



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 12:19 pm BST

PDB ID : 3EJ3
Title : Structural and mechanistic analysis of trans-3-chloroacrylic acid dehalogenase activity
Authors : Pegan, S.; Serrano, H.; Whitman, C.P.; Mesecar, A.D.
Deposited on : 2008-09-17
Resolution : 1.70 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

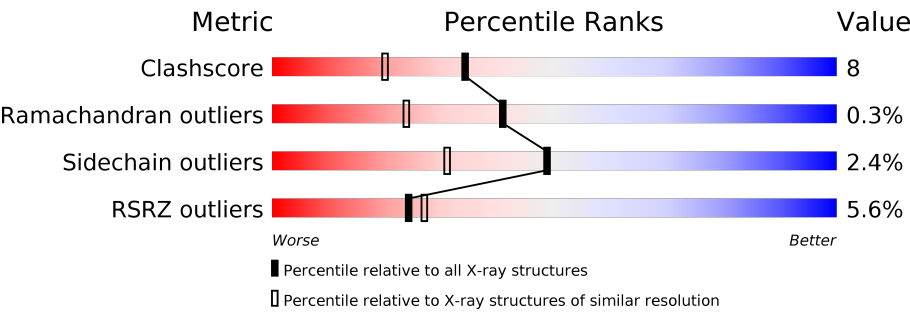
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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))
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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 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	76	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>68%13%18%</div></div>
1	C	76	<div><div>4%</div><div></div><div></div><div></div><div></div></div> <div>72%11%16%</div>
1	E	76	<div><div>4%</div><div></div><div></div><div></div><div></div></div> <div>70%12%18%</div>
1	G	76	<div><div>3%</div><div></div><div></div><div></div><div></div></div> <div>75%7%18%</div>
1	I	76	<div><div>4%</div><div></div><div></div><div></div><div></div></div> <div>70%13%16%</div>
1	K	76	<div><div>4%</div><div></div><div></div><div></div><div></div></div> <div>61%20%18%</div>
2	B	70	<div><div></div><div></div><div></div><div></div><div></div></div> <div>76%10%13%</div>

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Mol	Chain	Length	Quality of chain
2	D	70	<div><div></div><div>6%</div><div>69%</div><div>11%</div><div>19%</div></div>
2	F	70	<div><div></div><div>4%</div><div>74%</div><div>9%</div><div>17%</div></div>
2	H	70	<div><div></div><div>6%</div><div>69%</div><div>16%</div><div>16%</div></div>
2	J	70	<div><div></div><div>11%</div><div>59%</div><div>20%</div><div>17%</div></div>
2	L	70	<div><div></div><div>9%</div><div>74%</div><div>10%</div><div>14%</div></div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6413 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 Alpha-subunit of trans-3-chloroacrylic acid dehalogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	62	Total	C	N	O	S	0	2	0
			505	315	92	95	3			
1	C	64	Total	C	N	O	S	0	2	0
			521	326	92	100	3			
1	E	62	Total	C	N	O	S	0	2	0
			508	320	91	94	3			
1	G	62	Total	C	N	O	S	0	1	0
			499	312	91	93	3			
1	I	64	Total	C	N	O	S	0	2	0
			520	327	92	98	3			
1	K	62	Total	C	N	O	S	0	3	0
			513	325	91	94	3			

- Molecule 2 is a protein called Beta-subunit of trans-3-chloroacrylic acid dehalogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	61	Total	C	N	O	S	0	2	0
			470	294	85	89	2			
2	D	57	Total	C	N	O	S	0	2	0
			446	282	80	82	2			
2	F	58	Total	C	N	O	S	0	4	0
			466	294	84	86	2			
2	H	59	Total	C	N	O	S	0	1	0
			455	286	82	85	2			
2	J	58	Total	C	N	O	S	0	1	0
			447	280	81	84	2			
2	L	60	Total	C	N	O	S	0	2	0
			469	294	85	88	2			

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	E	1	Total	C	O	0	0
			4	2	2		
3	G	1	Total	C	O	0	0
			4	2	2		
3	I	1	Total	C	O	0	0
			4	2	2		
3	K	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	P	0	0
			5	4	1		
4	J	1	Total	O	P	0	0
			5	4	1		

