



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:41 AM UTC

PDB ID : 3EJ7 / pdb_00003ej7
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 : 1.90 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 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

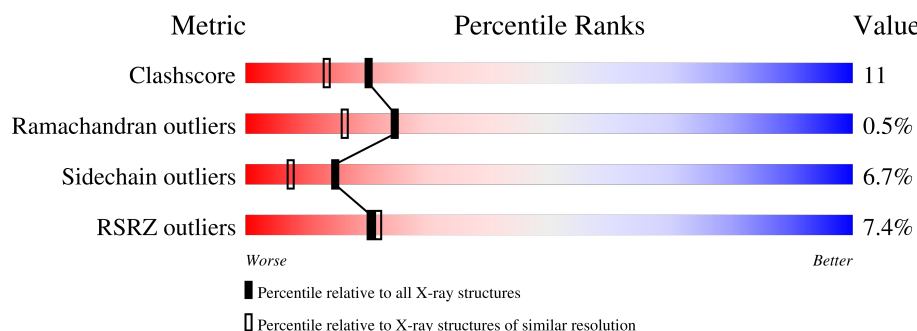
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	76	9% 55% 13% • 30%
1	C	76	3% 63% 11% • • 22%
1	E	76	% 59% 16% • 24%
1	G	76	8% 59% 9% 5% 26%
1	I	76	4% 51% 22% • 22%
1	K	76	9% 59% 17% • 22%

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Mol	Chain	Length	Quality of chain
2	B	70	3% 71% 10% 19%
2	D	70	9% 64% 16% 19%
2	F	70	3% 74% 9% 16%
2	H	70	11% 60% 16% 23%
2	J	70	9% 56% 11% 10% 20%
2	L	70	1% 61% 19% 17%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5887 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	53	Total	C	N	O	S	0	3	0
			430	268	80	79	3			
1	C	59	Total	C	N	O	S	0	1	0
			464	290	82	89	3			
1	E	58	Total	C	N	O	S	0	0	0
			451	281	81	86	3			
1	G	56	Total	C	N	O	S	0	0	0
			436	270	79	84	3			
1	I	59	Total	C	N	O	S	0	0	0
			459	285	82	89	3			
1	K	59	Total	C	N	O	S	0	0	0
			459	285	82	89	3			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	ALA	ARG	engineered mutation	UNP Q9EV85
C	8	ALA	ARG	engineered mutation	UNP Q9EV85
E	8	ALA	ARG	engineered mutation	UNP Q9EV85
G	8	ALA	ARG	engineered mutation	UNP Q9EV85
I	8	ALA	ARG	engineered mutation	UNP Q9EV85
K	8	ALA	ARG	engineered mutation	UNP Q9EV85

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

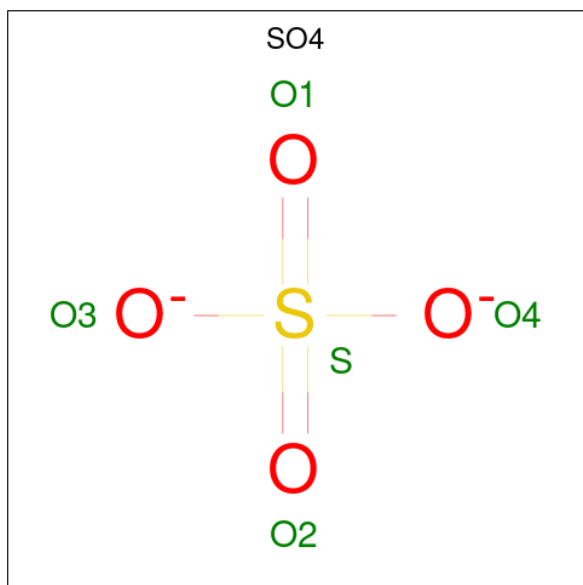
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	57	Total	C	N	O	S	0	1	0
			440	276	80	81	3			
2	D	57	Total	C	N	O	S	0	1	0
			441	277	80	82	2			
2	F	59	Total	C	N	O	S	0	0	0
			450	281	82	85	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	54	Total	C	N	O	S	0	1	0
			412	259	72	79	2			
2	J	56	Total	C	N	O	S	0	3	0
			440	280	77	81	2			
2	L	58	Total	C	N	O	S	0	1	0
			446	281	81	82	2			

