



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:31 PM GMT

PDB ID : 3ZO7
Title : Crystal structure of ClcFE27A with substrate
Authors : Roth, C.; Groening, J.A.D.; Kaschabek, S.R.; Schloemann, M.; Straeter, N.
Deposited on : 2013-02-20
Resolution : 2.22 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

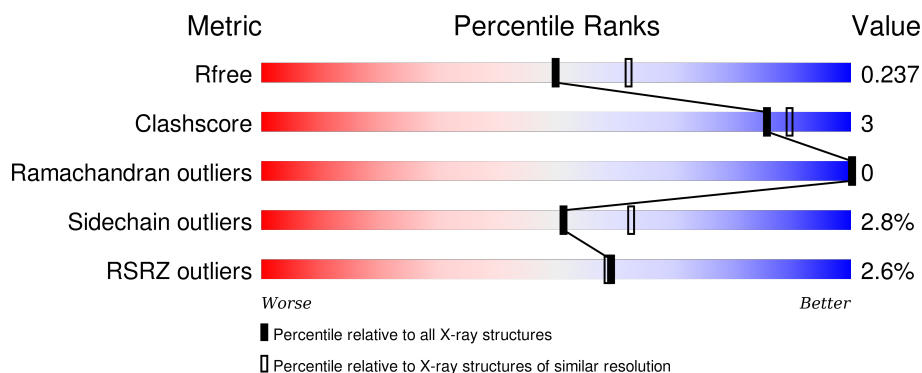
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.22 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	4405 (2.24-2.20)
Clashscore	102246	5146 (2.24-2.20)
Ramachandran outliers	100387	5065 (2.24-2.20)
Sidechain outliers	100360	5066 (2.24-2.20)
RSRZ outliers	91569	4414 (2.24-2.20)

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	94	<div> <div>87%</div> <div>10% ..</div> </div>
1	B	94	<div> <div>89%</div> <div>11%</div> </div>
1	C	94	<div> <div>88%</div> <div>12%</div> </div>
1	D	94	<div> <div>3%</div> <div>91%</div> <div>5% .</div> </div>
1	E	94	<div> <div>5%</div> <div>85%</div> <div>7% . 5%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	94	
1	G	94	
1	H	94	
1	I	94	
1	J	94	

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	K6H	A	1093	-	-	-	X
2	K6H	B	1095	-	-	-	X
2	K6H	C	1097	-	-	-	X
2	K6H	D	1092	-	-	-	X
2	K6H	E	1092	-	-	-	X
2	K6H	G	1095	-	-	-	X
2	K6H	H	1093	-	-	-	X
2	K6H	I	1094	-	-	-	X
2	K6H	J	1093	-	-	-	X
3	CL	E	1093	-	-	-	X

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 16157 atoms, of which 7764 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 5-CHLOROMUCONOLACTONE DEHALOGENASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	92	Total	C	H	N	O	S	0	1	0
			1544	495	769	140	138	2			
1	B	94	Total	C	H	N	O	S	0	1	0
			1579	505	786	143	143	2			
1	C	94	Total	C	H	N	O	S	0	1	0
			1579	505	786	143	143	2			
1	D	91	Total	C	H	N	O	S	0	1	0
			1537	493	766	139	137	2			
1	E	89	Total	C	H	N	O	S	0	1	0
			1498	482	745	134	135	2			
1	F	91	Total	C	H	N	O	S	0	1	0
			1544	495	773	139	135	2			
1	G	94	Total	C	H	N	O	S	0	1	0
			1579	505	786	143	143	2			
1	H	92	Total	C	H	N	O	S	0	1	0
			1543	494	770	140	137	2			
1	I	92	Total	C	H	N	O	S	0	1	0
			1544	495	769	140	138	2			
1	J	92	Total	C	H	N	O	S	0	2	0
			1552	497	774	140	139	2			

There are 10 discrepancies between the modelled and reference sequences:

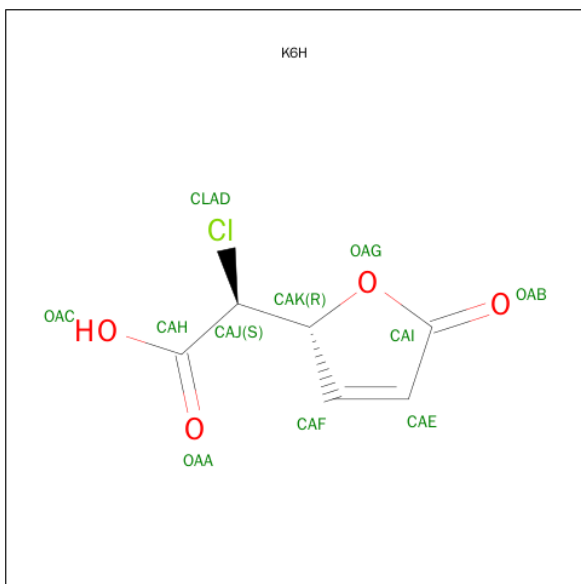
Chain	Residue	Modelled	Actual	Comment	Reference
A	27	ALA	GLU	ENGINEERED MUTATION	UNP Q8G9L0
B	27	ALA	GLU	ENGINEERED MUTATION	UNP Q8G9L0
C	27	ALA	GLU	ENGINEERED MUTATION	UNP Q8G9L0
D	27	ALA	GLU	ENGINEERED MUTATION	UNP Q8G9L0
E	27	ALA	GLU	ENGINEERED MUTATION	UNP Q8G9L0
F	27	ALA	GLU	ENGINEERED MUTATION	UNP Q8G9L0
G	27	ALA	GLU	ENGINEERED MUTATION	UNP Q8G9L0
H	27	ALA	GLU	ENGINEERED MUTATION	UNP Q8G9L0
I	27	ALA	GLU	ENGINEERED MUTATION	UNP Q8G9L0

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Chain	Residue	Modelled	Actual	Comment	Reference
J	27	ALA	GLU	ENGINEERED MUTATION	UNP Q8G9L0

- Molecule 2 is (2S)-2-CHLORANYL-2-[(2R)-5-OXIDANYLIDENE-2H-FURAN-2-YL]ETHANOIC ACID (three-letter code: K6H) (formula: C₆H₅ClO₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	H	O	0	0
			15	6	1	4	4		
2	B	1	Total	C	Cl	H	O	0	0
			15	6	1	4	4		
2	C	1	Total	C	Cl	H	O	0	0
			15	6	1	4	4		
2	D	1	Total	C	Cl	H	O	0	0
			15	6	1	4	4		
2	E	1	Total	C	Cl	H	O	0	0
			15	6	1	4	4		
2	F	1	Total	C	Cl	H	O	0	0
			15	6	1	4	4		
2	G	1	Total	C	Cl	H	O	0	0
			15	6	1	4	4		
2	H	1	Total	C	Cl	H	O	0	0
			15	6	1	4	4		
2	I	1	Total	C	Cl	H	O	0	0
			15	6	1	4	4		
2	J	1	Total	C	Cl	H	O	0	0
			15	6	1	4	4		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total Cl 1 1	0	0
3	J	1	Total Cl 1 1	0	0
3	D	1	Total Cl 1 1	0	0
3	E	1	Total Cl 1 1	0	0
3	H	1	Total Cl 1 1	0	0
3	B	3	Total Cl 3 3	0	0
3	I	1	Total Cl 1 1	0	0
3	C	2	Total Cl 2 2	0	0
3	A	2	Total Cl 2 2	0	0
3	F	1	Total Cl 1 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	76	Total O 76 76	0	0
4	B	80	Total O 80 80	0	0
4	C	56	Total O 56 56	0	0
4	D	27	Total O 27 27	0	0
4	E	35	Total O 35 35	0	0
4	F	47	Total O 47 47	0	0
4	G	51	Total O 51 51	0	0
4	H	51	Total O 51 51	0	0
4	I	22	Total O 22 22	0	0