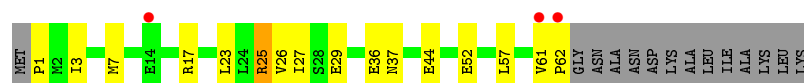
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	51	Total	O	0	0
			51	51		
5	B	48	Total	O	0	0
			48	48		
5	C	58	Total	O	0	0
			58	58		
5	D	37	Total	O	0	0
			37	37		
5	E	57	Total	O	0	0
			57	57		
5	F	42	Total	O	0	0
			42	42		
5	G	52	Total	O	0	0
			52	52		
5	H	41	Total	O	0	0
			41	41		
5	I	52	Total	O	0	0
			52	52		
5	J	30	Total	O	0	0
			30	30		

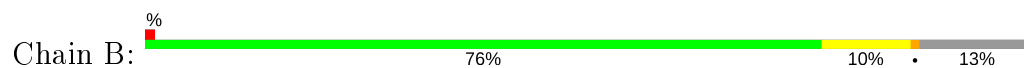
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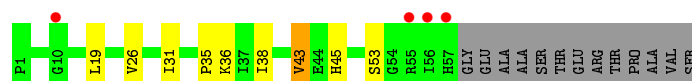
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	K	50	Total	O	0	0
			50	50		
5	L	42	Total	O	0	0
			42	42		



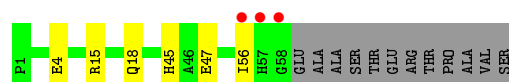
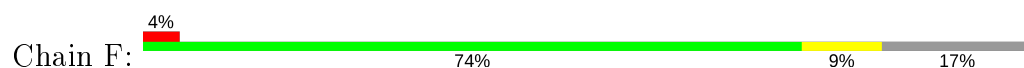
- Molecule 2: Beta-subunit of trans-3-chloroacrylic acid dehalogenase



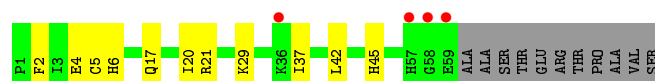
- Molecule 2: Beta-subunit of trans-3-chloroacrylic acid dehalogenase



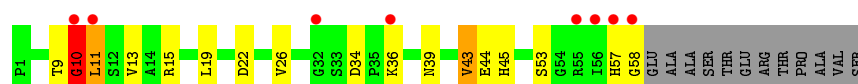
- Molecule 2: Beta-subunit of trans-3-chloroacrylic acid dehalogenase



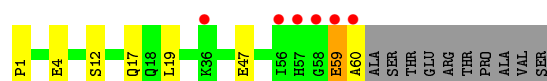
- Molecule 2: Beta-subunit of trans-3-chloroacrylic acid dehalogenase



- Molecule 2: Beta-subunit of trans-3-chloroacrylic acid dehalogenase



- Molecule 2: Beta-subunit of trans-3-chloroacrylic acid dehalogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	50.70Å 97.31Å 69.02Å 90.00° 96.12° 90.00°	Depositor
Resolution (Å)	68.68 – 1.70 28.57 – 1.70	Depositor EDS
% Data completeness (in resolution range)	96.9 (68.68-1.70) 96.8 (28.57-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.07 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.179 , 0.218 0.181 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	20.1	Xtriage
Anisotropy	0.543	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 49.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6413	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.18% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: PO4, ACT

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	0.62	0/518	0.69	0/696
1	C	0.60	0/535	0.75	0/720
1	E	0.69	0/525	0.94	2/706 (0.3%)
1	G	0.63	0/512	0.68	0/688
1	I	0.66	0/534	0.82	0/719
1	K	0.71	0/533	0.92	2/717 (0.3%)
2	B	0.59	0/481	0.70	0/649
2	D	0.58	0/457	0.69	0/617
2	F	0.57	0/477	0.66	0/643
2	H	0.60	0/463	0.71	0/624
2	J	0.50	0/455	0.81	1/613 (0.2%)
2	L	0.59	0/477	0.67	0/643
All	All	0.62	0/5967	0.76	5/8035 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1
1	K	0	1
2	J	0	1
All	All	0	3