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	38	Total	O	0	0
			38	38		
4	B	59	Total	O	0	0
			59	59		
4	C	59	Total	O	0	0
			59	59		
4	D	40	Total	O	0	0
			40	40		
4	E	54	Total	O	0	0
			54	54		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	F	53	Total 53	O 53	0	0
4	G	40	Total 40	O 40	0	0
4	H	40	Total 40	O 40	0	0
4	I	36	Total 36	O 36	0	0
4	J	48	Total 48	O 48	0	0
4	K	36	Total 36	O 36	0	0
4	L	51	Total 51	O 51	0	0

- Molecule 1: Alpha-subunit of trans-3-chloroacrylic acid dehalogenase



Number of proteins

MET P1 A7 M8 Y9 G10 R11 V26 L27 T31 G32 E33 T42 R43 E44 F50 H53 G54 H55 H56 D59 TVR VAL PRO GLY ASN ALA ASN ASP LYS ALA ILE ALA LYS LEU LYS

Category	Count
MET	1
P1	1
M7	1
R11	1
S20	1
A21	1
G22	1
L23	1
V26	1
E29	1
E33	1
P34	1
R35	1
E36	1
N37	1
I38	1
E44	1
H53	1
P58	1
ASP	1
TYR	1
VAL	1
PRO	1
GLY	1
ASN	1
ALA	1
ASN	1
ASP	1
LYS	1
ALA	1
LEU	1
ILE	1
ALA	1
LYS	1
LEU	1
LYS	1

MET
P1
R11
L19
L23
I27
S28
E29
A30
T31
G32
E33
V51
E52
H53
G54
E55
H56
LEU
PRO
ASP
TYR
VAL
PRO
GLY
ASN
ALA
ALA
ASN
ASP
LYS
ALA
LEU
ILE
ALA
LYS
LEU
LYS

Met	P1	Y9	G10	R11	T12	D13	R17	A18	L19	L23	L24	R25	V26	L27	E33	P34	R35	E36	N37	I38	E44	G47	F50	H53	H56	L57	P58	D59	Tyr	Val	Pro	Gly	Asn	Ala	Asn	Asp	Lys	Ala	Leu	Ile	Ala	Lys	Leu
Met	P1	Y9	G10	R11	T12	D13	R17	A18	L19	L23	L24	R25	V26	L27	E33	P34	R35	E36	N37	I38	E44	G47	F50	H53	H56	L57	P58	D59	Tyr	Val	Pro	Gly	Asn	Ala	Asn	Asp	Lys	Ala	Leu	Ile	Ala	Lys	Leu





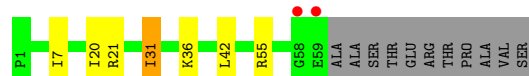
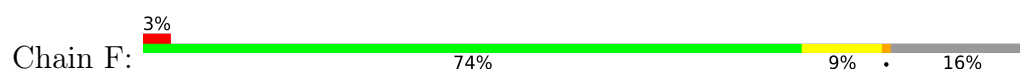
- Molecule 2: Beta-subunit of trans-3-chloroacrylic acid dehalogenase



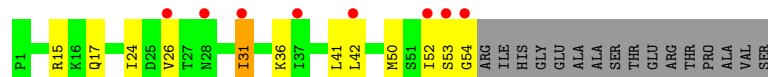
- Molecule 2: Beta-subunit of trans-3-chloroacrylic acid dehalogenase



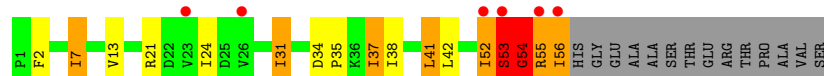
- Molecule 2: Beta-subunit of trans-3-chloroacrylic acid dehalogenase



