



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 10:21 PM UTC

PDB ID : 5VLC / pdb_00005vlc
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 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

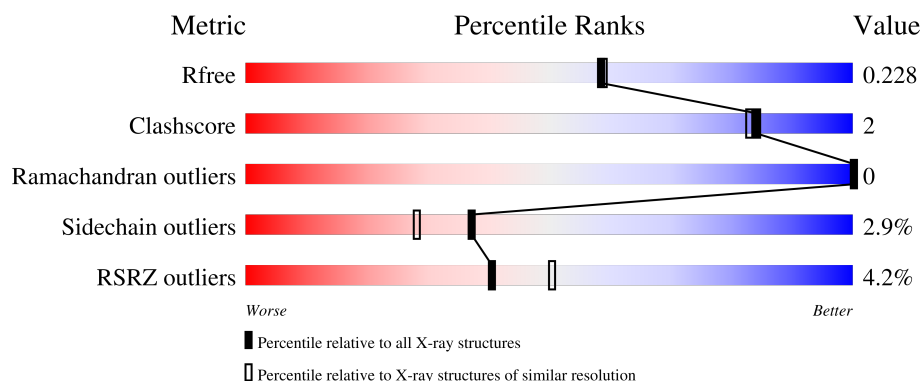
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.97 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}	180053	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	446	5% 90% 6% ..
1	B	446	2% 90% 6% .
1	C	446	% 89% 8% .
1	D	446	2% 88% 8% ..
1	E	446	10% 86% 10% ..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	446	6% 91% 6%

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:

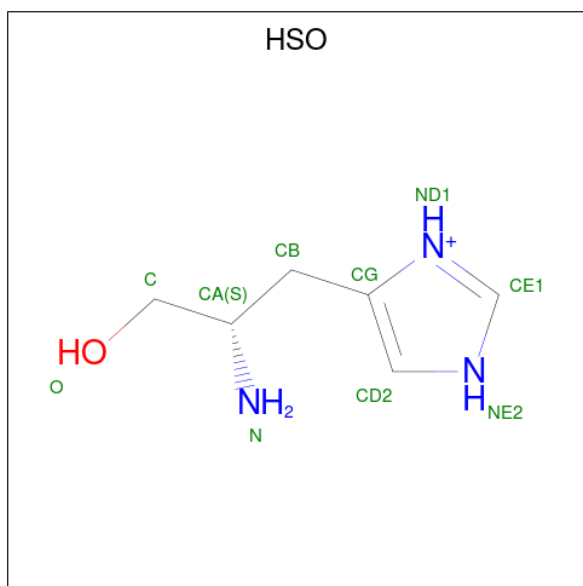
Chain	Residue	Modelled	Actual	Comment	Reference
A	33	SER	-	expression tag	UNP G7IKX3
A	34	ASN	-	expression tag	UNP G7IKX3
A	35	ALA	-	expression tag	UNP G7IKX3
B	33	SER	-	expression tag	UNP G7IKX3
B	34	ASN	-	expression tag	UNP G7IKX3
B	35	ALA	-	expression tag	UNP G7IKX3
C	33	SER	-	expression tag	UNP G7IKX3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

Continued on next page...

Continued from previous page...

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

- Molecule 2 is L-histidinol (CCD ID: HSO) (formula: C₆H₁₂N₃O).



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 (CCD ID: ZN) (formula: Zn).

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

Continued on next page...

Continued from previous page...

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

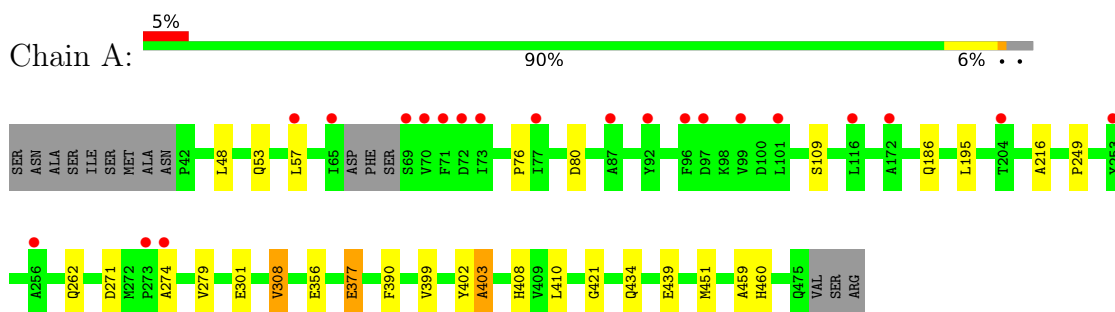
- Molecule 4 is water.