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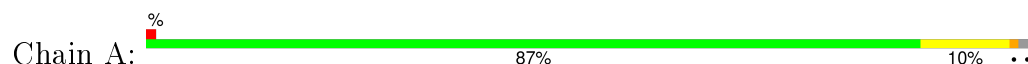
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	J	49	Total	O	0	0
			49	49		

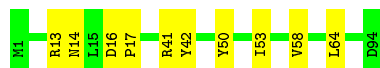
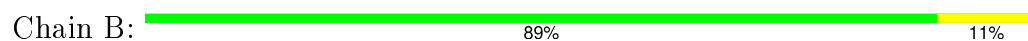
3 Residue-property plots [i](#)

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.

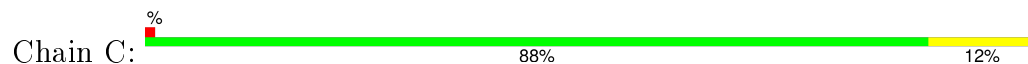
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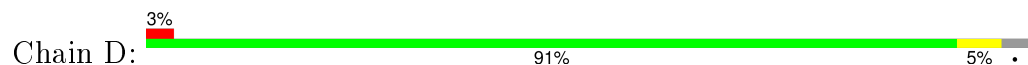
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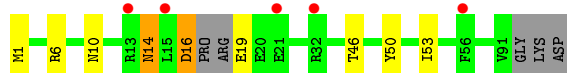
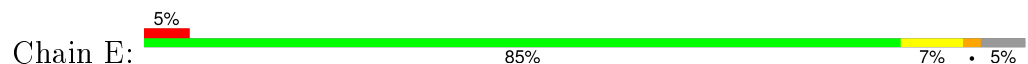
- Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE



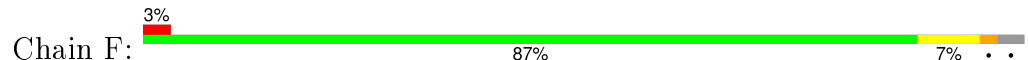
- Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE



- Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE

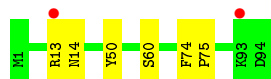


- Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE

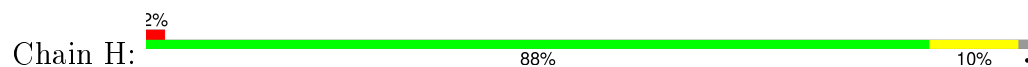




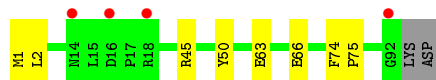
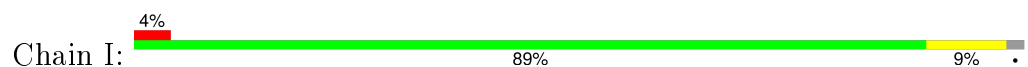
- Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE



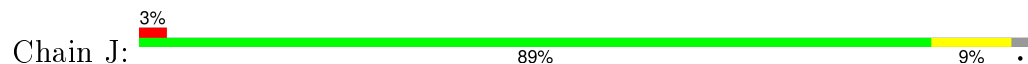
- Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE



- Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE



- Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	77.84Å 103.11Å 137.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.93 – 2.22 19.93 – 2.22	Depositor EDS
% Data completeness (in resolution range)	98.9 (19.93-2.22) 98.9 (19.93-2.22)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 2.23Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.186 , 0.232 0.186 , 0.237	Depositor DCC
R_{free} test set	1100 reflections (2.06%)	DCC
Wilson B-factor (Å ²)	34.7	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 41.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 54451 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16157	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 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: K6H, CL

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	0.22	0/800	0.42	0/1087
1	B	0.23	0/818	0.42	0/1109
1	C	0.23	0/818	0.42	0/1109
1	D	0.22	0/796	0.40	0/1082
1	E	0.22	0/776	0.40	0/1053
1	F	0.22	0/796	0.42	0/1082
1	G	0.22	0/818	0.40	0/1109
1	H	0.23	0/798	0.40	0/1084
1	I	0.22	0/800	0.39	0/1087
1	J	0.23	0/806	0.40	0/1095
All	All	0.22	0/8026	0.41	0/10897

There are no bond length outliers.