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	25	ARG	NE-CZ-NH2	-9.28	115.66	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	10	GLY	N-CA-C	-7.79	93.63	113.10
1	K	25	ARG	NE-CZ-NH2	-7.22	116.69	120.30
1	E	25	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	K	25	ARG	NE-CZ-NH1	5.97	123.29	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	37	ASN	Peptide
2	J	10	GLY	Peptide
1	K	37	ASN	Peptide

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	505	0	496	11	0
1	C	521	0	502	13	0
1	E	508	0	501	6	0
1	G	499	0	492	4	0
1	I	520	0	507	12	1
1	K	513	0	512	7	0
2	B	470	0	492	8	0
2	D	446	0	476	9	0
2	F	466	0	494	6	0
2	H	455	0	478	20	0
2	J	447	0	467	12	0
2	L	469	0	490	10	0
3	A	4	0	3	0	0
3	C	4	0	3	0	0
3	E	4	0	3	1	0
3	G	4	0	3	0	0
3	I	4	0	3	1	0
3	K	4	0	3	0	0
4	B	5	0	0	0	0
4	J	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	51	0	0	2	0
5	B	48	0	0	2	0
5	C	58	0	0	5	0
5	D	37	0	0	0	0
5	E	57	0	0	1	1
5	F	42	0	0	1	0
5	G	52	0	0	0	0
5	H	41	0	0	5	0
5	I	52	0	0	1	0
5	J	30	0	0	4	0
5	K	50	0	0	1	0
5	L	42	0	0	2	0
All	All	6413	0	5925	99	1

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 8.