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	60.25Å 83.62Å 124.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	69.30 – 1.90 69.30 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.9 (69.30-1.90) 99.0 (69.30-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.56 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.202 , 0.269 (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	24.7	Xtriage
Anisotropy	0.839	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 33.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5887	wwPDB-VP
Average B, all atoms (Å ²)	16.0	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 56.04 % 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 2.8982e-05. 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0/445	0.83	0/594
1	C	1.17	1/475 (0.2%)	0.95	0/638
1	E	0.79	0/459	0.92	0/616
1	G	0.79	0/443	0.94	0/593
1	I	0.74	0/467	0.92	0/627
1	K	1.38	3/467 (0.6%)	0.92	1/627 (0.2%)
2	B	0.83	0/448	0.86	0/604
2	D	0.83	0/449	0.91	0/606
2	F	0.79	0/455	0.92	2/613 (0.3%)
2	H	0.87	1/419 (0.2%)	0.99	1/566 (0.2%)
2	J	0.83	0/453	1.05	3/611 (0.5%)
2	L	0.85	1/454 (0.2%)	0.88	0/612
All	All	0.91	6/5434 (0.1%)	0.93	7/7307 (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
2	J	0	2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	56	HIS	CE1-NE2	22.00	1.54	1.32
1	C	55	GLU	CD-OE2	18.08	1.59	1.25
1	K	56	HIS	CG-ND1	11.26	1.50	1.38
1	K	56	HIS	CG-CD2	7.32	1.44	1.35
2	H	36	LYS	CD-CE	5.52	1.69	1.52
2	L	24	ILE	CA-CB	5.11	1.60	1.54

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	52	ILE	CA-C-N	7.09	134.47	121.70
2	J	52	ILE	C-N-CA	7.09	134.47	121.70
2	F	31	ILE	N-CA-CB	-6.58	104.98	112.21
2	J	54	GLY	N-CA-C	5.94	127.27	113.18
2	H	36	LYS	CG-CD-CE	-5.80	97.96	111.30
1	K	56	HIS	ND1-CG-CD2	5.25	111.35	106.10
2	F	31	ILE	CB-CA-C	5.21	117.35	110.84

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	J	53	SER	Peptide
2	J	54	GLY	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	430	0	437	6	0
1	C	464	0	457	11	0
1	E	451	0	442	8	0
1	G	436	0	424	16	0
1	I	459	0	446	16	0
1	K	459	0	446	19	0
2	B	440	0	463	4	0
2	D	441	0	465	11	0
2	F	450	0	467	6	0
2	H	412	0	434	9	0
2	J	440	0	478	26	0
2	L	446	0	472	17	0
3	A	5	0	0	0	0
4	A	38	0	0	4	0
4	B	59	0	0	0	0
4	C	59	0	0	1	0
4	D	40	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	54	0	0	0	0
4	F	53	0	0	1	0
4	G	40	0	0	0	0
4	H	40	0	0	4	0
4	I	36	0	0	1	0
4	J	48	0	0	4	0
4	K	36	0	0	2	0
4	L	51	0	0	1	0
All	All	5887	0	5431	122	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 11.