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

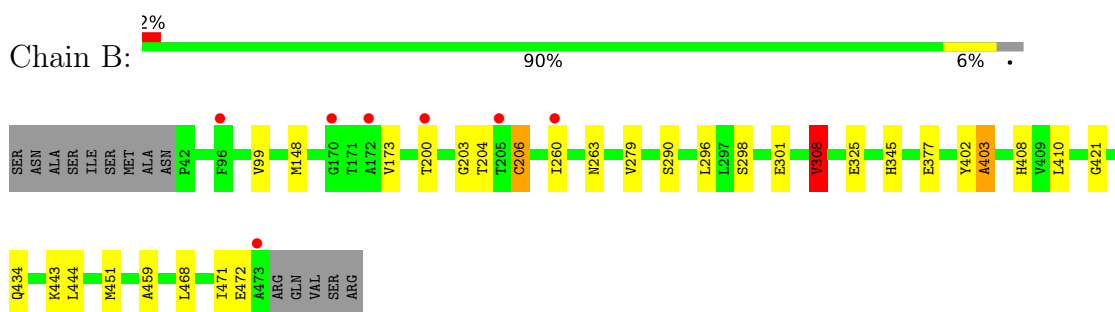
3 Residue-property plots

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

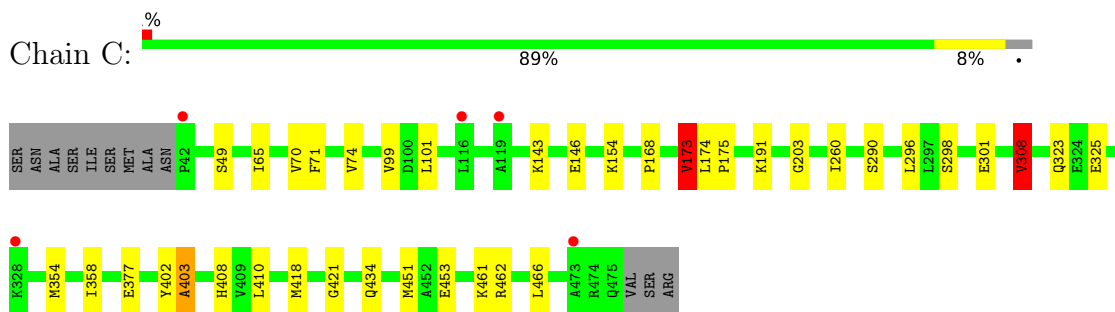
- Molecule 1: Histidinol dehydrogenase, chloroplastic



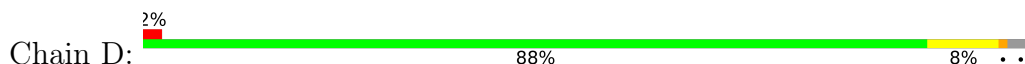
- Molecule 1: Histidinol dehydrogenase, chloroplastic

