



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 02:07 am BST

PDB ID : 5VLC
Title : Crystal Structure of Medicago truncatula L-Histidinol Dehydrogenase in Complex with L-Histidinol
Authors : Ruszkowski, M.; Dauter, Z.
Deposited on : 2017-04-25
Resolution : 1.97 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

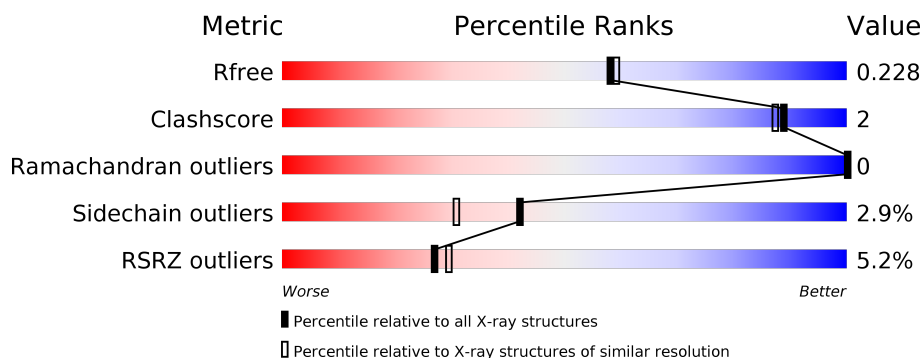
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.97 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}	130704	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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	446	<div> <div>2%</div> <div>90%</div> <div>6%</div> <div>.</div> </div>
1	B	446	<div> <div>2%</div> <div>91%</div> <div>5%</div> <div>.</div> </div>
1	C	446	<div> <div>2%</div> <div>90%</div> <div>7%</div> <div>.</div> </div>
1	D	446	<div> <div>4%</div> <div>91%</div> <div>5%</div> <div>..</div> </div>
1	E	446	<div> <div>9%</div> <div>87%</div> <div>10%</div> <div>.</div> </div>
1	F	446	<div> <div>11%</div> <div>93%</div> <div>.</div> <div>..</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 20385 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 Histidinol dehydrogenase, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	431	Total	C	N	O	S	0	1	0
			3278	2076	553	633	16			
1	B	432	Total	C	N	O	S	0	0	0
			3277	2077	550	634	16			
1	C	434	Total	C	N	O	S	0	0	0
			3297	2088	556	637	16			
1	D	432	Total	C	N	O	S	0	0	0
			3277	2077	550	634	16			
1	E	430	Total	C	N	O	S	0	0	0
			3268	2072	549	631	16			
1	F	434	Total	C	N	O	S	0	0	0
			3297	2088	556	637	16			

There are 18 discrepancies between the modelled and reference sequences:

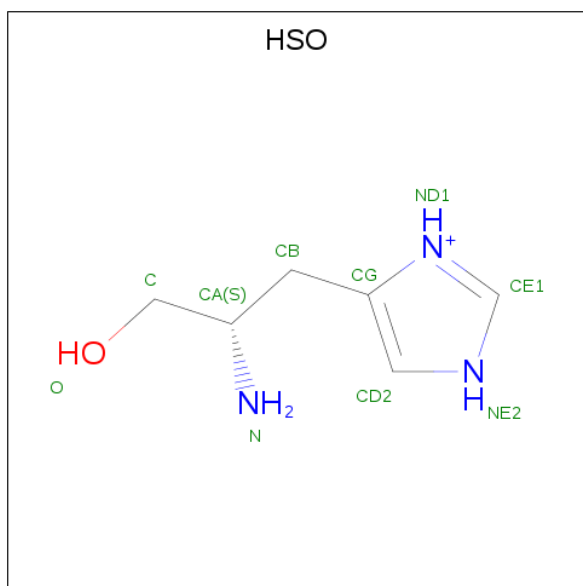
Chain	Residue	Modelled	Actual	Comment	Reference
A	33	SER	-	expression tag	UNP G7IKX3
A	34	ASN	-	expression tag	UNP G7IKX3
A	35	ALA	-	expression tag	UNP G7IKX3
B	33	SER	-	expression tag	UNP G7IKX3
B	34	ASN	-	expression tag	UNP G7IKX3
B	35	ALA	-	expression tag	UNP G7IKX3
C	33	SER	-	expression tag	UNP G7IKX3
C	34	ASN	-	expression tag	UNP G7IKX3
C	35	ALA	-	expression tag	UNP G7IKX3
D	33	SER	-	expression tag	UNP G7IKX3
D	34	ASN	-	expression tag	UNP G7IKX3
D	35	ALA	-	expression tag	UNP G7IKX3
E	33	SER	-	expression tag	UNP G7IKX3
E	34	ASN	-	expression tag	UNP G7IKX3
E	35	ALA	-	expression tag	UNP G7IKX3
F	33	SER	-	expression tag	UNP G7IKX3
F	34	ASN	-	expression tag	UNP G7IKX3

