076	260	0
1	G	3120	0	3088	269	0
1	H	3072	0	3039	224	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	24548	1660	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 34.

The worst 5 of 1660 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:LLP:H4'1	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:CG	1:C:152:ARG:HH21	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%)	9 8
1	B	383/390 (98%)	342 (89%)	35 (9%)	6 (2%)	7 6
1	C	386/390 (99%)	336 (87%)	43 (11%)	7 (2%)	6 4
1	D	379/390 (97%)	354 (93%)	22 (6%)	3 (1%)	16 16
1	E	381/390 (98%)	337 (88%)	37 (10%)	7 (2%)	6 4
1	F	384/390 (98%)	338 (88%)	41 (11%)	5 (1%)	9 8
1	G	385/390 (99%)	339 (88%)	40 (10%)	6 (2%)	7 6
1	H	379/390 (97%)	327 (86%)	46 (12%)	6 (2%)	7 6
All	All	3059/3120 (98%)	2725 (89%)	289 (9%)	45 (2%)	8 6

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%)	284 (84%)	56 (16%)	2	2
1	B	341/344 (99%)	274 (80%)	67 (20%)	1	1
1	C	344/344 (100%)	284 (83%)	60 (17%)	2	2
1	D	338/344 (98%)	287 (85%)	51 (15%)	3	2
1	E	339/344 (98%)	273 (80%)	66 (20%)	1	1
1	F	342/344 (99%)	275 (80%)	67 (20%)	1	1
1	G	343/344 (100%)	273 (80%)	70 (20%)	1	1
1	H	338/344 (98%)	265 (78%)	73 (22%)	1	1
All	All	2725/2752 (99%)	2215 (81%)	510 (19%)	1	1

5 of 510 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	383	LEU
1	H	29	THR
1	E	342	THR
1	H	20	GLN
1	H	224	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	354	ASN
1	G	324	ASN
1	G	36	GLN
1	G	140	ASN
1	G	372	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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	LLP	F	188	1	23,24,25	1.03	2 (8%)	25,32,34	1.15	1 (4%)
1	LLP	E	188	1	23,24,25	1.35	4 (17%)	25,32,34	1.16	1 (4%)
1	LLP	A	188	1	23,24,25	1.50	5 (21%)	25,32,34	1.30	2 (8%)
1	LLP	B	188	1	23,24,25	1.13	2 (8%)	25,32,34	1.16	2 (8%)
1	LLP	C	188	1	23,24,25	1.13	1 (4%)	25,32,34	0.99	2 (8%)
1	LLP	G	188	1	23,24,25	1.29	2 (8%)	25,32,34	1.22	2 (8%)
1	LLP	H	188	1	23,24,25	1.45	4 (17%)	25,32,34	1.21	2 (8%)
1	LLP	D	188	1	23,24,25	1.28	2 (8%)	25,32,34	1.04	3 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LLP	F	188	1	-	8/16/17/19	0/1/1/1
1	LLP	E	188	1	-	3/16/17/19	0/1/1/1
1	LLP	A	188	1	-	9/16/17/19	0/1/1/1
1	LLP	B	188	1	-	5/16/17/19	0/1/1/1
1	LLP	C	188	1	-	9/16/17/19	0/1/1/1
1	LLP	G	188	1	-	6/16/17/19	0/1/1/1
1	LLP	H	188	1	-	5/16/17/19	0/1/1/1
1	LLP	D	188	1	-	5/16/17/19	0/1/1/1

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	188	LLP	P-OP1	4.52	1.64	1.50
1	D	188	LLP	P-OP1	4.47	1.64	1.50
1	G	188	LLP	P-OP1	4.44	1.64	1.50
1	A	188	LLP	P-OP1	4.39	1.64	1.50
1	E	188	LLP	P-OP1	4.08	1.63	1.50

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	188	LLP	C4-C3-C2	-4.00	117.89	120.14
1	H	188	LLP	C4-C3-C2	-3.96	117.91	120.14
1	B	188	LLP	OP2-P-OP4	3.09	114.72	106.67
1	A	188	LLP	OP4-C5'-C5	-2.94	103.84	109.36
1	F	188	LLP	C5-C6-N1	-2.51	119.74	123.83

There are no chirality outliers.

5 of 50 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	188	LLP	C5'-OP4-P-OP3
1	A	188	LLP	N-CA-CB-CG
1	A	188	LLP	O-C-CA-CB
1	B	188	LLP	N-CA-CB-CG
1	B	188	LLP	O-C-CA-CB

There are no ring outliers.