All (99) 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:A:22:GLY:HA3	2:D:26:VAL:HG21	1.28	1.11
1:C:29:GLU:HG2	5:C:115:HOH:O	1.56	1.04
2:H:20:ILE:HG12	2:H:42[B]:LEU:HD21	1.38	1.04
1:C:63:GLY:HA2	1:C:64:ASN:HB3	1.41	1.01
2:H:20:ILE:CG1	2:H:42[B]:LEU:HD21	1.91	1.00
2:J:10:GLY:HA2	5:J:328:HOH:O	1.63	0.99
2:H:29:LYS:HD2	5:H:112:HOH:O	1.61	0.97
1:C:63:GLY:HA2	1:C:64:ASN:CB	1.94	0.96
2:H:20:ILE:HD11	2:H:42[B]:LEU:HD23	1.50	0.94
1:C:29:GLU:CG	5:C:115:HOH:O	2.13	0.90
1:A:22:GLY:HA3	2:D:26:VAL:CG2	2.08	0.84
1:A:22:GLY:CA	2:D:26:VAL:HG21	2.08	0.83
2:H:17:GLN:CD	5:H:108:HOH:O	2.23	0.76
2:H:20:ILE:CG1	2:H:42[B]:LEU:CD2	2.64	0.74
2:J:11:LEU:HB2	5:J:328:HOH:O	1.89	0.70
1:I:64:ASN:C	1:I:64:ASN:HD22	1.95	0.69
2:J:22:ASP:OD1	5:J:185:HOH:O	2.10	0.69
1:C:63:GLY:CA	1:C:64:ASN:CB	2.70	0.68
2:J:9:THR:HG22	2:J:44:GLU:HB3	1.76	0.68
2:F:4:GLU:OE1	5:F:101:HOH:O	2.12	0.67
2:L:4:GLU:OE2	5:L:123:HOH:O	2.12	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:63:GLY:HA3	1:I:64:ASN:HB3	1.75	0.67
2:H:20:ILE:HG12	2:H:42[B]:LEU:CD2	2.19	0.67
1:A:52:GLU:OE2	5:A:92:HOH:O	2.15	0.65
1:I:63:GLY:H	1:I:64:ASN:CG	2.01	0.64
1:C:25:ARG:O	1:C:29:GLU:HG3	1.97	0.63
2:J:34:ASP:OD2	2:J:36:LYS:HG2	2.00	0.62
3:I:76:ACT:H3	2:L:1:PRO:H3	1.65	0.61
2:H:20:ILE:CD1	2:H:42[B]:LEU:HD23	2.28	0.61
1:I:63:GLY:CA	1:I:64:ASN:HB3	2.30	0.61
1:K:3[A]:ILE:HD11	1:K:27:ILE:HG13	1.86	0.58
1:C:17:ARG:NE	5:C:126:HOH:O	1.92	0.57
1:K:17[B]:ARG:NH1	5:K:147:HOH:O	2.38	0.57
1:A:27:ILE:HD13	2:D:19:LEU:HD11	1.87	0.57
1:C:53:HIS:HE1	2:D:53:SER:OG	1.88	0.57
1:C:17:ARG:NH1	5:C:126:HOH:O	2.37	0.56
2:H:29:LYS:CD	5:H:112:HOH:O	2.34	0.56
2:H:37:ILE:HG22	1:K:52:GLU:HG2	1.88	0.56
2:H:20:ILE:HG13	2:H:42[B]:LEU:HD21	1.83	0.55
1:C:63:GLY:HA2	1:C:64:ASN:HB2	1.84	0.55
2:L:59:GLU:HA	2:L:59:GLU:OE2	2.05	0.55
2:B:9[A]:THR:OG1	2:L:12:SER:HB3	2.07	0.54
1:A:35:ARG:NH1	5:A:101:HOH:O	2.40	0.53
1:G:52:GLU:OE2	2:J:39:ASN:ND2	2.37	0.53
2:H:20:ILE:CD1	2:H:42[B]:LEU:CD2	2.87	0.53
2:B:6:HIS:HD2	2:B:45:HIS:NE2	2.08	0.52
2:L:17:GLN:NE2	5:L:126:HOH:O	2.44	0.51
2:H:6:HIS:HE1	5:J:249:HOH:O	1.92	0.51
2:F:15:ARG:HH21	2:F:18[B]:GLN:HE22	1.60	0.49
2:H:20:ILE:HD11	2:H:42[B]:LEU:CD2	2.29	0.49
2:B:6:HIS:HE1	5:B:95:HOH:O	1.96	0.49
2:B:17[B]:GLN:OE1	5:B:101:HOH:O	2.20	0.48
1:K:25:ARG:O	1:K:29:GLU:HG3	2.14	0.48
1:I:35:ARG:HA	1:I:38:ILE:HD12	1.94	0.47
1:E:36:GLU:H	1:E:36:GLU:CD	2.17	0.47
1:I:63:GLY:HA2	5:I:97:HOH:O	2.14	0.47
2:B:9[A]:THR:OG1	2:L:12:SER:CB	2.62	0.47
2:B:1:PRO:H3	3:E:76:ACT:H3	1.79	0.47
2:L:59:GLU:O	2:L:60:ALA:HB2	2.15	0.47
2:D:35:PRO:HA	2:D:38:ILE:HD12	1.97	0.46
2:J:11:LEU:HD22	2:J:15:ARG:HG2	1.97	0.45
1:E:36:GLU:HG3	5:E:127:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:43:VAL:HG22	2:J:45:HIS:NE2	2.31	0.45
1:E:34:PRO:HB2	1:E:36:GLU:OE2	2.17	0.45
2:H:6:HIS:HD2	2:H:45:HIS:NE2	2.14	0.45
1:A:54:GLY:O	1:E:35:ARG:NH2	2.44	0.45
1:A:7:MET:O	1:A:44:GLU:HA	2.17	0.45
1:C:34:PRO:HB2	1:C:36:GLU:OE1	2.17	0.45
1:K:7:MET:O	1:K:44:GLU:HA	2.16	0.45
1:I:25:ARG:O	1:I:29:GLU:HG3	2.17	0.45
2:J:57:HIS:HA	2:J:58:GLY:HA2	1.63	0.45
1:C:29:GLU:HG3	5:C:115:HOH:O	2.01	0.44
1:G:53:HIS:HE1	5:H:110:HOH:O	2.00	0.44
1:I:27:ILE:HD13	2:L:19:LEU:HD11	1.99	0.44
2:D:43:VAL:HG22	2:D:45:HIS:NE2	2.32	0.44
1:I:53:HIS:HE1	2:J:53:SER:OG	2.01	0.44
1:I:64:ASN:C	1:I:64:ASN:ND2	2.68	0.43
1:A:21:ALA:O	1:A:35:ARG:NH2	2.51	0.43
1:I:63:GLY:N	1:I:64:ASN:CG	2.68	0.43
1:G:7:MET:O	1:G:44:GLU:HA	2.18	0.43
2:F:15:ARG:NH2	2:F:18[B]:GLN:HE22	2.16	0.43
2:F:47:GLU:HG3	2:L:47:GLU:HB2	2.01	0.43
2:H:17:GLN:CG	5:H:108:HOH:O	2.66	0.42
2:H:2:PHE:CZ	2:H:4:GLU:HG2	2.54	0.42
1:C:53:HIS:CE1	2:D:53:SER:OG	2.71	0.42
1:K:61:VAL:HA	1:K:62:PRO:HD3	1.84	0.42
1:E:50:PHE:O	1:E:57:LEU:HD13	2.20	0.42
2:B:21:ARG:HH22	2:F:56:ILE:HG21	1.85	0.42
1:E:3:ILE:HD11	1:E:27:ILE:HG13	2.01	0.41
1:G:27:ILE:HD13	2:J:19:LEU:HD11	2.02	0.41
2:J:9:THR:HG22	2:J:44:GLU:CB	2.47	0.41
1:I:63:GLY:CA	1:I:64:ASN:CB	2.96	0.41
1:A:15:GLN:HB3	2:D:31:ILE:HG22	2.02	0.41
2:H:5:CYS:HB2	2:H:42[B]:LEU:HD13	2.03	0.41
1:K:23:LEU:HA	1:K:26:VAL:HG22	2.02	0.41
2:H:21:ARG:HE	2:L:60:ALA:HB1	1.86	0.40
2:B:41:LEU:HD11	2:F:45:HIS:CG	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:62:PRO:O	5:E:126:HOH:O[2_645]	2.07	0.13