All (122) 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:K:31:THR:HB	4:K:93:HOH:O	1.06	1.23
2:J:52:ILE:H	2:J:53:SER:HB2	1.17	1.09
2:H:31:ILE:HD12	1:K:19:LEU:HG	1.38	1.02
2:D:53:SER:HA	2:F:36:LYS:O	1.64	0.96
2:J:52:ILE:N	2:J:53:SER:HB2	1.81	0.95
2:B:37:ILE:HG22	1:E:53:HIS:HE1	1.33	0.94
2:H:17:GLN:HG2	4:H:102:HOH:O	1.70	0.92
1:C:27:ILE:O	1:C:31:THR:HB	1.69	0.91
1:A:35:ARG:NH1	4:A:80:HOH:O	2.02	0.90
1:C:31:THR:HG22	1:C:33:GLU:H	1.41	0.85
4:H:85:HOH:O	1:K:31:THR:HG21	1.74	0.85
2:F:7:ILE:HD11	2:F:42:LEU:HD21	1.59	0.82
2:J:21:ARG:NH2	4:J:108:HOH:O	2.13	0.80
1:K:35:ARG:HA	4:K:111:HOH:O	1.82	0.78
1:G:1:PRO:HD2	1:G:33:GLU:HG2	1.68	0.74
1:G:31:THR:CG2	1:G:33:GLU:HB2	2.18	0.74
1:G:31:THR:HG23	1:G:33:GLU:HB2	1.67	0.73
2:B:37:ILE:HG22	1:E:53:HIS:CE1	2.22	0.72
1:A:25:ARG:HB2	1:A:35:ARG:HH21	1.54	0.71
2:J:7[A]:ILE:HD12	2:J:42:LEU:HD11	1.72	0.71
2:H:31:ILE:CD1	1:K:19:LEU:HG	2.18	0.68
1:C:31:THR:CG2	1:C:33:GLU:H	2.06	0.68
2:H:50:MET:HG2	2:J:41:LEU:HD23	1.75	0.68
2:D:16:LYS:HE2	4:D:91:HOH:O	1.94	0.66
1:C:31:THR:CG2	1:C:33:GLU:HB2	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:11:ARG:HG2	2:J:31:ILE:HG13	1.76	0.65
1:I:27:ILE:HD13	2:L:19:LEU:HD11	1.80	0.64
1:I:13:ASP:O	1:I:17:ARG:HG3	1.97	0.64
1:I:9:TYR:HB3	4:I:105:HOH:O	1.98	0.64
2:H:54:GLY:HA2	2:J:24[B]:ILE:HD13	1.81	0.63
2:B:50:MET:HG2	2:D:41:LEU:HD23	1.82	0.62
2:J:56:ILE:HA	4:J:116:HOH:O	1.98	0.62
1:G:51:VAL:HG21	1:K:20:SER:OG	2.00	0.61
1:C:26:VAL:HG23	1:C:27:ILE:HD12	1.83	0.61
2:F:7:ILE:CD1	2:F:42:LEU:HD21	2.31	0.61
2:J:52:ILE:N	2:J:53:SER:CB	2.62	0.60
1:I:58:PRO:O	1:I:59:ASP:HB2	2.02	0.59
2:L:57:HIS:HD2	4:L:106:HOH:O	1.85	0.57
2:D:16:LYS:CE	4:D:91:HOH:O	2.52	0.57
4:H:72:HOH:O	1:K:31:THR:HG23	2.04	0.56
1:K:1:PRO:HD2	1:K:33:GLU:HG2	1.87	0.56
4:H:85:HOH:O	1:K:31:THR:CG2	2.43	0.56
1:I:36:GLU:H	1:I:36:GLU:CD	2.14	0.56
2:L:20[A]:ILE:HD11	2:L:42:LEU:HB2	1.88	0.56
1:K:19:LEU:HD13	1:K:40:PHE:HZ	1.71	0.55
1:G:27:ILE:O	1:G:31:THR:HB	2.07	0.54
2:J:7[A]:ILE:HD12	2:J:42:LEU:CD1	2.37	0.54
1:A:11[A]:ARG:HG3	1:A:15:GLN:OE1	2.07	0.54
2:H:26:VAL:HG11	1:K:22:GLY:HA3	1.91	0.53
2:J:56:ILE:HG23	4:J:84:HOH:O	2.08	0.53
1:A:51:VAL:HG21	1:E:20:SER:HB2	1.92	0.52
1:E:1:PRO:HD2	1:E:33:GLU:HG2	1.93	0.51
1:C:31:THR:HG21	1:C:33:GLU:HB2	1.92	0.51
2:D:9[A]:THR:HG22	2:D:44:GLU:HB3	1.93	0.51
1:C:11:ARG:HD2	4:C:92:HOH:O	2.10	0.51
1:I:1:PRO:HD2	1:I:33:GLU:HG2	1.94	0.50
1:I:47:GLY:H	1:I:59:ASP:C	2.19	0.50
2:L:7:ILE:HD11	2:L:42:LEU:HD21	1.93	0.50
2:L:24:ILE:CD1	2:L:40:VAL:CG2	2.90	0.50
1:E:22:GLY:O	1:E:26:VAL:HG13	2.12	0.50