There are no bond angle outliers.

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	775	769	765	6	0
1	B	793	786	782	6	0
1	C	793	786	782	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	771	766	762	4	0
1	E	753	745	741	9	0
1	F	771	773	769	6	0
1	G	793	786	782	4	0
1	H	773	770	766	7	0
1	I	775	769	765	6	0
1	J	778	774	770	5	0
2	A	11	4	4	0	0
2	B	11	4	4	0	0
2	C	11	4	4	0	0
2	D	11	4	4	0	0
2	E	11	4	4	0	0
2	F	11	4	4	0	0
2	G	11	4	4	0	0
2	H	11	4	4	1	0
2	I	11	4	4	1	0
2	J	11	4	4	0	0
3	A	2	0	0	0	0
3	B	3	0	0	0	0
3	C	2	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
4	A	76	0	0	0	0
4	B	80	0	0	0	0
4	C	56	0	0	0	0
4	D	27	0	0	0	0
4	E	35	0	0	0	0
4	F	47	0	0	0	0
4	G	51	0	0	0	0
4	H	51	0	0	0	0
4	I	22	0	0	0	0
4	J	49	0	0	0	0
All	All	8393	7764	7724	43	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (43) 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:B:14:ASN:OD1	1:D:13:ARG:NH1	2.23	0.72
1:B:13:ARG:NH1	1:G:14:ASN:OD1	2.23	0.71
1:E:14:ASN:O	1:F:13:ARG:NH2	2.28	0.66
1:D:65:HIS:CE1	1:H:45:ARG:HD3	2.32	0.65
1:H:65:HIS:CE1	1:I:45:ARG:HD3	2.33	0.64
1:A:13:ARG:HD2	1:J:12:PRO:HG2	1.88	0.56
1:B:16:ASP:HB2	1:B:17:PRO:HD2	1.92	0.52
1:E:46:THR:CG2	1:E:53:ILE:CD1	2.89	0.51
1:E:16:ASP:HB2	1:E:19:GLU:HB3	1.93	0.51
1:I:45:ARG:NH2	2:I:1094:K6H:OAA	2.44	0.50
1:G:13:ARG:HB3	1:G:13:ARG:CZ	2.42	0.50
1:E:6:ARG:NH1	1:E:53:ILE:HD11	2.28	0.49
1:E:46:THR:HG22	1:E:53:ILE:HD13	1.95	0.48
1:E:1:MET:SD	1:I:1:MET:CE	3.01	0.48
1:E:1:MET:SD	1:I:1:MET:HE2	2.53	0.48
1:J:74:PHE:N	1:J:75:PRO:HD2	2.29	0.47
1:F:13:ARG:C	1:F:13:ARG:CD	2.82	0.47
1:F:1:MET:SD	1:H:60:SER:HA	2.56	0.46
1:E:16:ASP:N	1:E:16:ASP:OD1	2.49	0.46
1:F:74:PHE:N	1:F:75:PRO:CD	2.79	0.46
1:I:74:PHE:N	1:I:75:PRO:HD2	2.30	0.46
1:H:45:ARG:NH2	2:H:1093:K6H:OAA	2.50	0.45
1:C:1:MET:SD	1:G:60:SER:HA	2.57	0.45