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Chain	Residue	Modelled	Actual	Comment	Reference
F	35	ALA	-	expression tag	UNP G7IKX3

- Molecule 2 is L-histidinol (three-letter code: HSO) (formula: $C_6H_{12}N_3O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			10	6	3	1		
2	B	1	Total	C	N	O	0	0
			10	6	3	1		
2	C	1	Total	C	N	O	0	0
			10	6	3	1		
2	D	1	Total	C	N	O	0	0
			10	6	3	1		
2	E	1	Total	C	N	O	0	0
			10	6	3	1		
2	F	1	Total	C	N	O	0	0
			10	6	3	1		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	A	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total 1	Zn 1	0	0
3	E	2	Total 2	Zn 2	0	0

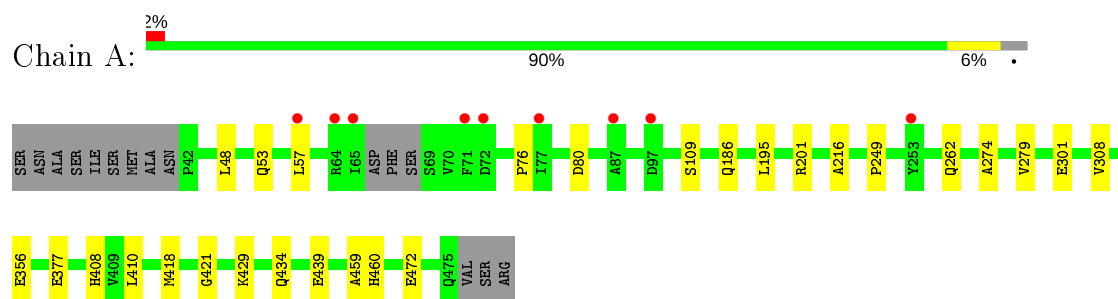
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	149	Total 149	O 149	0	0
4	B	133	Total 133	O 133	0	0
4	C	116	Total 116	O 116	0	0
4	D	98	Total 98	O 98	0	0
4	E	65	Total 65	O 65	0	0
4	F	64	Total 64	O 64	0	0

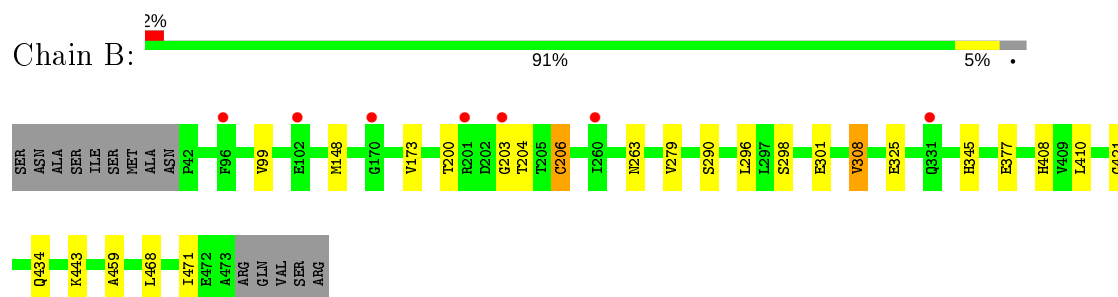
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