2:L:24:ILE:CD1	2:L:40:VAL:HG23	2.41	0.50
1:K:7:MET:SD	1:K:11:ARG:NH2	2.86	0.49
2:B:34:ASP:OD1	2:B:36:LYS:HB2	2.12	0.49
1:I:35:ARG:HA	1:I:38:ILE:HD12	1.95	0.48
1:C:50:PHE:O	1:C:56:HIS:HA	2.13	0.48
1:G:11:ARG:CG	2:J:31:ILE:HG13	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:31:THR:HG22	1:G:33:GLU:H	1.78	0.48
1:A:13:ASP:O	1:A:17[A]:ARG:HG3	2.13	0.48
2:J:53:SER:HB3	2:J:54:GLY:O	2.14	0.48
2:J:13:VAL:HG12	4:J:112:HOH:O	2.15	0.47
2:J:55:ARG:CD	2:J:55:ARG:O	2.62	0.47
2:L:24:ILE:HD11	2:L:40:VAL:HG23	1.95	0.47
1:K:19:LEU:HD13	1:K:40:PHE:CZ	2.49	0.47
2:D:56:ILE:HG13	2:F:21:ARG:HG3	1.97	0.47
2:L:24:ILE:HD13	2:L:40:VAL:CG2	2.45	0.47
1:I:34:PRO:HB2	1:I:36:GLU:HG2	1.96	0.47
1:E:7:MET:O	1:E:44:GLU:HA	2.15	0.47
1:I:25:ARG:HG3	1:I:35:ARG:NH2	2.31	0.46
2:F:36:LYS:HG3	4:F:88:HOH:O	2.16	0.46
2:L:35:PRO:HA	2:L:38:ILE:HD12	1.98	0.46
1:G:31:THR:CG2	1:G:33:GLU:H	2.28	0.46
2:L:13:VAL:O	2:L:17:GLN:HG3	2.17	0.45
1:I:19:LEU:HB2	2:L:31:ILE:HD13	1.97	0.45
1:G:56:HIS:CE1	1:K:17:ARG:HG2	2.52	0.45
2:H:26:VAL:CG1	1:K:22:GLY:HA3	2.47	0.45
2:J:55:ARG:O	2:J:55:ARG:HD3	2.17	0.45
1:K:1:PRO:CD	1:K:33:GLU:HG2	2.48	0.44
1:I:50:PHE:O	1:I:56:HIS:HA	2.18	0.44
2:D:8:ALA:HB2	2:D:50:MET:HE1	2.00	0.44
1:E:33:GLU:HG3	1:E:37:ASN:HB2	2.00	0.44
1:G:19:LEU:HD22	2:J:31:ILE:HD13	1.99	0.43
1:G:56:HIS:HE1	1:K:17:ARG:HA	1.82	0.43
1:C:7:MET:HE2	1:C:42:ILE:HG21	2.00	0.43
4:A:105:HOH:O	2:D:52:ILE:HD13	2.17	0.43
2:L:15:ARG:HD2	2:L:15:ARG:HA	1.73	0.43
2:D:51:SER:HB3	2:F:20:ILE:HG21	2.00	0.43
1:G:51:VAL:HB	1:K:40:PHE:HB3	2.01	0.43
2:L:24:ILE:HD11	2:L:40:VAL:CG2	2.49	0.43
2:J:34:ASP:O	2:J:37:ILE:HG12	2.19	0.43
4:A:103:HOH:O	1:C:55:GLU:HG2	2.18	0.42
1:E:35:ARG:HA	1:E:38:ILE:HD12	2.01	0.42
1:G:19:LEU:HB2	2:J:31:ILE:HD13	2.01	0.42
2:H:54:GLY:HA2	2:J:24[A]:ILE:HG21	2.02	0.42
1:I:9:TYR:CD1	1:I:44:GLU:HB3	2.55	0.42
1:I:11:ARG:CG	2:L:31:ILE:HG13	2.49	0.42
2:J:55:ARG:CD	2:J:55:ARG:C	2.92	0.42
2:J:52:ILE:CA	2:J:53:SER:HB2	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:31:THR:CG2	1:G:33:GLU:CB	2.94	0.42
1:I:36:GLU:CD	1:I:36:GLU:N	2.78	0.41
2:J:35:PRO:HA	2:J:38:ILE:HD12	2.02	0.41
1:C:7:MET:O	1:C:44:GLU:HA	2.20	0.41
1:I:11:ARG:HG2	2:L:31:ILE:HG13	2.01	0.41
2:J:53:SER:OG	2:J:56:ILE:CG2	2.68	0.41
1:K:23:LEU:O	1:K:27:ILE:HD13	2.20	0.41
1:A:23:LEU:O	1:A:27:ILE:HD13	2.20	0.41
2:J:2:PHE:HE1	2:J:41:LEU:HB2	1.86	0.41
2:D:2:PHE:HE1	2:D:41:LEU:HB2	1.86	0.41
2:J:53:SER:OG	2:J:56:ILE:HG21	2.21	0.41
1:G:51:VAL:HG11	1:G:55:GLU:HB2	2.03	0.41
4:A:105:HOH:O	2:D:52:ILE:CD1	2.70	0.40
2:H:24:ILE:HD13	2:L:54:GLY:HA2	2.03	0.40