1:A:6:ARG:CZ	1:A:53:ILE:HD11	2.47	0.45
1:F:6:ARG:NH1	1:F:53[B]:ILE:HD11	2.33	0.44
1:F:12:PRO:HD3	1:F:76:TYR:CD1	2.52	0.44
1:A:13:ARG:CD	1:J:12:PRO:HG2	2.48	0.44
1:I:63:GLU:O	1:I:66:GLU:HG3	2.19	0.43
1:B:41:ARG:HD3	1:B:42:TYR:CE2	2.53	0.43
1:J:27:ALA:HA	1:J:72:PRO:HG2	2.00	0.43
1:E:46:THR:HG22	1:E:53:ILE:CD1	2.49	0.42
1:C:74:PHE:N	1:C:75:PRO:CD	2.81	0.42
1:D:65:HIS:NE2	1:H:45:ARG:HD3	2.34	0.42
1:G:74:PHE:N	1:G:75:PRO:CD	2.83	0.42
1:D:6:ARG:CZ	1:D:53:ILE:HD11	2.50	0.42
1:C:12:PRO:HD3	1:C:76:TYR:CD1	2.55	0.41
1:H:53:ILE:HD12	1:J:84:LEU:CD2	2.50	0.41
1:H:74:PHE:N	1:H:75:PRO:HD2	2.36	0.41
1:A:16:ASP:HB2	1:A:17:PRO:HD2	2.02	0.41
1:A:74:PHE:N	1:A:75:PRO:HD2	2.35	0.40
1:B:58:VAL:HG21	1:B:64:LEU:HB2	2.04	0.40
1:A:41:ARG:HD3	1:A:42:TYR:CE2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:ILE:HG21	1:C:84:LEU:CD2	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	91/94 (97%)	91 (100%)	0	0	100	100
1	B	93/94 (99%)	93 (100%)	0	0	100	100
1	C	93/94 (99%)	93 (100%)	0	0	100	100
1	D	90/94 (96%)	90 (100%)	0	0	100	100
1	E	86/94 (92%)	85 (99%)	1 (1%)	0	100	100
1	F	90/94 (96%)	89 (99%)	1 (1%)	0	100	100
1	G	93/94 (99%)	91 (98%)	2 (2%)	0	100	100
1	H	91/94 (97%)	90 (99%)	1 (1%)	0	100	100
1	I	91/94 (97%)	90 (99%)	1 (1%)	0	100	100
1	J	92/94 (98%)	92 (100%)	0	0	100	100
All	All	910/940 (97%)	904 (99%)	6 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	85/86 (99%)	83 (98%)	2 (2%)	57	69
1	B	87/86 (101%)	86 (99%)	1 (1%)	80	89
1	C	87/86 (101%)	82 (94%)	5 (6%)	25	28
1	D	85/86 (99%)	84 (99%)	1 (1%)	78	88
1	E	83/86 (96%)	79 (95%)	4 (5%)	31	36
1	F	85/86 (99%)	82 (96%)	3 (4%)	43	52
1	G	87/86 (101%)	86 (99%)	1 (1%)	80	89
1	H	85/86 (99%)	82 (96%)	3 (4%)	43	52
1	I	85/86 (99%)	83 (98%)	2 (2%)	57	69
1	J	86/86 (100%)	84 (98%)	2 (2%)	58	70
All	All	855/860 (99%)	831 (97%)	24 (3%)	51	63