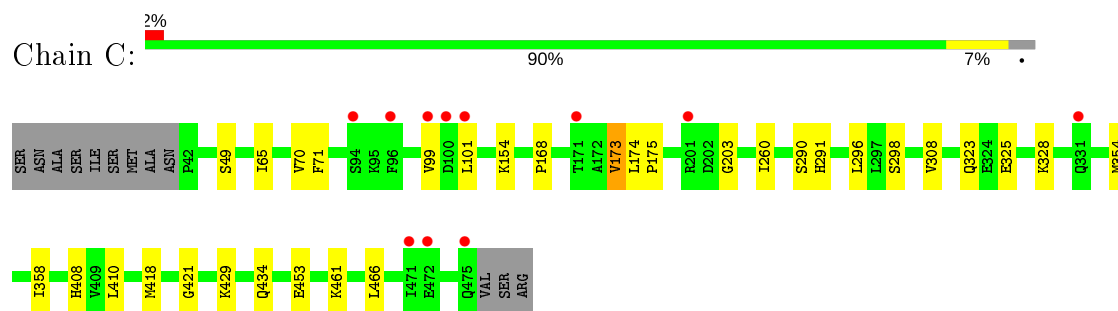
- Molecule 1: Histidinol dehydrogenase, chloroplastic



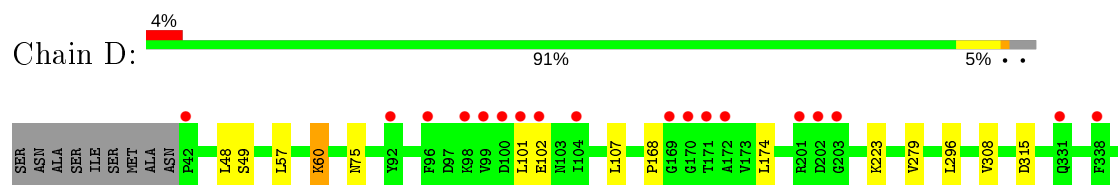
- Molecule 1: Histidinol dehydrogenase, chloroplastic



- Molecule 1: Histidinol dehydrogenase, chloroplastic

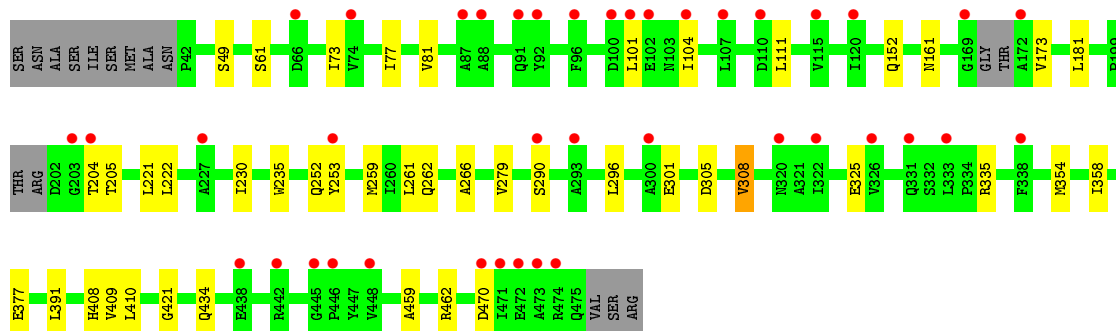
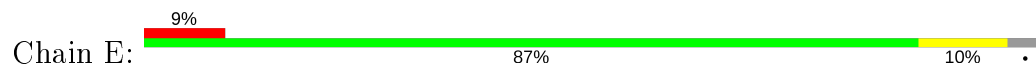