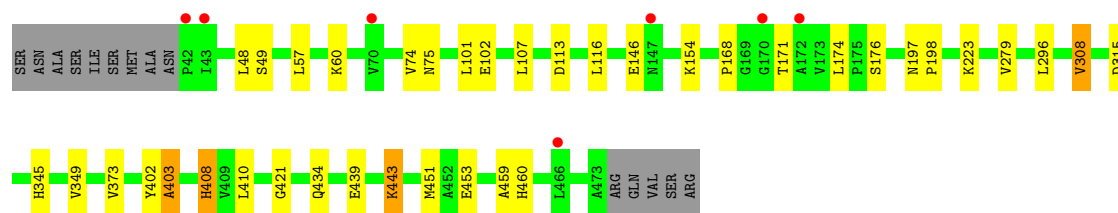


- Molecule 1: Histidinol dehydrogenase, chloroplastic

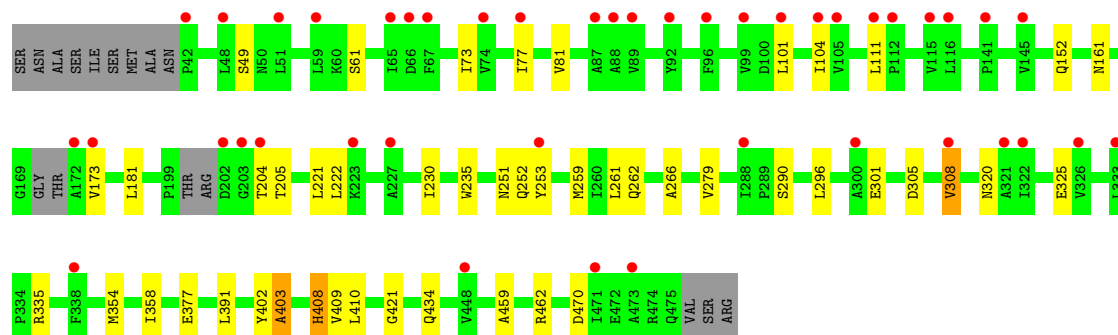
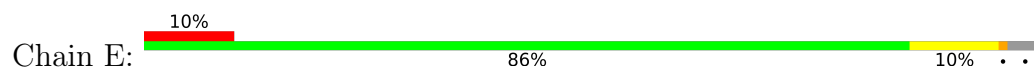


- Molecule 1: Histidinol dehydrogenase, chloroplastic

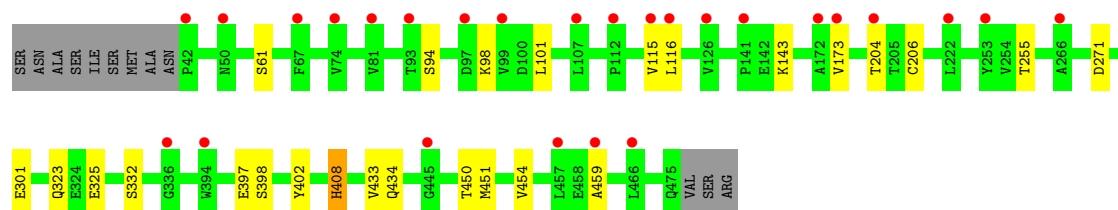




● Molecule 1: Histidinol dehydrogenase, chloroplastic



● 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 , 42.5	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	0.97	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	1.08	1/3346 (0.0%)	1.09	4/4547 (0.1%)
1	B	1.06	0/3344	1.04	3/4547 (0.1%)
1	C	0.97	0/3364	1.03	6/4573 (0.1%)
1	D	0.97	3/3344 (0.1%)	1.08	11/4547 (0.2%)
1	E	0.98	0/3333	1.06	3/4528 (0.1%)
1	F	0.94	1/3364 (0.0%)	1.02	3/4573 (0.1%)
All	All	1.00	5/20095 (0.0%)	1.05	30/27315 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	198	PRO	CA-C	5.86	1.56	1.52
1	A	390	PHE	C-O	-5.26	1.18	1.24
1	F	433	VAL	C-O	5.26	1.29	1.24
1	D	176	SER	N-CA	5.06	1.52	1.46
1	D	453	GLU	C-O	-5.04	1.18	1.24