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	62/76 (82%)	61 (98%)	1 (2%)	0	100	100
1	C	64/76 (84%)	61 (95%)	2 (3%)	1 (2%)	9	1
1	E	62/76 (82%)	61 (98%)	1 (2%)	0	100	100
1	G	61/76 (80%)	60 (98%)	1 (2%)	0	100	100
1	I	64/76 (84%)	64 (100%)	0	0	100	100
1	K	63/76 (83%)	62 (98%)	1 (2%)	0	100	100
2	B	61/70 (87%)	61 (100%)	0	0	100	100
2	D	57/70 (81%)	57 (100%)	0	0	100	100
2	F	60/70 (86%)	60 (100%)	0	0	100	100
2	H	58/70 (83%)	58 (100%)	0	0	100	100
2	J	57/70 (81%)	56 (98%)	0	1 (2%)	8	1
2	L	60/70 (86%)	59 (98%)	1 (2%)	0	100	100
All	All	729/876 (83%)	720 (99%)	7 (1%)	2 (0%)	41	24

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	J	11	LEU
1	C	63	GLY

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	55/63 (87%)	55 (100%)	0	100	100
1	C	56/63 (89%)	55 (98%)	1 (2%)	59	43
1	E	55/63 (87%)	55 (100%)	0	100	100
1	G	54/63 (86%)	54 (100%)	0	100	100
1	I	56/63 (89%)	52 (93%)	4 (7%)	14	3
1	K	56/63 (89%)	53 (95%)	3 (5%)	22	7
2	B	53/59 (90%)	50 (94%)	3 (6%)	20	6
2	D	52/59 (88%)	50 (96%)	2 (4%)	33	14
2	F	54/59 (92%)	54 (100%)	0	100	100
2	H	52/59 (88%)	52 (100%)	0	100	100
2	J	51/59 (86%)	48 (94%)	3 (6%)	19	6
2	L	53/59 (90%)	52 (98%)	1 (2%)	57	41
All	All	647/732 (88%)	630 (97%)	17 (3%)	49	28

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	9[A]	THR
2	B	9[B]	THR
2	B	42	LEU
1	C	61	VAL
2	D	36	LYS
2	D	43	VAL
1	I	23[A]	LEU
1	I	23[B]	LEU
1	I	61	VAL
1	I	64	ASN
2	J	13	VAL
2	J	26	VAL
2	J	43	VAL
1	K	1	PRO
1	K	36	GLU
1	K	57	LEU
2	L	59	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	6	HIS
2	B	57	HIS
1	C	53	HIS
2	D	17	GLN
2	F	17	GLN
2	H	6	HIS
2	H	28	ASN
1	I	53	HIS
2	L	17	GLN

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](#)

8 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	$\# Z > 2$
4	PO4	B	71	-	4,4,4	0.82	0	6,6,6	0.88	0
3	ACT	G	76	-	1,3,3	0.28	0	0,3,3	0.00	-
4	PO4	J	71	-	4,4,4	0.79	0	6,6,6	0.72	0
3	ACT	K	76	-	1,3,3	1.31	0	0,3,3	0.00	-
3	ACT	I	76	-	1,3,3	1.15	0	0,3,3	0.00	-
3	ACT	E	76	-	1,3,3	1.45	0	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	ACT	C	76	-	1,3,3	1.09	0	0,3,3	0.00	-
3	ACT	A	76	-	1,3,3	1.52	0	0,3,3	0.00	-

There are no bond length outliers.