- Molecule 1: Histidinol dehydrogenase, chloroplastic

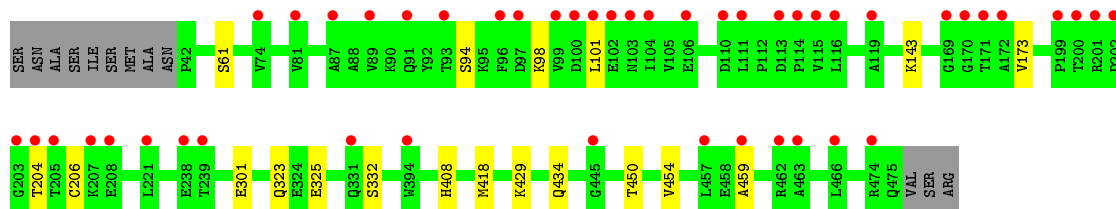
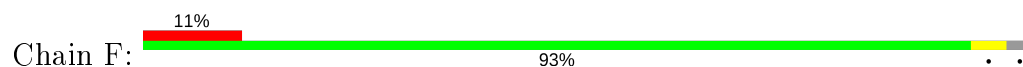




- Molecule 1: Histidinol dehydrogenase, chloroplastic



- Molecule 1: Histidinol dehydrogenase, chloroplastic



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	102.86Å 139.20Å 102.69Å 90.00° 119.18° 90.00°	Depositor
Resolution (Å)	48.73 – 1.97 48.73 – 1.97	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.73-1.97) 99.6 (48.73-1.97)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.03 (at 1.97Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.179 , 0.229 0.185 , 0.228	Depositor DCC
R_{free} test set	1232 reflections (0.70%)	wwPDB-VP
Wilson B-factor (Å ²)	36.1	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 51.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.022 for l,k,-h-l 0.022 for -h-l,k,h 0.033 for -h-l,-k,l 0.031 for h,-k,-h-l 0.039 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	20385	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.81	0/3346	0.84	0/4547
1	B	0.79	0/3344	0.84	0/4547
1	C	0.73	0/3364	0.83	0/4573
1	D	0.71	0/3344	0.85	0/4547
1	E	0.72	0/3333	0.81	0/4528
1	F	0.68	0/3364	0.79	0/4573
All	All	0.74	0/20095	0.83	0/27315

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 [i](#)

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	3278	0	3282	13	0
1	B	3277	0	3274	18	0
1	C	3297	0	3295	13	0
1	D	3277	0	3274	11	0
1	E	3268	0	3263	21	0
1	F	3297	0	3295	5	0
2	A	10	0	11	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	10	0	11	0	0
2	C	10	0	11	0	0
2	D	10	0	11	0	0
2	E	10	0	11	0	0
2	F	10	0	11	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	2	0	0	0	0
4	A	149	0	0	0	0
4	B	133	0	0	0	0
4	C	116	0	0	0	0
4	D	98	0	0	0	0
4	E	65	0	0	0	0
4	F	64	0	0	1	0
All	All	20385	0	19749	74	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 2.