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	271	ASP	N-CA-C	8.39	120.20	111.14
1	E	402	TYR	N-CA-C	8.26	123.91	112.93
1	B	402	TYR	N-CA-C	8.08	123.68	112.93
1	C	402	TYR	N-CA-C	7.80	123.30	112.93
1	A	402	TYR	N-CA-C	7.69	123.16	112.93
1	F	402	TYR	N-CA-C	7.59	123.02	112.93
1	D	113	ASP	CA-C-N	-7.35	112.75	120.03
1	D	113	ASP	C-N-CA	-7.35	112.75	120.03
1	D	402	TYR	N-CA-C	7.27	122.61	112.93
1	E	403	ALA	N-CA-C	6.44	124.13	113.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	146	GLU	CA-C-N	6.15	128.77	120.65
1	C	146	GLU	C-N-CA	6.15	128.77	120.65
1	A	399	VAL	N-CA-C	5.88	116.62	110.62
1	C	403	ALA	N-CA-C	5.72	122.94	113.50
1	C	173	VAL	CB-CA-C	5.72	118.68	110.33
1	B	403	ALA	N-CA-C	5.71	122.61	114.16
1	B	308	VAL	CB-CA-C	5.66	120.50	110.71
1	D	171	THR	N-CA-C	5.62	117.08	111.07
1	D	197	ASN	CA-C-N	-5.62	115.62	119.66
1	D	197	ASN	C-N-CA	-5.62	115.62	119.66
1	A	403	ALA	N-CA-C	5.60	122.74	113.50
1	F	271	ASP	N-CA-C	5.58	117.17	111.14
1	D	171	THR	CB-CA-C	-5.46	102.30	110.88
1	D	154	LYS	N-CA-CB	-5.21	103.48	111.56
1	D	403	ALA	N-CA-C	5.17	122.03	113.50
1	F	255	THR	N-CA-C	5.16	117.58	111.33
1	C	308	VAL	CB-CA-C	5.15	118.93	110.69
1	E	320	ASN	N-CA-C	5.10	116.53	111.07
1	D	146	GLU	CA-C-N	5.09	127.56	120.63
1	D	146	GLU	C-N-CA	5.09	127.56	120.63

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	3278	0	3282	15	0
1	B	3277	0	3274	22	0
1	C	3297	0	3295	18	0
1	D	3277	0	3274	14	0
1	E	3268	0	3263	25	0
1	F	3297	0	3295	9	0
2	A	10	0	11	0	0
2	B	10	0	11	0	0
2	C	10	0	11	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	90	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 (90) 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:E:354:MET:HE3	1:E:358:ILE:HD11	1.58	0.85
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:C:354:MET:HE3	1:C:358:ILE:HD11	1.78	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:A:403:ALA:HB2	1:B:451:MET:HE1	1.83	0.59
1:B:290:SER:HA	1:B:325:GLU:HG2	1.84	0.59
1:C:451:MET:HE1	1:D:403:ALA:HB2	1.85	0.59
1:B:148:MET:HE3	1:B:443:LYS:CG	2.33	0.57
1:B:99:VAL:HG21	1:B:203:GLY:HA2	1.87	0.57
1:A:301:GLU:CD	1:B:459:ALA:HB3	2.30	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:MET:HE3	1:B:443:LYS:HG2	1.88	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
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:E:459:ALA:HB3	1:F:301:GLU:CD	2.35	0.52
1:C:99:VAL:HG11	1:C:203:GLY:HA2	1.90	0.52
1:A:377:GLU:H	1:A:377:GLU:CD	2.18	0.51
1:E:235:TRP:CE2	1:E:266:ALA:HB2	2.46	0.51
1:B:377:GLU:H	1:B:377:GLU:CD	2.19	0.51
1:A:459:ALA:HB3	1:B:301:GLU:CD	2.36	0.50
1:C:403:ALA:HB2	1:D:451:MET:HE1	1.91	0.50
1:E:296:LEU:HD22	1:E:308:VAL:HG13	1.93	0.50
1:A:451:MET:HE1	1:B:403:ALA:HB2	1.94	0.50
1:F:173:VAL:HG13	1:F:206:CYS:SG	2.52	0.50
1:E:403:ALA:HB2	1:F:451:MET:HE1	1.94	0.50
1:B:410:LEU:HD23	1:B:421:GLY:HA3	1.94	0.49
1:E:354:MET:HE3	1:E:358:ILE:CD1	2.36	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:301:GLU:CD	1:F:459:ALA:HB3	2.39	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:279:VAL:HG12	1:A:308:VAL:HG22	1.97	0.45
1:B:148:MET:HE3	1:B:443:LYS:HG3	1.97	0.45
1:A:262:GLN:NE2	1:B:263:ASN:OD1	2.49	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:D:408:HIS:CD2	1:D:408:HIS:C	2.95	0.45
1:C:301:GLU:CD	1:D:459:ALA:HB3	2.41	0.45
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:B:200:THR:O	1:B:203:GLY:N	2.52	0.43
1:E:259:MET:O	1:E:262:GLN:HG2	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:377:GLU:H	1:C:377:GLU:CD	2.27	0.42
1:A:186:GLN:HB2	1:A:216:ALA:O	2.20	0.42
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:F:408:HIS:CD2	1:F:408:HIS:C	2.98	0.42
1:B:148:MET:HE1	1:B:444:LEU:HB2	2.01	0.42
1:C:410:LEU:HD23	1:C:421:GLY:HA3	2.01	0.42
1:E:377:GLU:H	1:E:377:GLU:CD	2.28	0.42
1:D:48:LEU:HD21	1:D:349:VAL:HG11	2.02	0.41
1:C:354:MET:HE3	1:C:358:ILE:CD1	2.46	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:F:115:VAL:C	1:F:116:LEU:HD12	2.45	0.41
1:E:408:HIS:CD2	1:E:408:HIS:C	2.98	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:F:397:GLU:O	1:F:398:SER:C	2.65	0.40
1:C:354:MET:CE	1:C:358:ILE:HD11	2.49	0.40
1:E:251:ASN:OD1	1:E:251:ASN:C	2.64	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	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%)	350 (98%)	7 (2%)	48	42
1	B	357/369 (97%)	349 (98%)	8 (2%)	45	38
1	C	359/369 (97%)	345 (96%)	14 (4%)	28	17
1	D	357/369 (97%)	344 (96%)	13 (4%)	31	20
1	E	356/369 (96%)	344 (97%)	12 (3%)	32	22
1	F	359/369 (97%)	350 (98%)	9 (2%)	42	33
All	All	2145/2214 (97%)	2082 (97%)	63 (3%)	37	28