There are no symmetry-related clashes.

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	23/76 (30%)	23 (100%)	0	0	100	100
1	C	58/76 (76%)	57 (98%)	1 (2%)	0	100	100
1	E	56/76 (74%)	56 (100%)	0	0	100	100
1	G	54/76 (71%)	53 (98%)	0	1 (2%)	6	1
1	I	57/76 (75%)	57 (100%)	0	0	100	100
1	K	57/76 (75%)	54 (95%)	3 (5%)	0	100	100
2	B	56/70 (80%)	56 (100%)	0	0	100	100
2	D	56/70 (80%)	55 (98%)	1 (2%)	0	100	100
2	F	57/70 (81%)	57 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	53/70 (76%)	52 (98%)	0	1 (2%)	6	1
2	J	57/70 (81%)	56 (98%)	0	1 (2%)	6	1
2	L	57/70 (81%)	57 (100%)	0	0	100	100
All	All	641/876 (73%)	633 (99%)	5 (1%)	3 (0%)	24	16

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	J	53	SER
2	H	53	SER
1	G	54	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	46/62 (74%)	43 (94%)	3 (6%)	15	8
1	C	50/62 (81%)	47 (94%)	3 (6%)	17	9
1	E	48/62 (77%)	45 (94%)	3 (6%)	16	8
1	G	46/62 (74%)	41 (89%)	5 (11%)	6	2
1	I	49/62 (79%)	45 (92%)	4 (8%)	10	5
1	K	49/62 (79%)	48 (98%)	1 (2%)	48	46
2	B	51/59 (86%)	48 (94%)	3 (6%)	18	10
2	D	51/59 (86%)	49 (96%)	2 (4%)	28	21
2	F	51/59 (86%)	49 (96%)	2 (4%)	28	21
2	H	48/59 (81%)	43 (90%)	5 (10%)	7	2
2	J	52/59 (88%)	45 (86%)	7 (14%)	4	1
2	L	51/59 (86%)	49 (96%)	2 (4%)	28	21
All	All	592/726 (82%)	552 (93%)	40 (7%)	15	7