All (74) 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:296:LEU:HD22	1:C:308:VAL:HG13	1.61	0.82
1:A:48:LEU:HD23	1:A:356[A]:GLU:HG2	1.67	0.76
1:E:290:SER:HA	1:E:325:GLU:HG2	1.72	0.71
1:B:279:VAL:HG12	1:B:308:VAL:HG22	1.72	0.69
1:A:48:LEU:HD23	1:A:356[A]:GLU:CG	2.24	0.66
1:B:296:LEU:HD22	1:B:308:VAL:HG13	1.80	0.63
1:D:101:LEU:HD21	1:D:223:LYS:HE3	1.82	0.61
1:E:252:GLN:NE2	1:E:305:ASP:OD2	2.35	0.60
1:B:290:SER:HA	1:B:325:GLU:HG2	1.84	0.59
1:B:99:VAL:HG21	1:B:203:GLY:HA2	1.87	0.57
1:C:290:SER:HA	1:C:325:GLU:HG2	1.88	0.55
1:B:290:SER:HA	1:B:325:GLU:CG	2.37	0.55
1:D:279:VAL:HG12	1:D:308:VAL:HG22	1.89	0.55
1:C:290:SER:HA	1:C:325:GLU:CG	2.37	0.54
1:E:77:ILE:O	1:E:81:VAL:HG23	2.08	0.54
1:E:279:VAL:HG12	1:E:308:VAL:HG22	1.89	0.53
1:B:279:VAL:CG1	1:B:308:VAL:HG22	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:VAL:HG13	1:B:206:CYS:SG	2.48	0.53
1:D:410:LEU:HD23	1:D:421:GLY:HA3	1.90	0.53
1:D:296:LEU:HD22	1:D:308:VAL:HG13	1.91	0.53
1:A:301:GLU:CD	1:B:459:ALA:HB3	2.30	0.52
1:C:99:VAL:HG11	1:C:203:GLY:HA2	1.90	0.52
1:E:235:TRP:CE2	1:E:266:ALA:HB2	2.46	0.51
1:B:148:MET:HE3	1:B:443:LYS:HG2	1.93	0.51
1:E:296:LEU:HD22	1:E:308:VAL:HG13	1.93	0.50
1:F:173:VAL:HG13	1:F:206:CYS:SG	2.52	0.50
1:B:410:LEU:HD23	1:B:421:GLY:HA3	1.94	0.49
1:E:354:MET:CE	1:E:358:ILE:HD11	2.43	0.49
1:C:453:GLU:OE2	1:C:461:LYS:NZ	2.44	0.49
1:E:161:ASN:HB2	4:F:662:HOH:O	2.12	0.48
1:E:181:LEU:HD21	1:E:409:VAL:HG21	1.96	0.47
1:E:279:VAL:CG1	1:E:308:VAL:HG22	2.44	0.47
1:D:57:LEU:O	1:D:60:LYS:HG2	2.15	0.47
1:A:377:GLU:CD	1:A:377:GLU:H	2.18	0.47
1:E:459:ALA:HB3	1:F:301:GLU:CD	2.35	0.47
1:A:459:ALA:HB3	1:B:301:GLU:CD	2.36	0.46
1:A:279:VAL:HG12	1:A:308:VAL:HG22	1.97	0.45
1:A:262:GLN:NE2	1:B:263:ASN:OD1	2.49	0.45
1:B:377:GLU:H	1:B:377:GLU:CD	2.19	0.45
1:E:104:ILE:HG22	1:E:222:LEU:HD12	1.98	0.45
1:E:410:LEU:HD23	1:E:421:GLY:HA3	1.98	0.45
1:C:65:ILE:HB	1:C:70:VAL:CG2	2.47	0.45
1:B:468:LEU:HD23	1:B:471:ILE:HD12	1.99	0.45
1:E:354:MET:HE3	1:E:358:ILE:HD11	1.99	0.44
1:A:410:LEU:HD23	1:A:421:GLY:HA3	1.99	0.44
1:D:168:PRO:HB2	1:D:174:LEU:HD12	2.00	0.44
1:E:377:GLU:HA	1:E:391:LEU:HD13	1.99	0.43
1:E:301:GLU:CD	1:F:459:ALA:HB3	2.39	0.43
1:B:200:THR:O	1:B:203:GLY:N	2.52	0.43
1:C:354:MET:CE	1:C:358:ILE:HD11	2.49	0.43
1:E:259:MET:O	1:E:262:GLN:HG2	2.18	0.43
1:A:460:HIS:CE1	1:B:298:SER:O	2.72	0.43
1:E:301:GLU:O	1:E:335:ARG:NH2	2.51	0.43
1:C:298:SER:O	1:D:460:HIS:CE1	2.72	0.42
1:D:296:LEU:HD22	1:D:308:VAL:CG1	2.49	0.42
1:B:148:MET:HE3	1:B:443:LYS:CG	2.49	0.42
1:C:354:MET:HE2	1:C:358:ILE:HD11	2.02	0.42
1:A:186:GLN:HB2	1:A:216:ALA:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:450:THR:O	1:F:454:VAL:HG23	2.20	0.42
1:F:94:SER:O	1:F:98:LYS:HA	2.20	0.42
1:E:73:ILE:HG21	1:E:253:TYR:CE1	2.54	0.42
1:C:410:LEU:HD23	1:C:421:GLY:HA3	2.01	0.42
1:D:48:LEU:HD21	1:D:349:VAL:HG11	2.02	0.41
1:C:71:PHE:HA	1:C:260:ILE:HD11	2.02	0.41
1:D:439:GLU:O	1:D:443:LYS:HG2	2.21	0.41
1:C:173:VAL:HG13	1:C:175:PRO:HD3	2.02	0.41
1:A:76:PRO:O	1:A:80:ASP:HB2	2.20	0.41
1:C:168:PRO:HB2	1:C:174:LEU:HD12	2.01	0.41
1:A:53:GLN:O	1:A:57:LEU:HG	2.20	0.41
1:E:205:THR:HG21	1:E:221:LEU:HD21	2.03	0.41
1:E:230:ILE:HG22	1:E:261:LEU:HD12	2.01	0.41
1:B:290:SER:CA	1:B:325:GLU:HG2	2.51	0.40
1:A:249:PRO:HB3	1:A:274:ALA:O	2.22	0.40
1:D:408:HIS:C	1:D:408:HIS:CD2	2.95	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	428/446 (96%)	416 (97%)	12 (3%)	0	100	100
1	B	430/446 (96%)	417 (97%)	13 (3%)	0	100	100
1	C	432/446 (97%)	418 (97%)	14 (3%)	0	100	100
1	D	430/446 (96%)	416 (97%)	14 (3%)	0	100	100
1	E	424/446 (95%)	409 (96%)	15 (4%)	0	100	100
1	F	432/446 (97%)	419 (97%)	13 (3%)	0	100	100
All	All	2576/2676 (96%)	2495 (97%)	81 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	357/369 (97%)	348 (98%)	9 (2%)	47	39
1	B	357/369 (97%)	351 (98%)	6 (2%)	60	53
1	C	359/369 (97%)	347 (97%)	12 (3%)	38	26
1	D	357/369 (97%)	345 (97%)	12 (3%)	37	25
1	E	356/369 (96%)	344 (97%)	12 (3%)	37	25
1	F	359/369 (97%)	348 (97%)	11 (3%)	40	28
All	All	2145/2214 (97%)	2083 (97%)	62 (3%)	42	31