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	109	SER
1	A	195	LEU
1	A	308	VAL
1	A	377	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	408	HIS
1	A	434	GLN
1	A	439	GLU
1	B	204	THR
1	B	206	CYS
1	B	260	ILE
1	B	308	VAL
1	B	345	HIS
1	B	408	HIS
1	B	434	GLN
1	B	472	GLU
1	C	49	SER
1	C	74	VAL
1	C	101	LEU
1	C	143	LYS
1	C	154	LYS
1	C	173	VAL
1	C	191	LYS
1	C	308	VAL
1	C	323	GLN
1	C	408	HIS
1	C	418	MET
1	C	434	GLN
1	C	462	ARG
1	C	466	LEU
1	D	49	SER
1	D	74	VAL
1	D	75	ASN
1	D	102	GLU
1	D	107	LEU
1	D	116	LEU
1	D	308	VAL
1	D	315	ASP
1	D	345	HIS
1	D	373	VAL
1	D	408	HIS
1	D	434	GLN
1	D	443	LYS
1	E	49	SER
1	E	61	SER
1	E	101	LEU
1	E	111	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	434	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	434	GLN
1	A	475	GLN
1	B	291	HIS
1	C	469	GLN
1	D	53	GLN
1	D	262	GLN
1	D	291	HIS
1	E	50	ASN
1	E	75	ASN
1	E	345	HIS
1	F	75	ASN
1	F	291	HIS
1	F	323	GLN

5.3.3 RNA ⓘ

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](#)

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	D	502	3	10,10,10	1.83	2 (20%)	10,12,12	1.90	3 (30%)
2	HSO	A	501	3	10,10,10	1.60	2 (20%)	10,12,12	1.89	3 (30%)
2	HSO	F	501	3	10,10,10	1.35	1 (10%)	10,12,12	1.98	3 (30%)
2	HSO	B	502	3	10,10,10	2.16	4 (40%)	10,12,12	2.05	5 (50%)
2	HSO	C	502	3	10,10,10	1.23	0	10,12,12	1.97	4 (40%)
2	HSO	E	502	3	10,10,10	2.06	4 (40%)	10,12,12	2.34	5 (50%)