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	ARG
1	A	50	TYR
1	B	50	TYR
1	C	13	ARG
1	C	15	LEU
1	C	18	ARG
1	C	19	GLU
1	C	50	TYR
1	D	50	TYR
1	E	10	ASN
1	E	14	ASN
1	E	16	ASP
1	E	50	TYR
1	F	1	MET
1	F	13	ARG
1	F	50	TYR
1	G	50	TYR
1	H	1	MET
1	H	19	GLU
1	H	50	TYR
1	I	2	LEU
1	I	50	TYR
1	J	33	THR
1	J	50	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	37	GLN
1	E	39	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 24 ligands modelled in this entry, 14 are monoatomic - leaving 10 for Mogul analysis.

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	K6H	A	1093	-	8,11,11	1.82	1 (12%)	8,15,15	3.54	6 (75%)
2	K6H	B	1095	-	8,11,11	1.82	1 (12%)	8,15,15	3.48	6 (75%)
2	K6H	C	1097	-	8,11,11	1.85	1 (12%)	8,15,15	3.47	6 (75%)
2	K6H	D	1092	-	8,11,11	1.85	1 (12%)	8,15,15	3.51	6 (75%)
2	K6H	E	1092	-	8,11,11	1.86	1 (12%)	8,15,15	3.54	6 (75%)
2	K6H	F	1093	-	8,11,11	1.85	1 (12%)	8,15,15	3.55	6 (75%)
2	K6H	G	1095	-	8,11,11	1.83	1 (12%)	8,15,15	3.42	6 (75%)
2	K6H	H	1093	-	8,11,11	1.84	1 (12%)	8,15,15	3.42	6 (75%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	K6H	I	1094	-	8,11,11	1.84	1 (12%)	8,15,15	3.51	6 (75%)
2	K6H	J	1093	-	8,11,11	1.84	1 (12%)	8,15,15	3.55	6 (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	K6H	A	1093	-	-	0/4/17/17	0/1/1/1
2	K6H	B	1095	-	-	0/4/17/17	0/1/1/1
2	K6H	C	1097	-	-	0/4/17/17	0/1/1/1
2	K6H	D	1092	-	-	0/4/17/17	0/1/1/1
2	K6H	E	1092	-	-	0/4/17/17	0/1/1/1
2	K6H	F	1093	-	-	0/4/17/17	0/1/1/1
2	K6H	G	1095	-	-	0/4/17/17	0/1/1/1
2	K6H	H	1093	-	-	0/4/17/17	0/1/1/1
2	K6H	I	1094	-	-	0/4/17/17	0/1/1/1
2	K6H	J	1093	-	-	0/4/17/17	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1095	K6H	OAG-CAI	4.87	1.45	1.36
2	A	1093	K6H	OAG-CAI	4.88	1.45	1.36
2	G	1095	K6H	OAG-CAI	4.90	1.45	1.36
2	J	1093	K6H	OAG-CAI	4.92	1.46	1.36
2	H	1093	K6H	OAG-CAI	4.93	1.46	1.36
2	I	1094	K6H	OAG-CAI	4.93	1.46	1.36
2	D	1092	K6H	OAG-CAI	4.94	1.46	1.36
2	C	1097	K6H	OAG-CAI	4.95	1.46	1.36
2	F	1093	K6H	OAG-CAI	4.96	1.46	1.36
2	E	1092	K6H	OAG-CAI	5.00	1.46	1.36