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	109	SER
1	A	195	LEU
1	A	201	ARG
1	A	408	HIS
1	A	418	MET
1	A	429	LYS
1	A	434	GLN
1	A	439	GLU
1	A	472	GLU
1	B	204	THR
1	B	206	CYS
1	B	308	VAL
1	B	345	HIS
1	B	408	HIS
1	B	434	GLN
1	C	49	SER
1	C	101	LEU
1	C	154	LYS
1	C	173	VAL

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Mol	Chain	Res	Type
1	C	291	HIS
1	C	323	GLN
1	C	328	LYS
1	C	408	HIS
1	C	418	MET
1	C	429	LYS
1	C	434	GLN
1	C	466	LEU
1	D	49	SER
1	D	60	LYS
1	D	75	ASN
1	D	102	GLU
1	D	107	LEU
1	D	315	ASP
1	D	345	HIS
1	D	373	VAL
1	D	408	HIS
1	D	429	LYS
1	D	434	GLN
1	D	443	LYS
1	E	49	SER
1	E	61	SER
1	E	101	LEU
1	E	111	LEU
1	E	152	GLN
1	E	173	VAL
1	E	204	THR
1	E	308	VAL
1	E	408	HIS
1	E	434	GLN
1	E	462	ARG
1	E	470	ASP
1	F	61	SER
1	F	101	LEU
1	F	143	LYS
1	F	204	THR
1	F	323	GLN
1	F	325	GLU
1	F	332	SER
1	F	408	HIS
1	F	418	MET
1	F	429	LYS

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Mol	Chain	Res	Type
1	F	434	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	345	HIS
1	E	50	ASN
1	E	82	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 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	HSO	F	501	3	6,10,10	1.46	1 (16%)	4,12,12	1.23	0
2	HSO	B	502	3	6,10,10	2.62	3 (50%)	4,12,12	1.00	0
2	HSO	E	502	3	6,10,10	2.35	2 (33%)	4,12,12	1.52	1 (25%)
2	HSO	C	502	3	6,10,10	1.13	0	4,12,12	1.16	1 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HSO	D	502	3	6,10,10	2.28	2 (33%)	4,12,12	0.95	0
2	HSO	A	501	3	6,10,10	1.98	2 (33%)	4,12,12	0.88	0