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

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	502	HSO	C-CA	4.78	1.60	1.52
2	D	502	HSO	CB-CA	4.56	1.60	1.53
2	E	502	HSO	C-CA	4.53	1.59	1.52
2	A	501	HSO	C-CA	3.39	1.58	1.52
2	A	501	HSO	CB-CA	-2.72	1.49	1.53
2	F	501	HSO	C-CA	2.63	1.56	1.52
2	D	502	HSO	CA-N	2.63	1.55	1.46
2	E	502	HSO	CD2-CG	2.52	1.41	1.36
2	B	502	HSO	CA-N	2.48	1.54	1.46
2	B	502	HSO	CB-CA	-2.46	1.49	1.53
2	E	502	HSO	CB-CA	-2.42	1.49	1.53
2	E	502	HSO	CE1-ND1	2.21	1.38	1.33
2	B	502	HSO	CE1-ND1	2.11	1.37	1.33

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	502	HSO	CG-CD2-NE2	4.44	113.35	106.54
2	C	502	HSO	CG-CD2-NE2	4.12	112.86	106.54
2	E	502	HSO	CD2-CG-ND1	-3.76	101.26	108.86
2	B	502	HSO	CG-CD2-NE2	3.74	112.28	106.54
2	F	501	HSO	CG-CD2-NE2	3.64	112.13	106.54
2	D	502	HSO	CD2-CG-ND1	-3.63	101.53	108.86
2	B	502	HSO	CD2-CG-ND1	-3.45	101.89	108.86
2	F	501	HSO	CD2-CG-ND1	-3.44	101.90	108.86
2	A	501	HSO	CG-CD2-NE2	3.35	111.69	106.54
2	D	502	HSO	CG-CD2-NE2	3.28	111.57	106.54
2	A	501	HSO	CD2-CG-ND1	-3.17	102.46	108.86
2	C	502	HSO	CD2-CG-ND1	-2.81	103.17	108.86
2	E	502	HSO	CB-CG-ND1	2.42	128.96	121.74
2	F	501	HSO	CE1-ND1-CG	2.32	111.07	105.80
2	E	502	HSO	CE1-ND1-CG	2.30	111.03	105.80
2	C	502	HSO	CA-CB-CG	2.27	117.26	113.13
2	E	502	HSO	CD2-NE2-CE1	-2.26	103.34	107.36
2	A	501	HSO	CE1-ND1-CG	2.25	110.91	105.80
2	B	502	HSO	CB-CG-ND1	2.21	128.34	121.74
2	B	502	HSO	CE1-ND1-CG	2.18	110.76	105.80
2	D	502	HSO	CE1-ND1-CG	2.16	110.71	105.80
2	C	502	HSO	CB-CG-ND1	2.14	128.12	121.74
2	B	502	HSO	CA-CB-CG	2.01	116.78	113.13

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	502	HSO	CA-CB-CG-ND1
2	E	502	HSO	CA-CB-CG-CD2

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%)	0.15	21 (4%)	35	44	20, 38, 76, 99	1 (0%)
1	B	432/446 (96%)	0.15	7 (1%)	70	79	22, 39, 67, 102	0
1	C	434/446 (97%)	0.12	5 (1%)	76	83	25, 42, 68, 106	0
1	D	432/446 (96%)	0.19	7 (1%)	70	79	25, 44, 72, 95	0
1	E	430/446 (96%)	0.80	43 (10%)	12	18	29, 54, 82, 115	0
1	F	434/446 (97%)	0.64	26 (5%)	27	36	28, 54, 86, 103	0
All	All	2593/2676 (96%)	0.34	109 (4%)	40	50	20, 44, 77, 115	1 (0%)