There are no bond angle outliers.

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
3	I	76	ACT	1	0
3	E	76	ACT	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	62/76 (81%)	0.07	1 (1%) 72 76	15, 19, 33, 37	0
1	C	64/76 (84%)	0.08	3 (4%) 31 35	14, 19, 32, 48	0
1	E	62/76 (81%)	0.10	3 (4%) 30 34	13, 20, 33, 46	0
1	G	62/76 (81%)	0.19	2 (3%) 47 52	14, 20, 35, 44	0
1	I	64/76 (84%)	0.02	3 (4%) 31 35	13, 19, 34, 50	0
1	K	62/76 (81%)	0.06	3 (4%) 30 34	13, 19, 32, 42	0
2	B	61/70 (87%)	-0.04	1 (1%) 72 76	14, 21, 33, 43	0
2	D	57/70 (81%)	0.43	4 (7%) 16 18	14, 23, 34, 41	0
2	F	58/70 (82%)	0.24	3 (5%) 27 30	14, 22, 35, 41	0
2	H	59/70 (84%)	0.24	4 (6%) 17 19	14, 22, 40, 54	0
2	J	58/70 (82%)	0.97	8 (13%) 2 3	18, 28, 41, 45	0
2	L	60/70 (85%)	0.25	6 (10%) 7 8	14, 21, 43, 53	0
All	All	729/876 (83%)	0.21	41 (5%) 24 27	13, 21, 37, 54	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	58	GLY	9.2
2	J	58	GLY	6.7
2	J	10	GLY	5.5
2	B	61	ALA	5.3
2	J	57	HIS	5.1
1	E	62	PRO	4.8
1	K	62	PRO	4.5
2	L	59	GLU	4.5
2	D	57	HIS	4.4
2	L	58	GLY	4.4
1	C	63	GLY	4.4

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Mol	Chain	Res	Type	RSRZ
1	G	62	PRO	4.2
2	J	56	ILE	4.1
1	G	61	VAL	4.1
2	F	58	GLY	4.1
2	L	60	ALA	3.9
1	C	64	ASN	3.5
2	H	59	GLU	3.4
2	F	57	HIS	3.3
1	I	64	ASN	3.1
2	J	11	LEU	3.1
2	D	56	ILE	3.0
2	H	57	HIS	3.0
2	J	32	GLY	2.9
2	J	36	LYS	2.9
2	D	10	GLY	2.8
1	I	63	GLY	2.7
2	J	55	ARG	2.7
1	I	9[A]	TYR	2.7
1	E	61	VAL	2.7
2	L	36	LYS	2.6
2	L	57	HIS	2.6
1	E	9[A]	TYR	2.5
2	L	56	ILE	2.5
2	H	36	LYS	2.4
2	F	56	ILE	2.4
1	C	9[A]	TYR	2.3
1	K	61	VAL	2.2
1	K	14	GLU	2.1
2	D	55	ARG	2.1
1	A	62	PRO	2.0

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

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

6.3 Carbohydrates ⓘ

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. 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
3	ACT	K	76	4/4	0.85	0.17	27,29,30,33	0
3	ACT	I	76	4/4	0.90	0.14	22,26,27,29	0
3	ACT	E	76	4/4	0.94	0.10	28,31,32,33	0
3	ACT	C	76	4/4	0.95	0.11	23,25,27,28	0
3	ACT	A	76	4/4	0.95	0.14	26,28,30,31	0
4	PO4	J	71	5/5	0.96	0.09	37,37,39,39	0
3	ACT	G	76	4/4	0.96	0.11	24,26,26,28	0
4	PO4	B	71	5/5	0.99	0.06	29,31,31,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.