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	HSO	F	501	3	-	2/6/6/6	0/1/1/1
2	HSO	B	502	3	-	1/6/6/6	0/1/1/1
2	HSO	E	502	3	-	1/6/6/6	0/1/1/1
2	HSO	C	502	3	-	1/6/6/6	0/1/1/1
2	HSO	D	502	3	-	1/6/6/6	0/1/1/1
2	HSO	A	501	3	-	1/6/6/6	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	502	HSO	C-CA	4.84	1.60	1.52
2	D	502	HSO	CB-CA	4.74	1.60	1.53
2	E	502	HSO	C-CA	4.59	1.59	1.52
2	A	501	HSO	C-CA	3.45	1.58	1.52
2	A	501	HSO	CB-CA	-2.96	1.49	1.53
2	F	501	HSO	C-CA	2.68	1.56	1.52
2	B	502	HSO	CB-CA	-2.68	1.49	1.53
2	E	502	HSO	CB-CA	-2.64	1.49	1.53
2	D	502	HSO	CA-N	2.59	1.55	1.46
2	B	502	HSO	CA-N	2.44	1.54	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	502	HSO	CG-CD2-NE2	2.45	113.35	108.80
2	C	502	HSO	CG-CD2-NE2	2.18	112.86	108.80

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	501	HSO	CA-CB-CG-ND1

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Mol	Chain	Res	Type	Atoms
2	B	502	HSO	CA-CB-CG-ND1
2	E	502	HSO	CA-CB-CG-ND1
2	C	502	HSO	CA-CB-CG-ND1
2	A	501	HSO	CA-CB-CG-ND1
2	D	502	HSO	CA-CB-CG-ND1
2	F	501	HSO	O-C-CA-N

There are no ring outliers.

No monomer is involved in short contacts.

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	431/446 (96%)	0.10	9 (2%) 63 65	21, 38, 76, 99	0
1	B	432/446 (96%)	-0.04	7 (1%) 72 73	22, 39, 67, 102	0
1	C	434/446 (97%)	0.19	11 (2%) 57 59	25, 42, 68, 106	0
1	D	432/446 (96%)	0.18	20 (4%) 32 34	25, 44, 72, 95	0
1	E	430/446 (96%)	0.57	40 (9%) 8 10	29, 54, 82, 115	0
1	F	434/446 (97%)	0.63	47 (10%) 5 6	28, 54, 86, 103	0
All	All	2593/2676 (96%)	0.27	134 (5%) 27 29	21, 44, 77, 115	0

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	101	LEU	6.7
1	F	204	THR	6.7
1	E	338	PHE	6.5
1	C	201	ARG	5.7
1	E	87	ALA	5.5
1	F	97	ASP	5.4
1	F	170	GLY	4.8
1	F	81	VAL	4.8
1	E	104	ILE	4.7
1	F	101	LEU	4.6
1	D	201	ARG	4.6
1	A	72	ASP	4.5
1	F	93	THR	4.5
1	A	87	ALA	4.4
1	E	102	GLU	4.4
1	E	88	ALA	4.3
1	F	116	LEU	4.3
1	A	65	ILE	4.3
1	E	96	PHE	4.2