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	65	ILE	5.6
1	E	101	LEU	5.4
1	A	70	VAL	4.3
1	E	42	PRO	4.0
1	A	71	PHE	3.9
1	E	300	ALA	3.7
1	A	69	SER	3.5
1	D	172	ALA	3.4
1	E	88	ALA	3.3
1	E	204	THR	3.2
1	A	274	ALA	3.2
1	B	473	ALA	3.2
1	A	57	LEU	3.2
1	E	473	ALA	3.1
1	F	115	VAL	3.0
1	A	72	ASP	2.9
1	E	99	VAL	2.9
1	E	173	VAL	2.9
1	C	42	PRO	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	104	ILE	2.9
1	A	101	LEU	2.9
1	E	87	ALA	2.9
1	F	42	PRO	2.8
1	A	87	ALA	2.8
1	E	338	PHE	2.8
1	B	260	ILE	2.7
1	E	471	ILE	2.7
1	D	42	PRO	2.7
1	E	145	VAL	2.7
1	E	448	VAL	2.7
1	F	266	ALA	2.6
1	F	74	VAL	2.6
1	B	96	PHE	2.6
1	E	141	PRO	2.6
1	E	65	ILE	2.6
1	D	170	GLY	2.6
1	F	173	VAL	2.6
1	D	147	ASN	2.6
1	E	89	VAL	2.6
1	F	172	ALA	2.6
1	A	92	TYR	2.5
1	E	48	LEU	2.5
1	F	107	LEU	2.5
1	B	170	GLY	2.5
1	E	322	ILE	2.5
1	A	172	ALA	2.5
1	E	333	LEU	2.5
1	E	321	ALA	2.5
1	E	326	VAL	2.5
1	E	92	TYR	2.5
1	E	253	TYR	2.5
1	A	253	TYR	2.4
1	F	253	TYR	2.4
1	E	111	LEU	2.4
1	A	96	PHE	2.4
1	C	473	ALA	2.4
1	F	141	PRO	2.4
1	E	74	VAL	2.4
1	F	336	GLY	2.4
1	A	77	ILE	2.3
1	F	99	VAL	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	204	THR	2.3
1	E	172	ALA	2.3
1	E	66	ASP	2.3
1	F	81	VAL	2.3
1	A	73	ILE	2.3
1	E	115	VAL	2.3
1	E	77	ILE	2.2
1	E	308	VAL	2.2
1	F	50	ASN	2.2
1	A	204	THR	2.2
1	B	200	THR	2.2
1	E	59	LEU	2.2
1	E	203	GLY	2.2
1	A	97	ASP	2.2
1	B	172	ALA	2.2
1	E	202	ASP	2.2
1	F	394	TRP	2.2
1	D	43	ILE	2.2
1	D	466	LEU	2.2
1	F	445	GLY	2.2
1	A	273	PRO	2.2
1	F	67	PHE	2.2
1	E	223	LYS	2.2
1	E	105	VAL	2.2
1	C	116	LEU	2.2
1	E	51	LEU	2.2
1	E	116	LEU	2.2
1	F	457	LEU	2.2
1	F	466	LEU	2.2
1	E	96	PHE	2.1
1	F	93	THR	2.1
1	F	97	ASP	2.1
1	F	126	VAL	2.1
1	E	112	PRO	2.1
1	F	116	LEU	2.1
1	F	222	LEU	2.1
1	A	256	ALA	2.1
1	E	67	PHE	2.1
1	D	70	VAL	2.1
1	C	119	ALA	2.1
1	E	288	ILE	2.1
1	A	99	VAL	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	227	ALA	2.1
1	F	459	ALA	2.1
1	B	205	THR	2.0
1	A	116	LEU	2.0
1	C	328	LYS	2.0
1	F	112	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
2	HSO	E	502	10/10	0.91	0.10	43,44,45,48	0
2	HSO	F	501	10/10	0.91	0.09	47,48,50,51	0
2	HSO	D	502	10/10	0.93	0.10	35,35,38,42	0
2	HSO	C	502	10/10	0.94	0.08	35,36,38,39	0
2	HSO	A	501	10/10	0.96	0.06	24,24,26,30	0
2	HSO	B	502	10/10	0.97	0.06	28,29,30,33	0
3	ZN	A	502	1/1	0.99	0.02	30,30,30,30	0
3	ZN	D	501	1/1	0.99	0.02	39,39,39,39	0
3	ZN	E	501	1/1	0.99	0.05	45,45,45,45	0
3	ZN	E	503	1/1	0.99	0.04	46,46,46,46	0
3	ZN	C	501	1/1	1.00	0.01	37,37,37,37	0
3	ZN	B	501	1/1	1.00	0.02	26,26,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.