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	24	LEU
1	A	33	GLU
2	B	11	LEU
2	B	42	LEU
2	B	52	ILE
1	C	11	ARG
1	C	31	THR
1	C	55	GLU
2	D	29	LYS
2	D	41	LEU
1	E	11	ARG
1	E	23	LEU
1	E	26	VAL
2	F	31	ILE
2	F	55	ARG
1	G	11	ARG
1	G	23	LEU
1	G	31	THR
1	G	55	GLU
1	G	56	HIS
2	H	15	ARG
2	H	31	ILE
2	H	41	LEU
2	H	42	LEU
2	H	52	ILE
1	I	1	PRO
1	I	11	ARG
1	I	23	LEU
1	I	36	GLU
2	J	7[A]	ILE
2	J	7[B]	ILE
2	J	31	ILE
2	J	37	ILE
2	J	41	LEU
2	J	55	ARG
2	J	56	ILE
1	K	19	LEU
2	L	3	ILE
2	L	31	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
2	B	17	GLN
1	E	53	HIS
1	G	53	HIS
2	H	17	GLN
2	J	17	GLN
2	J	39	ASN
2	J	49	ASN
2	L	39	ASN
2	L	57	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](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	A	76	-	4,4,4	0.43	0	6,6,6	0.36	0

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.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	53/76 (69%)	0.73	7 (13%) 7 7	7, 16, 28, 30	3 (5%)
1	C	59/76 (77%)	0.51	2 (3%) 48 51	6, 13, 25, 30	1 (1%)
1	E	58/76 (76%)	0.28	1 (1%) 69 72	5, 12, 18, 19	0
1	G	56/76 (73%)	0.76	6 (10%) 11 11	8, 15, 29, 39	0
1	I	59/76 (77%)	0.69	3 (5%) 33 36	9, 15, 22, 25	0
1	K	59/76 (77%)	1.10	7 (11%) 9 9	12, 18, 27, 28	0
2	B	57/70 (81%)	0.55	2 (3%) 47 50	7, 13, 22, 25	1 (1%)
2	D	57/70 (81%)	0.85	6 (10%) 11 12	8, 15, 21, 23	1 (1%)
2	F	59/70 (84%)	0.42	2 (3%) 48 51	8, 12, 20, 26	0
2	H	54/70 (77%)	1.10	8 (14%) 5 6	8, 17, 29, 31	1 (1%)
2	J	56/70 (80%)	1.03	6 (10%) 11 11	6, 16, 22, 26	3 (5%)
2	L	58/70 (82%)	0.53	1 (1%) 69 72	8, 14, 20, 23	1 (1%)
All	All	685/876 (78%)	0.71	51 (7%) 20 22	5, 15, 26, 39	11 (1%)

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	56	ILE	6.8
1	G	54	GLY	5.9
2	F	58	GLY	4.6
2	D	52	ILE	4.4
2	H	53	SER	4.3
1	G	55	GLU	4.3
2	D	53	SER	4.2
2	D	55	ARG	4.0
2	J	53	SER	3.7
2	H	52	ILE	3.6
1	A	53	HIS	3.5

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Mol	Chain	Res	Type	RSRZ
1	I	9	TYR	3.2
1	I	59	ASP	3.1
2	H	31	ILE	3.1
1	G	56	HIS	3.1
1	K	59	ASP	2.9
2	J	52	ILE	2.9
1	C	9	TYR	2.9
1	K	58	PRO	2.9
1	A	29	GLU	2.8
2	J	23	VAL	2.7
2	H	54	GLY	2.7
2	D	51	SER	2.7
1	A	14	GLU	2.7
1	G	53	HIS	2.7
1	A	32	GLY	2.7
1	K	36	GLU	2.7
2	J	55	ARG	2.6
2	D	57	HIS	2.6
2	H	26	VAL	2.6
1	C	53	HIS	2.6
1	E	29	GLU	2.5
2	H	28	ASN	2.5
1	K	51	VAL	2.5
1	G	29	GLU	2.5
2	H	37	ILE	2.3
2	J	26	VAL	2.3
1	K	10	GLY	2.3
2	B	37	ILE	2.3
2	L	57	HIS	2.3
1	A	38	ILE	2.2
1	K	37	ASN	2.2
1	A	35	ARG	2.2
1	G	27	ILE	2.1
1	I	53	HIS	2.1
2	H	42	LEU	2.1
2	B	52	ILE	2.1
2	F	59	GLU	2.1
2	D	56	ILE	2.0
1	K	8	ALA	2.0
1	A	34	PRO	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 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($\text{\AA}^2$)	Q<0.9
3	SO4	A	76	5/5	0.95	0.12	22,23,25,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.