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	1093	K6H	CAK-OAG-CAI	-8.24	105.38	109.30
2	A	1093	K6H	CAK-OAG-CAI	-8.23	105.39	109.30
2	F	1093	K6H	CAK-OAG-CAI	-8.21	105.40	109.30
2	E	1092	K6H	CAK-OAG-CAI	-8.21	105.40	109.30
2	D	1092	K6H	CAK-OAG-CAI	-8.15	105.42	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	1094	K6H	CAK-OAG-CAI	-8.12	105.44	109.30
2	B	1095	K6H	CAK-OAG-CAI	-8.04	105.48	109.30
2	C	1097	K6H	CAK-OAG-CAI	-8.00	105.50	109.30
2	G	1095	K6H	CAK-OAG-CAI	-7.93	105.53	109.30
2	H	1093	K6H	CAK-OAG-CAI	-7.89	105.55	109.30
2	F	1093	K6H	OAB-CAI-CAE	-2.73	125.69	130.99
2	I	1094	K6H	OAB-CAI-CAE	-2.72	125.71	130.99
2	E	1092	K6H	OAB-CAI-CAE	-2.71	125.73	130.99
2	H	1093	K6H	OAB-CAI-CAE	-2.71	125.74	130.99
2	B	1095	K6H	OAB-CAI-CAE	-2.70	125.75	130.99
2	C	1097	K6H	OAB-CAI-CAE	-2.69	125.76	130.99
2	J	1093	K6H	OAB-CAI-CAE	-2.69	125.77	130.99
2	D	1092	K6H	OAB-CAI-CAE	-2.69	125.77	130.99
2	G	1095	K6H	OAB-CAI-CAE	-2.62	125.91	130.99
2	A	1093	K6H	OAB-CAI-CAE	-2.62	125.91	130.99
2	F	1093	K6H	CAF-CAE-CAI	-2.39	107.31	108.72
2	J	1093	K6H	CAF-CAE-CAI	-2.35	107.33	108.72
2	A	1093	K6H	CAF-CAE-CAI	-2.33	107.34	108.72
2	D	1092	K6H	CAF-CAE-CAI	-2.33	107.34	108.72
2	B	1095	K6H	CAF-CAE-CAI	-2.33	107.34	108.72
2	C	1097	K6H	CAF-CAE-CAI	-2.29	107.36	108.72
2	I	1094	K6H	CAF-CAE-CAI	-2.28	107.37	108.72
2	G	1095	K6H	CAF-CAE-CAI	-2.24	107.39	108.72
2	E	1092	K6H	CAF-CAE-CAI	-2.21	107.41	108.72
2	H	1093	K6H	CAF-CAE-CAI	-2.12	107.46	108.72
2	G	1095	K6H	OAG-CAK-CAF	2.01	105.75	103.79
2	B	1095	K6H	OAG-CAK-CAF	2.01	105.75	103.79
2	C	1097	K6H	OAG-CAK-CAF	2.02	105.75	103.79
2	H	1093	K6H	OAG-CAK-CAF	2.03	105.77	103.79
2	F	1093	K6H	OAG-CAK-CAF	2.06	105.80	103.79
2	I	1094	K6H	OAG-CAK-CAF	2.08	105.82	103.79
2	E	1092	K6H	OAG-CAK-CAF	2.11	105.84	103.79
2	D	1092	K6H	OAG-CAK-CAF	2.11	105.85	103.79
2	J	1093	K6H	OAG-CAK-CAF	2.12	105.86	103.79
2	A	1093	K6H	OAG-CAK-CAF	2.20	105.93	103.79
2	A	1093	K6H	OAG-CAI-OAB	2.48	123.87	120.81
2	G	1095	K6H	OAG-CAI-OAB	2.57	123.98	120.81
2	H	1093	K6H	OAG-CAI-CAE	2.60	110.05	108.10
2	J	1093	K6H	OAG-CAI-OAB	2.61	124.03	120.81
2	D	1092	K6H	OAG-CAI-OAB	2.64	124.07	120.81
2	C	1097	K6H	OAG-CAI-CAE	2.67	110.10	108.10
2	B	1095	K6H	OAG-CAI-OAB	2.67	124.11	120.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1095	K6H	OAG-CAI-CAE	2.67	110.11	108.10
2	E	1092	K6H	OAG-CAI-OAB	2.68	124.12	120.81
2	F	1093	K6H	OAG-CAI-OAB	2.68	124.12	120.81
2	C	1097	K6H	OAG-CAI-OAB	2.69	124.13	120.81
2	I	1094	K6H	OAG-CAI-CAE	2.70	110.13	108.10
2	I	1094	K6H	OAG-CAI-OAB	2.71	124.16	120.81
2	B	1095	K6H	OAG-CAI-CAE	2.72	110.14	108.10
2	E	1092	K6H	OAG-CAI-CAE	2.74	110.16	108.10