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Mol	Chain	Res	Type	RSRZ
1	F	221	LEU	4.2
1	C	472	GLU	4.2
1	F	201	ARG	4.1
1	C	171	THR	4.1
1	F	169	GLY	4.1
1	B	201	ARG	4.0
1	E	115	VAL	4.0
1	F	115	VAL	3.9
1	F	171	THR	3.9
1	E	74	VAL	3.9
1	F	104	ILE	3.8
1	F	459	ALA	3.8
1	F	457	LEU	3.8
1	C	475	GLN	3.8
1	F	172	ALA	3.7
1	E	300	ALA	3.7
1	E	322	ILE	3.6
1	F	200	THR	3.6
1	C	99	VAL	3.6
1	D	331	GLN	3.6
1	C	100	ASP	3.5
1	E	66	ASP	3.5
1	D	170	GLY	3.5
1	F	91	GLN	3.4
1	E	472	GLU	3.4
1	F	111	LEU	3.4
1	E	474	ARG	3.4
1	D	99	VAL	3.4
1	E	326	VAL	3.4
1	C	96	PHE	3.3
1	C	101	LEU	3.3
1	F	99	VAL	3.3
1	E	92	TYR	3.3
1	F	203	GLY	3.3
1	F	331	GLN	3.3
1	D	171	THR	3.2
1	E	442	ARG	3.2
1	F	207	LYS	3.2
1	E	293	ALA	3.2
1	F	102	GLU	3.2
1	B	170	GLY	3.2
1	F	89	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	96	PHE	3.1
1	F	103	ASN	3.1
1	E	470	ASP	3.0
1	F	110	ASP	3.0
1	D	96	PHE	3.0
1	D	172	ALA	3.0
1	E	473	ALA	3.0
1	D	102	GLU	3.0
1	D	202	ASP	3.0
1	C	94	SER	3.0
1	D	101	LEU	3.0
1	E	203	GLY	2.9
1	D	338	PHE	2.9
1	D	203	GLY	2.9
1	E	227	ALA	2.9
1	E	446	PRO	2.8
1	F	96	PHE	2.8
1	E	331	GLN	2.8
1	E	172	ALA	2.7
1	E	253	TYR	2.7
1	E	333	LEU	2.7
1	F	205	THR	2.7
1	F	119	ALA	2.7
1	A	71	PHE	2.6
1	D	169	GLY	2.6
1	F	394	TRP	2.6
1	A	64	ARG	2.6
1	D	104	ILE	2.6
1	F	74	VAL	2.6
1	E	110	ASP	2.6
1	D	42	PRO	2.5
1	D	98	LYS	2.5
1	D	471	ILE	2.5
1	E	320	ASN	2.5
1	E	100	ASP	2.5
1	F	100	ASP	2.5
1	F	466	LEU	2.4
1	D	473	ALA	2.4
1	A	97	ASP	2.4
1	F	239	THR	2.4
1	F	202	ASP	2.4
1	F	114	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	102	GLU	2.4
1	A	253	TYR	2.4
1	F	87	ALA	2.4
1	E	169	GLY	2.4
1	E	91	GLN	2.3
1	E	445	GLY	2.3
1	E	438	GLU	2.3
1	F	113	ASP	2.3
1	B	203	GLY	2.3
1	E	120	ILE	2.3
1	F	462	ARG	2.3
1	F	199	PRO	2.3
1	F	238	GLU	2.2
1	E	290	SER	2.2
1	B	260	ILE	2.2
1	E	471	ILE	2.2
1	F	445	GLY	2.2
1	D	92	TYR	2.2
1	F	208	GLU	2.2
1	E	204	THR	2.2
1	F	463	ALA	2.2
1	E	448	VAL	2.2
1	A	57	LEU	2.1
1	F	106	GLU	2.1
1	A	77	ILE	2.1
1	D	100	ASP	2.1
1	E	107	LEU	2.1
1	B	331	GLN	2.1
1	C	471	ILE	2.1
1	F	474	ARG	2.0
1	C	331	GLN	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
2	HSO	E	502	10/10	0.94	0.18	43,44,45,48	0
2	HSO	C	502	10/10	0.95	0.13	35,36,38,39	0
2	HSO	D	502	10/10	0.95	0.12	35,35,38,42	0
2	HSO	F	501	10/10	0.96	0.10	47,48,50,51	0
2	HSO	B	502	10/10	0.98	0.09	28,29,30,33	0
2	HSO	A	501	10/10	0.98	0.14	24,24,26,30	0
3	ZN	A	502	1/1	0.99	0.10	30,30,30,30	0
3	ZN	E	503	1/1	0.99	0.07	46,46,46,46	0
3	ZN	D	501	1/1	0.99	0.10	39,39,39,39	0
3	ZN	E	501	1/1	0.99	0.04	45,45,45,45	0
3	ZN	C	501	1/1	1.00	0.11	37,37,37,37	0
3	ZN	B	501	1/1	1.00	0.13	26,26,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.