8 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	F	188	LLP	7	0
1	E	188	LLP	2	0
1	A	188	LLP	4	0
1	B	188	LLP	6	0
1	C	188	LLP	4	0
1	G	188	LLP	4	0
1	H	188	LLP	3	0
1	D	188	LLP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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
2	AKG	C	403	-	9,9,9	1.73	2 (22%)	11,11,11	1.85	5 (45%)
2	AKG	A	401	-	9,9,9	1.97	2 (22%)	11,11,11	1.55	3 (27%)
2	AKG	H	406	-	9,9,9	1.96	2 (22%)	11,11,11	2.37	5 (45%)
2	AKG	B	402	-	9,9,9	2.06	2 (22%)	11,11,11	1.62	3 (27%)
2	AKG	D	404	-	9,9,9	1.49	1 (11%)	11,11,11	1.58	1 (9%)
2	AKG	F	405	-	9,9,9	2.40	3 (33%)	11,11,11	1.66	2 (18%)

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	C	403	-	-	4/9/9/9	-
2	AKG	A	401	-	-	4/9/9/9	-
2	AKG	H	406	-	-	0/9/9/9	-
2	AKG	B	402	-	-	3/9/9/9	-
2	AKG	D	404	-	-	4/9/9/9	-
2	AKG	F	405	-	-	2/9/9/9	-

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	405	AKG	C2-C1	-5.97	1.44	1.53
2	B	402	AKG	C2-C1	-4.50	1.46	1.53
2	H	406	AKG	O3-C5	4.32	1.36	1.22
2	A	401	AKG	O3-C5	4.27	1.36	1.22
2	C	403	AKG	O3-C5	3.62	1.33	1.22

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	406	AKG	C4-C3-C2	-4.46	104.53	112.91
2	H	406	AKG	C3-C2-C1	3.96	122.58	115.86
2	F	405	AKG	C4-C3-C2	-3.75	105.86	112.91
2	B	402	AKG	C4-C3-C2	-3.19	106.92	112.91
2	D	404	AKG	C3-C4-C5	-2.81	106.20	113.67

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	AKG	C1-C2-C3-C4
2	B	402	AKG	O2-C1-C2-C3
2	C	403	AKG	O2-C1-C2-C3
2	D	404	AKG	C1-C2-C3-C4
2	A	401	AKG	O5-C2-C3-C4

There are no ring outliers.

5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	403	AKG	1	0
2	A	401	AKG	1	0
2	B	402	AKG	5	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%)	-1.98	0 100 100	11, 37, 67, 96	1 (0%)
1	B	384/390 (98%)	-1.98	0 100 100	14, 36, 70, 88	1 (0%)
1	C	387/390 (99%)	-1.98	0 100 100	10, 38, 73, 89	1 (0%)
1	D	380/390 (97%)	-1.98	0 100 100	11, 37, 66, 94	1 (0%)
1	E	382/390 (97%)	-1.97	0 100 100	13, 42, 72, 94	1 (0%)
1	F	385/390 (98%)	-1.97	0 100 100	13, 40, 73, 92	1 (0%)
1	G	386/390 (98%)	-1.96	0 100 100	15, 45, 74, 98	1 (0%)
1	H	380/390 (97%)	-1.96	0 100 100	14, 45, 77, 100	1 (0%)
All	All	3067/3120 (98%)	-1.97	0 100 100	10, 40, 73, 100	8 (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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	LLP	A	188	24/25	1.00	0.01	7,34,55,78	0
1	LLP	B	188	24/25	1.00	0.01	11,28,86,99	0
1	LLP	C	188	24/25	1.00	0.01	10,26,55,83	0
1	LLP	D	188	24/25	1.00	0.01	14,36,61,69	0
1	LLP	E	188	24/25	1.00	0.01	5,40,99,99	0
1	LLP	F	188	24/25	1.00	0.02	32,59,99,99	0
1	LLP	G	188	24/25	1.00	0.01	13,26,57,66	0
1	LLP	H	188	24/25	1.00	0.01	13,39,98,99	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	AKG	A	401	10/10	1.00	0.01	34,66,99,99	0
2	AKG	B	402	10/10	1.00	0.01	16,32,70,79	0
2	AKG	C	403	10/10	1.00	0.01	16,32,99,99	0
2	AKG	D	404	10/10	1.00	0.01	23,42,99,99	0
2	AKG	F	405	10/10	1.00	0.01	43,62,99,99	0
2	AKG	H	406	10/10	1.00	0.01	15,37,99,99	0

6.5 Other polymers [i](#)

There are no such residues in this entry.