2	D	1092	K6H	OAG-CAI-CAE	2.74	110.16	108.10
2	H	1093	K6H	OAG-CAI-OAB	2.75	124.21	120.81
2	F	1093	K6H	OAG-CAI-CAE	2.77	110.19	108.10
2	J	1093	K6H	OAG-CAI-CAE	2.81	110.21	108.10
2	A	1093	K6H	OAG-CAI-CAE	2.82	110.22	108.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	1093	K6H	1	0
2	I	1094	K6H	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	92/94 (97%)	-0.29	1 (1%) 82 82	22, 31, 48, 72	0
1	B	94/94 (100%)	-0.38	0 100 100	19, 29, 51, 75	0
1	C	94/94 (100%)	-0.29	1 (1%) 82 82	21, 30, 58, 81	0
1	D	91/94 (96%)	0.08	3 (3%) 50 49	23, 37, 77, 101	0
1	E	89/94 (94%)	0.16	5 (5%) 28 27	27, 41, 89, 105	0
1	F	91/94 (96%)	-0.13	3 (3%) 50 49	27, 38, 66, 103	0
1	G	94/94 (100%)	-0.25	2 (2%) 67 65	22, 34, 55, 97	0
1	H	92/94 (97%)	-0.04	2 (2%) 65 64	25, 36, 69, 93	0
1	I	92/94 (97%)	0.12	4 (4%) 39 38	28, 41, 81, 106	0
1	J	92/94 (97%)	-0.15	3 (3%) 50 49	26, 37, 57, 88	0
All	All	921/940 (97%)	-0.12	24 (2%) 59 59	19, 36, 71, 106	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	18	ARG	5.0
1	I	18	ARG	4.6
1	F	13	ARG	3.8
1	E	15	LEU	3.4
1	E	13	ARG	3.4
1	G	93	LYS	3.1
1	J	92	GLY	3.1
1	H	18	ARG	3.0
1	F	14	ASN	2.9
1	I	92	GLY	2.8
1	C	13	ARG	2.8
1	J	14	ASN	2.8
1	G	13	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	14	ASN	2.6
1	E	21	GLU	2.6
1	E	56	PHE	2.3
1	F	18	ARG	2.3
1	H	22	ARG	2.3
1	J	13	ARG	2.2
1	I	16	ASP	2.2
1	E	32	ARG	2.2
1	I	14	ASN	2.1
1	D	22	ARG	2.0
1	D	40	TRP	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
2	K6H	D	1092	11/11	0.86	0.29	5.07	47,49,59,60	15
2	K6H	C	1097	11/11	0.93	0.26	4.71	37,38,45,46	0
2	K6H	J	1093	11/11	0.96	0.27	4.32	37,39,46,47	0
2	K6H	H	1093	11/11	0.90	0.24	4.00	45,47,55,56	0
2	K6H	I	1094	11/11	0.90	0.24	3.66	45,47,56,57	15
2	K6H	A	1093	11/11	0.96	0.23	3.37	34,36,43,43	0
2	K6H	G	1095	11/11	0.95	0.24	3.22	39,40,48,48	0
3	CL	E	1093	1/1	0.96	0.25	2.47	48,48,48,48	0
2	K6H	B	1095	11/11	0.94	0.20	2.17	33,33,40,41	0
2	K6H	E	1092	11/11	0.92	0.21	2.02	39,42,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	CL	A	1094	1/1	0.99	0.16	1.58	27,27,27,27	0
3	CL	C	1095	1/1	1.00	0.14	1.00	33,33,33,33	0
3	CL	G	1096	1/1	0.99	0.14	0.85	29,29,29,29	0
2	K6H	F	1093	11/11	0.92	0.17	0.82	42,46,55,56	0
3	CL	H	1094	1/1	0.97	0.13	0.64	38,38,38,38	0
3	CL	D	1093	1/1	0.97	0.14	0.58	49,49,49,49	0
3	CL	F	1092	1/1	0.99	0.12	0.13	36,36,36,36	0
3	CL	I	1093	1/1	0.97	0.12	0.00	44,44,44,44	0
3	CL	B	1096	1/1	0.99	0.10	-0.06	27,27,27,27	0
3	CL	J	1094	1/1	0.98	0.11	-0.23	32,32,32,32	0
3	CL	C	1096	1/1	0.98	0.09	-0.82	41,41,41,41	0
3	CL	B	1097	1/1	0.99	0.04	-2.33	40,40,40,40	0
3	CL	A	1095	1/1	0.98	0.04	-	45,45,45,45	0
3	CL	B	1098	1/1	0.98	0.08	-	41,41,41,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.